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Surveys in Stochastic Processes

Jochen Blath
Peter Imkeller
Sylvie Rœlly
Editors

European Mathematical Society

Editors:

Jochen Blath
Institut für Mathematik
Technische Universität Berlin
Straße des 17. Juni 136
10623 Berlin
Germany

blath@math.tu-berlin.de

Peter Imkeller
Institut für Mathematik
Humboldt-Universität zu Berlin
Unter den Linden 6
10099 Berlin
Germany

imkeller@math.hu-berlin.de

Sylvie Rœlly
Institut für Mathematik der
Universität Potsdam
Am Neuen Palais, 10
14469 Potsdam
Germany

roelly@math.uni-potsdam.de

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Contact address:

European Mathematical Society Publishing House
Seminar for Applied Mathematics
ETH-Zentrum FLI C4
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Preface

In this volume many of the plenary lecturers of the *33rd Conference on Stochastic Processes and Their Applications* present their personal snapshots of recent important developments that they have been involved in within the area of stochastic processes and their applications. This reflects the idea leading us to compose this congress report: to present a collection of survey type articles that offer a glimpse of the state-of-the-art in many of the promising and thriving fields of the area of stochastic processes and their applications at the moment this SPA conference was held.

One of our hopes is that this collection may help young scientists in setting up research goals in the wide scope of fields represented in this volume.

To our knowledge, this is the first time that proceedings of an SPA conference has been published. The idea for this volume grew among the organizers in Spring 2009, and after a meeting with Professor Marta Sanz-Solé from the Bernoulli Society in Berlin and upon approval by both the CCSP[1] and the publishing committee of the Bernoulli Society we decided to go ahead with it. As a particularly welcome effect of this volume we could imagine starting a tradition for forthcoming SPA events.

We wish to thank all contributing plenary speakers, anonymous referees and the EMS publishing house for making this volume possible.

On behalf of the 33rd SPA organizing committee: Enjoy reading!

Berlin and Potsdam, June 2011

Jochen Blath
Peter Imkeller
Sylvie Rœlly

[1] 'Committee for conferences on stochastic processes' of the Bernoulli Society.

Contents

The 33rd SPA Conference 2009

The *33rd Conference on Stochastic Processes and Their Applications* (SPA) was held in Berlin from July 27 through July 31, 2009, with more than 600 participants from 49 countries[1].

The conference continued a successful series of SPA conferences in this prospering field of mathematics, which is both reflected in the growing number and internationality of participants, as well as in the size of the program and the recognition for the field within mathematics.

One indication of this might be seen in the felicitous fact that one of the plenary speakers, Professor Stanislav Smirnov from Geneva, was awarded with a *Fields Medal* in 2010.

The main aim behind the selection of the 20 plenary lectures at this conference was to give an overview of recent developments in the rich current active research fields in Stochastic Processes and Their Applications, in particular aimed at younger participants. They were also chosen to reflect the variety of the current probability community with respect to research topics, scientific age and diversity with respect to geography and gender. We think that this has worked very well, and hence our thanks go to the members of the scientific committee (see below).

We particularly encouraged young researchers and researchers from developing countries to participate. More than 300 talks and 40 poster presentations, many of them by young participants, reflected the vibrancy of the field and provided an international forum for scientific and cultural exchange.

One further major aim of this conference was to *make the stochastic processes community feel at home*. Hence, we put particular emphasis on the social and public program of the conference, a few highlights of which we would like to report about briefly here.

During a reception in the 'Lichthof' of TU Berlin on the first evening of the conference, following a welcome address by Staatssekretär Dr. Hans-Gerhard Husung on behalf of the Senate of the State of Berlin, Professor Alice Guionnet from Lyon was announced as winner of the 2009 Loève prize. The elegant musical background throughout the reception was provided by a classical trio with direct links to the probability community, namely Alice Adenot-Meyer[2] (Mezzo-Soprano), Thérèse Dourdent (Piano) and Professor Sylvie Rœlly (Cello). Professor Ruth Williams from San Diego provided a personal obituary, remembering the recently deceased Professor Kai Lai Chung (1917 – 2009).

On the second evening, Professor Marc Wouts from Paris was awarded with the Itô-Prize. The sad occasion of the recent passing away of one of the most influential probabilists, Professor Kiyoshi Itô (1915 – 2008), was remembered by a touching and

[1] Detailed conference information can be found at www.math.tu-berlin.de/SPA2009

[2] Alice Adenot-Meyer is a daughter of Paul-André Meyer

charming presentation of his life and work by Professor Masatoshi Fukushima from Osaka.

A large part of the evening was devoted to the work and tragic life of the Berlin-born mathematician Wolfgang Döblin. Wolfgang Döblin (1915 – 1940) was the second son of the famous Jewish-German novelist Alfred Döblin ('Berlin Alexanderplatz'), an eminent figure in German intellectual life during the Weimarer Republik. In 1933, his family escaped the Nazis to Paris, where Wolfgang became a French citizen and studied probability at the Institut Henri Poincaré. He wrote a brilliant dissertation under the supervision of Maurice Fréchet in 1938. One year later, Wolfgang Döblin was drafted for French military service. In May 1940, facing imminent capture by the Wehrmacht, he took his own life in Housseras (Vosges, France). Before, however, he was able to mail his last mathematical manuscript *"Sur l'équation de Kolmogoroff"* in a sealed envelope to the Académie des Sciences, which remained unopened for 60 years. It has only recently been discovered and investigated by Bernard Bru and Marc Yor, and it turned out that it contains spectacular results, in particular related to the work of Itô.

The screening of a recent documentary on Wolfgang Döblins life and mathematical legacy in the presence of the filmmakers Agnes Handwerk and Harry Willems followed an introduction to his mathematical work and life by Professor Hans Föllmer.

Figure 1. During the Monday reception at TU Lichthof.

The success of this conference would not have been possible without the tireless commitment of many people. First, we wish to thank all plenary, invited session and contributed session speakers and the poster presenters for their scientific contributions. We further wish to thank the scientific committee and the representatives of the Bernoulli

Society, in particular Professors Ruth Williams and Marta Sanz-Solé, for all their effort, dedication and advice. Many students, staff and faculty at TU Berlin, HU Berlin and U Potsdam contributed greatly to the smooth running of this conference. A special heartfelt ‘thank you’ goes to Ms Jean Downes, running the conference secretariat. The TU Berlin and its Mathematical Institute provided support in many ways – we particularly thank the TU President Professor Kurt Kutzler. Finally, thanks go to the ‘TU Servicegesellschaft’ and in particular to Ms Lisa Hertel.

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"Limit laws of directed last passage site percolation"

Sourav Chatterjee (Berkeley)
"Superconcentration"

Freddy Delbaen (Zürich)
"Monetary utility functions, BSDE and (non-) linear PDE"

Amir Dembo (Stanford) Lévy Lecture
"Statistical mechanics on sparse random graphs"

Saïd Hamadène (Le Mans)
"Switching problems and systems of reflected BSDEs"

Claudia Klüppelberg (Munich) IMS Medallion Lecture
"Lévy driven stochastic volatility models"

James Martin (Oxford)
"Multi-class particle systems, growth models, and queues"

Servet Martinez (Santiago)
"Quasi-stationary distributions in Markov chains and population models"

Pierre Mathieu (Marseille)
"Symmetric diffusions in a random environment: the Einstein relation"

Jonathan Mattingly (Durham, NC)
"What makes infinite dimensional Markov processes different?"

Peter Mörters (Bath)
"The parabolic Anderson model with heavy-tailed potential"

Ed Perkins (Vancouver) Doob Lecture
"Uniqueness and non-uniqueness in parabolic stochastic partial differential equations"

Gesine Reinert (Oxford)
"Gaussian approximation of functionals: Malliavin calculus and Stein's method"

Laurent Saloff-Coste (Ithaca, NY)
"Merging properties of time inhomogeneous Markov chains"

Alexander Schied (München)
"On the mathematics of illiquid markets"

Gordon Slade (Vancouver) IMS Medallion Lecture
"The self-avoiding walk"

Stanislav Smirnov (Genève)
"Conformal invariance and universality in the $2D$ *Ising model"*

Masayoshi Takeda (Tohoku)
"L^p*-independence of growth bounds of Feynman–Kac semigroups"*

Anton Wakolbinger (Frankfurt am Main)
"Random genealogies in diffusion processes"

Feng-Yu Wang (Beijing)
"Functional inequalitites and applications"

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Optimal switching, systems of reflected BSDEs and systems of variational inequalities with inter-connected obstacles

Saïd Hamadène

1 Introduction

Optimal control of multiple switching models arise naturally in many applied disciplines. The pioneering work by Brennan and Schwartz [3], proposing a two-modes switching model for the life cycle of an investment in the natural resource industry, is probably first to apply this special case of stochastic impulse control to questions related to the structural profitability of an investment project or an industry whose production depends on the fluctuating market price of a number of underlying commodities or assets. Within this discipline, Carmona and Ludkosvki [5] suggest a multiple switching model to price energy tolling agreements, where the commodity prices are modeled as continuous time processes, and the holder of the agreement exercises her managerial options by controlling the production modes of the assets. All these applications seem agree that reformulating these problems in a multiple switching dynamic setting is a promising (if not the only) approach to fully capture the interplay between profitability, flexibility and uncertainty.

The optimal two-modes switching problem is probably the most extensively studied in the literature starting with above mentioned work by Brennan and Schwartz [3], and Dixit [10] who considered a similar model, but without resource extraction – see Dixit and Pindyck [11] and Trigeorgis [30] for an overview, extensions of these models and extensive reference lists. Brekke and Øksendal [1] and [2], Shirakawa [27], Knudsen, Meister and Zervos [24], Duckworth and Zervos [12] and [13] and Zervos [31] use the framework of generalized impulse control to solve several versions and extensions of this model, in the case where the decision to start and stop the production process is done over an infinite time horizon and the market price process of the underlying commodity is a diffusion process, while Trigeorgis [29] models the market price process of the commodity as a binomial tree. Hamadène and Jeanblanc [20] consider a finite horizon optimal two-modes switching problem in the case of Brownian filtration setting while Hamadène and Hdhiri [19] extend the set up of the latter paper to the case where the processes of the underlying commodities are adapted to a filtration generated by a Brownian motion and an independent Poisson process. Porchet et al. [26] also study the same problem, where they assume the payoff function to be given by an exponential utility function and allow the manager to trade on the commodities market. Finally, let us mention the work by Djehiche and Hamadène [8] where it is shown that including

the possibility of abandonment or bankruptcy in the two-modes switching model over a finite time horizon, makes the search for an optimal strategy highly nonlinear and is not at all a trivial extension of previous results.

An example of the class of multiple switching models discussed in Carmona and Ludkovski [5] is related to the management strategies to run a power plant that converts natural gas into electricity (through a series of gas turbines) and sells it in the market. The payoff rate from running the plant is roughly given by the difference between the market price of electricity and the market price of gas needed to produce it.

Suppose that besides running the plant at full capacity or keeping it completely off (the two-modes switching model), there also exists a total of $m-2$ ($m \geq 3$) intermediate operating modes, corresponding to different subsets of turbines running.

Let ℓ_{ij} and Ψ_i denote respectively the switching costs from state i to state j, to cover the required extra fuel and various overhead costs and the payoff rate in mode i. A management strategy for the power plant is a combination of two sequences:

(i) a nondecreasing sequence of stopping times $(\tau_n)_{n\geq 1}$, where, at time τ_n, the manager decides to switch the production from its current mode to another one;

(ii) a sequence of indicators $(\xi_n)_{n\geq 1}$ taking values in $\{1,\ldots,m\}$ of the states the production is switched to. At τ_n, for $n \geq 1$, the station is switched from its current mode ξ_{n-1} to ξ_n. The value ξ_0 is deterministic and is the state of the station at time 0.

When the power plant is run under a strategy $\Sigma = ((\tau_n)_{n\geq 1}, (\xi_n)_{n\geq 1})$, over a finite horizon $[0, T]$, the total expected profit up to T for such a strategy is

$$J(\Sigma, i) = \mathbb{E}\bigg[\int_0^T \sum_{n\geq 0} \big(\Psi_{\xi_n}(s)\mathbb{1}_{(\tau_n,\tau_{n+1}]}(s)\big)\, ds - \sum_{n\geq 1} \ell_{\xi_{n-1},\xi_n}(\tau_n)\mathbb{1}_{[\tau_n<T]}\bigg],$$

where we set $\tau_0 = 0$ and $\xi_0 = i$. The optimal switching problem we will investigate is to find a management strategy Σ^* such that $J(\Sigma^*, i) = \sup_\Sigma J(\Sigma, i)$. This latter quantity is nothing else but the price of the power plant in the market.

We first provide a Verification Theorem that shapes the problem, via the Snell envelope of processes. We show that if the Verification Theorem is satisfied by a vector of continuous processes $(Y^1, \ldots, Y^m)$ such that

$$Y_t^i = \operatorname*{ess\,sup}_{\tau\geq t} \mathbb{E}\bigg[\int_t^\tau \Psi_i(s)ds + \max_{j\neq i}(-\ell_{ij}(\tau) + Y_\tau^j)1_{[\tau<T]}\big|\mathcal{F}_t\bigg], \tag{1}$$

$\forall\ i = 1,\ldots,m$, $\forall t \leq T$, then each Y_t^i is the value function of the optimal problem when the system is in mode i at time t, i.e.,

$$Y_t^i = \operatorname*{ess\,sup}_{\Sigma\in\mathcal{A}_t^i} \mathbb{E}\bigg[\int_t^T \sum_{n\geq 0} \big(\Psi_{\xi_n}(s)\mathbb{1}_{(\tau_n,\tau_{n+1}]}(s)\big)\, ds - \sum_{n\geq 1} \ell_{\xi_{n-1},\xi_n}(\tau_n)\mathbb{1}_{[\tau_n<T]}\big|\mathcal{F}_t\bigg],$$

where $\mathcal{A}_t^i$ is the set of admissible strategies such that $\tau_1 \geq t$ a.s. and $\xi_0 = i$. An optimal strategy Σ^* is then constructed using the relation (1). Moreover, it holds that $Y_0^i = \sup_\Sigma J(\Sigma, i)$.

The unique solution for the Verification Theorem is obtained as the limit of sequences of processes $(Y^{i,n})_{n\geq 0}$, where for any $t \leq T$, $Y_t^{i,n}$ is the value function (or the optimal yield) from t to T, when the system is in mode i at time t and only at most n switchings after t are allowed. This sequence of value functions will be defined recursively (see (9) and (10)). As a by-product, we obtain also existence and uniqueness of the solution of the system of backward stochastic differential equations (hereafter BSDEs for short) with oblique reflection (or inter-connected obstacles) associated with the switching problem.

In the second part of this paper we deal with the optimal switching problem within the Markovian framework. Actually we assume that the processes Ψ_i (resp. ℓ_{ij}) are given by $\psi_i(t, X_t)$ (resp. $\ell_{ij}(t, X_t)$) where X is an Itô diffusion and $\psi_i(t,x)$, $\ell_{ij}(t,x)$ are deterministic continuous with polynomial growth functions. In this case the Verification Theorem of the switching problem can be expressed by means of a system of variational inequalities with inter-connected obstacles. We prove existence of m deterministic continuous functions $v^1(t,x), \ldots, v^m(t,x)$ such that for any $i \in \{1, \ldots, m\}$, $Y_t^i = v^i(t, X_t)$. Moreover the vector $(v^1, \ldots, v^m)$ is the unique viscosity solution of the Verification Theorem system.

In the last part of the paper, we discuss the issue of existence and uniqueness of the solution for general systems of BSDEs with oblique reflection. Those systems are involved especially when dealing with optimal switching problems under Knightian uncertainty (see e.g. [22] for more details). At the end, the question of numerics for system of reflected BSDEs with oblique reflection, which is crucial for practitioners, is introduced.

2 Formulation of the problem, assumptions and preliminary results

Throughout this paper $(\Omega, \mathcal{F}, \mathbb{P})$ will be a fixed probability space on which is defined a standard d-dimensional Brownian motion $B = (B_t)_{0\leq t\leq T}$ whose natural filtration is $(\mathcal{F}_t^0 := \sigma\{B_s, s \leq t\})_{0\leq t\leq T}$. Let $\boldsymbol{\mathcal{F}} = (\mathcal{F}_t)_{0\leq t\leq T}$ be the completed filtration of $(\mathcal{F}_t^0)_{0\leq t\leq T}$ with the $\mathbb{P}$-null sets of $\mathcal{F}$. Hence $\boldsymbol{\mathcal{F}}$ satisfies the usual conditions, i.e., it is right continuous and complete. Furthermore, let:

- $\mathcal{P}$ be the σ-algebra on $[0,T] \times \Omega$ of $\boldsymbol{\mathcal{F}}$-progressively measurable sets;
- $\mathcal{M}^{p,k}$ be the set of $\mathcal{P}$-measurable and $\mathbb{R}^k$-valued processes $\zeta = (\zeta_t)_{t\leq T}$ such that the process $(|\zeta_t|^p)_{t\leq T}$ is $dt \otimes dP$-integrable and $\mathcal{S}^p$ be the set of $\mathcal{P}$-measurable, continuous, $\mathbb{R}$-valued processes $\zeta = (\zeta_t)_{t\leq T}$ such that $\mathbb{E}\left[\sup_{0\leq t\leq T} |\zeta_t|^p\right] < \infty$ ($p > 1$ is, throughout this paper, fixed);
- For any stopping time $\tau \in [0,T]$, $\mathcal{T}_\tau$ denotes the set of all stopping times θ such that $\tau \leq \theta \leq T$, $\mathbb{P}$-a.s. Next for $\tau \in \mathcal{T}_0$, we denote by $\mathcal{F}_\tau$ the σ-algebra of events prior to τ, i.e., the set $\{A \in \mathcal{F},\ A \cap \tau \leq t \in \mathcal{F}_t, \forall t \leq T\}$.

The finite horizon multiple switching problem can be formulated as follows. First assume *w.l.o.g* that the plant is in production mode 1 at $t = 0$ and let $\mathcal{J} := \{1, \ldots, m\}$

be the set of all possible activity modes of the production of the commodity. A management strategy of the project consists, on the one hand, of the choice of a sequence of nondecreasing $\mathcal{F}$-stopping times $(\tau_n)_{n\geq 1}$ (i.e., $\tau_n \leq \tau_{n+1}$) where the manager decides to switch the activity from its current mode, say i, to another one from the set $\mathcal{I}^{-i} \subseteq \{1,\ldots,i-1,i+1,\ldots,m\}$. On the other hand, it consists of the choice of the mode ξ_n to which the production is switched at τ_n from the current mode i. Therefore, we assume that for any $n \geq 1$, ξ_n is a random variable $\mathcal{F}_{\tau_n}$-measurable with values in $\mathcal{I}$.

Assume that a strategy of running the plant $\Sigma := ((\tau_n)_{n\geq 1}, (\xi_n)_{n\geq 1})$ is given. We denote by $(u_t)_{t\leq T}$ its associated indicator of the production activity mode at time $t \in [0,T]$. It is given by

$$u_t = \mathbb{1}_{[0,\tau_1]}(t) + \sum_{n\geq 1} \xi_n \mathbb{1}_{(\tau_n,\tau_{n+1}]}(t). \tag{2}$$

The strategy Σ will be called *admissible* if it satisfies $\lim_{n\to\infty} \tau_n = T$ $\mathbb{P}$-a.s. and the set of admissible strategies is denoted by $\mathcal{A}$.

Now for $i \in \mathcal{I}$, let $\Psi_i := (\Psi_i(t))_{0\leq t\leq T}$ be a stochastic process which belongs to $\mathcal{M}^{p,1}$. In the sequel, it stands for the payoff rate per unit time when the plant is in state i. On the other hand, for $i \in \mathcal{I}$ and $j \in \mathcal{I}^{-i}$ let $\ell_{ij} := (\ell_{ij}(t))_{0\leq t\leq T}$ be a continuous process of $\mathcal{S}^p$. It stands for the switching cost of the production at time t from its current mode i to another mode $j \in \mathcal{I}^{-i}$. For completeness we adopt the convention that $\ell_{ij} \equiv +\infty$ for any $i \in \mathcal{I}$ and $j \in \mathcal{I} - \mathcal{I}^{-i}$ $(j \neq i)$. This convention is set in order to exclude the switching from the state i to another state j which does not belong to $\mathcal{I}^{-i}$. Moreover we suppose that there exists a real constant $\gamma > 0$ such that for any $i, j \in \mathcal{I}$, and any $t \leq T$, $\ell_{ij}(t) \geq \gamma$. This assumption means that switching from a state to another one costs at least γ.

When a strategy $\Sigma := ((\tau_n)_{n\geq 1}, (\xi_n)_{n\geq 1})$ is implemented the optimal yield is given by

$$J(\Sigma) = J(1,\Sigma) := \mathbb{E}\left[\int_0^T \Psi_{u_s}(s)ds - \sum_{n\geq 1} \ell_{\xi_{n-1},\xi_n}(\tau_n)\mathbb{1}_{[\tau_n<T]}\right] \ (\xi_0 = 1).$$

We can now formulate the multi-regime switching problem as follows.

Problem. Find a strategy $\Sigma^* \equiv ((\tau_n^*)_{n\geq 1}, (\xi_n^*)_{n\geq 1}) \in \mathcal{A}$ such that

$$J(\Sigma^*) = \sup_{\Sigma\in\mathcal{A}} J(\Sigma).$$

An admissible strategy Σ is called *finite* if, during the time interval $[0,T]$, it allows the manager to make only a finite number of decisions, i.e., $\mathbb{P}[\omega, \tau_n(\omega) < T, \text{ for all } n \geq 0] = 0$. Hereafter the set of finite strategies will be denoted by $\mathcal{A}^f$. The next proposition tells us that the supremum of the expected total profit can only be reached over finite strategies .

Proposition 2.1. *The suprema over admissible strategies and finite strategies coincide:*

$$\sup_{\Sigma\in\mathcal{A}} J(\Sigma) = \sup_{\Sigma\in\mathcal{A}^f} J(\Sigma).$$

Proof. If Σ is an admissible strategy which does not belong to $\mathcal{A}^f$, then $J(\Sigma) = -\infty$. Indeed, let $B = \{\omega, \tau_n(\omega) < T, \text{ for all } n \geq 0\}$ and B^c be its complement. Since $\Sigma \in \mathcal{A} \setminus \mathcal{A}^f$, then $\mathbb{P}(B) > 0$. Recall that the processes Ψ_i belong to $\mathcal{M}^{p,1}$ (with $p > 1$). Therefore,

$$J(\Sigma) \leq \mathbb{E}\Big[\int_0^T \max_{i\in\mathcal{J}} |\Psi_i(s)|\, ds\Big] - \mathbb{E}\Big[\Big\{\sum_{n\geq 1} \ell_{\xi_{n-1},\xi_n}(\tau_n)\Big\}\mathbb{1}_B + \Big\{\sum_{n\geq 1} \ell_{\xi_{n-1},\xi_n}(\tau_n)\mathbb{1}_{[\tau_n<T]}\Big\}\mathbb{1}_{B^c}\Big] = -\infty,$$

since for any $t \leq T$ and $i, j \in \mathcal{J}$, $\ell_{ij}(t) \geq \gamma > 0$. This implies that $J(\Sigma) = -\infty$ and then (2.1) is proved. □

We finish this section by introducing the key ingredient of the proof of the main result, namely the notion of Snell envelope of processes and its properties. We refer to El Karoui [16], Cvitanic and Karatzas [6], Appendix D in Karatzas and Shreve [23] or Hamadène [18] for further details.

2.1 The Snell envelope. In the following proposition we summarize the main results on the Snell envelope of processes used in this paper.

Proposition 2.2. *Let $U = (U_t)_{0\leq t\leq T}$ be an $\boldsymbol{\mathcal{F}}$-adapted $\mathbb{R}$-valued càdlàg process that belongs to the class* [D]*, i.e., the set of random variables $\{U_\tau,\ \tau \in \mathcal{T}_0\}$ is uniformly integrable. Then, there exists an $\boldsymbol{\mathcal{F}}$-adapted $\mathbb{R}$-valued càdlàg process $Z := (Z_t)_{0\leq t\leq T}$ such that Z is the smallest super-martingale which dominates U, i.e., if $(\overline{Z}_t)_{0\leq t\leq T}$ is another càdlàg supermartingale of class* [D] *such that for all $0 \leq t \leq T$, $\overline{Z}_t \geq U_t$, then $\overline{Z}_t \geq Z_t$ for any $0 \leq t \leq T$. The process Z is called the Snell envelope of U. Moreover it enjoys the following properties:*

(i) *For any $\boldsymbol{\mathcal{F}}$-stopping time θ we have*

$$Z_\theta = \operatorname*{ess\,sup}_{\tau\in\mathcal{T}_\theta} \mathbb{E}[U_\tau|\mathcal{F}_\theta] \quad (\textit{and then } Z_T = U_T).$$

(ii) *The Doob–Meyer decomposition of Z implies the existence of a continuous martingale $(M_t)_{0\leq t\leq T}$ and two nondecreasing processes $(A_t)_{0\leq t\leq T}$ and $(B_t)_{0\leq t\leq T}$ which are respectively continuous and purely discontinuous predictable such that for all $t \in [0, T]$,*

$$Z_t = M_t - A_t - B_t \quad (\textit{with } A_0 = B_0 = 0).$$

Moreover, for any $0 \leq t \leq T$, $\{\Delta_t B > 0\} \subset \{\Delta_t U < 0\} \cap \{Z_{t-} = U_{t-}\}$.

(iii) *If U has only positive jumps then Z is a continuous process. Furthermore, if θ is an $\mathcal{F}$-stopping time and $\tau_\theta^* = \inf\{s \geq \theta, Z_s = U_s\} \wedge T$ then τ_θ^* is optimal after θ, i.e.,*

$$Z_\theta = \mathbb{E}[Z_{\tau_\theta^*}|\mathcal{F}_\theta] = \mathbb{E}[U_{\tau_\theta^*}|\mathcal{F}_\theta] = \operatorname*{ess\,sup}_{\tau \geq \theta} \mathbb{E}[U_\tau|\mathcal{F}_\theta].$$

(iv) *If $(U^n)_{n\geq 0}$ and U are càdlàg, of class* [D] *and such that the sequence $(U^n)_{n\geq 0}$ converges increasingly and pointwisely to U then $(Z^{U^n})_{n\geq 0}$ converges increasingly and pointwisely to Z^U; Z^{U_n} and Z^U are the Snell envelopes of respectively U_n and U. Finally, if U belongs to $\mathcal{S}^p$ then Z^U belongs to $\mathcal{S}^p$.*

For the sake of completeness, we give a proof of the stability result (iv), as we could not find it in the standard references mentioned above.

Proof of (iv). Since, for any $n \geq 0$, U^n converges increasingly and pointwisely to U, it follows that for all $t \in [0, T]$, $Z_t^{U_n} \leq Z_t^U$ $\mathbb{P}$-a.s. Therefore, $\mathbb{P}$-a.s., for any $t \in [0, T]$, $\lim_{n\to\infty} Z_t^{U_n} \leq Z_t^U$. Note that the process $(\lim_{n\to\infty} Z_t^{U^n})_{0\leq t\leq T}$ is a càdlàg supermartingale of class [D], since it is a limit of a nondecreasing sequence of supermartingales (see e.g. Dellacherie and Meyer [7], pp. 86). But $U^n \leq Z^{U_n}$ implies that $\mathbb{P}$-a.s., for all $t \in [0, T]$, $U_t \leq \lim_{n\to\infty} Z_t^{U^n}$. Thus, $Z_t^U \leq \lim_{n\to\infty} Z_t^{U^n}$ since the Snell envelope of U is the lowest supermartingale that dominates U. It follows that $\mathbb{P}$-a.s., for any $t \leq T$, $\lim_{n\to\infty} Z_t^{U^n} = Z_t^U$, whence the desired result. □

Assume now that U belongs to $\mathcal{S}^p$. Since, for any $0 \leq t \leq T$,

$$-\mathbb{E}\Big[\sup_{0\leq s\leq T} |U_s|\Big|\mathcal{F}_t\Big] \leq U_t \leq \mathbb{E}\Big[\sup_{0\leq s\leq T} |U_s|\Big|\mathcal{F}_t\Big],$$

using the Doob–Meyer inequality, it follows that Z^U also belongs to $\mathcal{S}^p$.

3 A Verification Theorem

In terms of a Verification Theorem, we show that this switching problem is reduced to the existence of m continuous processes $Y^1, \ldots, Y^m$ solutions of a system of equations expressed via Snell envelopes. The process Y_t^i, for $i \in \mathcal{J}$, will stand for the optimal expected profit if, at time t, the production activity is in the state i. So for τ an $\mathcal{F}$-stopping time and $(\zeta_t)_{0\leq t\leq T}$, $(\zeta'_t)_{0\leq t\leq T}$ two continuous $\mathcal{F}$-adapted and $\mathbb{R}$-valued processes let us set

$$D_\tau(\zeta = \zeta') := \inf\{s \geq \tau, \zeta_s = \zeta'_s\} \wedge T.$$

We have the following:

Theorem 1 (Verification Theorem). *Assume there exist m processes $(Y^i := (Y_t^i)_{0\leq t\leq T}$, $i = 1, \ldots, m)$ of $\mathcal{S}^p$ that satisfy* (1)*. Then:*

(i)
$$Y_0^1 = \sup_{\Sigma\in\mathcal{A}} J(\Sigma). \tag{3}$$

(ii) *Define the sequence of $\mathcal{F}$-stopping times $(\tau_n)_{n\geq 1}$ by*
$$\tau_1 = D_0\big(Y^1 = \max_{j\in\mathcal{J}^{-1}}(-\ell_{1j} + Y^j)\big) \tag{4}$$
and, for $n \geq 2$,
$$\tau_n = D_{\tau_{n-1}}\big(Y^{\xi_{n-1}} = \max_{k\in\mathcal{J}^{-\xi_{n-1}}}(-\ell_{\xi_{n-1}k} + Y^k)\big), \tag{5}$$
where

- $\xi_1 = \sum_{j\in\mathcal{J}} j\,\mathbb{1}_{\{\max_{k\in\mathcal{J}^{-1}}(-\ell_{1k}(\tau_1)+Y^k_{\tau_1}) = -\ell_{1j}(\tau_1)+Y^j_{\tau_1}\}}$;
- *for any $n \geq 1$ and $t \geq \tau_n$, $Y_t^{\xi_n} = \sum_{j\in\mathcal{J}} \mathbb{1}_{[\xi_n=j]} Y_t^j$;*
- *for $n \geq 2$, $\xi_n = l$ on the set*
$$\Big\{\max_{k\in\mathcal{J}^{-\xi_{n-1}}}(-\ell_{\xi_{n-1}k}(\tau_n) + Y^k_{\tau_n}) = -\ell_{\xi_{n-1}l}(\tau_n) + Y^l_{\tau_n}\Big\},$$

where
$$\ell_{\xi_{n-1}k}(\tau_n) = \sum_{j\in\mathcal{J}} \mathbb{1}_{[\xi_{n-1}=j]}\ell_{jk}(\tau_n) \;\text{ and }\; \mathcal{J}^{-\xi_{n-1}} = \sum_{j\in\mathcal{J}} \mathbb{1}_{[\xi_{n-1}=j]}\mathcal{J}^{-j}.$$

Then, the strategy $\Sigma^* = ((\tau_n)_{n\geq 1}, (\xi_n)_{n\geq 1})$ is optimal, i.e., $J(\Sigma^*) \geq J(v)$ for any $v \in \mathcal{A}$.

(iii) *The m-uplet of processes $(Y^1, \ldots, Y^m)$ is unique.*

Proof. Let us begin with points (i) and (ii).

Assume that at the initial time $t = 0$ the system is in mode 1. For any $t \leq T$, we have
$$Y_t^1 + \int_0^t \Psi_1(s)ds = \operatorname*{ess\,sup}_{\tau\geq t} \mathbb{E}\bigg[\int_0^\tau \Psi_1(s)ds + \max_{j\in\mathcal{J}^{-1}}(-\ell_{1j}(\tau) + Y^j_\tau)\mathbb{1}_{[\tau<T]}\big|\mathcal{F}_t\bigg].$$
But Y_0^1 is $\mathcal{F}_0$-measurable, therefore it is $\mathbb{P}$-a.s. constant and then $Y_0^1 = \mathbb{E}[Y_0^1]$.

On the other hand, according to Proposition 2.2 (iii), τ_1 as defined by (4) is optimal, and
$$\xi_1 = \sum_{j\in\mathcal{J}} j\,\mathbb{1}_{\{\max_{k\in\mathcal{J}^{-1}}(-\ell_{1k}(\tau_1)+Y^k_{\tau_1}) = -\ell_{1j}(\tau_1)+Y^j_{\tau_1}\}}.$$

Therefore,

$$Y_0^1 = \mathbb{E}\left[\int_0^{\tau_1} \Psi_1(s)ds + \max_{j\in\mathcal{J}^{-1}}(-\ell_{1j}(\tau_1) + Y_{\tau_1}^j)\mathbb{1}_{[\tau_1<T]}\right]$$
$$= \mathbb{E}\left[\int_0^{\tau_1} \Psi_1(s)ds + (-\ell_{1\xi_1}(\tau_1) + Y_{\tau_1}^{\xi_1})\mathbb{1}_{[\tau_1<T]}\right]. \quad (6)$$

Next, we claim that $\mathbb{P}$-a.s. for every $\tau_1 \le t \le T$,

$$Y_t^{\xi_1} = \operatorname*{ess\,sup}_{\tau\ge t} \mathbb{E}\Big[\int_t^{\tau} \Psi_{\xi_1}(s)ds + \max_{j\in\mathcal{J}^{-\xi_1}}(-\ell_{\xi_1 j}(\tau) + Y_\tau^j)\mathbb{1}_{[\tau<T]}\Big|\mathcal{F}_t\Big]. \quad (7)$$

To see this, remark that Eq. (1) means that the process $(Y_t^i + \int_0^t \Psi_i(s)ds)_{t\le T}$ is a supermartingale which dominates

$$\Big\{\int_0^t \Psi_i(s)ds + \max_{j\in\mathcal{J}^{-i}}(-\ell_{ij}(t) + Y_t^j)\mathbb{1}_{[t<T]},\ 0 \le t \le T\Big\}.$$

Since $\mathcal{J}$ is finite, the process $\sum_{i\in\mathcal{J}} \mathbb{1}_{[\xi_1=i]}\left(Y_t^i + \int_{\tau_1}^t \Psi_i(s)ds\right)$, for $t \ge \tau_1$, is a supermartingale which dominates

$$\sum_{i\in\mathcal{J}} \mathbb{1}_{[\xi_1=i]}\left(\int_{\tau_1}^t \Psi_i(s)ds + \max_{j\in\mathcal{J}^{-i}}(-\ell_{ij}(t) + Y_t^j)\mathbb{1}_{[t<T]}\right).$$

Thus the process $Y_t^{\xi_1} + \int_{\tau_1}^t \Psi_{\xi_1}(s)ds$, for $t \ge \tau_1$, is a supermartingale which is greater than

$$\int_{\tau_1}^t \Psi_{\xi_1}(s)ds + \max_{j\in\mathcal{J}^{-\xi_1}}(-\ell_{\xi_1 j}(t) + Y_t^j)\mathbb{1}_{[t<T]}.$$

To complete the proof it remains to show that it is the smallest one which has this property and use the characterization of the Snell envelope given in Proposition 2.2.

Indeed, let $(Z_t)_{t\in[0,T]}$ be a supermartingale of class [D] such that for any $t \ge \tau_1$,

$$Z_t \ge \int_{\tau_1}^t \Psi_{\xi_1}(s)ds + \max_{j\in\mathcal{J}^{-\xi_1}}(-\ell_{\xi_1 j}(t) + Y_t^j)\mathbb{1}_{[t<T]}.$$

It follows that for every $t \ge \tau_1$,

$$Z_t\mathbb{1}_{[\xi_1=i]} \ge \mathbb{1}_{[\xi_1=i]}\left(\int_{\tau_1}^t \Psi_i(s)ds + \max_{j\in\mathcal{J}^{-i}}(-\ell_{ij}(t) + Y_t^j)\mathbb{1}_{[t<T]}\right).$$

But the process $(Z_t\mathbb{1}_{[\xi_1=i]})_{t\in[0,T]}$ is a supermartingale for $t \ge \tau_1$ since $\mathbb{1}_{[\xi_1=i]}$ is $\mathcal{F}_{\tau_1}$-measurable and non-negative. Again with (1) it follows that for every $t \ge \tau_1$,

$$\mathbb{1}_{[\xi_1=i]}Z_t \ge \mathbb{1}_{[\xi_1=i]}\left(Y_t^i + \int_{\tau_1}^t \Psi_i(s)ds\right).$$

Summing over i, we get for every $t \geq \tau_1$,

$$Z_t \geq Y_t^{\xi_1} + \int_{\tau_1}^t \Psi_{\xi_1}(s)ds.$$

Hence, the process $Y_t^{\xi_1} + \int_{\tau_1}^t \Psi_{\xi_1}(s)ds$, $t \geq \tau_1$, is the Snell envelope of

$$\int_{\tau_1}^t \Psi_{\xi_1}(s)ds + \max_{j \in \mathcal{J}^{-\xi_1}} (-\ell_{\xi_1 j}(t) + Y_t^j)\mathbb{1}_{[t<T]},$$

whence Eq. (7).

Now from (7) and the definition of τ_2 in Eq. (5), we have

$$\begin{aligned} Y_{\tau_1}^{\xi_1} &= \mathbb{E}\left[\int_{\tau_1}^{\tau_2} \Psi_{\xi_1}(s)ds + \max_{j \in \mathcal{J}^{-\xi_1}} (-\ell_{\xi_1 j}(\tau_2) + Y_{\tau_2}^j)\mathbb{1}_{[\tau_2<T]}\big|\mathcal{F}_{\tau_1}\right] \\ &= \mathbb{E}\left[\int_{\tau_1}^{\tau_2} \Psi_{\xi_1}(s)ds + (-\ell_{\xi_1\xi_2}(\tau_2) + Y_{\tau_2}^{\xi_2})\mathbb{1}_{[\tau_2<T]}\big|\mathcal{F}_{\tau_1}\right]. \end{aligned}$$

Setting this characterization of $Y_{\tau_1}^{\xi_1}$ in (6) and noting that $\mathbb{1}_{[\tau_1<T]}$ is F_{τ_1}-measurable, it follows that

$$\begin{aligned} Y_0^1 &= \mathbb{E}\left[\int_0^{\tau_1} \Psi_1(s)ds - \ell_{1\xi_1}(\tau_1)\mathbb{1}_{[\tau_1<T]}\right] \\ &\quad + \mathbb{E}\left[\int_{\tau_1}^{\tau_2} \Psi_{\xi_1}(s)ds\mathbb{1}_{[\tau_1<T]} - \ell_{\xi_1\xi_2}(\tau_2)\mathbb{1}_{[\tau_2<T]} + Y_{\tau_2}^{\xi_2}\mathbb{1}_{[\tau_2<T]}\right] \\ &= \mathbb{E}\left[\int_0^{\tau_2} \Psi_{u_s}(s)ds - \ell_{1\xi_1}(\tau_1)\mathbb{1}_{[\tau_1<T]} - \ell_{\xi_1\xi_2}(\tau_2)\mathbb{1}_{[\tau_2<T]} + Y_{\tau_2}^{\xi_2}\mathbb{1}_{[\tau_2<T]}\right], \end{aligned}$$

since $[\tau_2 < T] \subset [\tau_1 < T]$. Repeating this procedure n times, we obtain

$$\mathbb{E}\left[\int_0^{\tau_n} \Psi_{u_s}(s)ds - \sum_{j=1}^n \ell_{\xi_{j-1}\xi_j}(\tau_j)\mathbb{1}_{[\tau_j<T]} + Y_{\tau_n}^{\xi_n}\mathbb{1}_{[\tau_n<T]}\right].$$

But the strategy $(\tau_n)_{n\geq 1}$ is finite, otherwise Y_0^1 would be equal to $-\infty$ since $\ell_{ij} \geq \gamma > 0$ contradicting the assumption that the processes Y^j belong to $\mathcal{S}^p$. Therefore, taking the limit as $n \to \infty$ we obtain $Y_0^1 = J(\Sigma^*)$.

To complete the proof it remains to show that $J(\Sigma^*) \geq J(v)$ for any other finite admissible strategy $v := ((\theta_n)_{n\geq 1}, (\zeta_n)_{n\geq 1})$ ($\tau_0 = 0$ and $\zeta_0 = 1$). The definition of the Snell envelope yields

$$\begin{aligned} Y_0^1 &\geq \mathbb{E}\left[\int_0^{\theta_1} \Psi_1(s)ds + \max_{j \in \mathcal{J}^{-1}} (-\ell_{1j}(\theta_1) + Y_{\theta_1}^j)\mathbb{1}_{[\theta_1<T]}\right] \\ &\geq \mathbb{E}\left[\int_0^{\theta_1} \Psi_1(s)ds + (-\ell_{1\zeta_1}(\theta_1) + Y_{\theta_1}^{\zeta_1})\mathbb{1}_{[\theta_1<T]}\right]. \end{aligned}$$

But once more using a similar characterization as (7), we get

$$Y_{\theta_1}^{\zeta_1} \geq \mathbb{E}\Big[\int_{\theta_1}^{\theta_2} \Psi_{\zeta_1}(s)ds + \max_{j\in\mathcal{I}^{-\zeta_1}}(-\ell_{\zeta_1 j}(\theta_2) + Y_{\theta_2}^{j})\mathbb{1}_{[\theta_2<T]}\big|\mathcal{F}_{\theta_1}\Big]$$
$$\geq \mathbb{E}\Big[\int_{\theta_1}^{\theta_2} \Psi_{\zeta_1}(s)ds + (-\ell_{\zeta_1\zeta_2}(\theta_2) + Y_{\theta_2}^{\zeta_2})\mathbb{1}_{[\theta_2<T]}\big|\mathcal{F}_{\theta_1}\Big].$$

Therefore,

$$Y_0^1 \geq \mathbb{E}\Big[\int_0^{\theta_1} \Psi_1(s)ds - \ell_{1\zeta_1}(\theta_1)\mathbb{1}_{[\theta_1<T]}\Big]$$
$$+ \mathbb{E}\Big[\mathbb{1}_{[\theta_1<T]}\int_{\theta_1}^{\theta_2} \Psi_{\zeta_1}(s)ds - \ell_{\zeta_1\zeta_2}(\theta_2)\mathbb{1}_{[\theta_2<T]} + Y_{\theta_2}^{\zeta_2}\mathbb{1}_{[\theta_2<T]}\Big]$$
$$= \mathbb{E}\Big[\int_0^{\theta_2} \Psi_{v_s}(s)ds - \ell_{1\zeta_1}(\theta_1)\mathbb{1}_{[\theta_1<T]} - \ell_{\zeta_1\zeta_2}(\theta_2)\mathbb{1}_{[\theta_2<T]} + Y_{\theta_2}^{\zeta_2}\mathbb{1}_{[\theta_2<T]}\Big],$$

where v_s, $s \leq T$, is the indicator of the mode of the plant at s associated with the strategy v (see (2)). Repeat this argument n times to obtain

$$Y_0^1 \geq \mathbb{E}\Big[\int_0^{\theta_n} \Psi_{v_s}(s)ds - \sum_{j=1}^{n} \ell_{\zeta_{j-1}\zeta_j}(\theta_j)\mathbb{1}_{[\theta_j<T]} + Y_{\theta_n}^{\zeta_n}\mathbb{1}_{[\theta_n<T]}\Big].$$

Finally, thanks to the dominated convergence theorem, taking the limit as $n \to \infty$ yields

$$Y_0^1 \geq \mathbb{E}\Big[\int_0^{T} \Psi_{v_s}(s)ds - \sum_{j\geq 1} \ell_{\zeta_{j-1}\zeta_j}(\theta_j)\mathbb{1}_{[\theta_j<T]}\Big] = J(v)$$

since the strategy v is finite. Hence, the strategy Σ^* is optimal.

Next, in order to prove uniqueness of the m-uplet $(Y^1, \ldots, Y^m)$ it is enough to show that Y_t^i, as defined by (1), is nothing but the expected total profit or the value function of the optimal problem, given that the system is in mode i at time t. More precisely we have

$$Y_t^i = \operatorname*{ess\,sup}_{\Sigma\in\mathcal{A}_t^{f,i}} \mathbb{E}\Big[\int_t^{T} \Psi_{u_s}(s)ds - \sum_{j\geq 1} \ell_{\xi_{j-1}\xi_j}(\tau_j)\mathbb{1}_{[\tau_j<T]}\big|\mathcal{F}_t\Big], \quad t \leq T, \tag{8}$$

where $\mathcal{A}_t^{f,i}$ is the set of finite strategies such that $\tau_1 \geq t$, $\mathbb{P}$-a.s. and $u_t = i$ (at time t the system is in mode i). The proof of this claim is obtained in the same way as we did above. This characterization implies in particular that the processes $Y^1, \ldots, Y^m$ are unique. The proof is now complete. □

4 Existence of the processes $(Y^1, \dots, Y^m)$

We will now establish existence of the processes $(Y^1, \dots, Y^m)$. They will be obtained as a limit of a sequence of processes $(Y^{1,n}, \dots, Y^{m,n})_{n\geq 0}$ defined recursively by means of the Snell envelope notion as follows:

For $i \in \mathcal{J}$, let us set, for any $0 \leq t \leq T$,

$$Y_t^{i,0} = \mathbb{E}\Big[\int_0^T \Psi_i(s)ds\big|\mathcal{F}_t\Big] - \int_0^t \Psi_i(s)ds, \tag{9}$$

and for $n \geq 1$,

$$Y_t^{i,n} = \operatorname*{ess\,sup}_{\tau\geq t} \mathbb{E}\Big[\int_0^\tau \Psi_i(s)ds + \max_{k\in\mathcal{J}^{-i}}(-\ell_{ik}(\tau)+Y_\tau^{k,n-1})\mathbb{1}_{[\tau<T]}\big|\mathcal{F}_t\Big] - \int_0^t \Psi_i(s)ds. \tag{10}$$

In the next proposition we collect some useful properties of $Y^{1,n}, \dots, Y^{m,n}$. In particular we show that the limit processes $\widetilde{Y}^i := \lim_{n\to\infty} Y^{i,n}$ exist and are only càdlàg but have the same characterization (1) as the Y^i's. Thus the existence proof of the Y^i's will consist in showing that $\widetilde{Y}^i$'s are continuous and hence satisfy the Verification Theorem. This will be done in Theorem 2 below.

Proposition 4.1. (i) *For each $n \geq 0$, the processes $Y^{1,n}, \dots, Y^{m,n}$ are continuous and belong to $\mathcal{S}^p$.*

(ii) *For any $i \in \mathcal{J}$, the sequence $(Y^{i,n})_{n\geq 0}$ converges increasingly and pointwisely $\mathbb{P}$-a.s. for any $0 \leq t \leq T$ and in $\mathcal{M}^{p,1}$ to a càdlàg processes $\widetilde{Y}^i$. Moreover these limit processes $\widetilde{Y}^i = (\widetilde{Y}_t^i)_{0\leq t\leq T}$, $i = 1, \dots, m$, satisfy the following:*

(a) $\mathbb{E}\big[\sup_{0\leq t\leq T} |\widetilde{Y}_t^i|^p\big] < \infty$, $i \in \mathcal{J}$.

(b) *For any $0 \leq t \leq T$ we have,*

$$\widetilde{Y}_t^i = \operatorname*{ess\,sup}_{\tau\geq t} \mathbb{E}\Big[\int_t^\tau \Psi_i(s)ds + \max_{k\in\mathcal{J}^{-i}}(-\ell_{ik}(\tau) + \widetilde{Y}_\tau^k)\mathbb{1}_{[\tau<T]}\big|\mathcal{F}_t\Big].$$

Proof. (i) Let us show by induction that for any $n \geq 0$ and every $i \in \mathcal{J}$, $Y^{i,n} \in \mathcal{S}^p$. For $n = 0$ the property holds true since we can write $Y^{i,0}$ as the sum of a continuous process and a martingale w.r.t. to the Brownian filtration. Therefore $Y^{i,0}$ is continuous and since the process $(\Psi_i(s))_{0\leq s\leq T}$ belongs to $\mathcal{M}^{p,1}$, using Doob's inequality, we obtain that $Y^{i,0}$ belongs to $\mathcal{S}^p$. Suppose now that the property is satisfied for some n. By Proposition 2.2, for every $i \in \mathcal{J}$ and up to a term, $Y^{i,n+1}$ is the Snell envelope of the process $(\int_0^t \Psi_i(s)ds + \max_{k\in\mathcal{J}^{-i}}(-\ell_{ik}(t) + Y_t^{k,n})\mathbb{1}_{[t<T]})_{0\leq t\leq T}$. But $\max_{k\in\mathcal{J}^{-i}}(-\ell_{ik}(t) + Y_t^{k,n})\big|_{t=T} < 0$ because $\ell_{ij} \geq \gamma$ and $Y_T^{n,k} = 0$, then the process $(\max_{k\in\mathcal{J}^{-i}}(-\ell_{ik}(t) + Y_t^{k,n})\mathbb{1}_{[t<T]})_{t\leq T}$ is continuous on $[0, T[$ and have a positive jump

at T since $Y^{n,k}$ is continuous. Hence $Y^{i,n+1}$ is continuous (Proposition 2.2 (iii)) and belongs to $\mathcal{S}^p$. This shows that, for every $i \in \mathcal{J}$, $Y^{i,n} \in \mathcal{S}^p$ for any $n \geq 0$.

(ii) Let us now set

$$\mathcal{A}_t^{i,n} = \big\{\Sigma = ((\tau_n)_{n\geq 1}, (\xi_n)_{n\geq 1}) \in \mathcal{A}\ (\tau_0 = 0,\ \xi_0 = i),\ \tau_1 \geq t \text{ and } \tau_{n+1} = T\big\}.$$

Using the same arguments as the ones of the Verification Theorem 1, the following characterization of the processes $Y^{i,n}$ holds true:

$$Y_t^{i,n} = \operatorname*{ess\,sup}_{\Sigma\in\mathcal{A}_t^{i,n}} \mathbb{E}\Big[\int_t^T \Psi_{u_s}(s)ds - \sum_{j=1}^{n} \ell_{\xi_{j-1}\xi_j}(\tau_j)\mathbb{1}_{[\tau_j<T]}\big|\mathcal{F}_t\Big]. \tag{11}$$

Since $\mathcal{A}_t^{i,n} \subset \mathcal{A}_t^{i,n+1}$, we have $\mathbb{P}$-a.s. for all $t \in [0,T]$, $Y_t^{i,n} \leq Y_t^{i,n+1}$ thanks to the continuity of $Y^{i,n}$. Using once more (11) and since $\ell_{ij} \geq \gamma > 0$, we obtain for each $i \in \mathcal{J}$:

$$\forall\ 0 \leq t \leq T, \quad Y_t^{i,n} \leq \mathbb{E}\Big[\int_t^T \max_{i=1,\ldots,m} |\Psi_i(s)|ds\big|\mathcal{F}_t\Big]. \tag{12}$$

Therefore, for every $i \in \mathcal{J}$, the sequence $(Y^{i,n})_{n\geq 0}$ is convergent and then let us set $\widetilde{Y}_t^i := \lim_{n\to\infty} Y_t^{i,n}$, for $t \leq T$. The process $\widetilde{Y}^i$ satisfies

$$Y_t^{i,0} \leq \widetilde{Y}_t^i \leq \mathbb{E}\Big[\int_t^T \max_{i=1,\ldots,m} |\Psi_i(s)|ds\big|\mathcal{F}_t\Big], \quad 0 \leq t \leq T. \tag{13}$$

Let us now show that $\widetilde{Y}^i$ is càdlàg. Actually, for each $i \in \mathcal{J}$ and $n \geq 1$, by Eq. (10), the process $(Y_t^{i,n} + \int_0^t \Psi_i(s)ds)_{0\leq t\leq T}$ is a continuous supermartingale. Hence its limit process $(\widetilde{Y}_t^i + \int_0^t \Psi_i(s)ds)_{0\leq t\leq T}$ is càdlàg as a limit of increasing sequence of continuous supermartingales (see Dellacherie and Meyer [7], pp. 86). Therefore $\widetilde{Y}^i$ is càdlàg. Next using (13), the L^p-properties of Ψ_i and Doob's Maximal Inequality yield, for each $i \in \mathcal{J}$,

$$\mathbb{E}\big[\sup_{0\leq t\leq T} |\widetilde{Y}_t^i|^p\big] < \infty.$$

By the Lebesgue dominated convergence theorem, the sequence $(Y^{i,n})_{n\geq 0}$ also converges to $\widetilde{Y}^i$ in $\mathcal{M}^{p,1}$.

Finally, the càdlàg processes $\widetilde{Y}^1, \ldots, \widetilde{Y}^m$ satisfy Eq. (1), since they are limits of the increasing sequence of processes $Y^{i,n}$, $i \in \mathcal{J}$, that satisfy (10). We use Proposition 2.2 (iv) to conclude. □

We will now prove that the processes $\widetilde{Y}^1, \ldots, \widetilde{Y}^m$ are continuous and satisfy the Verification Theorem 1.

Theorem 2. *The limit processes $\widetilde{Y}^1, \ldots, \widetilde{Y}^m$ satisfy the Verification Theorem.*

Proof. Recall from Proposition 4.1 that the processes $\widetilde{Y}^1, \dots, \widetilde{Y}^m$ are càdlàg, uniformly L^p-integrable and satisfy (1). It remains to prove that they are continuous.

Indeed note that, for $i \in \mathcal{J}$, the process $(\widetilde{Y}^i_t + \int_0^t \Psi_i(s)ds)_{0\le t\le T}$ is the Snell envelope of

$$\left(\int_0^t \Psi_i(s)ds + \max_{k\in\mathcal{J}^{-i}} (-\ell_{ik}(t) + \widetilde{Y}^k_t)\mathbb{1}_{[t<T]} \right)_{0\le t\le T}.$$

Of course the processes $\left(\int_0^t \Psi_i(s)ds \right)_{0\le t\le T}$ are continuous. Therefore from the property of the jumps of the Snell envelope (Proposition 2.2 (ii)), when there is a jump of $\widetilde{Y}^i$ at t (which is necessarily negative), there is a jump, at the same time t, of the process $(\max_{k\in\mathcal{J}^{-i}}(-\ell_{ik}(s) + \widetilde{Y}^k_s))_{0\le s\le T}$. Since ℓ_{ij} are continuous, there is $j \in \mathcal{J}^{-i}$ such that $\Delta_t \widetilde{Y}^j < 0$ and $\widetilde{Y}^i_{t-} = -\ell_{ij}(t) + \widetilde{Y}^j_{t-}$.

Suppose now there is an index $i_1 \in \mathcal{J}$ for which there exists $t \in [0,T]$ such that $\Delta_t \widetilde{Y}^{i_1} < 0$. This implies that there exists another index $i_2 \in \mathcal{J}^{-i_1}$ such that $\Delta_t \widetilde{Y}^{i_2} < 0$ and $\widetilde{Y}^{i_1}_{t-} = -\ell_{i_1 i_2}(t) + \widetilde{Y}^{i_2}_{t-}$. But given i_2, there exists an index $i_3 \in \mathcal{J}^{-i_2}$ such that $\Delta_t \widetilde{Y}^{i_3} < 0$ and $\widetilde{Y}^{i_2}_{t-} = -\ell_{i_2 i_3}(t) + \widetilde{Y}^{i_3}_{t-}$. Repeating this argument many times, we get a sequence of indices $i_1, \dots, i_j, \dots \in \mathcal{J}$ that have the property that $i_k \in \mathcal{J}^{-i_{k-1}}$, $\Delta_t \widetilde{Y}^{i_k} < 0$ and $\widetilde{Y}^{i_{k-1}}_{t-} = -\ell_{i_{k-1} i_k}(t) + \widetilde{Y}^{i_k}_{t-}$.

As $\mathcal{J}$ is finite there exist two indices $m < r$ such that $i_m = i_r$ and $i_m, i_{m+1}, \dots, i_{r-1}$ are mutually different. It follows that

$$\begin{aligned}\widetilde{Y}^{i_m}_{t-} &= -\ell_{i_m i_{m+1}}(t) + \widetilde{Y}^{i_{m+1}}_{t-} = -\ell_{i_m i_{m+1}}(t) - \ell_{i_{m+1} i_{m+2}}(t) + \widetilde{Y}^{i_{m+2}}_{t-} \\ &= \dots = -\ell_{i_m i_{m+1}}(t) - \dots - \ell_{i_{r-1} i_r}(t) + \widetilde{Y}^{i_r}_{t-}.\end{aligned}$$

As $i_m = i_r$ we get

$$-\ell_{i_m i_{m+1}}(t) - \dots - \ell_{i_{r-1} i_r}(t) = 0$$

which is impossible since for any $i \neq j$, all $0 \le t \le T$, $\ell_{ij}(t) \ge \gamma > 0$. Therefore there is no $i \in \mathcal{J}$ for which there is a $t \in [0,T]$ such that $\Delta_t \widetilde{Y}^i < 0$. This means that the processes $\widetilde{Y}^1, \dots, \widetilde{Y}^m$ are continuous. Since they satisfy (1), then by uniqueness, $Y^i = \widetilde{Y}^i$, for any $i \in \mathcal{J}$. Thus, the Verification Theorem 1 is satisfied by $Y^1, \dots, Y^m$. □

Remark 1. As an immediate consequence of Dini's theorem and the Lebesgue dominated convergence theorem, it holds true that

$$\forall i \in \mathcal{J}, \quad \mathbb{E}\big[\sup_{s\le T} |Y^{i,n}_s - Y^i_s|^p\big] \to 0 \quad \text{as } n \to +\infty.$$

5 Connection with systems of BSDEs with oblique reflection

In this section we take $p = 2$. Next let us introduce the notion of a reflected backward stochastic differential equation. For this let us consider:

(i) $f:[0,T]\times\Omega\times\mathbb{R}^{1+d}\to\mathbb{R}$ such that the process $(f(t,\omega,0,0))_{t\leq T}$ belongs to $\mathcal{M}^{2,1}$ and the mapping $(y,z)\mapsto f(t,\omega,y,z)$ is Lipschitz continuous uniformly in (t,ω);

(ii) ξ a square integrable $\mathcal{F}_T$-measurable random variable;

(iii) $S:=(S_t)_{t\leq T}$ a process of $\mathcal{S}^2$ which satisfies also $S_T\leq\xi$, $\mathbb{P}$-a.s.

Then we have the following result related to the existence and uniqueness of a solution of the reflected BSDE associated with (f,ξ,S).

Theorem 3 ([17], Thm. 5.2). *There exists a unique triple of processes $(Y_t,Z_t,K_t)_{t\leq T}$ with values in $\mathbb{R}^{1+d+1}$ such that*

$$\begin{cases} Y,K\in\mathcal{S}^2 \text{ and } Z\in\mathcal{M}^{2,d};\ K \text{ is non-decreasing and } K_0=0,\\ Y_s=\xi+\int_s^T f(r,Y_r,Z_r)dr-\int_s^T Z_r dB_r+K_T-K_s,\ \forall s\leq T,\\ Y_s\geq S_s,\ \forall s\leq T \text{ and } \int_0^T(Y_r-S_r)dK_r=0. \end{cases} \tag{14}$$

Moreover the following characterization of the process Y as a Snell envelope holds true:

$$\forall s\leq T,\ Y_s=\ \text{ess sup}_{\tau\in\mathcal{T}_s}E\left[\int_s^\tau f(r,Y_r,Z_r)dr+S_\tau\mathbb{1}_{[\tau<T]}+\xi\mathbb{1}_{[\tau=T]}\big|\mathcal{F}_s\right]. \tag{15}$$

Therefore from (15) and Theorem 2 we have the following result related the solution of the system of BSDEs obliquely reflected associated with the switching problem.

Theorem 4. *There exist processes (K^i,Z^i), $i\in\mathcal{J}$, such that the triples (Y^i,Z^i,K^i), $i\in\mathcal{J}$, is the unique solution of the following system of oblique reflected BSDEs: $\forall i\in\mathcal{J}$,*

$$\begin{cases} Y^i,K^i\in\mathcal{S}^2 \text{ and } Z^i\in\mathcal{M}^{2,d};\ K^i \text{ is non-decreasing and } K^i_0=0,\\ Y^i_s=\int_s^T\Psi_i(r)dr-\int_s^T Z^i_r dB_r+K^i_T-K^i_s,\ \forall s\leq T\ (Y^i_T=0);\\ Y^i_s\geq\max_{j\in\mathcal{J}^{-i}}(-\ell_{ij}(s)+Y^j_s),\ \forall s\leq T,\\ \int_0^T(Y^i_r-\max_{j\in\mathcal{J}^{-i}}(-\ell_{ij}(r)+Y^j_r))dK^i_r=0. \end{cases} \tag{16}$$

6 The Markovian framework of the optimal switching problem and its associated system of variational inequalities

6.1 Preliminaries. Let us introduce the following deterministic functions:

(i) $b:[0,T]\times\mathbb{R}^k\to\mathbb{R}^k$ and $\sigma:[0,T]\times\mathbb{R}^k\to\mathbb{R}^{k\times d}$ are two continuous functions and there exists a constant $C\geq 0$ such that for any $t\in[0,T]$ and $x,x'\in\mathbb{R}^k$

$$\begin{aligned} &|b(t,x)|+|\sigma(t,x)|\leq C(1+|x|)\quad\text{and}\\ &|\sigma(t,x)-\sigma(t,x')|+|b(t,x)-b(t,x')|\leq C|x-x'|. \end{aligned} \tag{17}$$

(ii) For $i, j \in \mathcal{J} = \{1, \dots, m\}$, $\ell_{ij} : [0,T] \times \mathbb{R}^k \to \mathbb{R}$ and $\psi_i : [0,T] \times \mathbb{R}^k \to \mathbb{R}$ are continuous functions and of polynomial growth, i.e., there exist some positive constants C and λ such that for each $i, j \in \mathcal{J}$,

$$|\psi_i(t,x)| + |\ell_{ij}(t,x)| \leq C(1 + |x|^\lambda), \quad \forall (t,x) \in [0,T] \times \mathbb{R}^k.$$

Moreover we assume that there exists a constant $\gamma > 0$ such that for any $(t,x) \in [0,T] \times \mathbb{R}^k$,

$$\min\{\ell_{ij}(t,x), i, j \in \mathcal{J},\ i \neq j\} \geq \gamma. \tag{18}$$

We now consider the following system of m variational inequalities with interconnected obstacles: $\forall\ i \in \mathcal{J}$,

$$\begin{cases} \min\big\{v_i(t,x) - \max\limits_{j \in \mathcal{J}^{-i}} (-\ell_{ij}(t,x) + v_j(t,x)); \\ \qquad\qquad -\partial_t v_i(t,x) - \mathcal{A}v_i(t,x) - \psi_i(t,x)\big\} = 0, \\ v_i(T,x) = 0, \end{cases} \tag{19}$$

where, for the sake of simplicity, we take $\mathcal{J}^{-i} := \mathcal{J} - \{i\}$ and $\mathcal{A}$ is the following infinitesimal generator:

$$\mathcal{A} = \frac{1}{2} \sum_{i,j=1,k} (\sigma\sigma^\top)_{ij}(t,x) \partial^2_{x_i x_j} + \sum_{i=1,k} b_i(t,x) \partial_{x_i}; \tag{20}$$

here the superscript "$\top$" stands for the transpose. This system is the deterministic version of the Verification Theorem associated with the optimal switching problem in the Markovian framework.

The main objective of this part is to focus on the existence and uniqueness of the solution in viscosity sense of (19) whose definition is as follows:

Definition 1. Let $(v_1, \dots, v_m)$ be a m-uplet of continuous functions defined on $[0,T] \times \mathbb{R}^k$, $\mathbb{R}$-valued and such that $v_i(T,x) = 0$ for any $x \in \mathbb{R}^k$ and $i \in \mathcal{J}$. The m-uplet $(v_1, \dots, v_m)$ is called:

(i) a viscosity supersolution (resp. subsolution) of the system (19) if for each fixed $i \in \mathcal{J}$, for any $(t_0, x_0) \in [0,T] \times \mathbb{R}^k$ and any function $\varphi_i \in C^{1,2}([0,T] \times \mathbb{R}^k)$ such that $\varphi_i(t_0,x_0) = v_i(t_0,x_0)$ and (t_0,x_0) is a local maximum of $\varphi_i - v_i$ (resp. minimum), we have

$$\begin{aligned} \min\big\{&v_i(t_0,x_0) - \max_{j \in \mathcal{J}^{-i}} (-\ell_{ij}(t_0,x_0) + v_j(t_0,x_0)), \\ &-\partial_t \varphi_i(t_0,x_0) - \mathcal{A}\varphi_i(t_0,x_0) - \psi_i(t_0,x_0)\big\} \geq 0 \quad (\text{resp. } \leq 0); \end{aligned} \tag{21}$$

(ii) a viscosity solution if it is both a viscosity supersolution and subsolution.

Let $(t,x)\in[0,T]\times\mathbb{R}^k$ and let $(X_s^{t,x})_{s\leq T}$ be the solution of the following standard SDE:

$$dX_s^{t,x}=b(s,X_s^{t,x})ds+\sigma(s,X_s^{t,x})dB_s \text{ for } t\leq s\leq T, \text{ and } X_s^{t,x}=x \text{ for } s\leq t, \quad (22)$$

where the functions b and σ are the ones of (17). These properties of σ and b imply in particular that the process $(X_s^{t,x})_{0\leq s\leq T}$ solution of the standard SDE (22) exists and is unique, for any $t\in[0,T]$ and $x\in\mathbb{R}^k$. The operator $\mathcal{A}$ that is appearing in (20) is the infinitesimal generator associated with $X^{t,x}$.

In the following result we collect some properties of $X^{t,x}$.

Proposition 6.1 (see e.g. [25]). *The process $X^{t,x}$ satisfies the following estimates:*

(i) *For any $q\geq 2$, there exists a constant C such that*

$$\mathbb{E}[\sup_{0\leq s\leq T}|X_s^{t,x}|^q]\leq C(1+|x|^q). \quad (23)$$

(ii) *There exists a constant C such that for any $t,t'\in[0,T]$ and $x,x'\in\mathbb{R}^k$,*

$$\mathbb{E}[\sup_{0\leq s\leq T}|X_s^{t,x}-X_s^{t',x'}|^2]\leq C(1+|x|^2)(|x-x'|^2+|t-t'|). \quad (24)$$

□

We are going now to make the connection between solutions of reflected BSDEs of type (14) and viscosity solutions of variational inequalities.

For this we introduce deterministic functions $\varphi:[0,T]\times\mathbb{R}^{k+1+d}\to\mathbb{R}$, $h:[0,T]\times\mathbb{R}^k\to\mathbb{R}$ and $g:\mathbb{R}^k\to\mathbb{R}$ continuous, of polynomial growth and such that $h(x,T)\leq g(x)$. Additionally we assume that for any $(t,x)\in[0,T]\times\mathbb{R}^k$, the mapping $(y,z)\in\mathbb{R}^{1+d}\mapsto\varphi(t,x,y,z)$ is Lipschitz continuous uniformly in $(t,x)\in[0,T]\times\mathbb{R}^k$. Then we have:

Theorem 5 ([17], Thm. 8.5). *For any $(t,x)\in[0,T]\times\mathbb{R}^k$, let $(Y^{t,x},Z^{t,x},K^{t,x})$ be the solution of the reflected BSDE associated with $(\varphi(s,X_s^{t,x},y,z),g(X_T^{t,x}),h(s,X_s^{t,x}))$, i.e.,*

$$\begin{cases} Y^{t,x},K^{t,x}\in\mathcal{S}^2 \text{ and } Z^{t,x}\in\mathcal{M}^{2,d};\ K^{t,x} \text{ is non-decreasing and } K_0^{t,x}=0,\\ Y_s^{t,x}=g(X_T^{t,x})+\int_s^T\varphi(r,X_r^{t,x},Y_r^{t,x},Z_r^{t,x})dr-\int_s^T Z_r^{t,x}dB_r+K_T^{t,x}-K_s^{t,x}, \quad s\leq T,\\ Y_s^{t,x}\geq h(s,X_s^{t,x}),\ \forall s\leq T \text{ and } \int_0^T(Y_r^{t,x}-h(r,X_r^{t,x}))dK_r^{t,x}=0. \end{cases}$$

Then there exists a deterministic continuous with polynomial growth function $u:[0,T]\times\mathbb{R}^k\to\mathbb{R}$ such that for any $s\in[t,T]$, $Y_s^{t,x}=u(s,X_s^{t,x})$. Moreover the function u is solution in viscosity sense of the following variational inequality:

$$\begin{cases} \min\{u(t,x)-h(t,x);\\ \qquad -\partial_t u(t,x)-\mathcal{A}u(t,x)-f(t,x,u(t,x),\sigma(t,x)^\top\nabla_x u(t,x))\}=0,\\ u(T,x)=g(x) \end{cases}$$

where ∇_x is the gradient w.r.t. x. □

6.2 Existence of a solution for the system of variational inequalities (19). Let $(Y_s^{1,t,x},\dots,Y_s^{m,t,x})_{0\le s\le T}$ be the processes that satisfy the Verification Theorem 1 in the case when $\Psi_i(s,\omega)=\psi_i(s,X_s^{t,x}(\omega))$ and $\ell_{ij}(s,\omega)=\ell_{ij}(s,X_s^{t,x}(\omega))$, $s\le T$ and $i,j\in\mathcal{J}$. Note that in this case, thanks to the above assumptions on the deterministic functions ψ_i and ℓ_{ij}, the processes $(\psi_i(s,X_s^{t,x}(\omega)))_{s\le T}$ and $(\ell_{ij}(s,X_s^{t,x}(\omega)))_{s\le T}$, $i,j\in\mathcal{J}$, belong to $\mathcal{M}^{p,1}$ and $\mathcal{S}^p$ respectively for any $p>1$. Therefore using Theorem 4, there exist processes $K^{i,t,x}$ and $Z^{i,t,x}$, $i\in\mathcal{J}$, such that the triples $(Y^{i,t,x},Z^{i,t,x},K^{i,t,x})$, $i\in\mathcal{J}$, is the unique solution of the following system of reflected BSDEs: $\forall i\in\mathcal{J}$,

$$\begin{cases} Y^{i,t,x},K^{i,t,x}\in\mathcal{S}^2 \text{ and } Z^{i,t,x}\in\mathcal{M}^{2,d}\,;\ K^{i,t,x} \text{ is non-decreasing and } K_0^{i,t,x}=0,\\ Y_s^{i,t,x}=\int_s^T\psi_i(r,X_r^{t,x})du-\int_s^T Z_r^{i,t,x}dB_r+K_T^{i,t,x}-K_s^{i,t,x},\\ \qquad\qquad\qquad\qquad\qquad\qquad \forall s\le T\ (Y_T^{i,t,x}=0),\\ Y_s^{i,t,x}\ge\max\limits_{j\in\mathcal{J}^{-i}}(-\ell_{ij}(s,X_s^{t,x})+Y_s^{j,t,x}),\ \forall s\le T,\\ \int_0^T(Y_r^{i,t,x}-\max\limits_{j\in\mathcal{J}^{-i}}(-\ell_{ij}(r,X_r^{t,x})+Y_r^{j,t,x}))dK_r^{i,t,x}=0. \end{cases}$$

Moreover we have:

Proposition 6.2. *There exist deterministic functions $v^1,\dots,v^m\colon[0,T]\times\mathbb{R}^k\to\mathbb{R}$ such that*

$$\forall(t,x)\in[0,T]\times\mathbb{R}^k,\ \forall s\in[t,T],\quad Y_s^{i,t,x}=v^i(s,X_s^{t,x}),\quad i=1,\dots,m.$$

Additionally the functions v^i, $i=1,\dots,m$, are lower semi-continuous and of polynomial growth.

Proof. For $n\ge0$ let $(Y_s^{n,1,t,x},\dots,Y_s^{n,m,t,x})_{0\le s\le T}$ be the processes constructed in (9) and (10) when $\Psi_i(s,\omega)=\psi_i(s,X_s^{t,x}(\omega))$ and $\ell_{ij}(s,\omega)=\ell_{ij}(s,X_s^{t,x}(\omega))$, $s\le T$ and $i,j\in\mathcal{J}$. Then using an induction argument and Theorems 3 and 5, there exist deterministic continuous with polynomial growth functions $v^{i,n}$ $(i=1,\dots,m)$ such that for any $(t,x)\in[0,T]\times\mathbb{R}^k$, $\forall s\in[t,T]$, $Y_s^{n,i,t,x}=v^{i,n}(s,X_s^{t,x})$. Using now inequality (12) we get

$$Y_t^{n,i,t,x}\le Y_t^{n+1,i,t,x}\le\mathbb{E}\Big[\int_t^T\big\{\max_{i=1,\dots,m}|\psi_i(s,X_s^{t,x})|\big\}ds\Big]$$

since $Y_t^{n,i,t,x}$ is deterministic. Therefore combining the polynomial growth of ψ_i and estimate (23) for $X^{t,x}$ we obtain

$$v^{i,n}(t,x)\le v^{i,n+1}(t,x)\le C(1+|x|^\lambda)$$

for some constants C and λ independent of n. In order to complete the proof it is enough now to set $v^i(t,x):=\lim_{n\to\infty}v^{i,n}(t,x)$, $(t,x)\in[0,T]\times\mathbb{R}^k$ since $Y^{i,n,t,x}\nearrow Y^{i,t,x}$ as $n\to\infty$. □

We are now going to focus on the continuity of the functions $v^1, \dots, v^m$. For this we first deal with some properties of the optimal strategy which exist thanks to Theorem 1.

Proposition 6.3. *Let $(\delta, \xi) = ((\tau_n)_{n\geq 1}, (\xi_n)_{n\geq 1})$ be an optimal strategy, then there exist two positive constant C and p which do not depend on t and x such that*

$$\forall n \geq 1, \quad \mathbb{P}[\tau_n < T] \leq \frac{C(1+|x|^p)}{n}. \tag{25}$$

Proof. Recall the characterization of (8) that reads as follows:

$$Y_0^{1,t,x} = \sup_{(\delta,\xi)\in\mathcal{A}^f} \mathbb{E}\Big[\int_0^T \psi_{u_r}(r, X_r^{t,x})dr - \sum_{k\geq 1} \ell_{\xi_{k-1}\xi_k}(\tau_k, X_{\tau_k}^{t,x})\mathbb{1}_{[\tau_k<T]}\Big].$$

Now if $(\delta, \xi) = ((\tau_n)_{n\geq 1}, (\xi_n)_{n\geq 1})$ $(\tau_0 = 0, \xi_0 = 1)$ is the optimal strategy then we have

$$Y_0^{1,t,x} = \mathbb{E}\Big[\int_0^T \psi_{u_r}(r, X_r^{t,x})dr - \sum_{k\geq 1} \ell_{\xi_{k-1}\xi_k}(\tau_k, X_{\tau_k}^{t,x})\mathbb{1}_{[\tau_k<T]}\Big].$$

Taking into account that $\ell_{ij} \geq \gamma > 0$ for any $i \neq j$ we obtain

$$\begin{aligned}\mathbb{E}\Big[\sum_{k=1,n} \gamma \mathbb{1}_{[\tau_k<T]}\Big] + Y_0^{1,t,x} \\ \leq \mathbb{E}\Big[\int_0^T \psi_{u_r}(r, X_r^{t,x})dr - \sum_{k\geq n+1} \ell_{\xi_{k-1}\xi_k}(\tau_k, X_{\tau_k}^{t,x})\mathbb{1}_{[\tau_k<T]}\Big].\end{aligned}$$

But for any $k \leq n$, $[\tau_n < T] \subset [\tau_k < T]$, so

$$\gamma n \mathbb{P}[\tau_n < T] + Y_0^{1,t,x} \leq \mathbb{E}\Big[\int_0^T \psi_{u_r}(r, X_r^{t,x})dr\Big].$$

and hence

$$\begin{aligned}n\gamma\mathbb{P}[\tau_n < T] &\leq \mathbb{E}\Big[\int_0^T \mid \psi_{u_r}(r, X_r^{t,x}) \mid dr\Big] - Y_0^{1,t,x} \\ &\leq \mathbb{E}\Big[\int_0^T \mid \psi_{u_r}(r, X_r^{t,x}) \mid dr\Big] - Y_0^{1,0,t,x}.\end{aligned}$$

Finally taking into account the facts that ψ_i and $Y^{1,0,t,x}$ are of polynomial growth and estimate (23) for $X^{t,x}$ to obtain the desired result. Note that the polynomial growth of $Y^{1,0,t,x}$ stems from (13). □

Remark 2. The estimate (25) is also valid for the optimal strategy if at the initial time the state of the plant is an arbitrary $i \in \mathcal{I}$. □

Next for $i \in \mathcal{J}$ let $(y_s^{i,t,x}, z_s^{i,t,x}, k_s^{i,t,x})_{s\le T}$ be the processes defined as follows:

$$\begin{cases} y^{i,t,x}, k^{i,t,x} \in \mathcal{S}^2 \text{ and } z^{i,t,x} \in \mathcal{M}^{2,d};\ k^{i,t,x} \text{ is non-decreasing and } k_0^{i,t,x} = 0, \\ y_s^{i,t,x} = \displaystyle\int_s^T \psi_i(r, X_r^{t,x})\mathbb{1}_{[r\ge t]}dr - \int_s^T z_r^{i,t,x}dB_r + k_T^{i,t,x} - k_s^{i,t,x},\ \ \forall\, s \le T, \\ y_s^{i,t,x} \ge l_s^{i,t,x} := \max\limits_{j\in\mathcal{J}^{-i}} \{-\ell_{ij}(t\vee s, X_{t\vee s}^{t,x}) + y_s^{j,t,x})\},\ \ \forall s \le T, \\ \displaystyle\int_0^T (y_r^{i,t,x} - l_r^{i,t,x})dk_r^{i,t,x} = 0. \end{cases}$$

The existence of $(y^{i,t,x}, z^{i,t,x}, k^{i,t,x}), i \in \mathcal{J}$, is obtained through Theorem 4. On the other hand, once more thanks to uniqueness in Theorem 4, for any $(t,x) \in [0,T]\times\mathbb{R}^k$, for any $s \in [0,t]$ we have $y_s^{i,t,x} = Y_t^{i,t,x}$, $z_s^{i,t,x} = 0$ and $k_s^{i,t,x} = 0$.

We are now ready to give the main result of this section.

Theorem 6. *For any $i = 1,\dots,m$, the function $v^i : [0,T]\times\mathbb{R}^k \to \mathbb{R}$ is continuous and $(v^1,\dots,v^m)$ is solution in viscosity sense of the system of variational inequalities with inter-connected obstacles* (19).

Proof. First let us focus on continuity and let us show that v^1 is continuous. The same proof will be valid for the continuity of the other functions v^i $(i = 2,\dots,m)$.

First the characterization (8) implies that

$$y_0^{1,t,x} = \sup_{(\delta,\xi)\in\mathcal{A}^f} \mathbb{E}\Big[\int_0^T \psi_{u_s}(s, X_s^{t,x})\mathbb{1}_{[s\ge t]}ds - \sum_{n\ge 1} \ell_{\xi_{n-1}\xi_n}(\tau_n\vee t, X_{\tau_n\vee t}^{t,x})\mathbb{1}_{[\tau_n<T]}\Big].$$

On the other hand an optimal strategy $(\delta_{t,x}^*, \xi_{t,x}^*)$ exists and satisfies the estimates (25) with the same constants C and p. Next let $\epsilon > 0$ and $(t',x') \in B((t,x),\epsilon)$ and let us consider the following set of strategies:

$$\widetilde{\mathcal{D}} := \{(\delta,\xi) = ((\tau_n)_{n\ge1}, (\xi_n)_{n\ge1}) \in \mathcal{A}^f \quad (\tau_0 = 0,\ \xi_0 = 1)$$

such that

$$\forall n \ge 1, \quad \mathbb{P}[\tau_n < T] \le \frac{C(1 + (\epsilon + |x|)^p)}{n}\}.$$

Therefore the strategies $(\delta_{t,x}^*, \xi_{t,x}^*)$ and $(\delta_{t',x'}^*, \xi_{t',x'}^*)$ belong to $\widetilde{\mathcal{D}}$ and then we have

$$\begin{aligned} y_0^{1,t,x} &= \sup_{(\delta,\xi)\in\widetilde{\mathcal{D}}} \mathbb{E}\Big[\int_0^T \psi_{u_s}(s, X_s^{t,x})\mathbb{1}_{[s\ge t]}ds \\ &\qquad - \sum_{n\ge1} \ell_{\xi_{n-1}\xi_n}(\tau_n\vee t, X_{\tau_n\vee t}^{t,x})\mathbb{1}_{[\tau_n<T]}\Big] \\ &= \sup_{(\delta,\xi)\in\widetilde{\mathcal{D}}} \mathbb{E}\Big[\int_0^{\tau_n} \psi_{u_s}(s, X_s^{t,x})\mathbb{1}_{[s\ge t]}ds \\ &\qquad - \sum_{1\le k\le n} \ell_{\xi_{k-1}\xi_k}(t\vee\tau_k, X_{t\vee\tau_k}^{t,x})\mathbb{1}_{[\tau_k<T]} + \mathbb{1}_{[\tau_n<T]}y_{\tau_n}^{\xi_n,t,x}\Big] \end{aligned}$$

and

$$
\begin{aligned}
y_0^{1,t',x'} &= \sup_{(\delta,\xi)\in\widetilde{\mathcal{D}}} \mathbb{E}\Big[\int_0^T \psi_{u_s}(s, X_s^{t',x'})\mathbb{1}_{[s\geq t']}ds \\
&\qquad - \sum_{n\geq 1} \ell_{\xi_{n-1}\xi_n}(\tau_n \vee t', X_{\tau_n\vee t'}^{t',x'})\mathbb{1}_{[\tau_n<T]}\Big] \\
&= \sup_{(\delta,\xi)\in\widetilde{\mathcal{D}}} \mathbb{E}\Big[\int_0^{\tau_n} \psi_{u_s}(s, X_s^{t',x'})\mathbb{1}_{[s\geq t']}ds \\
&\qquad - \sum_{1\leq k\leq n} \ell_{\xi_{k-1}\xi_k}(t' \vee \tau_k, X_{t'\vee\tau_k}^{t',x'})\mathbb{1}_{[\tau_k<T]} + \mathbb{1}_{[\tau_n<T]}y_{\tau_n}^{\xi_n,t',x'}\Big].
\end{aligned}
$$

The second equalities are obtained in using the dynamical programming principle [14]. It follows that

$$
\begin{aligned}
&y_0^{1,t',x'} - y_0^{1,t,x} \\
&\leq \sup_{(\delta,\xi)\in\widetilde{\mathcal{D}}} \mathbb{E}\Big[\int_0^{\tau_n} \{\psi_{u_s}(s, X_s^{t',x'})\mathbb{1}_{[s\geq t']} - \psi_{u_s}(s, X_s^{t,x})\mathbb{1}_{[s\geq t]}\}ds \\
&\qquad - \sum_{1\leq k\leq n} \{\ell_{\xi_{k-1}\xi_k}(t' \vee \tau_k, X_{t'\vee\tau_k}^{t',x'}) - \ell_{\xi_{k-1}\xi_k}(t \vee \tau_k, X_{t\vee\tau_k}^{t,x})\}\mathbb{1}_{[\tau_k<T]} \\
&\qquad + \mathbb{1}_{[\tau_n<T]}\{y_{\tau_n}^{\xi_n,t',x'} - y_{\tau_n}^{\xi_n,t,x}\}\Big].
\end{aligned} \tag{26}
$$

Next w.l.o.g. we assume that $t' < t$. Then from (26) we deduce that

$$
\begin{aligned}
&y_0^{1,t',x'} - y_0^{1,t,x} \\
&\leq \sup_{(\delta,\xi)\in\widetilde{\mathcal{D}}} \mathbb{E}\Big[\int_0^{\tau_n} \{(\psi_{u_s}(s, X_s^{t',x'}) - \psi_{u_s}(s, X_s^{t,x}))\mathbb{1}_{[s\geq t]} + \psi_{u_s}(s, X_s^{t',x'})\mathbb{1}_{[t'\leq s<t]}\}ds \\
&\qquad - \sum_{1\leq k\leq n} \{\ell_{\xi_{k-1}\xi_k}(t' \vee \tau_k, X_{t'\vee\tau_k}^{t',x'}) - \ell_{\xi_{k-1}\xi_k}(t \vee \tau_k, X_{t\vee\tau_k}^{t,x})\}\mathbb{1}_{[\tau_k<T]} \\
&\qquad + \mathbb{1}_{[\tau_n<T]}\{y_{\tau_n}^{\xi_n,t',x'} - y_{\tau_n}^{\xi_n,t,x}\}\Big] \\
&\leq \mathbb{E}\Big[\int_0^T \max_{j=1,m} |(\psi_j(s, X_s^{t',x'}) - \psi_j(s, X_s^{t,x}))|\mathbb{1}_{[s\geq t]} \\
&\qquad + \max_{j=1,m} |\psi_j(s, X_s^{t',x'})|\mathbb{1}_{[t'\leq s<t]}\}ds \\
&\qquad + n \max_{i\neq j\in\mathcal{J}} \{\sup_{s\leq T} |\ell_{ij}(t' \vee s, X_{t'\vee s}^{t',x'}) - \ell_{ij}(t \vee s, X_{t\vee s}^{t,x})|\} \\
&\qquad + \sup_{(\delta,u)\in\widetilde{D}} (\mathbb{P}[\tau_n < T])^{\frac{1}{2}} (2\mathbb{E}[(y_{\tau_n}^{\xi_n,t',x'})^2 + (y_{\tau_n}^{\xi_n,t,x})^2])^{\frac{1}{2}}\Big].
\end{aligned} \tag{27}
$$

In the right-hand side of (27) the first term converges to 0 as $(t', x') \to (t, x)$. Next let us show that for any $i \neq j \in \mathcal{J}$,

$$\mathbb{E}[\sup_{s\leq T} |\ell_{ij}(t' \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t,x}_{t\vee s})|] \to 0 \quad \text{as } (t', x') \to (t, x).$$

Actually for any $\varrho > 0$ we have

$$\begin{aligned}
&|\ell_{ij}(t' \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t,x}_{t\vee s})| \\
&\quad \leq |\ell_{ij}(t \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t,x}_{t\vee s})| \\
&\qquad + |\ell_{ij}(t' \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t',x'}_{t'\vee s})| \mathbb{1}_{[|X^{t',x'}_{t'\vee s}| \geq \varrho]} \\
&\qquad + |\ell_{ij}(t' \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t',x'}_{t'\vee s})| \mathbb{1}_{[|X^{t',x'}_{t'\vee s}| \leq \varrho]}.
\end{aligned}$$

Therefore we have

$$\begin{aligned}
&\mathbb{E}\big[\sup_{s\leq T} |\ell_{ij}(t' \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t,x}_{t\vee s})|\big] \\
&\quad \leq \mathbb{E}\big[\sup_{s\leq T} \big\{|\ell_{ij}(t' \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t',x'}_{t'\vee s})| \mathbb{1}_{[|X^{t',x'}_{t'\vee s}| \leq \varrho]}\big\}\big] \\
&\qquad + \mathbb{E}\big[\sup_{s\leq T} \big\{|\ell_{ij}(t' \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t',x'}_{t'\vee s})|\big\} \mathbb{1}_{[\sup_{s\leq T} |X^{t',x'}_{t'\vee s}| \geq \varrho]}\big] \\
&\qquad + \mathbb{E}\big[\sup_{s\leq T} \big\{|\ell_{ij}(t \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t,x}_{t\vee s})|\big\} \mathbb{1}_{[\sup_{s\leq T} |X^{t',x'}_{t'\vee s}| + \sup_{s\leq T} |X^{t,x}_{t\vee s}| \geq \varrho]}\big] \\
&\qquad + \mathbb{E}\big[\sup_{s\leq T} \big\{|\ell_{ij}(t \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t,x}_{t\vee s})|\big\} \mathbb{1}_{[\sup_{s\leq T} |X^{t',x'}_{t'\vee s}| + \sup_{s\leq T} |X^{t,x}_{t\vee s}| \leq \varrho]}\big]
\end{aligned}$$

But since ℓ_{ij} is continuous then it is uniformly continuous on $[0, T]\times\{x \in \mathbb{R}^k, |x| \leq \varrho\}$. Henceforth for any $\epsilon_1 > 0$ there exists $\eta_{\epsilon_1} > 0$ such that for any $|t - t'| < \eta_{\epsilon_1}$ we have

$$\sup_{s\leq T} \big\{|\ell_{ij}(t' \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t',x'}_{t'\vee s})| \mathbb{1}_{[|X^{t',x'}_{t'\vee s}| \leq \varrho]}\big\} \leq \epsilon_1. \tag{28}$$

Next using Cauchy–Schwarz's inequality and then Markov's one with the second term we obtain

$$\mathbb{E}\big[\sup_{s\leq T} \big\{|\ell_{ij}(t' \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t',x'}_{t'\vee s})|\big\} \mathbb{1}_{[\sup_{s\leq T} |X^{t',x'}_{t'\vee s}| \geq \varrho]}\big] \leq C(1 + |x'|^p)\varrho^{-\frac{1}{2}}, \tag{29}$$

where C and p are real constants which are bound to the polynomial growth of ℓ_{ij} and estimate (23). In the same way we have:

$$\begin{aligned}
&\mathbb{E}\big[\sup_{s\leq T} \big\{|\ell_{ij}(t \vee s, X^{t',x'}_{t'\vee s}) - \ell_{ij}(t \vee s, X^{t,x}_{t\vee s})|\big\} \mathbb{1}_{[\sup_{s\leq T} |X^{t',x'}_{t'\vee s}| + \sup_{s\leq T} |X^{t,x}_{t\vee s}| \geq \varrho]}\big] \\
&\qquad \leq C(1 + |x|^p + |x'|^p)\varrho^{-\frac{1}{2}}.
\end{aligned} \tag{30}$$

Finally using the uniform continuity of ℓ_{ij} on compact subsets, the continuity property (24) and the Lebesgue dominated convergence theorem to obtain that

$$\mathbb{E}\Big[\sup_{s\leq T}\big\{|\ell_{ij}(t\vee s,X^{t',x'}_{t'\vee s})-\ell_{ij}(t\vee s,X^{t,x}_{t\vee s})|\big\}\mathbb{1}_{[\sup_{s\leq T}|X^{t',x'}_{t'\vee s}|+\sup_{s\leq T}|X^{t,x}_{t\vee s}|\leq\varrho]}\Big]\to 0 \tag{31}$$

as $(t',x')\to(t,x)$. Taking now into account (28)–(31) we have

$$\limsup_{(t',x')\to(t,x)}\mathbb{E}\Big[\sup_{s\leq T}|\ell_{ij}(t'\vee s,X^{t',x'}_{t'\vee s})-\ell_{ij}(t\vee s,X^{t,x}_{t\vee s})|\Big]\leq\epsilon_1+C(1+|x|^p)\varrho^{-\frac{1}{2}}.$$

As ϵ_1 and ϱ are arbitrary then making $\epsilon_1\to 0$ and $\varrho\to+\infty$ to obtain that

$$\lim_{(t',x')\to(t,x)}\mathbb{E}\Big[\sup_{s\leq T}|\ell_{ij}(t'\vee s,X^{t',x'}_{t'\vee s})-\ell_{ij}(t\vee s,X^{t,x}_{t\vee s})|\Big]=0.$$

Thus the claim is proved.

Finally let us focus on the last term in (27). Since $(\delta,\xi)\in\widetilde{\mathcal{D}}$ then:

$$\begin{aligned}&\sup_{(\delta,\xi)\in\widetilde{\mathcal{D}}}\big(\mathbb{P}[\tau_n<T]\big)^{\frac{1}{2}}\big(2\mathbb{E}\big[(y^{\xi_n,t',x'}_{\tau_n})^2+(y^{\xi_n,t,x}_{\tau_n})^2\big]\big)^{\frac{1}{2}}\\&\leq n^{-\frac{1}{2}}\sup_{(\delta,\xi)\in\widetilde{\mathcal{D}}}\big(2\mathbb{E}\big[(y^{\xi_n,t',x'}_{\tau_n})^2+(y^{\xi_n,t,x}_{\tau_n})^2\big]\big)^{\frac{1}{2}}\\&\leq Cn^{-\frac{1}{2}}(1+|x|^p+|x'|^p),\end{aligned}$$

where C and p are appropriate constants which come from the polynomial growth of ψ_i, $i\in\mathcal{J}$, estimate (23) for the process $X^{t,x}$ and inequality (13). Going back now to (27), taking the limit as $(t',x')\to(t,x)$ we obtain

$$\limsup_{(t',x')\to(t,x)}y_0^{1,t',x'}\leq y_0^{1,t,x}+Cn^{-\frac{1}{2}}(1+2|x|^p).$$

As n is arbitrary then putting $n\to+\infty$ we obtain

$$\limsup_{(t',x')\to(t,x)}y_0^{1,t',x'}\leq y_0^{1,t,x}.$$

This implies that

$$\limsup_{(t',x')\to(t,x)}y_0^{1,t',x'}=\limsup_{(t',x')\to(t,x)}Y_{t'}^{1,t',x'}=\limsup_{(t',x')\to(t,x)}v^1(t',x')\leq y_0^{1,t,x}=Y_t^{1,t,x}$$

and then v^1 is upper semi-continuous since $Y_t^{1,t,x}=v^1(t,x)$. But v^1 is also lower semi-continuous, therefore it is continuous. In the same way we can show that $v^2,\ldots,v^m$ are continuous. As they are of polynomial growth, then taking into account Theorem 5 to obtain that $(v^1,\ldots,v^m)$ is a viscosity solution for the system of variational inequalities with inter-connected obstacles (19). □

Remark 3. The solution in viscosity sense of the system of variational inequalities with inter-connected obstacles (19) is unique in the space of continuous functions on $[0,T]\times R^k$ which satisfy a polynomial growth condition, i.e., in the space

$$\mathcal{C} := \{\varphi\colon [0,T]\times\mathbb{R}^k \to \mathbb{R},\ \text{continuous and for any } (t,x),\ |\varphi(t,x)| \le C(1+|x|^\gamma) \text{ for some constants } C \text{ and } \gamma\}.$$

Therefore for any $i \in \mathcal{J}$, v^i has the following representation: $\forall (t,x)\in[0,T]\times\mathbb{R}^k$,

$$v^i(t,x) = \sup_{(\delta,\xi)\in\mathcal{A}_t^{f,i}} \mathbb{E}\Big[\int_t^T \psi_{u_s}(s,X_s^{t,x})ds - \sum_{n\ge 1}\ell_{\xi_{n-1}\xi_n}(\tau_n, X_{\tau_n}^{t,x})\mathbb{1}_{[\tau_n<T]}\Big].$$

For more details one can see [14]. □

7 Extension and numerical schemes

7.1 General systems of BSDEs with oblique reflection. The problem which we deal with now is to what extent can we provide a solution for systems of types (16) where the generators ψ_i, which depend only on (t,ω), are replaced by functions which depend also on y^i, z^i, $i\in\mathcal{J}$. Namely let us consider the following system of BSDEs with oblique reflection: for $i\in\mathcal{J}$,

$$\begin{cases} Y^i, K^i \in \mathcal{S}^2,\ Z^i\in\mathcal{M}^{2,d}\,; K^i \text{ non-decreasing and } K_0^i = 0,\\ Y_t^i = \xi_i + \displaystyle\int_t^T f_i(s,Y_s^1,\dots,Y_s^m,Z_s^i)ds - \int_t^T Z_s^i dB_s + K_T^i - K_t^i,\ t\le T,\\ Y_t^i \ge \max\limits_{j\in A_i} h_{i,j}(t,Y_t^j);\quad [Y_t^i - \max\limits_{j\in A_i} h_{i,j}(t,Y_t^j)]dK_t^i = 0. \end{cases} \tag{32}$$

Here ξ_i are $\mathcal{F}_T$-measurable, the coefficients f_i, $h_{i,j}$ can depend on ω, and $A_i\subset\{1,\dots,m\}-\{j\}$. For simplicity we denote $\vec{Y}_t := (Y_t^1,\dots,Y_t^m)$, and similarly for other vectors. The constraint A_i means that from mode i the plant can only be switched to those modes in A_i. We emphasize that A_j can be empty and if so we take the convention that the maximum over the empty set, denoted as $\emptyset$, is $-\infty$. Then in this case Y^i has no lower barrier and then we take $K^i=0$. Consequently, Y^i satisfies the following BSDE without reflection:

$$Y_t^i = \xi_i + \int_t^T f_i(s,\vec{Y}_s,Z_s^i)ds - \int_t^T Z_s^i dB_s,\ 0\le t\le T.$$

Also, for any i we define

$$h_{i,i}(t,y) := y.$$

Then a solution of (32) always satisfies

$$Y_t^i \ge \max_{j\in A_i\cup\{i\}} h_{i,j}(t,Y_t^j).$$

The general barrier $h_{i,j}$ allows one to consider more general switching costs. In fact, even if the original cost takes the form $h_{i,j}(t,\omega,y) = y - \ell_{i,j}(t,\omega)$, in the risk-sensitive switching problem (see e.g. [21]) one needs to take the standard exponential transformation and then the barrier becomes $\tilde{h}_{i,j}(t,\tilde{y}) := e^{-\ell_{i,j}}\tilde{y}$. Finally let us point out that systems of types (32) are involved when dealing with optimal switching problems under Knightian uncertainty (see e.g. [21], [22]).

Let us now introduce the following assumptions:

Assumptions [A]. For any $i = 1,\dots,m$, it holds that

(i) $E\{\int_0^T (\sup_{\vec{y}:y_i=0} |f_i(t,\vec{y},0)|^2)dt + |\xi_i|^2\} < \infty$.

(ii) $f_i(t,\vec{y},z)$ is uniformly Lipschitz continuous in (y_i,z) and is continuous in y_j for any $j \neq i$; and $h_{i,j}(t,y)$ is continuous in (t,y) for $j \in A_i$.

(iii) $f_i(t,\vec{y},z)$ is increasing in y_j for $j \neq i$, and $h_{i,j}(t,y)$ is increasing in y for $j \in A_i$.

(iv) For $j \in A_i$, $h_{i,j}(t,y) \leq y$. Moreover, there is no sequence $i_2 \in A_{i_1},\dots,i_k \in A_{i_{k-1}}$, $i_1 \in A_{i_k}$, and $(y_1,\dots,y_k)$ such that

$$y_1 = h_{i_1,i_2}(t,y_2),\ y_2 = h_{i_2,i_3}(t,y_3),\dots,y_{k-1} = h_{i_{k-1},i_k}(t,y_k),\ y_k = h_{i_k,i_1}(t,y_1).$$

(v) For any $i = 1,\dots,m$, $\xi_i \geq \max_{j\in A_i} h_{i,j}(T,\xi_j)$.

We note that (i), (ii) and (v) are standard. The assumption (iv) means that it is not free to make a circle of instantaneous switchings.

Our main result, stated by Hamadène–Zhang in [22] where we can find all the details, is:

Theorem 7. *Assume Assumptions* [A] *hold. Then the system of RBSDEs* (32) *has a solution.* □

The solution is unique if we strengthen slightly the assumptions on the data of the problem. Actually we have:

Theorem 8 ([22]). *Besides Assumptions* [A], *assume moreover that*

(i) *f_i is uniformly Lipschitz continuous in all y_j.*

(ii) *If $j \in A_i, k \in A_j$, then $k \in A_i \cup \{i\}$. Moreover,*

$$h_{i,j}(t,h_{j,k}(t,y)) < h_{i,k}(t,y).$$

(iii) *For any $j \in A_i$,*

$$|h_{i,j}(t,y_1) - h_{i,j}(t,y_2)| \leq |y_1 - y_2|.$$

Then the solution of system (32) *is unique.* □

7.2 Numerical schemes. As it has been pointed out previously, those systems of reflected BSDEs with oblique reflection arise in several applied disciplines of mathematics especially in finance. Therefore the issue of finding their solution becomes crucial but a tough task as well. An alternative is to provide numerical schemes which converge to the solution of the system with a good rate. There are actually some works in this sense of which we can quote [4] where the authors deal with numerics of the following system:

$$\begin{cases} Y_s^{i,t,x} = g_i(X_T^{t,x}) + \int_s^T f_i(r, X_r^{t,x}, Y_r^{t,x}, Z_r^{t,x})du \\ \qquad\qquad - \int_s^T Z_r^{i,t,x} dB_r + K_T^{i,t,x} - K_s^{i,t,x}, \\ Y_s^{i,t,x} \geq \max_{j \in \mathcal{J}^{-i}} (-\ell_{ij}(s, X_s^{t,x}) + Y_s^{j,t,x}), \\ \int_0^T (Y_r^{i,t,x} - \max_{j \in \mathcal{J}^{-i}} (-\ell_{ij}(r, X_r^{t,x}) + Y_r^{j,t,x}))dK_r^{i,t,x} = 0. \end{cases} \tag{33}$$

They have introduced a discrete time system of reflected BSDEs associated with (33) in using an oblique projection operator. Further they provide a control of the error which is especially significant in the case when the coefficients $(f_i)_{i=1,\dots,m}$ do not depend on z since they show that it is of order $\frac{1}{2} - \epsilon$, $\epsilon > 0$.

The case $m = 2$ is particular and has been considered in [20].

Finally note that there is another point of view which uses the link of the solutions of the above system and minimal solutions of constrained BSDEs with jumps, which is developed in [15].

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The COGARCH: a review, with news on option pricing and statistical inference

Claudia Klüppelberg, Ross Maller and Alexander Szimayer

1 Introduction

Mathematical Finance and Econometrics can be viewed as two sides of a coin. Econometrics concentrates on finding optimal models concerning statistical properties like correlations and prediction. Mathematical Finance, on the other side is mainly concerned with finding good models which allow for hedging and derivatives pricing.

Two major innovations revolutionised the theory and practise of econometrics in the latter part of the last century. The first was the development of the unit root and related cointegration concepts in the analysis of time series data, and the associated Dickie–Fuller test (cf. [11]) and its various generalisations. Soon after came the idea of conditional heteroscedasticity models to capture the empirically observed feature of apparently randomly varying volatility[1] fluctuations in time series. Landmark models include Taylor's stochastic volatility model [47] and the ARCH and GARCH models of Engle [16] and Bollerslev [4]. These innovations and their subsequent rapid development and application in many directions were particularly appropriate for high frequency time series financial data, which became easily accessible in large quantities over the period, with the introduction of modern computer technology.

Rigorous hedging and pricing of financial derivatives started with the seminal paper by Black and Scholes [3] using the complete model of geometric Brownian motion and its explicit unique option price. After it became clear that this model cannot capture all realistic features of market conditions, incomplete models entered the scene. Characterization of no arbitrage pricing by martingale measures came into focus in the important papers by Harrison and Kreps [22] and Harrison and Pliska [23]. The problem of non-unique martingale measures was met by a specific approach of Föllmer and Schweizer [18]. Exponential Lévy models were a first step towards more realistic modelling promoted early on by Eberlein and collaborators; cf. Eberlein [15] for a review. Pricing measures were suggested for normal mixture models such as the variance gamma model due to Madan and Seneta [35] and the normal inverse Gaussian model, which was originally suggested by Barndorff-Nielsen [1].

This paper aims at a reconciliation between certain econometric models and pricing models. Our econometrics motivation comes from the availability of high frequency data, which are often sampled at irregular time points, making continuous-time modelling necessary. Our motivation for derivatives pricing originates in the need for more realistic pricing models.

[1] The "volatility" is simply the square root of the variance.

The paper is organised as follows. In Section 2 we recall the discrete time ARCH and GARCH models and some of their properties. We further summarize some continuous-time limits of such models from the literature and explain their drawbacks. Section 3 is devoted to the continuous time GARCH (COGARCH) model as suggested in Klüppelberg, Lindner and Maller [30]. Section 4 presents new material on option pricing within the COGARCH model. As an explicit example we treat the variance gamma driven COGARCH and compare it to the Heston model via implicit volatilities. It turns out that the COGARCH can produce higher implied volatilities for short maturities deep in-the-money and far out of-the-money; desirable properties in applications. Section 5 is devoted to statistical estimation of the COGARCH parameters. Besides classical moment estimators we also present a method to obtain a GARCH skeleton within the COGARCH model, which allows for the use of existing software for estimation. This involves functional limit theorems in various modes of convergence.

2 Background in discrete time ARCH and GARCH models

AutoRegressive Conditional Heteroscedasticity (ARCH) models were introduced by Engle [16] and soon generalised to GARCH (Generalised AutoRegressive Conditional Heteroscedasticity) models by Bollerslev [4]. Nowadays they are seen as particular kinds of stochastic volatility models, in which the variance of time series innovations is itself assumed to vary randomly, conditional on past information.

A special feature of ARCH and GARCH models is that they incorporate feedback between an observation and its volatility, whereby a large fluctuation in an innovation triggers a corresponding large fluctuation in the variance of the series, which in the absence of further large fluctuations, then reverts to a steady state level, as long as the process is in a stationary regime. This is an attractive concept, which accords well with intuition and empirical observation of, especially, financial time series. As it turns out, the models also display further desirable features from the modelling point of view. In particular, they typically induce long tailedness of marginal distributions, and serial correlations, not in the innovations themselves, but in the *squared* innovations. These features again accord well with empirical observation. We expand further on them later.

The simplest GARCH model, the GARCH$(1,1)$, is a discrete time process with three parameters, $\beta > 0$, $\phi \geq 0$, $\delta \geq 0$, specifying the variance as a discrete time stochastic recursion, or difference equation. We write it using two equations, one specifying the "mean level" process (the observed data, perhaps after removal of trend or other deterministic feature, to approximate stationarity) and the other specifying the variance process, which is time dependent and randomly fluctuating. Thus, for $i = 1, 2, \ldots,$

$$Y_i = \varepsilon_i \sigma_i, \tag{2.1}$$

with

$$\sigma_i^2 = \beta + \phi Y_{i-1}^2 + \delta \sigma_{i-1}^2 = \beta + (\phi \varepsilon_{i-1}^2 + \delta)\sigma_{i-1}^2. \tag{2.2}$$

Here the starting values ε_0 and σ_0 are given quantities, possibly random, and usually assumed independent of the $(\varepsilon_i)_{i=1,2,\ldots}$, which are the sole source of variation in the

model. The ε_i, $i = 1, 2, \ldots$, are assumed to be independent identically distributed (i.i.d.) random variables (rvs) centered at 0. Serial dependence between the Y_i is introduced via the dependence of the σ_i^2 on their past values. Conditional on σ_i, Y_i simply has the distribution of ε_i, scaled by σ_i, which in general (as long as $\phi, \delta > 0$) is time dependent, hence the "conditional heteroscedasticity" part of the terminology. The "autoregressive" aspect refers to the form of the dependence of σ_i^2 on σ_{i-1}^2, as in an autoregressive time series model.

When $\delta = 0$ this term in σ_{i-1}^2 disappears, but volatility remains stochastic via the dependence of σ_i^2 on Y_{i-1}, as long as $\phi > 0$. We then have the ARCH(1) model of Engle [16]. Such a model was generally found to be inadequate, however, to describe observed data, in which variance tends to be highly persistent and mean reverting. The introduction of the σ_{i-1}^2 term in (2.2) when $\delta > 0$ improves the modelling of such data substantially, and gives rise to the highly successful GARCH(1, 1) model of Bollerslev [4]. A very natural extension of this model is to add further autoregressive terms to (2.2), thus defining a GARCH(p, q) model, and, similarly, the ARCH(p) model is defined.

Of course if $\phi = \delta = 0$ in (2.2) the model simply reduces to one of i.i.d. observations for the Y_i, with variance $\beta > 0$.

2.1 Stationarity and tail behaviour in GARCH models. Often, in a practical regression situation, the ε_i might be assumed $N(0, 1)$ for the purposes of model fitting. Such a short tailed distribution for the ε_i, however, does not necessarily translate into a short tailed marginal distribution for the observations Y_i. Eq. (2.2) specifies the sequence $(\sigma_i^2)_{i=1,2,\ldots}$ as a *stochastic recurrence equation*, studied in some depth in the probability literature, especially, see Kesten [28], Vervaat [49] and Goldie [19]; see also the readable overview paper by Diaconis and Freedman [10]. In a stationary regime, or otherwise, the resulting Y_i will usually have a heavy tailed distribution. This comes about as follows. Necessary and sufficient conditions for the "stability" (existence of an almost sure (a.s.) limit for large times) of a discrete time stochastic perpetuity given in Goldie and Maller [20] can be applied directly to give necessary and sufficient conditions in terms of log moments of the ε_i and the parameters ϕ and δ, for the stability of the ARCH(1) and GARCH(1, 1) models. Specifically, Theorem 2.1 of Klüppelberg, Lindner and Maller [30] shows that we have stability of the mean and variance processes, that is, $Y_i \xrightarrow{D} Y_\infty$ and $\sigma_i \xrightarrow{D} \sigma_\infty$ as $i \to \infty$, for finite rvs Y_∞ and σ_∞, if and only if

$$E|\log(\delta + \phi\varepsilon_1^2)| < \infty \quad \text{and} \quad E\log(\delta + \phi\varepsilon_1^2) < 0.$$

These then constitute conditions for stationarity of $(Y_i, \sigma_i^2)_{i=1,2,\ldots}$ if the sequence is started with the values $(Y_\infty, \sigma_\infty)$. Then, further results transferable from the theory of stochastic difference equations show that, under certain fairly general conditions, Y_∞ will have a long tailed distribution, specifically, a distribution with a Pareto (power law) tail. A good exposition of this is in Lindner [32].

Thus, even with a short tailed distribution such as the normal assumed for the innovations ε_i, we may expect a heavy tailed marginal distribution for the Y_i. This

accords with observed features of, especially, financial data, cf. Klüppelberg [29], Mikosch [37]. More recently, Platen and Sidorowicz [42], for example, in a very extensive investigation, suggest that much financial returns data has a very heavy tailed distribution, such as a t-distribution with 4 degrees of freedom.

2.2 Continuous time limits of GARCH models. Motivated, in particular, by the availability of high-frequency data and by a need for option pricing technologies, classical diffusion limits have been used in a natural way to suggest continuous time limits of discrete time processes, including for the GARCH models. The best known of these is due to Nelson [40]. His limiting diffusion model is:

$$\mathrm{d}Y_t = \sigma_t \mathrm{d}B_t^{(1)}, \quad t \geq 0, \tag{2.3}$$

where σ_t, the volatility process, satisfies

$$\mathrm{d}\sigma_t^2 = \left(\beta - \eta\sigma_t^2\right)\mathrm{d}t + \phi\sigma_t^2 \mathrm{d}B_t^{(2)}, \quad t > 0, \tag{2.4}$$

with $B^{(1)}$ and $B^{(2)}$ independent Brownian motions, and $\beta > 0$, $\eta \geq 0$ and $\phi \geq 0$ constants.

Unfortunately, in these situations, the limiting models can lose certain essential properties of the discrete time GARCH models. It is surprising and counter-intuitive, for example, that Nelson's diffusion limit of the GARCH process is driven by two independent Brownian motions, i.e. has two independent sources of randomness[2], whereas the discrete time GARCH process is driven only by a single white noise sequence. One of the features of the GARCH process is the idea that large innovations in the price process are almost immediately manifested as innovations in the volatility process; but this feedback mechanism is lost in models such as the Nelson continuous time version. Further, the appearance of an extra source of variation can have implications for completeness considerations in options pricing models, for example.

The phenomenon that a diffusion limit may be driven by two independent Brownian motions, while the discrete time model is given in terms of a single white noise sequence, is not restricted to the classical GARCH process. Duan [13] has shown that this occurs for many GARCH-like processes. On the other hand, Corradi [8] modified Nelson's method to obtain a diffusion limit depending only on a single Brownian motion - but then the equation for σ_t^2 degenerates to an ordinary differential equation. Using a Brownian bridge between discrete time observations, Kallsen and Taqqu [26] found a complete model driven by only one Brownian motion.

Moreover, the continuous time limits found in such a way can have distinctly different statistical properties to the original discrete time processes. As was shown by Wang [50], parameter estimation in the discrete time GARCH and the corresponding continuous time limit stochastic volatility model may yield different estimates (see also

[2]Dependence has been introduced in the literature in an ad hoc way by allowing $B^{(1)}$ and $B^{(2)}$ in (2.3) and (2.4) to be correlated, but such models still rely on two sources of randomness.

Brown, Wang and Zhao [6]). Thus these kinds of continuous time models are probabilistically and statistically different from their discrete time progenitors. See Lindner [31] for a recent overview of continuous time approximations to GARCH processes.

In Klüppelberg, Lindner and Maller [30], the authors proposed a radically different approach to obtaining a continuous time model. Their "COGARCH" (continuous time GARCH) model is a direct analogue of the discrete time GARCH, based on a single background driving Lévy process, and generalises the essential features of the discrete time GARCH process in a natural way. In the next section we review this model.

Throughout this article, by the "COGARCH" model we will always mean the COGARCH(1, 1) model.

3 The COGARCH model

The COGARCH model is specified by two equations, the mean and variance equations, analogous to (2.1) and (2.2). The single source of variation is a so-called *background driving Lévy process* $L = (L_t)_{t\geq 0}$ with characteristic triplet (γ, σ^2, Π); we refer to Sato [43] for background on Lévy processes. The continuous time process L has i.i.d. increments, which are analogous to the i.i.d. innovations ε_i in (2.1) and (2.2). Then the COGARCH process $(G_t)_{t\geq 0}$ is defined in terms of its stochastic differential, $\mathrm{d}G$, such that

$$\mathrm{d}G_t = \sigma_{t-}\mathrm{d}L_t, \quad t \geq 0, \tag{3.1}$$

where σ_t, the volatility process, satisfies

$$\mathrm{d}\sigma_t^2 = \left(\beta - \eta\sigma_{t-}^2\right)\mathrm{d}t + \phi\sigma_{t-}^2\mathrm{d}[L, L]_t, \quad t > 0, \tag{3.2}$$

for constants $\beta > 0$, $\eta \geq 0$ and $\phi \geq 0$. Here $[L, L]_t$ denotes the quadratic variation process of L, defined for $t > 0$ by

$$[L, L]_t := \sigma^2 t + \sum_{0<s\leq t} (\Delta L_s)^2 = \sigma^2 t + [L_t, L_t]^d, \tag{3.3}$$

with $[L_t, L_t]^d$ denoting the pure jump component of $[L, L]$. (There should be no confusion between the constant σ^2 specifying the variance of the Gaussian component of L and the COGARCH variance process $(\sigma_t^2)_{t\geq 0}$. In (3.3), $\Delta L_t = L_t - L_{t-}$ for $t \geq 0$ (with $L_{0-} = 0$) and similarly for other processes throughout. All processes are cádlág)

To see the analogy with (2.1) and (2.2), note from (2.2) that

$$\sigma_i^2 - \sigma_{i-1}^2 = \beta - (1-\delta)\sigma_{i-1}^2 + \phi\sigma_{i-1}^2\varepsilon_{i-1}^2,$$

which corresponds to (3.2) (with a reparameterisation from η to $\delta = 1 - \eta$) when the time increment $\mathrm{d}t$ is taken as a unit, or at least fixed, interval of time. But an advantage of the continuous time setup is that non-equally spaced observations are easily catered for, as we demonstrate later (Section 5.4).

Just as an understanding of discrete time perpetuities is the key to stability, stationarity and tail behaviour of the discrete time GARCH, so kinds of continuous time perpetuities are instrumental in the analysis of the COGARCH. The solution of the stochastic differential equation (SDE) (3.2) can be obtained with the help of an auxiliary Lévy process $X = (X_t)_{t\geq 0}$ defined by

$$X_t = \eta t - \sum_{0<s\leq t} \log(1+\phi(\Delta L_s)^2), \quad t \geq 0.$$

X is a spectrally negative Lévy process of bounded variation arising in a natural way in Klüppelberg et al. [30], where the COGARCH(1, 1) is motivated directly as an analogue to the discrete time GARCH(1, 1) process. Using Ito's lemma, it can be verified that the solution of (3.2) can be written in terms of X as

$$\sigma_t^2 = e^{-X_t}\left(\beta\int_0^t e^{X_s}\mathrm{d}s + \sigma_0^2\right), \quad t \geq 0,$$

which reveals σ_t^2 as a kind of generalised Ornstein–Uhlenbeck (GOU) process, parameterised by (β, η, φ), and driven by the Lévy process L. For results on the GOU, and associated studies of *Lévy integrals*, see Lindner and Maller [33] and their references. An understanding of stability, stationarity and tail behaviour properties for the GOU is essential for such issues relating to G.

Klüppelberg et al. [30], Theorem 3.2, show that the variance process $(\sigma_t^2)_{t\geq 0}$ for the COGARCH is a time homogeneous Markov process, and, further, that the bivariate process $(G_t, \sigma_t^2)_{t\geq 0}$ is Markovian. A finite random variable σ_∞^2 exists as the limit in distribution of σ_t^2 as $t \to \infty$ if and only if

$$\int_{\mathbb{R}} \log\left(1+\frac{\phi}{\delta}y^2\right)\Pi(\mathrm{d}y) < -\log\delta. \tag{3.4}$$

σ_∞^2 has the same distribution as β times the stochastic integral $\int_0^\infty e^{-X_t}\mathrm{d}t$, which exists as a finite rv a.s. under (3.4) (see Theorem 3.1 of [30]). If this is the case and $(\sigma_t^2)_{t\geq 0}$ is started with value σ_∞^2, i.e., σ_0^2 is taken to have the distribution of σ_∞^2, independent of L, then $(\sigma_t^2)_{t\geq 0}$ is strictly stationary and $(G_t)_{t\geq 0}$ is a process with stationary increments (Theorem 3.2 and Corollary 3.1 of [30]).

Moments of the COGARCH process can be calculated using the Laplace transform of the auxiliary process X, which satisfies $\mathbb{E}e^{-\theta X_t} = e^{t\Psi(\theta)}$, with

$$\Psi(\theta) = -\eta\theta + \int_{\mathbb{R}} \left((1+\phi x^2)^\theta - 1\right)\Pi(dx), \quad \theta \geq 0. \tag{3.5}$$

Returns over time intervals of fixed length $r > 0$ we denote by

$$G_t^{(r)} := G_t - G_{t-r} = \int_{(t-r,t]} \sigma_{s-}\, dL_s, \quad t \geq r, \tag{3.6}$$

so that $(G_{ri}^{(r)})_{i\in\mathbb{N}}$ describes an equidistant sequence of non-overlapping returns. Calculating the corresponding quantity for the volatility yields

$$\begin{aligned}\sigma_{ri}^{2(r)} &:= \sigma_{ri}^2 - \sigma_{r(i-1)}^2 = \int_{(r(i-1),ri]} \left((\beta - \eta\sigma_s^2)\,\mathrm{d}s + \varphi\,\sigma_{s-}^2\,\mathrm{d}[L,L]_s\right) \\ &= \beta r - \eta \int_{(r(i-1),ri]} \sigma_s^2\,ds + \varphi \int_{(r(i-1),ri]} \sigma_{s-}^2\,\mathrm{d}[L,L]_s. \end{aligned} \tag{3.7}$$

Note that the stochastic process

$$\int_{(0,t]} \sigma_{s-}^2\,\mathrm{d}[L,L]_s = \sigma^2 \int_0^t \sigma_{s-}^2 ds + \sum_{0<s\le t} \sigma_{s-}^2 (\Delta L_s)^2, \quad t \ge 0,$$

is the quadratic variation $[G,G]_t$ of G, which satisfies

$$[G,G]_t = \int_0^t \sigma_{s-}^2\,d\,[L,L]_s, \quad t \ge 0;$$

thus $\int_{(r(i-1),ri]} \sigma_{s-}^2\,\mathrm{d}[L,L]_s^d$ in (3.7) corresponds to the jump part of the quadratic variation of G accumulated during $(r(i-1),ri]$.

The following result (Proposition 2.1 of Haug et al. [24]) shows that the COGARCH has a similar moment structure as the GARCH model; in particular, increments are uncorrelated, but squared increments are positively correlated. We shall need these results in Section 5.1 when we present a method of moment estimation of the COGARCH parameters.

Proposition 3.1. *Suppose that $(L_t)_{t\ge0}$ has finite variance and zero mean, and that the Gaussian component has variance σ^2. Suppose also that $\Psi(1) < 0$ for Ψ as given in (3.5). Let $(\sigma_t^2)_{t\ge0}$ be the stationary volatility process, so that $(G_t)_{t\ge0}$ has stationary increments. Then $\mathbb{E}(G_t^2) < \infty$ for all $t \ge 0$, and for every $t, h \ge r > 0$ we have*

$$\mathbb{E}(G_t^{(r)}) = 0, \quad \mathbb{E}(G_t^{(r)})^2 = \frac{\beta r}{|\Psi(1)|}\mathbb{E}L_1^2, \quad \mathrm{Cov}(G_t^{(r)}, G_{t+h}^{(r)}) = 0.$$

If, further, $\mathbb{E}(L_1^4) < \infty$ and $\Psi(2) < 0$, then $\mathbb{E}(G_t^4) < \infty$ for all $t \ge 0$ and, if, additionally, the Lévy measure Π of L is such that $\int_{\mathbb{R}} x^3\Pi(dx) = 0$, then for every $t, h \ge r > 0$, we have

$$\begin{aligned}\mathbb{E}(G_t^{(r)})^4 = {} & 6\mathbb{E}(L_1^2)\frac{\beta^2}{\Psi(1)^2}\left(\frac{2\eta}{\varphi} + 2\sigma^2 - \mathbb{E}L_1^2\right)\left(\frac{2}{|\Psi(2)|} - \frac{1}{|\Psi(1)|}\right) \\ & \left(r - \frac{1-e^{-r|\Psi(1)|}}{|\Psi(1)|}\right) + \frac{2\beta^2}{\varphi^2}\left(\frac{2}{|\Psi(2)|} - \frac{1}{|\Psi(1)|}\right)r + \frac{3\beta^2}{\Psi(1)^2}(\mathbb{E}L_1^2)^2 r^2,\end{aligned}$$

and

$$\begin{aligned}\mathrm{Cov}\big((G_t^{(r)})^2, (G_{t+h}^{(r)})^2\big) = {} & \frac{\mathbb{E}(L_1^2)\beta^2}{|\Psi(1)|^3}\left(\frac{2\eta}{\varphi} + 2\sigma^2 - \mathbb{E}L_1^2\right)\left(\frac{2}{|\Psi(2)|} - \frac{1}{|\Psi(1)|}\right) \\ & \left(1 - e^{-r|\Psi(1)|}\right)\left(e^{r|\Psi(1)|} - 1\right) e^{-h|\Psi(1)|} > 0.\end{aligned}$$

Motivated by the generalization of the GARCH$(1,1)$ to the GARCH(p,q) model, Brockwell, Chadraa, and Lindner [5] introduced a COGARCH(p,q) model. In it, the volatility follows a CARMA (continuous-time ARMA) process driven by a Lévy process (cf. Doob [12], Todorov and Tauchen [48]).

In Stelzer [45] multivariate COGARCH$(1,1)$ processes are introduced, constituting a dynamical extension of normal mixture models and again incorporating such features as dependence of returns (but without autocorrelation), jumps, heavy tailed distributions, etc. Stelzer's definition agrees for $d = 1$ with the COGARCH$(1,1)$ process. As in the univariate case, the model has only one source of randomness, a single multivariate Lévy process. The time-varying covariance matrix is modelled as a stochastic process in the class of positive semi-definite matrices. In [45] Stelzer analyses the probabilistic properties of the model and gives a sufficient condition for the existence of a stationary distribution for the stochastic covariance matrix process, and criteria ensuring the finiteness of moments.

4 A COGARCH option pricing model

A potentially important application of the COGARCH model is to option pricing. Traditionally, and for mathematical tractability, option pricing models are based on continuous time models for an underlying stock price process. The discrete-time GARCH reproduces features commonly observed in financial data, especially relating to the so-called stylized facts (volatility clustering, mean reversion of volatility, negative skew, and heavy tails). Consequently, the COGARCH, as a continuous time limit of the discrete GARCH (see Section 5.3), can be expected to result in more accurate option valuation than standard models. In this section we propose an option pricing framework, where the stock price return is driven by COGARCH, thus allowing for stochastic volatility, and we also include the possibility of default in the model. Combining these features is not new; however, our framework is parsimonious in its parameterisation and as we will see can reproduce observed kinds of volatility smile and skew quite well. Further, the default probability in the model can be expressed as a function of the volatility.[3]

The financial market is defined on a filtered probability space $(\Omega, \mathcal{F}, P, (\mathcal{F}_t)_{t\geq 0})$ satisfying the usual hypothesis, which is large enough to support a Lévy process $L = (L_t)_{t\geq 0}$ with characteristic function given for every $t \geq 0$ by $E[e^{izL_t}] = e^{t\psi(z)}$ for $z \in \mathbb{R}$ where

$$\psi(z) = i\gamma z - \frac{\sigma^2}{2}z^2 + \int_{\mathbb{R}\setminus\{0\}} \left(1 - e^{izx} - izh(x)\right) \Pi(\mathrm{d}x).$$

As usual (γ, σ^2, Π) is the characteristic triplet, with related truncation function $h(x) = x\,\mathbf{1}_{\{|x|\leq 1\}}$. As a technical prerequisite we assume that the fourth moment of L exists,

[3] As is also the case with the expected default frequency in Moody's KMV (Kealhofer, McQuown and Vasicek) EDF (Expected Default Frequency) proprietary credit measures model, the KMV EDF$^{\mathrm{TM}}$; see, e.g., www.moodyskmv.com/newsevents/files/EDF_Overview.pdf.

i.e. $\int x^4\,\Pi(\mathrm{d}x) < \infty$. The investment opportunities considered here are the risk-free money market account and the risky company stock. The *risk-free money market account* has the price process $B = (B_t)_{t\geq 0}$ with dynamics

$$\mathrm{d}B_t = rB_t\,\mathrm{d}t, \quad B_0 = 1,$$

where $r \in \mathbb{R}$ is the instantaneous risk-free rate; hence $B_t = e^{rt}$ for $t \geq 0$. The *stock price process* is denoted by $S = (S_t)_{t\geq 0}$ and bears two kinds of related risks. The stock price fluctuation is driven by a COGARCH process $G = (G_t)_{t\geq 0}$ with its accompanying volatility process $(\sigma_t)_{t\geq 0}$, and, further, the stock price is assumed to fall to zero at a default time τ, if default occurs, after which it stays at that level. Before default the stock price process satisfies

$$\mathrm{d}S_t = S_{t-}\,\mathrm{d}R_t, \quad S_0 > 0,$$

where $R = (R_t)_{t\geq 0}$, the cumulative return process, is driven by the COGARCH process G in the following sense:

$$\mathrm{d}R_t = [r + \lambda(\sigma_{t-})\,\sigma_{t-}]\,\mathrm{d}t + \sigma_{t-}\,\mathrm{d}L_t. \tag{4.1}$$

Here the scaled innovation $\sigma_{t-}\,\mathrm{d}L_t$ is a COGARCH increment, $\mathrm{d}G_t$, $\lambda\colon [0,\infty) \to \mathbb{R}$ is the risk premium, and the volatility $(\sigma_t^2)_{t\geq 0}$ follows the dynamics in (3.2), namely

$$\mathrm{d}\sigma_t^2 = \left(\beta - \eta\,\sigma_{t-}^2\right)\mathrm{d}t + \phi\,\sigma_{t-}^2\,\mathrm{d}[L,L]_t, \quad t > 0. \tag{4.2}$$

The default time τ is defined as the first time at which the cumulative return R exhibits a jump ΔR_t below $-100\% = -1$:

$$\tau = \inf\{t > 0 : \Delta R_t \leq -1\} = \inf\{t > 0 : \sigma_{t-}\,\Delta L_t \leq -1\}.$$

At default the stock price drops to zero and stays there, thus we can write

$$S_t = S_0\,\mathcal{E}(R)_t\,\mathbf{1}_{\{t<\tau\}},$$

where $\mathcal{E}(X)$ denotes the stochastic exponential of X.

4.1 Relationship to other stochastic volatility models. To compare our model to other SV models, we reparameterise (4.1) and (4.2) as follows. Let us first assume that L in (4.1) is an error term satisfying $\mathbb{E}L_t = 0$ and $\mathbb{E}[L_t^2] = t$, or, equivalently,

$$\gamma + \int_{|x|>1} x\,\Pi(\mathrm{d}x) = 0, \quad \text{and} \quad \sigma^2 + \int_{\mathbb{R}} x^2\,\Pi(\mathrm{d}x) = 1. \tag{4.3}$$

This assumption is in fact no restriction, but ensures that the parameters can be identified. (Note that the function λ can be adjusted when centering L, and the scaling to unit variance of L affects only the variance parameters.)

The bracket process $[L, L]$ drives the volatility process σ. We center and scale $[L, L]$ to a martingale M with unit variance rate

$$M_t = \frac{[L,L]_t - \mathbb{E}[L,L]_t}{\sqrt{\mathbb{E}\left[([L,L]_1 - \mathbb{E}[L,L]_1)^2\right]}} = \frac{[L,L]_t^d - t\int_{\mathbb{R}} x^2\,\Pi(\mathrm{d}x)}{\sqrt{\int_{\mathbb{R}} x^4\,\Pi(\mathrm{d}x)}}, \quad t \geq 0.$$

Then we can write the variance equation (4.2) as

$$\mathrm{d}\sigma_t^2 = \kappa\left(\bar{\sigma}^2 - \sigma_{t-}^2\right)\mathrm{d}t + \nu\,\sigma_{t-}^2\,\mathrm{d}M_t, \quad t > 0, \tag{4.4}$$

where

$$\kappa = \eta - \phi, \quad \bar{\sigma}^2 = \frac{\beta}{\eta - \phi} \quad \text{and} \quad \nu = \phi\sqrt{\int_{\mathbb{R}} x^4\,\Pi(\mathrm{d}x)}.$$

The variance process is thus seen to be mean-reverting with mean level $\bar{\sigma}^2$, mean-reversion speed κ, and volatility $(\nu\sigma_t^2)_{t\geq 0}$, implying an average volatility of the variance process of $\nu\,\bar{\sigma}^2$. This enables us to benchmark our model to other SV models. We compare the COGARCH with the stochastic volatility model of Heston [25] (other related models include a Heston extension allowing for jumps of Bates [2], the SABR model of Hagan et al. [21], etc.). The dynamics of the Heston model are

$$\begin{aligned}\mathrm{d}S_t^H &= \mu_t^H\,S_t^H\mathrm{d}t + \sigma_t^H\,S_t^H\,\mathrm{d}W_t^{H,1},\\ \mathrm{d}(\sigma_t^H)^2 &= \kappa^H\left((\bar{\sigma}^H)^2 - (\sigma_t^H)^2\right)\mathrm{d}t + \nu^H\sqrt{(\sigma_t^H)^2}\,\mathrm{d}W_t^{H,2},\end{aligned}$$

with expected return rate μ^H, mean-reversion speed κ^H, mean level $(\bar{\sigma}^H)^2$, volatility of volatility parameter ν^H, and leverage ρ^H. Here, the leverage ρ^H is in fact the correlation of the standard Brownian motions $W^{H,1}$ and $W^{H,2}$.

Our model features the so-called option pricing leverage effect that is also included in the Heston model. However, in our setup leverage is not a free parameter, but is determined by the skew and kurtosis of the jump measure of L. Formally, leverage is quantified by the instantaneous correlation between the increments of the price equation $\mathrm{d}R_t$ and the increments of the variance equation $\mathrm{d}\sigma_t^2$. By scaling this reduces to the correlation of L_t and M_t, and leverage is given by

$$\rho = \mathrm{cor}(L_t, M_t) = \frac{\mathbb{E}[L_t\,M_t]}{t} = \frac{1}{t}\,\mathbb{E}\,[[L,M]_t] = \frac{\int_{\mathbb{R}} x^3\,\Pi(\mathrm{d}x)}{\sqrt{\int_{\mathbb{R}} x^4\,\Pi(\mathrm{d}x)}}. \tag{4.5}$$

We see that ρ is restricted by more than just $|\rho| \leq 1$; the Cauchy–Schwarz inequality implies

$$|\rho| \leq \sqrt{\int_{\mathbb{R}} x^2\,\Pi(\mathrm{d}x)} = \sqrt{1-\sigma^2} \quad (\text{cf. } (4.3)).$$

The COGARCH and Heston models are compared in Table 1.

Table 1. Specifications of the variance processes for COGARCH and Heston models ("f.v." stands for "finite variation").

	Drift	Volatility	Noise	Leverage
COGARCH	$\kappa\left(\bar{\sigma}^2 - \sigma_t^2\right)$	$\nu\,\sigma_t^2$	f.v. pure jump	$\dfrac{\int_{\mathbb{R}} x^3\,\Pi(\mathrm{d}x)}{\sqrt{\int_{\mathbb{R}} x^4\,\Pi(\mathrm{d}x)}}$
Heston	$\kappa^H\left((\bar{\sigma}^H)^2 - (\sigma_t^H)^2\right)$	$\nu^H\sqrt{\left(\sigma_t^H\right)^2}$	Brownian	$\rho^H \in [-1,1]$

4.2 Default time and default adjusted return dynamics. The default time τ admits a predictable intensity $\hat{\mu} = (\hat{\mu}_t)_{t\geq 0}$ driven by the variance process $(\sigma_t^2)_{t\geq 0}$. Using the Markov property of $(\sigma_t^2)_{t\geq 0}^2$ and the independent and stationary increments property of L, we can establish that $\hat{\mu}_t = \hat{\mu}(\sigma_{t-})$, where the function $\hat{\mu}$ is given by

$$\hat{\mu}(x) = \Pi\left(\left(-\infty, -\frac{1}{x}\right]\right) = \int_{-\infty}^{-1/x} \Pi(\mathrm{d}y), \quad x > 0. \tag{4.6}$$

Then the process $N = (N_t)_{t\geq 0}$ defined by

$$N_t = \mathbf{1}_{\{\tau \leq t\}} - \int_0^{t\wedge\tau} \hat{\mu}(\sigma_{u-})\,\mathrm{d}u$$

is a martingale. The unconditional probability $\mathrm{PD} = (\mathrm{PD}_t)_{t\geq 0}$ of default prior to time t can then be calculated as

$$\mathrm{PD}_t = P(\tau \leq t) = 1 - \mathbb{E}\left[\exp\left(-\int_0^t \hat{\mu}(\sigma_u)\,\mathrm{d}u\right)\right], \quad t \geq 0.$$

We now turn to the effect of the default on the dynamics of the driving Lévy process L.

Theorem 4.1. *The bivariate process (S, σ^2) is a Markov process and the stochastic differential of S is given by*

$$\mathrm{d}S_t = S_{t-}\,[r + \lambda(\sigma_{t-})\,\sigma_{t-}]\,\mathrm{d}t + S_{t-}\,\sigma_{t-}\,\mathrm{d}\widehat{L}_t,$$

where $\widehat{L}$ is the stopped version of L with default adjustment

$$\widehat{L}_t = L_t^\tau + \mathbf{1}_{\{t\geq\tau\}}(-\Delta L_\tau - 1/\sigma_{\tau-}), \quad t \geq 0.$$

With $\hat{\lambda}$ defined by

$$\hat{\lambda}(x) = -\int_{-\infty}^{-1/x} \left(y + \frac{1}{x}\right)\Pi(\mathrm{d}y), \quad x > 0,$$

the compensated version $(\widehat{L}_t - \int_0^{t\wedge\tau} \hat{\lambda}(\sigma_{u-})\,\mathrm{d}u)_{t\geq 0}$ is a martingale.

Next, define the default adjusted return process $\widehat{R} = (\widehat{R}_t)_{t\geq 0}$ by

$$\widehat{R}_t = \int_0^{t\wedge\tau} (r + \lambda(\sigma_{u-})\,\sigma_{u-})\,\mathrm{d}u + \int_0^t \sigma_{u-}\,\mathrm{d}\widehat{L}_u. \tag{4.7}$$

By construction it is clear that that $S = S_0\,\mathcal{E}(\widehat{R})$, where $\mathcal{E}$ denotes the stochastic exponential. It follows that the discounted price process $Z = S/B$ is a local martingale if and only if $(\widehat{R}_t - r\,(t\wedge\tau))_{t\geq 0}$ is a local martingale. (Note that the processes $\widehat{R}$ and S are both stopped at τ.) The next theorem states the semimartingale characteristics of $\widehat{R}$ and is useful for identifying martingale measures. In our setting, the characteristics $(B_t^{\widehat{R}}, C_t^{\widehat{R}}, \Pi_t^{\widehat{R}})_{t\geq 0}$ of $\widehat{R}$ can be expressed as functions of σ_{t-}^2 using the Markov property, see also Kallsen and Vesenmayer [27].

Theorem 4.2. *The semimartingale characteristics $(B_t^{\widehat{R}}, C_t^{\widehat{R}}, \Pi_t^{\widehat{R}})$ of $\widehat{R}$ for the truncation function $h(x) = x\,\mathbf{1}_{\{|x|\leq 1\}}$ are for $t \geq 0$ given by*

$$\begin{aligned}
B_t^{\widehat{R}} &= \mathbf{1}_{\{t<\tau\}}\left(r + \sigma_{t-}\left[\lambda(\sigma_{t-}) + \hat{\lambda}(\sigma_{t-}) - \int_{1/\sigma_{t-}}^{\infty} x\,\Pi(\mathrm{d}x)\right]\right),\\
C_t^{\widehat{R}} &= \mathbf{1}_{\{t<\tau\}}\,\sigma_{t-}^2\,\sigma^2,\\
\Pi_t^{\widehat{R}}(A) &= \mathbf{1}_{\{t<\tau\}}\int \mathbf{1}_{\{\sigma_{t-}\,x\in(A\cap(-1,\infty))\}}\,\Pi(\mathrm{d}x) + \mathbf{1}_{\{t<\tau\}}\,\mathbf{1}_{\{-1\in A\}}\,\hat{\mu}(\sigma_t),
\end{aligned}$$

for Borel sets $A \subset \mathbb{R}\setminus\{0\}$.

Under a martingale measure Q, the drift of $\widehat{R}$ has to reduce to

$$B_t^{\widehat{R},Q} = \mathbf{1}_{\{t<\tau\}}\left(r - \sigma_{t-}\int_{1/\sigma_{t-}}^{\infty} x\,\Pi_t^Q(\mathrm{d}x)\right), \quad t \geq 0, \tag{4.8}$$

where Π_t^Q is the jump measure of L_t, and the correction results from our choice of truncation function $h(x) = x\,\mathbf{1}_{\{|x|\leq 1\}}$.

Remark 4.3. In the following we adopt the martingale modeling approach. Madan, Carr, and Chang [34] and Panayotov [41] also use this approach in related settings. Formally, the market model can be investigated for arbitrage using the results provided by Delbaen and Schachermayer [9]. Such a thoroughgoing investigation is beyond the scope of this paper.

4.3 The risk-neutral dynamics and option pricing. In the following we assume we are given a measure $Q \sim P$ such that L is a Lévy process with characteristic triplet $(\gamma^Q, (\sigma^Q)^2, \Pi^Q)$ and finite fourth moment. Further, assume that $(\sigma_t^2)_{t\geq 0}$ follows the dynamics given in (4.4). (Note that we can assume without loss of generality that L is centered to 0 and scaled to have a unit variance rate.)

The Q-dynamics of $(\sigma_t^2)_{t\geq 0}$ are given by the risk-neutral version of (4.4), i.e.,

$$\mathrm{d}\sigma_t^2 = \kappa^Q\,\left((\bar{\sigma}^Q)^2 - \sigma_{t-}^2\right)\mathrm{d}t + \nu^Q\,\sigma_{t-}^2\,\mathrm{d}M_t^Q, \quad t > 0, \tag{4.9}$$

where κ^{Q}, $(\bar{\sigma}^{Q})^2$, and ν^{Q} are the potentially adjusted parameters, and M^{Q} is the bracket process of L centered to 0 and scaled to unit variance rate. With $\hat{\lambda}^{Q}$ defined as in Theorem 4.1 by

$$\hat{\lambda}^{Q}(x) = -\int_{-\infty}^{-1/x} \left(y + \frac{1}{x}\right) \Pi^{Q}(\mathrm{d}y),$$

the compensated version $\hat{L}_t - \int_0^{t\wedge\tau} \hat{\lambda}^{Q}(\sigma_{u-})\,\mathrm{d}u$ is then a Q-martingale. The risk-neutral return process is then given by the risk-neutral version of (4.7), i.e.,

$$\hat{R}_t = \int_0^{t\wedge\tau} \left(r - \hat{\lambda}^{Q}(\sigma_{u-})\,\sigma_{u-}\right) \mathrm{d}u + \int_0^{t} \sigma_{u-}\,\mathrm{d}\hat{L}_u. \tag{4.10}$$

The expression $\hat{\lambda}^{Q}(\sigma_{t-})\,\sigma_{t-}$ can be conceptualised as the premium for the limited liability option, i.e. the premium paid by equity for protecting it from losses larger than 100%. The stock price process is given by $S = S_0\,\mathcal{E}(\hat{R})$.

Under the measure Q, denote by $\pi^{Q}(\cdot;\chi)$ the price process of a T-claim χ that is suitably integrable, i.e. the random variable χ is $\mathcal{F}_T$-measurable and $\mathbb{E}^{Q}|\chi| < \infty$. Then π^{Q} is given by

$$\pi^{Q}(t;\chi) = e^{-r\,(T-t)}\,\mathbb{E}^{Q}\left[\chi \mid \mathcal{F}_t\right].$$

4.4 Variance-Gamma COGARCH. In this section we take the Variance-Gamma (VG) process proposed by Madan and Seneta [35] and Madan, Carr, and Chang [34], and construct the VG-COGARCH model directly under a martingale measure Q, see discussion in the previous section. We examine the model for its suitability to reflect stylized facts, such as volatility clustering, leptokurtosis and skew, and incorporate as a new feature, possible default. We then compute option prices, and, using the implied Black–Scholes volatility, compare the results to those obtained from a corresponding Heston model. Finally, we discuss our stochastic exponential setup in relation to the exponential VG-COGARCH of Panayotov [41], see Remark 4.4 below.

Under the martingale measure Q the VG process L is defined by $L_t = \theta_{VG}\,\Gamma_t + \sigma_{VG}\,W_{\Gamma_t}$ for $t \geq 0$, where Γ is a Gamma process with variance rate ν_{VG} and unit mean rate carrying the market time. W is a standard Brownian motion independent of Γ, $\sigma_{\mathrm{VG}} > 0$ the volatility, and $\theta_{\mathrm{VG}} \in \mathbb{R}$ the drift. The VG process is a pure jump process having characteristic triplet $(\gamma^{Q}, 0, \Pi^{Q})$ with Lévy measure

$$\Pi^{Q}(\mathrm{d}x) = \frac{\exp(\theta_{\mathrm{VG}}\,x/\sigma^2_{\mathrm{VG}})}{|x|\,\nu_{\mathrm{VG}}} \exp\left(-\frac{\sqrt{2\,\sigma^2_{\mathrm{VG}}/\nu_{\mathrm{VG}} + \theta^2_{\mathrm{VG}}}}{\sigma^2_{\mathrm{VG}}}\,|x|\right) \mathrm{d}x, \tag{4.11}$$

and drift

$$\gamma^{Q} = \theta_{\mathrm{VG}} - \int_{|x|>1} x\,\Pi^{Q}(\mathrm{d}x). \tag{4.12}$$

With this parametrisation, the moments of the Lévy measure are

$$\int x\,\Pi^{Q}(\mathrm{d}x) = \theta_{\mathrm{VG}},$$
$$\int x^2\,\Pi^{Q}(\mathrm{d}x) = \theta_{\mathrm{VG}}^2\nu_{\mathrm{VG}} + \sigma_{\mathrm{VG}}^2,$$
$$\int x^3\,\Pi^{Q}(\mathrm{d}x) = 2\,\theta_{\mathrm{VG}}^3\nu_{\mathrm{VG}}^2 + 3\,\sigma_{\mathrm{VG}}^2\,\theta_{\mathrm{VG}}\,\nu_{\mathrm{VG}},$$
$$\int x^4\,\Pi^{Q}(\mathrm{d}x) = 6\,\theta_{\mathrm{VG}}^4\,\nu_{\mathrm{VG}}^3 + 12\,\sigma_{\mathrm{VG}}^2\,\theta_{\mathrm{VG}}^2\,\nu_{\mathrm{VG}}^2 + 3\,\sigma_{\mathrm{VG}}^4\,\nu_{\mathrm{VG}}.$$

Using the normalisation $\int x^2\,\Pi^{Q}(\mathrm{d}x) = 1$, which forces $\sigma_{\mathrm{VG}}^2 < 1$, the third and fourth moments can be written in the form

$$\int x^3\,\Pi^{Q}(\mathrm{d}x) = \mathrm{sign}(\theta_{\mathrm{VG}})\,\sqrt{\nu_{\mathrm{VG}}\,(1-\sigma_{\mathrm{VG}}^2)}\,(2+\sigma_{\mathrm{VG}}^2),$$
$$\int x^4\,\Pi^{Q}(\mathrm{d}x) = 3\,\nu_{\mathrm{VG}}\,(2-\sigma_{\mathrm{VG}}^4).$$

Then the leverage in (4.5) is obtained as a function of the VG parameter σ_{VG} and the sign of θ_{VG}:

$$\rho = \mathrm{sign}(\theta_{\mathrm{VG}})\,\frac{\sqrt{1-\sigma_{\mathrm{VG}}^2}\,(2+\sigma_{\mathrm{VG}}^2)}{\sqrt{3\,(2-\sigma_{\mathrm{VG}}^4)}}.$$

The risk-neutral default intensity $\hat{\mu}^{Q}(x)$ can then be derived from (4.6) as:

$$\hat{\mu}^{Q}(x) = \frac{1}{\nu_{\mathrm{VG}}}\,E_1\left(\frac{\theta_{\mathrm{VG}} + \sqrt{2\,\sigma_{\mathrm{VG}}^2/\nu_{\mathrm{VG}} + \theta_{\mathrm{VG}}^2}}{\sigma_{\mathrm{VG}}^2\,x}\right), \quad x > 0,$$

where $E_1(x) = \int_x^{\infty} y^{-1}\,e^{-y}\,\mathrm{d}y$ for $x > 0$.

Figure 1 displays the default intensity $\hat{\mu}^{Q}$ depending on the volatility $(\sigma_t)_{t\geq 0}$ for three different parameterisations. The structural parameters of the volatility SDE are $\kappa^{Q} = 1, \bar{\sigma}^{Q} = 0.30, \nu^{Q} = 1$. The first set of VG-parameters is given by $\theta_{\mathrm{VG}} = -1.64$, $\nu_{\mathrm{VG}} = 0.01$, $\sigma_{\mathrm{VG}}^2 = 0.99$, and reproduces a skew of -0.77 and a kurtosis of 7.90 for daily return data as is typically observed for liquidly traded single stocks (see blue/solid). The second parameter set is given by $\theta_{\mathrm{VG}} = -1.62$, $\nu_{\mathrm{VG}} = 0.02$, $\sigma_{\mathrm{VG}}^2 = 0.97$, and reproduces a skew of -1.51 and a kurtosis of 16.54 for daily return data (black/dotted). This parameter set shows more asymmetries and heavier tails and potentially proxies for rather illiquid mid-cap stocks. The third parameter set is given by $\theta_{\mathrm{VG}} = -1.60$, $\nu_{\mathrm{VG}} = 0.03$, $\sigma_{\mathrm{VG}}^2 = 0.96$, and reproduces a skew of -2.22 and a kurtosis of 25.83 for daily return data (red/dashed). As expected, the default intensity $\hat{\mu}^{Q}$ is increasing in the volatility and the kurtosis of the returns.

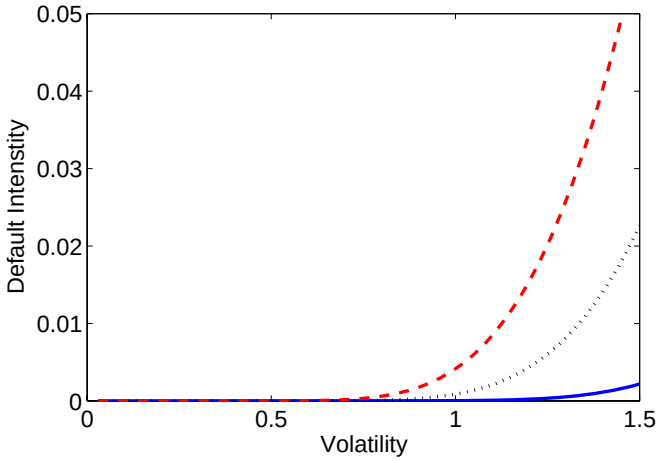

Figure 1. Risk-neutral default intensities $\hat{\mu}^{Q}$ for volatility parameters $\kappa^{Q} = 1$, $\bar{\sigma}^{Q} = 0.30$, $\nu^{Q} = 1$, and three different sets of VG parameters: (i) $\theta_{\mathrm{VG}} = -1.64$, $\nu_{\mathrm{VG}} = 0.01$, $\sigma^2_{\mathrm{VG}} = 0.99$ (blue/solid), (ii) $\theta_{\mathrm{VG}} = -1.62$, $\nu_{\mathrm{VG}} = 0.02$, $\sigma^2_{\mathrm{VG}} = 0.97$ (black/dotted), or (iii) $\theta_{\mathrm{VG}} = -1.60$, $\nu_{\mathrm{VG}} = 0.03$, $\sigma^2_{\mathrm{VG}} = 0.96$ (red/dashed).

The compensator $\hat{\lambda}^{Q}$ of $\widehat{L}$ can be calculated fairly explicitly as

$$\hat{\lambda}^{Q}(x) = \frac{\sigma^2_{\mathrm{VG}} \exp\left(-\frac{\theta_{\mathrm{VG}} + \sqrt{2\sigma^2_{\mathrm{VG}}/\nu_{\mathrm{VG}} + \theta^2_{\mathrm{VG}}}}{\sigma^2_{\mathrm{VG}}\, x}\right)}{\nu_{\mathrm{VG}}\left(\theta_{\mathrm{VG}} + \sqrt{2\sigma^2_{\mathrm{VG}}/\nu_{\mathrm{VG}} + \theta^2_{\mathrm{VG}}}\right)} - \frac{\hat{\mu}^{Q}(x)}{x}, \quad x > 0. \tag{4.13}$$

Figure 2 displays the risk-neutral default premium $\hat{\lambda}^{Q}(x)$ depending on the volatility for three different parameterisations. The risk-neutral default premium is as expected increasing in the volatility and the kurtosis. The parameterisations are identical to those of Figure 1 discussed above.

The option pricing model is now completely specified under the martingale measure Q. The driving Lévy process is VG with characteristic triplet $(\gamma^{Q}, 0, \Pi^{Q})$ defined in (4.11) and (4.12). The volatility dynamics are given according to (4.9) for some κ^{Q}, $(\bar{\sigma}^{Q})^2$, and ν^{Q}. The risk-neutral default adjusted return process $\widehat{R}$ is then defined according to (4.10) where $\hat{\lambda}^{Q}$ is given by (4.13).

Now, we compare the VG-COGARCH to the Heston model. We produce for both models the prices of European call options with varying strike prices and maturities. For the VG-COGARCH we apply Monte-Carlo simulation using a simple Euler discretisation scheme. The Heston call prices are computed by numerical integration of the characteristic function of the log-price process at maturity date. Both prices are then converted to corresponding implied Black–Scholes volatilities. The volatility dynamics is mean reverting around a level of $\bar{\sigma}^{Q} = \bar{\sigma}^{H,Q} = 0.30$ with mean reversion rate $\kappa^{Q} = \kappa^{H,Q} = 1$, for both VG-COGARCH and Heston, and a volatility of volatility pa-

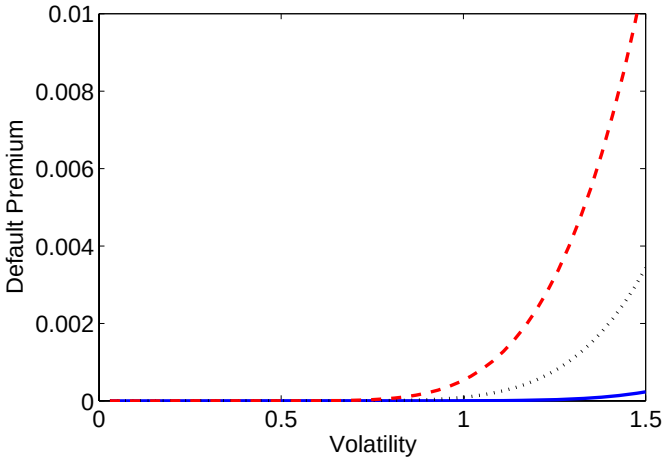

Figure 2. Risk-neutral default premium $\hat{\lambda}^{Q}(x)\,x$ for volatility parameters $\kappa^{Q} = 1$, $\bar{\sigma}^{Q} = 0.30$, $\nu^{Q} = 1$, and three different sets of VG parameters: (i) $\theta_{\mathrm{VG}} = -1.64$, $\nu_{\mathrm{VG}} = 0.01$, $\sigma^2_{\mathrm{VG}} = 0.99$ (blue/solid), (ii) $\theta_{\mathrm{VG}} = -1.62$, $\nu_{\mathrm{VG}} = 0.02$, $\sigma^2_{\mathrm{VG}} = 0.97$ (black/dotted), or (iii) $\theta_{\mathrm{VG}} = -1.60$, $\nu_{\mathrm{VG}} = 0.03$, $\sigma^2_{\mathrm{VG}} = 0.96$ (red/dashed).

rameter of $\nu^{Q} = 1$ for the VG-COGARCH and $\nu^{H,Q} = 0.30$ for Heston, respectively. With this setup we ensure that the volatility dynamics are comparable for both models, see Table 1. The VG parameters are set to $\theta_{\mathrm{VG}} = -1.64$, $\nu_{\mathrm{VG}} = 0.01$, and $\sigma^2_{\mathrm{VG}} = 0.99$ implying a leverage of $\rho = -0.275$ and skewness of -0.77 and kurtosis of 7.90 for the innovations on a daily basis. For the Heston model we have set $\rho^{H} = -0.275$ as well to keep the results comparable.

The implied volatility surface for the VG-COGARCH is displayed in Figure 3. The jumps and accordingly the high kurtosis lead to rather steep smile patterns for short dated options. At the long end the skewness dominates, and the typical smirk can be observed with declining implied volatilities for increasing strike prices. For the corresponding Heston model the implied volatility surface is graphed in Figure 4. Here, the smile for short dated options is of rather mild extent. This finding is well-known and can be attributed to the continuous price paths inherent in the Heston model. For longer maturities the skewness generated by the negative correlation $\rho^{H} = -0.275$ produces an implied volatility smirk approximately of the same extent as observed for VG-COGARCH. A difference plot for both volatilities is given in Figure 5. One may summarise that the VG-COGARCH can produce higher implied volatilities for short maturities deep in-the-money and far out-of-the-money.

Remark 4.4. We conclude this section by mentioning that a similar option pricing procedure for the COGARCH model has also been suggested by Panayotov [41]. In contrast to us he models the risk-neutral dynamics of the log price by a VG-COGARCH

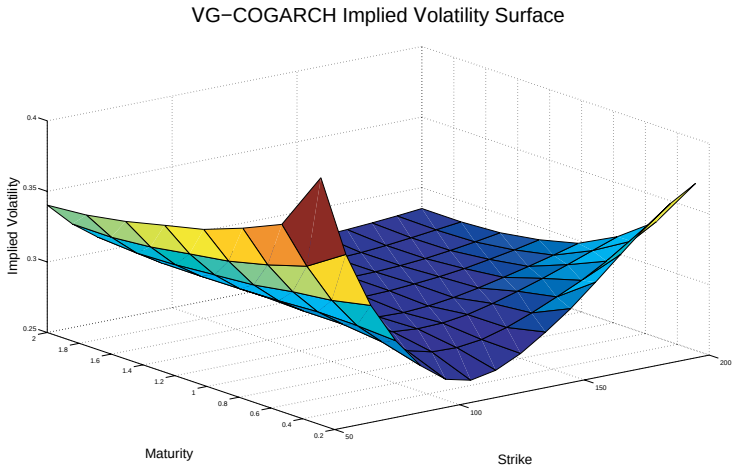

Figure 3. Implied Black–Scholes volatilities from VG-COGARCH call option prices. The risk-neutral parameters are $S_0 = 100$, $r = 0.05$, $\sigma_0^2 = 0.30^2$, $\kappa^Q = 1$, $\bar{\sigma}^Q = 0.30$, $\nu^Q = 1$, $\theta_{\mathrm{VG}} = -1.64$, $\nu_{\mathrm{VG}} = 0.01$, $\sigma_{\mathrm{VG}}^2 = 0.99$.

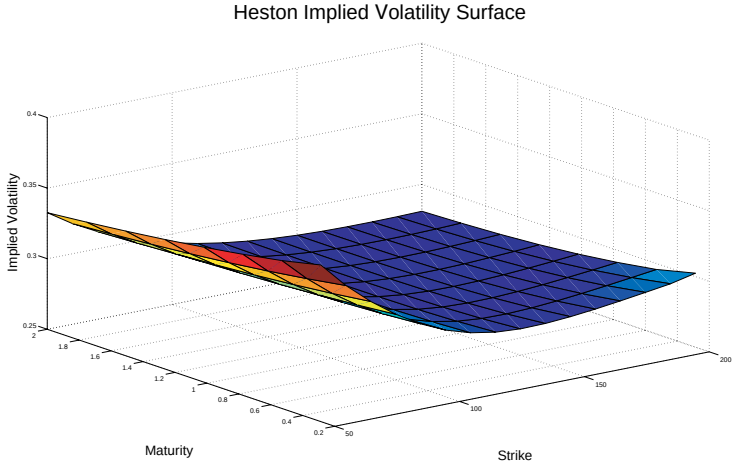

Figure 4. Implied Black–Scholes volatilities from Heston call option prices. The risk-neutral parameters are $S_0 = 100$, $r = 0.05$, $(\sigma_0^H)^2 = 0.30^2$, $\kappa^{H,Q} = 1$, $\bar{\sigma}^{H,Q} = 0.30$, $\nu^{H,Q} = 0.30$, $\rho^H = -0.275$.

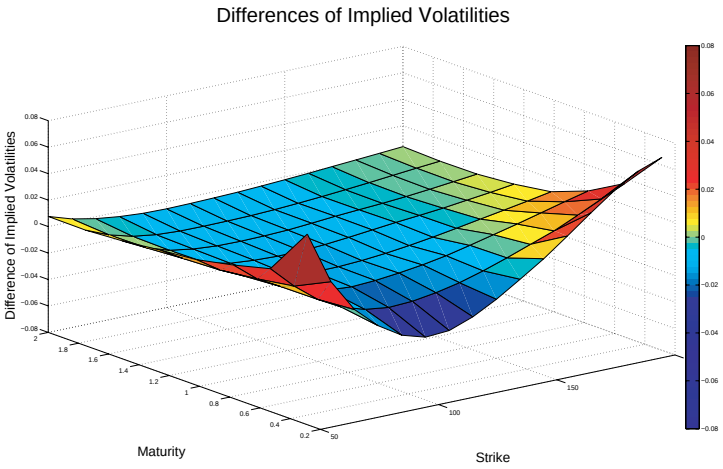

Figure 5. Difference of implied volatilities in Figure 3 and Figure 4.

process leading to a stock price process

$$\widetilde{S}_t = \widetilde{S}_0 \exp\Big(\int_0^t a_u \mathrm{d}u + \int_0^t \sigma_{u-} \, \mathrm{d}L_u \Big),$$

where $(\sigma_t)_{t\geq 0}$ is the COGARCH volatility driven by the VG process L, see Panayotov [41], Eq. (3.3.1). The expression $\int_0^t a_u \mathrm{d}u$ is a convexity correction which guarantees that the stock price has the proper risk-neutral expectation. According to (3.3.4) in Panayotov [41] the density of the correction a can be computed as follows

$$a_t = r - \int_{-\infty}^{\infty} \left(e^{\sigma_t x} - 1\right) \Pi^{Q}(\mathrm{d}x), \quad t \geq 0.$$

The log price process can be derived from this, and, using the fact that, together with the volatility process, it is jointly Markovian, the option price is calculated by numerically solving a PIDE. Possibility of default is not included in his model.

5 Statistical estimation of COGARCH

We present two different estimation procedures. The first is a simple method of moments estimation, which works only for equally spaced data. The second method is more sophisticated and handles unequally spaced data. It needs some preliminary results concerning the pathwise approximation of Lévy processes which we outline in this section. Throughout this section we assume that the driving Lévy process has no Gaussian part, i.e. that $\sigma^2 = 0$.

5.1 A method of moments estimation. For practical purposes, we need to discretise the continuous-time COGARCH onto a discrete grid over a finite time interval, and with a finite state space. Assume first that our data are given as described in (3.6). The goal of this section is to estimate the model parameters β, η, φ. Moreover, we shall present a simple estimate of the volatility.

5.1.1 Identifiability of the model parameters. We aim at estimation of the model parameters (β, η, φ) from a sample of equally spaced returns by matching empirical autocorrelation function and moments to their theoretical counterparts given in Proposition 3.1. The next result shows that the parameters are identifiable by this estimation procedure for driving Lévy processes L as in Proposition 3.1. We assume throughout that $\mathbb{E}(L_1) = 0$ and $\mathbb{E}(L_1^2) = 1$. For the sake of simplicity we set $r = 1$.

Theorem 5.1. *Suppose $(L_t)_{t\geq 0}$ is a Lévy process such that $\mathbb{E}(L_1) = 0$, $\mathbb{E}(L_1^2) = 1$, $\mathbb{E}(L_1^4) < \infty$ and $\int_{\mathbb{R}} x^3\, \Pi(dx) = 0$. Assume also that $\Psi(2) < 0$, and denote by $(G_i^{(1)})_{i\in\mathbb{N}}$ the stationary increment process of the* COGARCH(1, 1) *process with parameters $\beta, \eta, \varphi > 0$. Let $\mu, \gamma(0), k, p > 0$ be constants such that*

$$\begin{aligned} \mathbb{E}((G_i^{(1)})^2) &= \mu, \\ \mathrm{Var}((G_i^{(1)})^2) &= \gamma(0), \\ \rho(h) = \mathrm{corr}((G_i^{(1)})^2, (G_{i+h}^{(1)})^2) &= k e^{-hp}, \quad h \in \mathbb{N}. \end{aligned}$$

Define

$$\begin{aligned} M_1 &:= \gamma(0) - 2\mu^2 - 6\frac{1 - p - e^{-p}}{(1 - e^{p})(1 - e^{-p})}\, k\, \gamma(0), \\ M_2 &:= \frac{2k\gamma(0)p}{M_1(e^{p} - 1)(1 - e^{-p})}. \end{aligned} \tag{5.1}$$

Then $M_1, M_2 > 0$, and the parameters β, η, φ are uniquely determined by μ, $\gamma(0)$, k and p and are given by the formulas

$$\beta = p\,\mu, \tag{5.2}$$

$$\varphi = p\,\sqrt{1 + M_2} - p, \tag{5.3}$$

$$\eta = p + \varphi(1 - \mathrm{Var}(L_1)). \tag{5.4}$$

We conclude from (5.2)–(5.4) that our model parameter vector (β, η, φ) is a continuous function of the first two moments $\mu, \gamma(0)$ and the parameters of the autocorrelation function p and k. Hence, by continuity, consistency of the moments will immediately imply consistency of the corresponding plug-in estimates for (β, η, φ).

5.1.2 The estimation algorithm. The parameters are estimated under the following assumptions:

(H1) We have equally spaced observations G_i, $i = 0, \ldots, n$, on the integrated COGARCH as defined and parameterised in (3.1) and (3.2), assumed to be in its stationary regime. This gives return data $G_i^{(1)} = G_i - G_{i-1}$, $i = 1, \ldots, n$.

(H2) $\mathbb{E}(L_1) = 0$ and $\mathbb{E}(L_1^2) = 1$, i.e. $(\sigma_t^2)_{t\geq 0}$ can be interpreted as the volatility.

(H3) The driving Lévy process has no Gaussian part.

(H4) $\int_{\mathbb{R}} x^3\, \Pi(dx) = 0$, $\mathbb{E}(L_1^4) < \infty$ and $\Psi(2) < 0$.

We proceed as follows.

(1) Calculate the moment estimator $\hat{\mu}_n$ of μ as

$$\hat{\mu}_n := \frac{1}{n}\sum_{i=1}^{n}(G_i^{(1)})^2,$$

and for fixed $d \geq 2$ the empirical autocovariances $\hat{\boldsymbol{\gamma}}_n := (\hat{\gamma}_n(0), \hat{\gamma}_n(1), \ldots, \hat{\gamma}_n(d))^T$ as

$$\hat{\gamma}_n(h) := \frac{1}{n}\sum_{i=1}^{n-h}\big((G_{i+h}^{(1)})^2 - \hat{\mu}_n\big)\big((G_i^{(1)})^2 - \hat{\mu}_n\big), \quad h = 0, \ldots, d.$$

(2) Compute the empirical autocorrelations

$$\hat{\boldsymbol{\rho}}_n := (\hat{\gamma}_n(1)/\hat{\gamma}_n(0), \ldots, \hat{\gamma}_n(d)/\hat{\gamma}_n(0))^T.$$

(3) For fixed $d \geq 2$ define the mapping $H : \mathbb{R}_+^{d+2} \to \mathbb{R}$ by

$$H(\hat{\boldsymbol{\rho}}_n, \boldsymbol{\theta}) := \sum_{h=1}^{d}(\log(\hat{\rho}_n(h)) - \log k + ph)^2.$$

Compute the least squares estimator[4]

$$\hat{\boldsymbol{\theta}}_n := \operatorname{argmin}_{\boldsymbol{\theta}\in\mathbb{R}_+^2} H(\hat{\boldsymbol{\rho}}_n, \boldsymbol{\theta}).$$

(4) Define the mapping $J : \mathbb{R}_+^4 \to [0, \infty)^3$ by

$$J(\mu, \gamma(0), \boldsymbol{\theta}) := \begin{cases} (p\mu,\ p\sqrt{1+M_2} - p,\ p\sqrt{1+M_2} + p) & \text{if } p, M_2 > 0, \\ (0, 0, 0) & \text{otherwise,} \end{cases}$$

where M_2 is defined as in (5.1). Finally, compute the estimator

$$\hat{\boldsymbol{\vartheta}}_n = J(\hat{\mu}_n, \hat{\gamma}_n(0), \hat{\boldsymbol{\theta}}_n).$$

[4]We note the known robustness issues associated with least squares estimators. There is no difficulty in substituting for $\hat{\boldsymbol{\theta}}_n$ a more robust estimator, for instance, by replacing the $\mathcal{L}^2$-norm by the $\mathcal{L}^1$-norm, or invoking a weighted Huber estimator.

In Haug et al. [24] asymptotic normality of the estimated parameter vector was proved. This is essentially a consequence of the geometric ergodicity of the returns process $(G_i^{(1)})_{i\in\mathbb{N}}$.

To conclude this section we mention that Müller [38] developed an MCMC estimation procedure for the COGARCH(1, 1) model, which works also for irregularly spaced observations. The approach is, however, restricted to driving processes L of finite variation. Alternatively, Fasen [17] presents results on the non-parametric estimation of the autocovariance function of the volatility process and the COGARCH process by invoking point process methods. In the next section, we outline a more sophisticated way of dealing with unequally spaced data. It applies some results concerning the pathwise approximation of Lévy processes.

5.2 The "first jump" approximation for a Lévy process. In this section we review a "first jump" approximation to the underlying Lévy process which preserves certain crucial features of the process.

Suppose again that the Lévy process $(L_t)_{t\geq 0}$ has characteristic triplet of the form $(\gamma, 0, \Pi)$, where $\gamma \in \mathbb{R}$ and Π is the Lévy measure. As usual, denote the jumps of L_t by $\Delta L_t = L_t - L_{t-}$ for $t \geq 0$ (with $L_{0-} = 0$), and let

$$\bar{\Pi}(x) = \Pi((x, \infty)) + \Pi((-\infty, -x]), \quad x > 0, \tag{5.5}$$

denote the tail of $\Pi(\cdot)$.

We wish to approximate L on a finite time interval $[0, T]$, $0 < T < \infty$, partitioned into N_n not necessarily equally spaced intervals. Let $(N_n)_{n\in\mathbb{N}}$ be an increasing sequence of integers diverging to infinity as $n \to \infty$. For each $n \in \mathbb{N}$, form a deterministic partition $0 = t_0(n) < t_1(n) < \cdots < t_{N_n}(n) = T$ of $[0, T]$. In Maller and Szimayer [46], two approximating processes to L are constructed.

The first approximation, $\bar{L}_t(n)$ for $n \in \mathbb{N}$ is formed by taking the first jump, if one occurs, of L_t in each time subinterval $(t_{j-1}(n), t_j(n)]$, $j = 1, 2, \ldots, N_n$, where the jump sizes are bounded away from 0, then discretizing ("binning") these jumps to get an approximating process which takes only a finite number of values on a finite state space. The state space does not include 0, as we must avoid the possible singularity in Π at 0. If no jump occurs in a subinterval, $\bar{L}_t(n)$ remains constant in that subinterval.

A second approximating process, $L_t(n)$, $n \in \mathbb{N}$, is then taken as the discrete skeleton of $\bar{L}_t(n)$ on the time grid $(t_j(n))_{j=0,1,\ldots,N_n}$.

The time and space intervals are allowed to shrink and the state space to expand at appropriate rates, so as to get convergence of $\bar{L}_t(n)$ and $L_t(n)$ to L_t, as $n \to \infty$, in various modes.

To see how this works, take two sequences of real numbers $(m_n)_{n\in\mathbb{N}}$ and $(M_n)_{n\in\mathbb{N}}$, satisfying $1 > m_n \downarrow 0$ and $1 < M_n \uparrow \infty$ as $n \to \infty$. The first approximating process, $\bar{L}_t(n)$, takes discrete values in the set

$$J(n) = [-M_n, -m_n) \cup (m_n, M_n], \quad n \in \mathbb{N}.$$

To construct it, let

$$\tau_j(n) := \inf\{t : t_{j-1}(n) < t \le t_j(n); \Delta L_t \in J(n)\} \quad \text{for } 1 \le j \le N_n$$

(where the infimum over the empty set is defined as ∞) be the time of the first jump of L with magnitude in $(m_n, M_n]$ in interval j. Then decompose L_t as

$$L_t = \gamma_n t + L_t^{(1)}(n) + L_t^{(2)}(n) + L_t^{(3)}(n) \quad \text{for } 0 \le t \le T, \tag{5.6}$$

where for all $n \ge 1$ and $0 \le t \le T$:

$$L_t^{(1)}(n) = \text{a.s.} \lim_{\varepsilon \downarrow 0} \Big(\sum_{0<s\le t} \Delta L_s \, \mathbf{1}_{\{\varepsilon < |\Delta L_s| \le m_n\}} - t \int_{\varepsilon < |x| \le m_n} x \, \Pi(\mathrm{d}x) \Big),$$

$$L_t^{(2)}(n) = \sum_{0<s\le t} \Delta L_s \, \mathbf{1}_{\{M_n < |\Delta L_s|\}}, \quad L_t^{(3)}(n) = \sum_{0<s\le t} \Delta L_s \, \mathbf{1}_{\{m_n < |\Delta L_s| \le M_n\}},$$

and

$$\gamma_n = \gamma - \int_{m_n < |x| \le 1} x \, \Pi(\mathrm{d}x).$$

Decomposition (5.6) is a variant of the Lévy–Ito decomposition (Sato [44], Theorem 19.2, p. 120), in which, for each n, $L_t^{(1)}(n)$ is a compensated "small jump" martingale, and $L_t^{(2)}(n)$ and $L_t^{(3)}(n)$ might be thought of as "large jumps" and "medium jumps", respectively.

With no assumptions on L, Szimayer and Maller [46] show that, for $j = 1, 2$, $\lim_{n\to\infty} \sup_{0\le t\le T} L_t^{(j)}(n) = 0$ a.s. $L_t^{(3)}(n)$ can be further decomposed as follows:

$$L_t^{(3)}(n) = L_t^{(3,1)}(n) + L_t^{(3,2)}(n),$$

where

$$L_t^{(3,2)}(n) = \sum_{j=1}^{N_n} \mathbf{1}_{\{\tau_j(n) \le t\}} \Delta L^{(3)}_{\tau_j(n)}.$$

Thus $L_t^{(3,2)}(n)$ is the sum of the sizes of the first jump of L_t in each subinterval whose magnitude is in $(m_n, M_n]$, where such jumps occur, while $L_t^{(3,1)}(n)$ collects, over all subintervals, the sizes of those jumps with magnitudes in $(m_n, M_n]$ (except for the first jump), provided at least two such jumps occur in a subinterval.

Since we allow for the possibility that L has "infinite activity", that is, that $\Pi(\mathbb{R} \setminus \{0\}) = \infty$, we need a restriction on how fast m_n may tend to the possible singularity of Π at 0, by comparison with the speed at which the time mesh shrinks. With appropriate assumptions, $\lim_{n\to\infty} \sup_{0\le t\le T} |L_t^{(3,1)}(n)| = 0$ in probability, in $\mathcal{L}_1$, or, alternatively, in the almost sure sense. This leaves $L^{(3,2)}(n)$ as the predominant component, asymptotically, of L, and the penultimate step is to approximate it by a process $\bar{L}(n)$ that lives

on a finite state space. So we discretize the state space $J(n)$ with a grid of mesh size $\Delta(n) > 0$, where $\Delta(n) \searrow 0$ as $n \to \infty$, and set

$$\bar{L}_t(n) = \gamma_n t + \sum_{j=1}^{N_n} \mathbf{1}_{\{\tau_j(n) \le t\}} \left\lfloor \frac{\Delta L^{(3)}_{\tau_j(n)}}{\Delta(n)} \right\rfloor \Delta(n).$$

(The symbol $\lfloor x \rfloor$ denotes the integer part of $x \in \mathbb{R}$). Again under certain conditions, the difference between $L^{(3,2)}(n)$ and $\bar{L}(n)$ disappears, asymptotically, in the $\mathcal{L}_1$ or almost sure sense, uniformly in $0 \le t \le T$. Thus $\bar{L}(n)$ approximates L, in the sense that the distance between them as measured by the supremum metric tends to 0 in $\mathcal{L}_1$ or almost surely, in our setup.

The second approximation, $L(n)$, is obtained by evaluating $\bar{L}(n)$ on the same discrete time grid as we have used so far. Thus $L(n)$ is the piecewise constant process defined by

$$L_t(n) = \bar{L}_{t_{j-1}(n)}(n) \quad \text{when } t_{j-1}(n) \le t < t_j(n),\ j = 1, 2, \ldots, N_n, \tag{5.7}$$

and with $L_T(n) = \bar{L}_T(n)$. Because the original jumps are displaced in time in $L(n)$, we no longer expect convergence to L in the supremum metric. Instead, we get that $\lim_{n\to\infty} \rho(L(n), L) = 0$, where $\rho(\cdot,\cdot)$ denotes the Skorokhod J_1 distance in $\mathbb{D}[0, T]$. The processes $L(n)$ approximate L, *pointwise*, in probability, but not uniformly in $0 \le t \le T$. However, the convergence in probability in the Skorokhod topology suffices for certain applications that we discuss later.

Now we state the theorems from [46], which give the convergence of $\bar{L}_t(n)$ and $L_t(n)$ to L_t. Recall from (5.5) that $\bar{\Pi}$ denotes the tail of the Lévy measure of L_t. Let

$$\Delta t(n) := \max_{1\le j\le n} \left(t_j(n) - t_{j-1}(n)\right).$$

The main result for $\bar{L}_t(n)$ is:

Theorem 5.2. *Suppose*

$$\lim_{n\to\infty} \Delta t(n)\, \bar{\Pi}^2(m_n) = 0 \quad \text{and} \quad \lim_{n\to\infty} \Delta(n)\, \bar{\Pi}(m_n) = 0. \tag{5.8}$$

Then

$$\sup_{0\le t\le T} \left|\bar{L}_t(n) - L_t\right| \xrightarrow{P} 0 \quad \text{as } n \to \infty.$$

Next we consider the second approximating process, $L_t(n)$, as defined in (5.7). With a view to applications, we need the following property. The processes $(L_t(n))_{n\in\mathbb{N}}$ are said to satisfy *Aldous' criterion for tightness* if

$$\forall \varepsilon > 0 : \lim_{\delta \searrow 0} \limsup_{n\to\infty} \sup_{\substack{\sigma,\tau \in \mathcal{S}_{0,T}(n) \\ \sigma \le \tau \le \sigma+\delta}} \mathbb{P}\left(|L_\tau(n) - L_\sigma(n)| \ge \varepsilon\right) = 0,$$

where $\mathcal{S}_{t,T}(n)$ is the set of $\mathbb{F}^{L(n)}$-stopping times taking values in $[t, T]$, for $0 \le t \le T$. Let $\mathbb{D}[0, T]$ be the space of càdlàg real-valued functions on $[0, T]$ and $\rho(\cdot,\cdot)$ the Skorokhod J_1 distance between two processes in $\mathbb{D}[0, T]$.

Theorem 5.3. *Assume that Condition* (5.8) *of Theorem* 5.2 *holds. Then:*

(i) $\rho(L(n), L) \xrightarrow{P} 0$ *as* $n \to \infty$*;*

(ii) *the sequence* $(L_t(n))_{n\in\mathbb{N}}$ *satisfies Aldous' criterion for tightness.*

We conclude this section with some comments on the filtrations. Let $\mathbb{F}^L$, $\mathbb{F}^{\bar{L}(n)}$ and $\mathbb{F}^{L(n)}$ be the natural filtrations generated by the processes $(L_t)_{t\geq 0}$, $(\bar{L}_t(n))_{t\geq 0}$ and $(L_t(n))_{t\geq 0}$, respectively. Our construction clearly gives inclusion of the filtrations, that is, for each $n \geq 1$

$$\mathbb{F}^{L(n)} \subseteq \mathbb{F}^{\bar{L}(n)} \subseteq \mathbb{F}^L,$$

so, having demonstrated convergence of the approximating processes, we will have sufficient structure to prove convergence in some optimal stopping problems using recent results of Coquet and Toldo [7]. More discussion and possible applications of this can be found in Maller and Szimayer [46].

5.3 A discrete approximation to the COGARCH. In this section we show how to approximate a COGARCH pair $(G_t, \sigma_t)_{t\geq 0}$ with an embedded sequence of discrete time GARCH pairs, $(G_n(t), \sigma_n(t))_{t\geq 0}$, using the first jump technology developed in Section 5.2. The discrete approximating sequence, after appropriate rescaling, converges to the continuous time model in probability, in the Skorokhod metric, as the discrete approximating grid grows finer. This construction opens the way to using, for the COGARCH, similar statistical techniques to those already worked out for GARCH models, and useful applications can be made to options pricing, and to the modelling of irregularly spaced time series data.

For these kinds of applications L is usually assumed to have finite variance and mean 0, as we will do throughout this section.

Thus, we take as given the continuous time COGARCH pair $(G_t, \sigma_t)_{t\geq 0}$ defined in (3.1) and (3.2), and form a discrete approximating sequence as follows. Fix $T > 0$, and take deterministic sequences $(N_n)_{n\in\mathbb{N}}$ with $\lim_{n\to\infty} N_n = \infty$ and $0 = t_0(n) < t_1(n) < \cdots < t_{N_n}(n) = T$, and, for each $n \in \mathbb{N}$, divide $[0, T]$ into N_n subintervals of length $\Delta t_i(n) := t_i(n) - t_{i-1}(n)$, for $i = 1, 2, \ldots, N_n$. Assume $\Delta t(n) := \max_{i=1,\ldots,N_n} \Delta t_i(n) \to 0$ as $n \to \infty$, and define, for each $n \in \mathbb{N}$, a discrete time process $(G_{i,n})_{i=1,\ldots,N_n}$ satisfying

$$G_{i,n} = G_{i-1,n} + \sigma_{i-1,n}\sqrt{\Delta t_i(n)}\varepsilon_{i,n}, \quad i = 1, 2, \ldots, N_n, \tag{5.9}$$

where $G_{0,n} = G_0 := 0$, and the variance $\sigma^2_{i,n}$ follows the recursion

$$\sigma^2_{i,n} = \beta\Delta t_i(n) + \left(1 + \varphi\Delta t_i(n)\varepsilon^2_{i,n}\right) e^{-\eta\Delta t_i(n)}\sigma^2_{i-1,n}, \quad i = 1, 2, \ldots, N_n. \tag{5.10}$$

Here the innovations $(\varepsilon_{i,n})_{i=1,\ldots,N_n}$, $n \in \mathbb{N}$, are constructed using the "first jump" approximation outlined in Section 5.2. Since we assume a finite variance for L, we need only a single sequence $1 \geq m_n \downarrow 0$ bounding the jumps of L away from 0. We

assume it satisfies $\lim_{n\to\infty} \Delta t(n)\bar{\Pi}_L^2(m_n) = 0$. Such a sequence always exists, as $\lim_{x\downarrow 0} x^2\,\bar{\Pi}_L(x) = 0$. Fix $n \geq 1$ and define stopping times $\tau_{i,n}$ by

$$\tau_{i,n} = \inf\{t \in [t_{i-1}(n), t_i(n)) : |\Delta L(t)| \geq m_n\}, \quad i = 1, \ldots, N_n.$$

Thus $\tau_{i,n}$ is the time of the first jump of L in the ith interval whose magnitude exceeds m_n, if such a jump occurs.

By the strong Markov property, $\left(\mathbf{1}_{\{\tau_{i,n}<\infty\}}\Delta L(\tau_{i,n})\right)_{i=1,\ldots,N_n}$ is for each $n \in \mathbb{N}$ a sequence of independent rvs, with distribution specified by

$$\frac{\Pi(\mathrm{d}x)\mathbf{1}_{\{|x|>m_n\}}}{\bar{\Pi}(m_n)}\left(1 - e^{-\Delta t_i(n)\,\bar{\Pi}(m_n)}\right), \quad x \in \mathbb{R}\setminus\{0\},\ i = 1, 2, \ldots, N_n,$$

and with mass $e^{-\Delta t_i(n)\bar{\Pi}(m_n)}$ at 0. These rvs have finite mean, $\nu_i(n)$, and variance, $\xi_i(n)$, say. The innovations series $(\varepsilon_{i,n})_{i=1,\ldots,N_n}$ required for (5.9) is now defined by

$$\varepsilon_{i,n} = \frac{\mathbf{1}_{\{\tau_{i,n}<\infty\}}\,\Delta L(\tau_{i,n}) - \nu_i(n)}{\xi_i(n)}, \quad i = 1, 2, \ldots, N_n.$$

For each $n \in \mathbb{N}$, the $\varepsilon_{i,n}$ are independent rvs with $\mathbb{E}\varepsilon_{1,n} = 0$ and $\mathrm{Var}(\varepsilon_{1,n}) = 1$. Finally, in (5.10), we take $\sigma_{0,n}^2 = \sigma_0^2$, independent of the $\varepsilon_{i,n}$.

Remark 5.4. Equations (5.9) and (5.10) specify a GARCH(1, 1)-type recursion in the following sense. In the ordinary discrete time GARCH(1, 1) series, the volatility sequence satisfies (2.2), viz.,

$$\sigma_i^2 = \beta + \left(1 + (\phi/\delta)\varepsilon_{i-1}^2\right)\delta\sigma_{i-1}^2. \tag{5.11}$$

When the time grid is equally spaced, so $\Delta t_i(n) = \Delta t(n)$, $i = 1, 2, \ldots, N_n$, (5.10) is equivalent to (5.11), after rescaling by $\Delta t(n)$ and a reparametrisation from (β, φ, η) to (β, φ, δ), and (5.9) becomes a rescaled GARCH equation for the differenced sequence $G_{i,n} - G_{i-1,n}$. More generally, with an unequally spaced grid, if the series are scaled as in (5.9) and (5.10), convergence to the COGARCH is obtained as follows.

Embed the discrete time processes $G_{\cdot,n}$ and $\sigma_{\cdot,n}^2$ into continuous time versions G_n and σ_n^2 defined for $0 \leq t \leq T$ by

$$G_n(t) := G_{i,n} \quad \text{and} \quad \sigma_n^2(t) := \sigma_{i,n}^2, \quad \text{when } t \in [t_{i-1}(n), t_i(n)), \tag{5.12}$$

with $G_n(0) = 0$. The processes G_n and σ_n are in $\mathbb{D}[0, T]$. The next result is proved in Theorem 2.1 of Maller, Müller and Szimayer [36].

Theorem 5.5. *In the above setup, the Skorokhod distance between the processes (G, σ^2) defined by (3.1) and (3.2), and the discretised, piecewise constant processes $(G_n, \sigma_n^2)_{n\geq 1}$ defined by (5.12), converges in probability to 0 as $n \to \infty$; that is,*

$$\rho\left((G_n, \sigma_n^2), (G, \sigma^2)\right) \xrightarrow{\mathbb{P}} 0 \quad \text{as } n \to \infty.$$

Consequently, we also have convergence in distribution in $\mathbb{D}[0, T] \times \mathbb{D}[0, T]$:

$$(G_n, \sigma_n^2) \xrightarrow{D} (G, \sigma^2) \quad \text{as } n \to \infty.$$

Remark 5.6. Kallsen and Vesenmayer [27] derive the infinitesimal generator of the bivariate Markov process representation of the COGARCH model and show that any COGARCH process can be represented as the limit in law of a sequence of GARCH(1, 1) processes. The result of Theorem 5.5 is stronger in that it gives convergence to the continuous-time model in a strong sense (in probability, in the Skorokhod metric), as the discrete approximating grid grows finer. Whereas the diffusion limit in law established by Nelson [40] occurs from GARCH by aggregating its innovations, the COGARCH limit arising in Kallsen and Vesenmayer [27] and Maller et al. [36] both occur when the innovations are randomly thinned.

5.4 GARCH analysis of irregularly spaced data. Maller, Müller and Szimayer [36] apply the discrete approximation of the continuous time GARCH process to develop a method of fitting the model to unequally spaced times series data, using the methodology worked out for the discrete time GARCH.

5.4.1 The estimation algorithm. The parameters are estimated under the following assumptions:

(H1) Suppose given observations G_{t_i}, $0 = t_0 < t_1 < \cdots < t_N = T$, on the integrated COGARCH as defined and parameterised in (3.1) and (3.2), assumed to be in its stationary regime.

(H2) The (t_i) are assumed fixed (non-random) time points.

(H3) $\mathbb{E}L(1) = 0$ and $\mathbb{E}L^2(1) = 1$; i.e. σ^2 can be interpreted as the volatility.

(H4) The driving Lévy process has no Gaussian part.

Then we proceed as follows.

(1) Let $Y_i = G_{t_i} - G_{t_{i-1}}$ denote the observed increments and put $\Delta t_i := t_i - t_{i-1}$. Then from (3.1) we can write

$$Y_i = \int_{t_{i-1}}^{t_i} \sigma_{s-} \mathrm{d}L(s).$$

(2) We can use a pseudo-maximum likelihood (PML) method to estimate the parameters (β, η, φ) from the observed $Y_1, Y_2, \ldots, Y_N$. The pseudo-likelihood function can be derived as follows. Because $(\sigma_t)_{t\geq 0}$ is Markovian, Y_i is conditionally independent of $Y_{i-1}, Y_{i-2}, \ldots$, given $\mathcal{F}_{t_{i-1}}$. We have $\mathbb{E}(Y_i \mid \mathcal{F}_{t_{i-1}}) = 0$ for the conditional expectation of Y_i, and, for the conditional variance,

$$\rho_i^2 := \mathbb{E}(Y_i^2 \mid \mathcal{F}_{t_{i-1}}) = \left(\sigma_{t_{i-1}}^2 - \frac{\beta}{\eta - \varphi}\right)\left(\frac{e^{(\eta-\varphi)\Delta t_i} - 1}{\eta - \varphi}\right) + \frac{\beta \Delta t_i}{\eta - \varphi}. \tag{5.13}$$

Eq. (5.13) follows from the calculation in the third display on p. 618 of Klüppelberg et al. [30]. To ensure stationarity, we take $\mathbb{E}\sigma_0^2 = \beta/(\eta - \varphi)$, with $\eta > \varphi$, in that formula.

(3) Applying the PML method, then, we assume that the Y_i are conditionally $N(0, \rho_i^2)$, and use recursive conditioning to write a pseudo-log-likelihood function for the observations $Y_1, Y_2, \ldots, Y_N$ as

$$\mathcal{L}_N = \mathcal{L}_N(\beta, \varphi, \eta) = -\frac{1}{2}\sum_{i=1}^{N}\left(\frac{Y_i^2}{\rho_i^2}\right) - \frac{1}{2}\sum_{i=1}^{N}\log(\rho_i^2) - \frac{N}{2}\log(2\pi). \tag{5.14}$$

(4) We must substitute in (5.14) a calculable quantity for ρ_i^2, hence we need such for $\sigma_{t_{i-1}}^2$ in (5.13). For this, we discretise the continuous time volatility process just as was done in Theorem 5.5. Thus, (5.10) reads, in the present notation,

$$\sigma_i^2 = \beta\Delta t_i + e^{-\eta\Delta t_i}\sigma_{i-1}^2 + \varphi e^{-\eta\Delta t_i} Y_i^2. \tag{5.15}$$

(5) Finally, note that (5.15) is a GARCH-type recursion, so, after substituting σ_{i-1}^2 for $\sigma_{t_{i-1})}^2$ in (5.13), and the resulting modified ρ_i^2 in (5.14), we can think of (5.14) as the pseudo-log-likelihood function for fitting a GARCH model to the unequally spaced series.

The recursion in (5.15) is easily programmed, and, taking as starting value for σ_0^2 the stationary value $\beta/(\eta - \varphi)$, we can maximise the function $\mathcal{L}_N$ to get PMLEs of (β, η, φ). The small sample behaviour of these estimates are investigated in a simulation study in Durand, Maller and Müller [14]. Moreover, Müller, Maller and Durand [39] and Durand, Maller and Müller [14] apply this method to various financial data sets.

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Some properties of quasi-stationary distributions for finite Markov chains

Servet Martínez and Jaime San Martín

1 Introduction

Quasi-stationary distributions (q.s.d. for short) for Markov chains have been extensively studied since the pioneering work of Yaglom for the branching process in [11] and the classification of positive matrices introduced by Vere-Jones in [10]. We recommend the web site [6] at Philip Pollet's homepage for an extensive list of references on q.s.d. for countable Markov chains and related topics. In particular, the infinitesimal description of q.s.d. (as a probability eigenmeasure) on countable spaces was done in [5], for birth and death chains see [8] among others, and the more general existence result in the countable case was shown in [2].

The first study of q.s.d. for finite state Markov chains was done in [1]. In this work we remain in this setting. We supply some of the basic tools and results as well as some new properties. For example, we use the martingale property to give three equalities involving hitting times, this is done in Proposition 2.4. Based upon the geometrical property of the killing time we give in Proposition 2.5 a lumping result in terms of q.s.d.

Jointly with P. Collet we are preparing a monograph on q.s.d. for Markov processes, one dimensional diffusions and dynamical systems. There we give a much more general setting for the main properties of this paper.

2 Definitions and results

Let $X = (X_n : n \geq 0)$ be a discrete time Markov chain taking values on the finite set I, with transition matrix $P = (P_{ij} : i, j \in I)$. We denote by $\mathbb{P}_i$ the distribution of the chain when it starts from $X_0 = i$ and by $\mathbb{E}_i$ the corresponding mean value operator. We will assume that X is the canonical Markov chain, so the variable X_n is the projection of $I^{\mathbb{N}}$ onto its n-th coordinate.

Let $\partial I \subset I$ be a proper nonempty subset of I which we call set of forbidden states, and let $T = \inf\{n \geq 0 : X_n \in \partial I\}$ be the hitting time of this set. Let $\widehat{I} = I \setminus \partial I$ be the set of allowed states and $\widehat{P} = (P_{ij} : i, j \in \widehat{I})$. We will assume that $X_0 \in \widehat{I}$ and we shall consider the killed chain $X^{T-} = (X_n : n < T)$. A q.s.d. ν for X^{T-} is a probability distribution on $\widehat{I}$ that is conditionally invariant, that is, it verifies

$$\forall i \in \widehat{I},\ \forall n \geq 1 : \quad \mathbb{P}_\nu(X_n = i \mid T > n) = \nu(i). \tag{1}$$

Since the points in ∂I can be assumed to be absorbing, we can take $P_{ii} = 1$ for $i \in \partial I$. Then:

$$\forall i, j \in \widehat{I} : \quad P_{ij}^{(n)} = (\widehat{P}^n)_{ij}.$$

A necessary condition for the existence of q.s.d. is that the set of forbidden states can be hit from the set of allowed states, that is, there exists some $i_0 \in \widehat{I}$ such that $\mathbb{P}_{i_0}(T = 1) > 0$. To avoid technical problems that could make this presentation unnecessary heavy, we shall assume that $\widehat{P}$ is irreducible (that is, for all pairs $i, j \in \widehat{I}$ there exists $n > 0$ such that $P_{ij}^{(n)} > 0$).

2.1 Exponential killing. Let us write the q.s.d. condition in terms of $\widehat{P}$. First let us state the following property: if ν is a q.s.d., then when the process starts from ν, the killing time is geometrically distributed with parameter $1 - \theta(\nu)$. More precisely,

$$\forall\, n \geq 1: \quad \mathbb{P}_\nu(T > n) = \theta(\nu)^n \quad \text{with } \theta(\nu) = \mathbb{P}_\nu(T > 1). \tag{2}$$

Indeed, from the definition of q.s.d. and since the points of ∂I are absorbing we get

$$\begin{aligned}\mathbb{P}_\nu(T > n+m) &= \sum_{i\in\widehat{I}} \mathbb{P}_\nu(X_n = i, T > n+m)\\ &= \sum_{i\in\widehat{I}} \mathbb{P}_\nu(T > n+m \mid X_n = i)\mathbb{P}_\nu(X_n = i)\\ &= \sum_{i\in\widehat{I}} \mathbb{P}_i(T > m)\nu(i)\mathbb{P}_\nu(T > n) = \mathbb{P}_\nu(T > n)\mathbb{P}_\nu(T > m),\end{aligned}$$

and so the property (2) holds. The coefficient $\theta(\nu)$ is known as the rate of survival. Hence the property (1) can be written as

$$\forall i \in \widehat{I},\ \forall n \geq 1: \quad \sum_{j\in\widehat{I}} \nu(j) P_{ji}^{(n)} = \theta(\nu)^n \nu(i),$$

or equivalently $\nu' \widehat{P}^n = \theta(\nu)^n \nu'$ for all $n \geq 1$, which is equivalent to

$$\nu' \widehat{P} = \theta(\nu)\nu'.$$

Finally, observe that when ν is a probability eigenmeasure on $\widehat{I}$, that is, for some number θ,

$$\nu' \widehat{P} = \theta \nu',$$

then, by multiplying at the right by $\mathbb{1}$, we get $\theta = \theta(\nu)$. In particular,

$$\mathbb{P}_\nu(T > n) = \theta^n.$$

We have shown that a q.s.d. ν is any normalized positive eigenfunction of $\widehat{P}$.

We observe that if $Q = (Q_{ij} : i, j \in J)$ is an irreducible strictly substochastic matrix then for each state $j \in J_0 := \{j \in J : \sum_{k\in J} Q_{jk} < 1\}$ we add a state $\partial_j \notin J$. Let us define $I = J \cup \{\partial_j : j \in J_0\}$ and consider the following stochastic matrix P on I:

$$P_{ij} = Q_{ij} \quad \text{if } i, j \in J; \qquad P_{j\,\partial_j} = 1 - \sum_{k\in J} Q_{jk} \quad \text{if } j \in J_0; \qquad P_{\partial_j\,\partial_j} = 1,$$

and $P_{ij} = 0$ for any other pair of elements of I. When the set of forbidden states is $\partial I = \{\partial_j : j \in J_0\}$, then $\widehat{I} = J$ and $\widehat{P} = Q$. In the usual extension we collapse all the states ∂_j in a single state ∂.

Since $\widehat{P}$ is strictly substochastic, the Perron–Frobenius theory (see Theorem 1.2 in [7]) asserts that there exists a strictly positive eigenvalue $\theta \in (0,1)$ of $\widehat{P}$ which is its spectral radius. It is simple (because of irreducibility) and its left and right eigenvectors ν and h can be chosen to be strictly positive, hence

$$\nu' \widehat{P} = \theta \nu', \quad \widehat{P} h = \theta h, \quad \nu > 0,\ h > 0.$$

Here ν' denotes the row vector associated to ν. We can impose the following two normalizing conditions:

$$\nu' h = 1, \quad \nu' \mathbb{1} = 1,$$

where $\nu' f = \sum_{i \in \widehat{I}} f(i)\, \nu(i)$. In particular ν is a probability vector. From the above discussion the vector ν is a q.s.d. and the spectral radius θ is the rate of survival. The Perron–Frobenius theorem also guarantees that

$$\exists\, 0 \le \chi < \theta \ \text{ such that } \ \widehat{P}^n = \theta^n h\, \nu' + o(\chi^n),$$

or, equivalently,

$$P_{ij}^{(n)} = \theta^n h(i) \nu(j) + o(\chi^n).$$

So

$$\forall i \in \widehat{I} : \quad \mathbb{P}_i(T > n) = \sum_{j \in \widehat{I}} P_{ij}^{(n)} = \theta^n h(i) + o(\chi^n). \tag{3}$$

Remark 2.1. Assume that starting from the probability distribution η on $\widehat{I}$, the killing time T is geometrically distributed. Then from (3) we get that its parameter is necessarily $1 - \theta$, that is,

$$\mathbb{P}_\eta(T > n) = \eta' \widehat{P}^n \mathbb{1} = \theta^n \eta' \mathbb{1} = \theta^n.$$

Remark 2.2. In general it is not sufficient to assume that T has the geometrical distribution under the initial distribution η to conclude that η is a q.s.d. This occurs, for example, when the row sums of $\widehat{P}$ are a constant $c \in (0,1)$. In this case $h = \mathbb{1}$ where $\mathbb{1}$ is the vector with all its components equal to 1, and the spectral radius (rate of survival) is $\theta = c$. Moreover, for all probability measures η on $\widehat{I}$ we have the geometrical property $\mathbb{P}_\eta(T > n) = \theta^n$.

2.2 Exit independence between time and state. Let us show that when the process starts from a q.s.d., then the absorption time and the state where it is absorbed are independent random variables (see [3] for a general statement). Observe that the random variable X_T depends on the trajectories of $X^T = (X_n : n \le T)$.

Proposition 2.3. *Let ν be a q.s.d. Then T and X_T are $\mathbb{P}_\nu$-independent random variables.*

Proof. We already proved in (2) that the q.s.d. property implies $\mathbb{P}_\nu(T > n) = \theta(\nu)^n$. Take $k \in \partial I$. The Markov property and the q.s.d. equality $\mathbb{P}_\nu(X_n = i \mid T > n) = \nu(i)$ imply that for all real $n \geq 0$ it holds that

$$\begin{aligned}\mathbb{P}_\nu\,(T = n+1,\, X_T = \partial_k) &= \mathbb{P}_\nu\,(T > n,\, X_{n+1} = \partial_k)\\ &= \mathbb{P}_\nu\,(X_{n+1} = \partial_k \mid T > n)\;\mathbb{P}_\nu\,(T > n)\\ &= \mathbb{P}_\nu\,(X_1 = \partial_k)\;\theta(\nu)^n.\end{aligned}$$

We sum over $n \geq 0$ to get

$$\mathbb{P}_\nu(X_T = \partial_k) = \frac{1}{1-\theta(\nu)}\mathbb{P}_\nu(X_1 = \partial_k).$$

Thus

$$\begin{aligned}\mathbb{P}_\nu\,(T = n+1,\, X_T = \partial_k) &= \mathbb{P}_\nu(X_T = \partial_k)(1-\theta(\nu))\theta(\nu)^n\\ &= \mathbb{P}_\nu(X_T = \partial_k)\mathbb{P}_\nu(T = n+1),\end{aligned}$$

and the result follows. □

2.3 The martingale property. The process $W = (W_n : n \geq 0)$ defined by $W_n = \theta^{-n}h(X_n)$ is a $\mathbb{P}$-martingale. In fact, since $\widehat{P}h = \theta h$ we find

$$\begin{aligned}\mathbb{E}(\theta^{-n}h(X_n) \mid \sigma(X_0,\ldots,X_{n-1}) &= \mathbb{E}_{X_{n-1}}(\theta^{-n}h(X_1))\\ &= \theta^{-n}\,\widehat{P}h(X_{n-1}) = \theta^{-(n-1)}h(X_{n-1}),\end{aligned}$$

where as usual $\sigma(X_0,\ldots,X_{n-1})$ is the σ-field generated by $X_0,\ldots,X_{n-1}$. From Doob's sampling theorem we find that for all stopping times S and all n,

$$h(i) = \mathbb{E}_i(\theta^{-S\wedge n}h(X_{S\wedge n})) = \mathbb{E}_i(\theta^{-S}h(X_S),\, S \leq n) + \mathbb{E}_i(\theta^{-n}h(X_n),\, S > n).$$

Using the monotone convergence theorem we conclude that

$$h(i) = \mathbb{E}_i(\theta^{-S}h(X_S),\, S < \infty). \tag{4}$$

Consider the operator $\widetilde{\mathbb{E}}_i$ defined by the equality

$$\widetilde{\mathbb{E}}_i(G_n(X_1,\ldots,X_n)) = \frac{1}{h(i)}\mathbb{E}_i(G_n(X_1,\ldots,X_n)\theta^{-n}h(X_n)),$$

for all $G_n\colon I^n \to \mathbb{R}$. When G_n is an indicator function this defines a probability measure $\widetilde{\mathbb{P}}_i$ on $\widehat{I}^{\mathbb{N}}$. It is said that $\widetilde{\mathbb{P}}_i$ is induced by the martingale W.

Using the same ideas as in the proof of (4) we obtain for all stopping times S and all bounded functions $G\colon \bigcup_{n\in\mathbb{N}} I^n \to \mathbb{R}$ that

$$\widetilde{\mathbb{E}}_i(G(X_1,\ldots,X_S),\, S < \infty) = \frac{1}{h(i)}\mathbb{E}_i(G(X_1,\ldots,X_S)\theta^{-S}h(X_S),\, S < \infty). \tag{5}$$

Consider the transition matrix $\widetilde{P} = (\widetilde{P}_{ij} : i, j \in \widehat{I})$ given by

$$\widetilde{P}_{ij} := \frac{h(j)}{\theta h(i)} P_{ij}, \tag{6}$$

which is stochastic because h is a right eigenfunction with eigenvalue θ. We have that $\widetilde{\mathbb{P}}_i$ is the law of the canonical Markov chain with transition matrix $\widetilde{P}$. Since $\widetilde{P}$ is finite and irreducible, it is positive recurrent, and a direct computation shows that $(\nu h)' \widetilde{P} = (\nu h)'$. So the stationary distribution of $\widetilde{P}$ is given by

$$\nu h = (\nu(i)h(i) : i \in \widehat{I}).$$

Consider the random variables

$$T^i = \inf\{n \geq 0 : X_n = i\}.$$

Proposition 2.4. *For all $i, j \in \widehat{I}$ the following relations are satisfied:*

$$\begin{aligned} 1 &= \mathbb{E}_i(\theta^{-T^i}, T^i < \infty); \\ h(i) &= h(j)\mathbb{E}_i(\theta^{-T^j}, T^j < \infty); \\ \nu(i)h(i) &= \left(\mathbb{E}_i(\theta^{-T^i} T^i, T^i < \infty)\right)^{-1}. \end{aligned}$$

Proof. Since the law $\widetilde{\mathbb{P}}_i$ is the one of a positive recurrent Markov chain with stationary distribution given by νh, we obtain straightforwardly from (5) that the above three relations are respectively equivalent to

$$\widetilde{\mathbb{P}}_i(T^i < \infty) = 1; \quad \widetilde{\mathbb{E}}_i(h(T^j), T^j < \infty) = h(j); \quad \left(\widetilde{\mathbb{E}}_i(T^i)\right)^{-1} = \nu(i)h(i). \quad \square$$

2.4 Trajectories that are never killed. Let us observe that from relation (3) the following quasi-limiting behavior is obtained:

$$\forall i \in \widehat{I} : \quad \lim_{n\to\infty} \mathbb{P}_i(X_n = j \mid T > n) = \lim_{n\to\infty} \frac{\mathbb{P}_i(X_n = j)}{\mathbb{P}_i(T > n)} = \nu(j) \quad \text{for all } j \in I. \tag{7}$$

This property was shown in [1]. When $\nu \in \mathcal{P}(\widehat{I})$ satisfies property (7) it is called a quasi-limiting distribution or a Yaglom limit.

On the other hand (3) implies the following relation on the ratio of survival probabilities:

$$\forall i, j \in \widehat{I} : \quad \lim_{n\to\infty} \frac{\mathbb{P}_i(T > n)}{\mathbb{P}_j(T > n)} = \frac{h(i)}{h(j)}.$$

The same estimations give:

$$\forall i, j \in \widehat{I} : \quad \lim_{n\to\infty} \frac{\mathbb{P}_i(T > n - m)}{\mathbb{P}_j(T > n)} = \theta^{-m} \frac{h(i)}{h(j)}.$$

We now show that the trajectories that are never killed constitute a Markov chain and supply its law (see [4]). Let $i_0, \dots, i_k \in \widehat{I}$. Take $n > k$. From the Markov property we get

$$\mathbb{P}_{i_0}(X_1 = i_1, \dots, X_k = i_k,\ T > n) = \mathbb{P}_{i_0}(X_1 = i_1, \dots, X_k = i_k)\mathbb{P}_{i_k}(T > n-k).$$

Hence,

$$\begin{aligned}
&\lim_{n\to\infty} \mathbb{P}_{i_0}(X_1 = i_1, \dots, X_k = i_k \,|\, T > n) \\
&\quad = \mathbb{P}_{i_0}(X_1 = i_1, \dots, X_k = i_k) \lim_{n\to\infty} \frac{\mathbb{P}_{i_k}(T > n-k)}{\mathbb{P}_{i_0}(T > n)} \\
&\quad = \theta^{-k} \frac{h(i_k)}{h(i_0)} \mathbb{P}_{i_0}(X_1 = i_1, \dots, X_k = i_k) = \prod_{l=1}^{k} \left(\frac{h(i_l)}{\theta h(i_{l-1})} P_{i_{l-1}\, i_l} \right).
\end{aligned}$$

Then the process $Z = (Z_n : n \geq 0)$ whose law starting from $i \in \widehat{I}$ is given by

$$\mathbb{P}_i(Z_1 = i_1, \dots, Z_k = i_k) := \lim_{n\to\infty} \mathbb{P}_i(X_1 = i_1, \dots, X_k = i_k \,|\, T > n)$$

is a well-defined Markov chain taking values on $\widehat{I}$ with transition probability matrix $\widetilde{P} = (\widetilde{P}_{ij} : i, j \in \widehat{I})$ given by (6). This Markov chain is recurrent and its stationary distribution is νh.

Observe also that from the quasi-limiting behavior (7) we get the convergence of the final piece of the trajectory. Indeed, for any fixed $k \geq 0$, all $i_1, \dots i_k \in \widehat{I}$ and every initial distribution η on $\widehat{I}$ we have

$$\lim_{n\to\infty} \mathbb{P}_\eta \left(X_{n+1} = i_1, \dots, X_{n+k} = i_k \,|\, T > n\right) = \mathbb{P}_\nu \left(X_1 = i_1, \dots, X_k = i_k\right).$$

Here ν is the quasi-limiting distribution which, for irreducible finite Markov chains, coincides with the unique q.s.d.

2.5 Lumping. Finally let us state some conditions for lumping based upon the hypothesis that the killing time is geometrically distributed. This occurs for example when the initial distribution is a q.s.d., see (2) and Remark 2.2.

We briefly introduce the notion of a lumping process. Assume $X = (X_n : n \geq 0)$ is a finite state irreducible Markov chain on a finite set I with transition matrix $P = (P_{ij} : i, j \in I)$. Consider a partition $I_0, \dots, I_s$ of I. Define $\widetilde{I} = \{0, \dots, s\}$ and take the function $\psi : I \to \widetilde{I}$ given by $\psi(i) = a$ when $i \in I_a$. It is said that the process $\widetilde{X} = (\widetilde{X}_n : n \geq 0)$ with $\widetilde{X}_n = \psi(X_n)$ satisfies the lumping condition when it is a Markov chain.

The usual lumping condition is

$$\forall r, r' \in \{0, \dots, s\},\ \forall i, j \in I_r : \quad \sum_{k \in I_{r'}} P_{ik} = \sum_{k \in I_{r'}} P_{jk}. \tag{8}$$

Hence all the states in I_t are collapsed in a single state for $t = 0, \dots, s$. In this situation $\widetilde{X}$ satisfies the lumping condition, so it is a Markov chain and its stochastic kernel $\widetilde{P} = (\widetilde{P}_{ab} : a, b \in \widetilde{I})$ is given by

$$\widetilde{P}_{ab} = \sum_{k \in I_b} P_{ik}, \quad \text{where } i \in I_a.$$

In what follows we consider a two state lumping process. For this purpose we take $I = \{0, \dots, \ell\}$ with $\ell \geq 1$ and we assume $X = (X_n : n \geq 0)$ is an irreducible Markov chain taking values on I with transition matrix $P = (P_{ij} : i, j \in I)$. Consider the partition $I_0 = \{0\}$, $I_1 = \{1, \dots, \ell\}$, so $\psi(0) = 0$ and $\psi(i) = 1$ for all $i \in I_1$. In our Proposition 2.5 (see below) we shall give a condition in order that $\widetilde{X} = (\psi(X_n) : n \geq 0)$ verifies the lumping condition, that is, it is a Markov chain. This condition is related to geometrical absorption to the state 0. For this purpose let us consider $\partial I = \{0\}$ as the set of forbidden states. So $\widehat{I} = I_1$ and $T = \inf\{n \geq 0 : X_n = 0\}$ is the hitting time of 0 for the process X.

Our result will contain as a particular case the condition (8) which in this context reduces to:

$$\forall i \in I_1 : \quad P_{i0} = P_{10}.$$

In this special case $\widetilde{X}$ is a Markov chain with transition matrix $\widetilde{P}$ given by $\widetilde{P}_{00} = P_{00}$, $\widetilde{P}_{01} = 1 - P_{00}$, $\widetilde{P}_{10} = P_{10}$, $\widetilde{P}_{11} = 1 - P_{10}$. A key observation is that $\widehat{P}$, which is the restriction of P to $\widehat{I}$, has constant row sums $c = 1 - P_{10}$. Therefore, starting from any initial distribution on $\widehat{I}$, the random time T is geometrically distributed with parameter P_{10} (see Remark 2.2).

To state our generalization we need the following notion. The entrance distribution from 0 to $\widehat{I}$ is

$$e = (e_i : i \in \widehat{I}) \quad \text{with } e_i = \mathbb{P}_0(X_1 = i) = \frac{P_{0i}}{\sum_{j \in \widehat{I}} P_{0j}}.$$

We are in an irreducible finite case and as before we denote by θ the spectral radius. We also note that there exists a unique q.s.d. and its rate of survival is precisely θ.

Proposition 2.5. *Assume that under the entrance distribution e the random time T is geometrically distributed* (*this is satisfied when e is a q.s.d.*). *If the distribution of X_0 is a combination of δ_0 and e, then the process $\widetilde{X} = (\widetilde{X}_n : n \geq 0)$ is a Markov chain taking values in $\{0, 1\}$ with transition kernel $\widetilde{P}$ given by*

$$\widetilde{P}_{00} = P_{00}, \quad \widetilde{P}_{01} = 1 - P_{00}, \quad \widetilde{P}_{10} = 1 - \theta, \quad \widetilde{P}_{11} = 1 - P_{10}.$$

Proof. Since under e the killing time T is geometrically distributed, from Remark 2.1 its parameter is necessarily $1 - \theta$. We define by ζ the distribution on $\{0, 1\}$ given by $\zeta(0) = \mathbb{P}(X_0 = 0)$, $\zeta(1) = \mathbb{P}(X_0 \neq 0) = 1 - \zeta(0)$.

There is a unique (in distribution) Markov chain $Y = (Y_n : n \geq 0)$ taking values in $\{0, 1\}$ such that the initial distribution is ζ and the transition matrix Q is given by

$Q_{00} = P_{00} = 1 - Q_{01}$, $Q_{11} = \theta = 1 - Q_{10}$. This process is characterized by the sequence of independent sojourn times at 0 and 1, which are geometrically distributed with parameters $1 - P_{00}$ and $1 - \theta$ respectively.

On the other hand, the process $\widetilde{X}$ is realized as follows. Since the initial state of X is chosen at random with the distribution $\zeta(0)\delta_0 + \zeta(1)e$, the initial distribution of $\widetilde{X}$ is ζ. If $X_0 = 0$, then $\widetilde{X}$ remains at 0 according to a geometric distribution with parameter $1 - P_{00}$. If $X_0 \neq 0$ then, conditionally on this event, this initial state has a distribution e. By hypothesis $\widetilde{X}$ remains at 1 a time whose distribution is geometric with parameter $1 - \theta$. The process $\widetilde{X}$ then continues afresh. In this way $\widetilde{X}$ and Y have the same distribution and the result is shown. □

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The parabolic Anderson model with heavy-tailed potential

Peter Mörters

1 The parabolic Anderson problem

We consider the heat equation with random potential on the integer lattice $\mathbb{Z}^d$ and study the Cauchy problem with localised initial datum,

$$\begin{aligned} \partial_t u(t,z) &= \Delta u(t,z) + \xi(z)u(t,z), && \text{for } (t,z) \in (0,\infty) \times \mathbb{Z}^d, \\ \lim_{t \downarrow 0} u(t,z) &= \mathbf{1}_0(z), && \text{for } z \in \mathbb{Z}^d, \end{aligned} \tag{1}$$

where

$$(\Delta f)(z) = \sum_{\substack{y \in \mathbb{Z}^d \\ |y-z|=1}} [f(y) - f(z)], \quad \text{for } z \in \mathbb{Z}^d, \ f : \mathbb{Z}^d \to \mathbb{R}$$

is the discrete Laplacian, and the potential $(\xi(z) \colon z \in \mathbb{Z}^d)$ is a collection of independent identically distributed random variables. This problem appears in the context of chemical kinetics and population dynamics, and also provides a simplified qualitative approach to problems in magnetism and turbulence. Its name of *parabolic Anderson problem* goes back to the work of the nobel-prize winning physicist P. W. Anderson on entrapment of electrons in crystals with impurities, see [1]. The references [21], [28] and [11] provide applications, background and heuristics around the parabolic Anderson model and its relatives.

Interesting recent mathematical progress not discussed here can be found, for example, in [23], [20], [8], [17] and [13], two survey articles emphasising recent work on a range of potentials are [19] and [18]. Note that in some of these references the potential field is allowed to have a nontrivial time-dependence, a feature which we shall exclude from the discussions of the present paper.

The parabolic Anderson problem has a unique nonnegative solution if

$$E[(\xi(0) \vee 0)^{d+\epsilon}] < \infty \quad \text{for some } \epsilon > 0,$$

see [21]. Under this condition, the solution has a probabilistic representation known as the *Feynman–Kac formula*. Indeed, suppose the potential $(\xi(z) \colon z \in \mathbb{Z}^d)$ is fixed and let $(X_s \colon s \geq 0)$ be a continuous time random walk with generator Δ started at the origin. Let a particle following this walk have a mass, which is initially set to one. Suppose the particle mass grows with rate $\xi(z)$ when the particle sits at a site z with positive potential, and shrinks with rate $-\xi(z)$ when the particle sits at a site z with

nonpositive potential. The solution $u(t,z)$ of the parabolic Anderson problem is then given as the expected mass of particles at site z at time t. In other words,

$$u(t,z) = \mathbb{E}_0\Big[\mathbf{1}_{\{X_t=z\}} \exp\Big(\int_0^t \xi(X_s)\,ds\Big)\Big], \tag{2}$$

where the expectation refers only to the random walk, so that the solution is random due to its dependence on the potential $(\xi(z)\colon z \in \mathbb{Z}^d)$.

The main reason for the great interest the parabolic Anderson model has received over the past ten years is due to the *intermittency effect* which is believed to be present in the model as soon as the potential random variables $\xi(z)$ are truly random. Loosely speaking, intermittency means that, as time progresses, the bulk of the mass of the solution is not spreading in a regular fashion, but becomes concentrated in a small number of spatially separated connected sets of moderate size, whose location is determined by the potential, which are called intermittent islands. This means that there is a marked contrast between the behaviour of a diffusion in a constant potential, which, by the central limit theorem, spreads the bulk of its mass at time t over a ball of radius of order $\sqrt{t}$, and the behaviour of a random potential with even the slightest randomness. For example, in the case of a potential given by $P\{\xi(0) = 0\} = \varepsilon$, $P\{\xi(0) = -\delta\} = 1-\varepsilon$, for $\varepsilon, \delta > 0$, Biskup and König [9] provide evidence that the mass is almost surely concentrated in a small number of islands with diameter of order $(\log t)^{1/d}$ located in areas where the potential has a high concentration of zeroes.

On a heuristical level, the reason for this intermittent behaviour is the *competition* between the benefits of the random walk path spending much time at sites with large potential values, which is manifest from the exponential term in (2), and the unlikeliness of such paths. Even in the case of an only mildly random potential, there is an exponential advantage in spending most of the time in an area with maximal potential and therefore exponentially unlikely random walk paths make the dominant contribution to the expectation in (2). The strength of this effect depends on the distribution of the potential values $\xi(0)$, more precisely on the tail of the distribution of $\xi(0)$ at infinity. If the distribution has a *bounded support*, the main contribution will come from walks confined to islands consisting of sites with near maximal potential values. There will be a careful balance between the probability that a random walk reaches such an island in time $o(t)$ and stays there for the remaining time on the one hand, and the height of the potential on the island on the other hand. We expect that as time progresses the walk can reach larger and larger islands. Such behaviour also prevails if $\xi(0)$ has a *very light tail* at infinity. If the upper tail of $\xi(0)$ is *sufficiently heavy* however, we expect that only random walks that go to certain optimal sites in time $o(t)$ and remain at such a site for almost the entire time will contribute to the expectation. In this case the solution is localised in islands which are single sites and, in particular, do not grow in time.

It is a very hard problem to make the above heuristics rigorous, confirm the geometric picture of intermittency and study the precise time-dependence of the size of the islands as a function of the distribution of the potential values. Worse even, hardly anything is known about the number of islands on which the solutions are concentrated. Apart from the work described here, we note that progress on the geometry of the solutions has been

made on the one hand in the work of Sznitman for the closely related continuous model of a Brownian motion with Poissonian obstacles, the work of his group is surveyed in the monograph [29], and on the other hand in the seminal paper of Gärtner et al. [20], which treats the vicinity of the double-exponential distribution. The bulk of the literature however offers an alternative, less explicit, approach to the problem, by giving a rigorous expansion of the growth rate of the total mass of the solution in the time variable. This can then be interpreted in terms of geometric quantities like the size of the islands, and the height and profile of the solution on an island, see Section 2 for some more detail. In this context it was shown in [23] that there are four universality classes in the parabolic Anderson model, dividing potentials into classes corresponding to qualitatively different types of intermittent behaviour.

Roughly speaking, we can learn from this analysis that we can expect islands to be growing over time if the tails are light enough to satisfy

$$\text{(A)}\quad \frac{1}{x}\,\log\big|\log \mathbb{P}\{\xi(0) > x\}\big| \longrightarrow \infty \quad \text{as } x \uparrow \infty,$$

whereas the islands consist of single sites if

$$\text{(B)}\quad \frac{1}{x}\,\log\big|\log \mathbb{P}\{\xi(0) > x\}\big| \longrightarrow 0 \quad \text{as } x \uparrow \infty.$$

Class (A) covers all bounded potentials and some incredibly light-tailed unbounded ones, most of the unbounded potentials (in particular the class of Gaussian potentials) belong to class (B). Note that the rigorous results about this classification require mild additional regularity assumptions, which we neglect for the purpose of this introduction.

The present paper reports on the progress obtained in the attempt to study the geometry of the solutions for potentials which lead to islands consisting of single sites. Apart from the author of this survey, the researchers involved in various stages of this project were Remco van der Hofstad (Eindhoven), Wolfgang König (Berlin), Hubert Lacoin (Paris), Marcel Ortgiese (Berlin) and Nadia Sidorova (London). For our analysis we chose the potentials with the heaviest possible tails. In fact we assumed that the potentials follow the Pareto distribution

$$P\{\xi(0) \geq x\} = x^{-\alpha} \qquad \text{for all } x \geq 1.$$

We assumed that the parameter α is strictly bigger than the lattice dimension d, which is necessary and sufficient for the existence of a nonnegative solution to the parabolic Anderson problem.

While the choice of a potential with only polynomial decay at infinity was expected to make the possible qualitative effects of the random environment very pronounced, we were facing the technical challenge that much of the established techniques to study the parabolic Anderson problem were not available to us, as they require finiteness of some moments of the solution. As a result, new techniques had to be developed. I will give a flavour of these techniques when presenting the results of this project in the following sections.

2 The growth rate of the total mass

For comparison, we start by looking at the situation in the case of potential with milder irregularities, more precisely we assume that all exponential moments (with positive rate) of the random variable $\xi(0)$ are finite. Then the function

$$H(t) := \log E e^{t\,\xi(0)}, \quad \text{for } t > 0,$$

is well defined and finite. Define

$$U(t) := \sum_{z \in \mathbb{Z}^d} u(t,z)$$

to be the total mass of the system at time t. A large deviation heuristic (detailed, for example, in [23]) suggests that the following almost sure expansion holds as $t \uparrow \infty$:

$$\frac{1}{t} \log U(t) = \frac{H(\beta_t \alpha(\beta_t)^{-d})}{\beta_t \alpha(\beta_t)^{-d}} - \alpha(\beta_t)^2\,(\kappa + o(1)),$$

where α and β are positive scale-functions and $\alpha(\beta_t)$ plays the rôle of the order of the diameter of the intermittent islands at time t. The first order term describes the height of the potential on an island at time t and therefore the growth rate of the solution. The number κ in the second order term is the minimiser in a variational problem whose optimiser describes the profile of the solution on an island scaled to diameter of constant order. As indicated above, the papers [22], [9], [23] give rigorous asymptotic expansions of $\frac{1}{t} \log U(t)$ up to the second order term, which can then be interpreted in terms of these heuristics. Between them they cover all potentials with finite exponential moments, subject to mild regularity assumptions.

Note that the heuristics above predicts that the two leading terms in the expansion of the random variable $\frac{1}{t} \log U(t)$ are deterministic. In [24] we have shown that this does not apply in the case of the Pareto potential, as already the leading term is random.

Theorem 2.1 (Weak asymptotics of the growth rate, Theorem 1.2 in [24]). *Suppose that the random variable $\xi(0)$ is Pareto distributed with parameter $\alpha > d$. Then, as $t \uparrow \infty$,*

$$\frac{(\log t)^{\frac{d}{\alpha-d}}}{t^{\frac{\alpha}{\alpha-d}}} \log U(t) \Rightarrow Y, \quad \textit{where } P\{Y \le y\} = \exp\big(-\theta y^{d-\alpha}\big)$$

and

$$\theta := \frac{(\alpha-d)^d\, 2^d\, B(\alpha-d, d)}{d^d\,(d-1)!},$$

where B denotes the beta function.

Remark 2.2. (a) The limit law Y is of extremal Fréchet type with shape parameter $\alpha - d$.

(b) The fact that already the first term in the expansion of $\frac{1}{t}\log U(t)$ is random is due to the extreme irregularity of the Pareto potentials. The main result of [24] is an expansion for the case of the Weibull potentials, which shows that in this case the leading term in the expansion is still deterministic. Starting from the second term we have a discrepancy between the almost sure liminf and limsup behaviour. A weak limit theorem with nondegenerate limit distribution can only be observed for the fourth term, in which case we see a limit variable of Gumbel type.

We can also describe the fluctuations in the growth rate in an almost sure sense. To this end, we use the abbreviation

$$L_t := \tfrac{1}{t}\,\log U(t).$$

Theorem 2.3 (Almost sure asymptotics of the growth rate, Theorem 1.1 in [24]). *Suppose that the random variable $\xi(0)$ is Pareto distributed with parameter $\alpha > d$. Then, almost surely,*

$$\limsup_{t\to\infty} \frac{\log L_t - \frac{d}{\alpha-d}\log t}{\log\log t} = -\frac{d-1}{\alpha-d}, \quad \text{for } d > 1,$$
$$\limsup_{t\to\infty} \frac{\log L_t - \frac{d}{\alpha-d}\log t}{\log\log\log t} = \frac{1}{\alpha-d}, \quad \text{for } d = 1,$$

and

$$\liminf_{t\to\infty} \frac{\log L_t - \frac{d}{\alpha-d}\log t}{\log\log t} = -\frac{d}{\alpha-d}, \quad \text{for } d \geq 1.$$

Remark 2.4. Theorem 2.1 shows that the liminf above is indeed a limit in probability, which demonstrates that the differing limsup behaviour is due to a small number of exceptional time scales where the growth rate is slightly bigger than typical.

We postpone the discussion of proof techniques to Section 4 where we give a considerable strengthening of Theorem 2.1.

3 Localisation: The one- and the two-cities theorem

Having looked at the total mass $U(t)$, we now shift our interest to the *profile* of the solution defined as

$$v(t,z) := \frac{u(t,z)}{U(t)} \qquad \text{for } t > 0, z \in \mathbb{Z}^d.$$

In other words, for any time t, we define $v(t,z)$ as the proportion of mass allocated to the site z. Suppose that our potential is of class (B) and islands are expected to consist of

single lattice sites. Apart from confirming this rigorously, the most interesting question in this situation is how many islands are required to support the bulk of the solution.

Question. *Find $n = n(t)$ as small as possible such that, for suitable (pairwise distinct) random points $Z_t^{(1)}, \dots, Z_t^{(n)} \in \mathbb{Z}^d$, we have*

$$\lim_{t\uparrow\infty} \sum_{i=1}^{n} v(t, Z_t^{(i)}) = 1,$$

where the limit could be (a) *in probability, or* (b) *almost surely.*

This problem is essentially open for all nontrivial potentials in class (B) except for the Pareto potential, where it is solved in [25], a result we now present. We suppose from this point on in all our theorems that the random variable $\xi(0)$ is Pareto distributed with parameter $\alpha > d$.

Theorem 3.1 (One point localisation in probability, Theorem 1.2 in [25]). *There exists a càdlàg process $(Z_t : t > 0)$ with values in $\mathbb{Z}^d$, depending only on the potential field, such that*

$$\lim_{t\to\infty} v(t, Z_t) = 1 \quad \textit{in probability.}$$

Remark 3.2. (i) The solution is concentrated in just one site with high probability, a phenomenon often called *complete localisation*. To the best of our knowledge this has not been observed in any lattice-based model of mathematical physics so far, but it is not uncommon in mean-field models, see, for example, [15], [16].

(ii) We conjecture that the one-point localisation phenomenon holds for a wider class of heavy-tailed potentials, including the Weibull potentials, but does *not* hold for *all* potentials in class (A). In particular, it would be interesting to learn whether in the case of exponential distributions one needs $n(t) \to \infty$ points to cover the bulk of the solution.

An investigation of the proof of Theorem 2.1 given in [24] shows that

$$\frac{(\log t)^{\frac{d}{\alpha-d}}}{t^{\frac{\alpha}{\alpha-d}}} \log v(t, Z_t) \implies 0.$$

Note that this together with the asymptotics in Theorem 2.1 does not yield the concentration property in Theorem 3.1 since the asymptotics are only logarithmic. Much more precise techniques are required to prove the full strength of Theorem 3.1.

We describe the philosophy behind the proof, sketching the argument detailed in [26]. To guess the right choice of $(Z_t : t \geq 0)$ assume for the moment that the competition between the paths contributing to the expectation

$$U(t) = \mathbb{E}_0\Big[\exp\Big(\int_0^t \xi(X_s)\, ds\Big)\Big]$$

is only between paths that go to a site z in time $o(t)$ and stay there. While the exponential factor in this case yields $\exp(t\xi(z)\,(1+o(1))$, for z sufficiently far away from the origin the probability of such a path is essentially given by the probability that a random walk makes the minimum number of steps required to reach site z, which is the ℓ^1-norm $\|z\|_1$. As the number of steps of the walk in t time units is a Poisson random variable with mean $2dt$ the cost of reaching z is approximately

$$\frac{(2dt)^{\|z\|_1}}{\|z\|_1!}\,e^{-2dt} = \exp\big(-\|z\|_1\,\log\tfrac{\|z\|_1}{2dte}\,(1+o(1))\big).$$

Therefore we choose Z_t as the maximiser of the function

$$\Psi_t(z) = \xi(z) - \frac{\|z\|_1}{t}\,\log\frac{\|z\|_1}{2dte}, \quad \text{for } z \in \mathbb{Z}^d.$$

Note that the subtracted 'penalty term' depends increasingly on the ℓ^1-norm of the site z. Therefore, for the proof of Theorem 3.1, we can construct a centred ℓ^1-ball of random, time-dependent radius h_t so that Z_t is the site of maximal potential value in that box. Note that $\|Z_t\|_1$ would be a possible choice of such a radius, but in fact we can typically make it a bit larger. Given a site z and large time t we split $u(t,z)$ into three terms, which correspond to the contributions to the Feynman–Kac formula coming from paths that

(1) by time t have left the ball $\{z\colon \|z\|_1 \le h_t\}$,

(2) stay inside this ball up to time t but do not visit Z_t, and

(3) stay inside this ball and do visit Z_t.

It turns out that the total mass of the first two terms is negligible. For the first contribution this comes from an analysis, based on extreme value techniques, that shows that the radius h_t is very large at time t with high probability, so that it is very unlikely for random walk paths to leave this ball before time t. The argument for the second term is based on the fact, also obtained from extreme value analysis, that with high probability there is a large gap between the largest and the second-largest value of $\{\Psi_t(z)\colon z \in \mathbb{Z}^d\}$. Hence the contribution of paths avoiding Z_t is small compared to paths that spend a significant amount of time there.

It finally remains to show that there is only a negligible contribution from paths that stay in the box, visit Z_t but do not end up in Z_t at time t. The argument for this is based on a spectral analytical device, which is used in a similar manner as in [20]: We show that the third term above can be controlled in terms of the principal eigenfunction of the Anderson Hamiltonian, $\Delta + \xi$, in the ball with zero boundary conditions. This eigenfunction turns out to be exponentially concentrated in the maximal potential point in the ball, which by construction is Z_t. Hence the total mass U must be concentrated in Z_t, completing the sketch of the proof of Theorem 3.1.

Remark 3.3. The convergence in Theorem 3.1 cannot hold in the almost-sure sense. Indeed, assume that $v(t,Z_t) > 2/3$ for all $t \ge t_0$. As $v(\cdot\,,z)$ is continuous for

any $z \in \mathbb{Z}^d$, at any jump time $t \geq t_0$ of the process $(Z_t : t \geq 0)$ we have $v(t, Z_t-) + v(t, Z_t) > 4/3$, a contradiction. From the growth of $U(t)$ one can see that $(Z_t : t \geq 0)$ is not eventually constant, and thus has jumps at arbitrarily large times.

By the previous remark, at least *two sites* are needed to carry the total mass in an *almost sure* limit theorem. The main result of [25] shows that, in the case of Pareto distributed potentials, we have indeed almost sure localisation of the solution $u(t, \cdot)$ in two distinct lattice points $Z_t^{(1)}$ and $Z_t^{(2)}$, as $t \to \infty$.

Theorem 3.4 (Two cities theorem, Theorem 1.1 in [25]). *There exist processes $(Z_t^{(1)} : t > 0)$ and $(Z_t^{(2)} : t > 0)$ with values in $\mathbb{Z}^d$, depending only on the potential field, such that $Z_t^{(1)} \neq Z_t^{(2)}$ for all $t > 0$, and*

$$\lim_{t\to\infty} v(t, Z_t^{(1)}) + v(t, Z_t^{(2)}) = 1 \quad \textit{almost surely.}$$

Remark 3.5. The term two cities theorem was suggested by S. A. Molchanov. The underlying intuition is that at a typical large time the mass, which is thought of as a population, inhabits one site, interpreted as a city. At some rare times, however, the entire population moves to the new city, so that at the transition times part of the population still lives in the old city, while part has already moved to the new one.

Again we sketch the philosophy behind the proof. The main reason why this result is much harder than Theorem 3.1 is that the approximation of $\frac{1}{t} \log U(t)$ by the maximum of Ψ_t is not good enough at all large times t and a more complex variational problem has to be built to describe the cost and benefit of paths spending their time predominantly at a site z.

To this end, we look at the event that, for some $\rho > 0$, the random walk wanders directly to a site z during the time interval $[0, \rho t]$ and stays there throughout $[\rho t, t]$. Denoting $\eta(z) := \log \#\{$ paths of length $\|z\|_1$ from origin to $z\}$, this event has probability

$$\begin{aligned}\frac{e^{\eta(z)}}{(2d)^{\|z\|_1}} \frac{(2d\rho t)^{\|z\|_1}}{\|z\|_1!}\, e^{-2d\rho t}\, e^{-2d(1-\rho)t} \\ = \exp\big(- \|z\|_1 \log \tfrac{\|z\|_1}{\rho t e} - 2dt + \eta(z) + o(t)\big).\end{aligned}$$

The reward for this behaviour is $\exp(t(1-\rho)\xi(z)(1+o(1)))$ and therefore we look at those (ρ, z) which maximise

$$\sup_{z\in\mathbb{Z}^d} \sup_{\rho\in(0,1)} \big\{(1-\rho)\xi(z) - \tfrac{\|z\|_1}{t} \log \tfrac{\|z\|_1}{\rho t e} + \tfrac{\eta(z)}{t}\big\}$$

Looking for the global maximimiser of the inner variational problem we get $\rho = \|z\|_1/(t\xi(z))$, which for large t becomes smaller than 1. Hence $Z_t^{(1)}$ and $Z_t^{(2)}$ are chosen as the two largest values of

$$\Phi_t(z) := \xi(z) - \frac{\|z\|_1}{t} \log \xi(z) + \frac{\eta(z)}{t}.$$

We are then able to show that, almost surely,

$$\tfrac{1}{t}\log U(t) \sim \max_{z\in\mathbb{Z}^d} \Phi_t(z).$$

The proof of Theorem 3.4 is, just as in the case of the one-point localisation, based on a decomposition of paths, this time five rather than three cases need to be distinguished, and a similar, albeit slightly refined, arsenal of techniques. Without going into detail, the big difference is that in the almost-sure sense we can only expect a gap between the largest and the third-largest value of $\{\Phi_t(z)\colon z \in \mathbb{Z}^d\}$, because whenever t_0 is such that the maximiser z_1 for all large $t < t_0$ is different from the maximiser z_2 for all small $t > t_0$, we necessarily have $\Phi_t(z_1) = \Phi_t(z_2)$ by continuity of the mapping $t \mapsto \Phi_t(z)$. This requires a different treatment of cases where the gap is between the largest and second-largest value, or between the second-largest and third-largest value, respectively.

4 Scaling limit theorems

Having seen that the solution of the parabolic Anderson problem with Pareto distributed potential field is concentrated in a single point at most times, it is natural to ask how the location of that point moves as time progresses. Theorem 1.3 (a) of [27] gives a functional scaling limit theorem for the localisation point, together with the value of the potential in that point. For definiteness of the formulation define X_t by the property that $v(t, X_t)$ is the maximum value of the profile at time t. For the (countably many) times where this *peak* is not unique we choose the one with the smallest ℓ^1-norm.

Theorem 4.1 (Functional scaling limit theorem, Theorem 1.3 of [27]). *There exists a time-inhomogeneous Markov process* $((Y_t^{(1)}, Y_t^{(2)}) : t > 0)$ *on* $\mathbb{R}^d \times \mathbb{R}$ *such that, as* $T \to \infty$, *we have*

$$\Big(\big(\tfrac{\log T}{T}\big)^{\frac{\alpha}{\alpha-d}} X_{tT}, \big(\tfrac{\log T}{T}\big)^{\frac{d}{\alpha-d}} \xi(X_{tT})\Big) : t > 0\Big) \\ \Longrightarrow \Big(\big(Y_t^{(1)}, Y_t^{(2)} + \tfrac{d}{\alpha-d}\|Y_t^{(1)}\|_1\big) : t > 0\Big),$$

in distribution on the space of càdlàg functions $f : (0,\infty) \to \mathbb{R}^d \times \mathbb{R}$ *with respect to the Skorokhod topology on compact subintervals of* $(0,\infty)$.

Before we give a detailed description of the limiting process and comment on the proof of this result, we discuss some of its interesting consequences.

Remark 4.2. (i) Projecting onto the first coordinate at time $t = 1$ we obtain, as $T \to \infty$,

$$\big(\tfrac{\log T}{T}\big)^{\frac{\alpha}{\alpha-d}} X_T \implies Y$$

in distribution. This means that the contributing random walks move with *superlinear speed* to the optimal point, a very remarkable fact. This result was also obtained as

Theorem 1.3 in [25] where the limiting random variable was characterised by its density

$$p(x) = \alpha \int_0^\infty \frac{\exp(-\theta y^{d-\alpha})\, \mathrm{d}y}{(y + \frac{d}{\alpha-d}\|x\|_1)},$$

where θ is the same constant as in Theorem 2.1.

(ii) Using that $\frac{1}{t}\log U(t) \sim \max_{z\in\mathbb{Z}^d} \Psi_t(z)$ in probability, we can derive from Theorem 4.1 a functional version of Theorem 2.1: As $T \to \infty$, we have

$$\Big(\big(\tfrac{\log T}{T}\big)^{\frac{d}{\alpha-d}} \tfrac{\log U(tT)}{tT} \,:\, t>0\Big) \implies \big(Y_t^{(2)} + \tfrac{d}{\alpha-d}\big(1-\tfrac{1}{t}\big)\|Y_t^{(1)}\|_1 \,:\, t>0\big).$$

As all involved processes are continuous, this convergence holds in distribution on the space of continuous functions $f\colon (0,\infty) \to \mathbb{R}$ with respect to the uniform topology on compact subintervals.

(iii) To formulate a more classical (but weaker) scaling limit theorem we extend the profile to $(0,\infty)\times\mathbb{R}^d$ by taking the integer parts of the second coordinate, letting $v(t,x) := v(t,\lfloor x\rfloor)$. Taking nonnegative measurable functions on $\mathbb{R}^d$ as densities with respect to the Lebesgue measure, we can interpret $a^d v(t,ax)$ for any $a,t>0$ as an element of the space $\mathcal{M}(\mathbb{R}^d)$ of probability measures on $\mathbb{R}^d$. Denoting by $\delta(y)\in\mathcal{M}(\mathbb{R}^d)$ the Dirac point mass located in $y\in\mathbb{R}^d$ we obtain, as $T\uparrow\infty$,

$$\Big(\big(\tfrac{T}{\log T}\big)^{\frac{\alpha d}{\alpha-d}}\, v\big(tT, \big(\tfrac{T}{\log T}\big)^{\frac{\alpha}{\alpha-d}} x\big)\colon t>0\Big) \implies \big(\delta(Y_t^{(1)})\colon t>0\big),$$

in the sense of convergence of finite dimensional distributions on the space $\mathcal{M}(\mathbb{R}^d)$ equipped with the weak topology. In other words, the scaled solution profile converges to a wandering point mass whose path is given by the process $(Y_t^{(1)}\colon t\ge 0)$. This formulation of the result is intuitive, but has two drawbacks: first it cannot be improved to convergence on a standard path space, and second it only contains the information that the mass a time t is concentrated in an island of size $o((t/\log t)^{\frac{\alpha}{\alpha-d}})$ and hides the fact that this island is indeed a single site.

In order to describe the limit process we need to introduce some notation. Denote by Π a Poisson point process on the cone

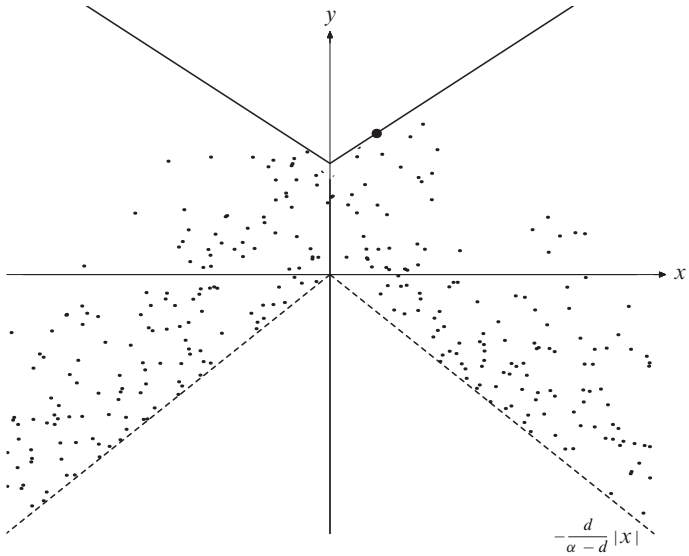
$$H^0 := \big\{(x,y)\in\mathbb{R}^d\times\mathbb{R}\colon y > -\tfrac{d}{\alpha-d}\|x\|_1\big\}$$

with intensity measure

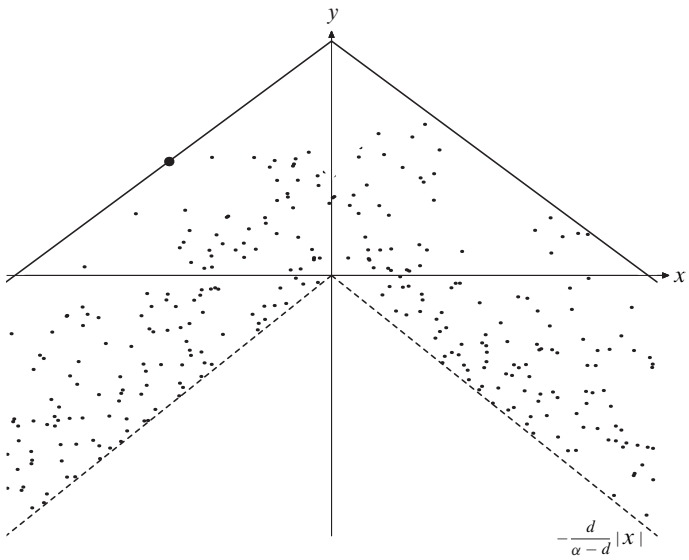
$$\nu(\mathrm{d}x\ \mathrm{d}y) = \mathrm{d}x \otimes \frac{\alpha\,\mathrm{d}y}{(y+\frac{d}{\alpha-d}\|x\|_1)^{\alpha+1}}.$$

Given this point process, we can define an $\mathbb{R}^d$-valued process $Y_t^{(1)}$ and an $\mathbb{R}$-valued process $Y_t^{(2)}$ in the following way. Fix $t>0$ and define the open cone with tip $(0,z)$ as

$$\mathcal{C}_t(z) = \big\{(x,y)\in\mathbb{R}^d\times\mathbb{R} \,:\, y + \tfrac{d}{\alpha-d}(1-\tfrac{1}{t})\|x\|_1 > z\big\},$$



(a) $t < 1$.



(b) $t > 1$.

Figure 1. The definition of the process $(Y_t^{(1)}, Y_t^{(2)})$ in terms of the point process Π. Note that t parametrises the opening angle of the cone, see (a) for $t < 1$ and (b) for $t > 1$.

and let

$$\mathcal{C}_t = \operatorname{cl} \bigcup_{z>0} \big\{ \mathcal{C}_t(z) \,:\, \Pi(\mathcal{C}_t(z)) = 0 \big\}.$$

Informally, $\mathcal{C}_t$ is the closure of the first cone $\mathcal{C}_t(z)$ that 'touches' the point process as we decrease z from infinity. Since $\mathcal{C}_t \cap \Pi$ contains at most two points, we can define $(Y_t^{(1)}, Y_t^{(2)})$ as the point in this intersection whose projection on the first component has the largest ℓ^1-norm, see Figures 1(a) and 1(b) for an illustration. The resulting process $((Y_t^{(1)}, Y_t^{(2)}) \colon t > 0)$ is an element of $D(0,\infty)$, the space of càdlàg functions on $(0,\infty)$ taking values in $\mathbb{R}^d \times \mathbb{R}$.

Remark 4.3 (Time evolution of the process). (i) $(Y_1^{(1)}, Y_1^{(2)})$ is the 'highest' point of the Poisson point process Π.

(ii) Given $(Y_t^{(1)}, Y_t^{(2)})$ and $s \geq t$ we consider the surface given by all $(x, y) \in \mathbb{R}^d \times \mathbb{R}$ such that

$$y = Y_t^{(2)} - \tfrac{d}{\alpha - d}\big(1 - \tfrac{1}{s}\big)(\|x\|_1 - \|Y_t^{(1)}\|_1).$$

For $s = t$ there are no points of Π above this surface, while $(Y_t^{(1)}, Y_t^{(2)})$ (and possibly one further point) is lying on it. We now increase the parameter s until the surface hits a further point of Π. At this time $s > t$ the process jumps to this new point $(Y_s^{(1)}, Y_s^{(2)})$. Geometrically, increasing s means opening the cone further keeping the point $(Y_t^{(1)}, Y_t^{(2)})$ on the boundary and moving the tip upwards on the y-axis.

(iii) Similarly, given the point $(Y_t^{(1)}, Y_t^{(2)})$ one can go backwards in time by decreasing s, or equivalently closing the cone and moving the tip downwards on the y-axis. The independence properties of Poisson processes ensure that this procedure yields a process $((Y_t^{(1)}, Y_t^{(2)}) \colon t > 0)$ which is Markovian in both the forward and backward direction. Note however that the projection $(Y_1^{(1)} \,:\, t > 0)$ is not Markovian (in either time direction).

(iv) An animation of the process $((Y_t^{(1)}, Y_t^{(2)}) \colon t > 0)$ provided by Marcel Ortgiese can be found at http://people.bath.ac.uk/maspm/animation_ageing.pdf

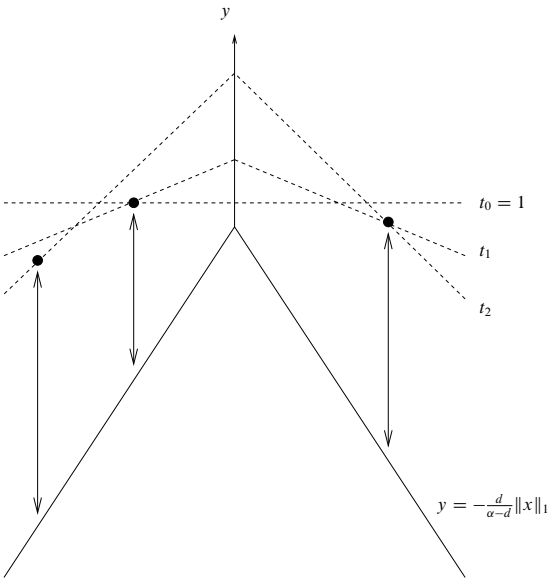
Remark 4.4. The process which describes the asymptotics of the scaled potential value in the peak,

$$\big(Y_t^{(2)} + \tfrac{d}{\alpha - d}\|Y_t^{(1)}\|_1 : t > 0\big),$$

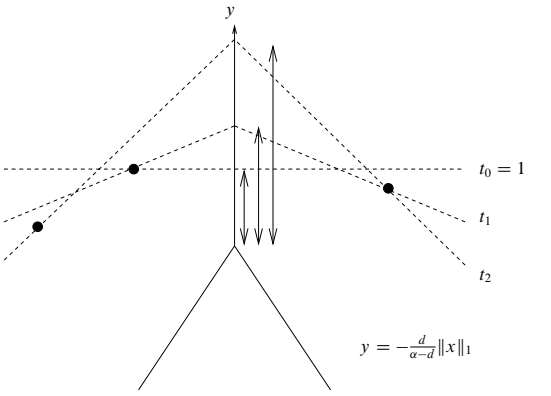
corresponds to the vertical distance of the point $(Y_t^{(1)}, Y_t^{(2)})$ to the boundary of the domain H_0 given by $y = -\frac{d}{\alpha - d}\|x\|_1$, see Figure 2(a). The process which describes the asymptotics of the scaled growth rate of the solution,

$$\big(Y_t^{(2)} + (1 - \tfrac{1}{t})\|Y_t^{(1)}\|_1 : t > 0\big)$$

corresponds to the y-coordinate of the tip of the cone $\mathcal{C}_t$, see Figure 2(b).



(a) The process describing the potential in the peak.



(b) The process describing the growth rate of the solution.

Figure 2. The position of the cone $\mathcal{C}_t$ at three times $1 = t_0 < t_1 < t_2$ is indicated by the three dashed contours. The maximal point of the Poisson process is marked by the bold dot on the dashed horizontal line. The two times t_1 and t_2 are jump times for the process $(Y_t^{(1)} : t \geq 1)$ with the Poisson points triggering the jumps marked. The vertical positions of the three dots represent the value of this process. (a) The length of the arrows indicate the value of the process $(Y_t^{(2)} + \frac{d}{\alpha - d}\|Y_t^{(1)}\|_1 : t > 0)$ at the three times corresponding to the dots at the end of the arrows. (b) The length of the arrows indicate the value of the process $(Y_t^{(2)} + (1 - \frac{1}{t})\|Y_t^{(1)}\|_1 : t > 0)$ at the three times, increasing from left to right.

The proof of this result uses the point process technique developed in [24]. We briefly describe the main idea here. Recall that at most times the peak X_t equals the maximiser Z_t of the variational problem given by Ψ_t. We have seen that, in probability,

$$\frac{1}{T}\log U(T) \sim \max_{z\in\mathbb{Z}^d} \Psi_T(z).$$

For $r_T = (T/\log T)^{\frac{\alpha}{\alpha-d}}$ and $a_T = (T/\log T)^{\frac{d}{\alpha-d}}$ the point process

$$\Pi_T = \sum_{z\in\mathbb{Z}^d} \delta_{(\frac{z}{r_T}, \frac{\Psi_T(z)}{a_T})},$$

where δ_x denotes the Dirac measure in x, converges to a Poisson point process Π with intensity measure $\nu(\mathrm{d}x\ \mathrm{d}y)$, as defined in the description of the limiting process. For fixed t and large T we obtain, when z/r_T is of constant order,

$$\frac{\Psi_{tT}(z)}{a_T} \approx \frac{\Psi_T(z)}{a_T} + \tfrac{d}{\alpha-d}\left(1-\tfrac{1}{t}\right)\frac{\|z\|_1}{r_T}.$$

Note further that

$$\frac{\xi(z)}{a_T} \approx \frac{\Psi_T(z)}{a_T} + \tfrac{d}{\alpha-d}\frac{\|z\|_1}{r_T}.$$

This allows us to approximate the events of interest with events involving only the point process Π_T. Informally, we obtain

$$\begin{aligned} &P\left\{\tfrac{Z_{tT}}{r_T}\in A,\ \tfrac{\xi(Z_{tT})}{a_T}\in B\right\} \\ &\quad\approx \iint_{x\in A, y+\frac{d}{\alpha-d}x\in B} P\Big\{\Pi_T(\mathrm{d}x\ \mathrm{d}y)>0, \\ &\qquad\qquad \Pi_T\big\{(\bar{x},\bar{y})\colon \bar{y}-y > \tfrac{d}{\alpha-d}\left(1-\tfrac{1}{t}\right)(\|x\|_1-\|\bar{x}\|_1)\big\}=0\Big\}, \end{aligned}$$

where the first line of conditions on the right means that there is a site $z/r_T \in A$ with $\Psi_T(z)/a_T = y$ and $\xi(z)/a_T \in B$, and the second line means that $\Psi_{tT}(z)$ is not surpassed by $\Psi_{tT}(\bar{z})$ for any other site $\bar{x} = \bar{z}/r_T$. We can now use the convergence of Π_T to Π inside the formula to give the limit theorem for the finite-dimensional distributions of

$$\Big(\big(\tfrac{X_{tT}}{r_T}, \tfrac{\xi(X_{tT})}{a_T}\big)\ :\ t>0\Big).$$

Checking a tightness criterion in Skorokhod space completes the argument.

5 Ageing in the parabolic Anderson model

In a physical system which changes over time we are naturally interested in the time scales in which we experience significant changes of the system. If the system has randomness we may, for example, try to find a function $s(t)$ such that the probability that the state at time t remains unchanged up to time $t + s(t)$ remains bounded from

zero and one, as $t \uparrow \infty$. We may say that the system exhibits *ageing* if $s(t)$ goes to infinity as $t \uparrow \infty$, while in typical cases of ageing we even observe a linear dependence of $s(t)$ on t. Hence, as time goes on, in an ageing system changes become less likely and the typical time scales of the system are increasing. Therefore, ageing can be associated to the existence of infinitely many time-scales that are inherently relevant to the system. This is in marked contrast to metastable systems, which are characterised by a finite number of well separated time-scales, corresponding to the lifetimes of different metastable states.

Ageing has been the subject of extensive research. Some interesting papers exhibiting the ageing phenomenon include the case of spherical spin glasses [7], the random energy model with Glauber dynamics [2] and interacting diffusions [12]. The bulk of the research however is on very simple *trap models* which give a phenomenological description of a particle moving in an energy landscape getting trapped in deeper and deeper energy wells. Interest for trap models in the mathematical community was created through the pioneering work of [14] and [6], and a survey is provided in the lecture notes of [3]. Recent work of Ben Arous and Černý [5] shows that in the case of trap models ageing is naturally linked with the arcsine law for stable subordinators, and this connection is believed to be of a universal nature.

Coming back to the parabolic Anderson model with Pareto tails, we can conjecture on the basis of the scaling limit theorem that the system exhibits some form of ageing: doubling the length of the observation window asymptotically doubles the length of periods of near constancy of the solution profile. However, the statement of the scaling limit theorem is not strong enough to verify a full ageing result, which can be obtained by other means.

Theorem 5.1 (Ageing in probability, Theorem 1.1 in [27].). *For any $\theta > 0$ there exists $0 < I(\theta) < 1$ such that, for all $0 < \varepsilon < \frac{1}{2}$,*

$$\begin{aligned}\lim_{t\uparrow\infty} P\Big\{ \sup_{z\in\mathbb{R}^d} \sup_{s\in[t,t+t\theta)]} \big|v(t,z) - v(s,z)\big| < \varepsilon\Big\}\\ = \lim_{t\uparrow\infty} P\Big\{ \sup_{z\in\mathbb{R}^d} \big|v(t,z) - v(t+t\theta,z)\big| < \varepsilon\Big\}\\ = I(\theta).\end{aligned}$$

Remark 5.2. As discussed in [4] in trap models it is often the case that a particle is in the same state at times t and $t + s(t)$ but has left this state briefly several times during the interval $[t, t + s(t)]$. This can lead to different relevant scales for the two limits above. For the parabolic Anderson model this is not the case, the profile never returns to an earlier state.

Remark 5.3. The constant $I(\theta) \in (0, 1)$ can be given explicitly in terms of an integral. The most interesting fact is that it does *not* come from a generalised arcsine law as in the paradigm cases described in [5]. We can also describe its tails at infinity and zero as

$$I(\theta) \sim C\,\theta^{-d} \quad \text{as } \theta \uparrow \infty, \qquad \text{and} \qquad 1 - I(\theta) \sim c\,\theta \quad \text{as } \theta \downarrow 0,$$

for explicit constants $0 < c, C < \infty$.

Let us briefly discuss the proof of Theorem 5.1. We first show that

$$\lim_{t\uparrow\infty} P\Big\{ \sup_{z\in\mathbb{R}^d} \sup_{s\in[t,t+t\theta]} \big|v(t,z) - v(s,z)\big| < \varepsilon \Big\} = \lim_{t\uparrow\infty} P\big\{Z_t = Z_{t+t\theta}\big\},$$

where Z_t can be taken to be the maximiser in the variational problem given by Ψ_t. To discuss the limit on the right hand side we again approximate the probability on the right hand side in terms of the point process Π_t. We are able to write

$$\frac{\Psi_{t+\theta t}(z)}{a_t} = \frac{\Psi_t(z)}{a_t} + \frac{\theta}{1+\theta}\,\frac{d}{\alpha-d}\,\frac{|z|}{r_t} + \text{error}, \tag{3}$$

where the error can be suitably controlled. Hence (in symbolic notation)

$$\begin{aligned} &P\big\{Z_t = Z_{t+t\theta}\big\} \\ &\approx \iint P\big\{\Pi_t(\delta x\,\delta y) > 0, \Pi_t\{(\bar x,\bar y)\colon \bar y > y\} = 0, \\ &\qquad\qquad \Pi_t\{(\bar x,\bar y)\colon |\bar x| > |x| \text{ and } \bar y > y - \tfrac{d}{\alpha-d}\tfrac{\theta}{1+\theta}(|\bar x| - |x|)\} = 0\big\}, \end{aligned}$$

where the first line of conditions on the right means that x is a maximizer of Ψ_t with maximum y, and the second line means that x is also a maximizer of $\Psi_{t+\theta t}$. As $t \uparrow \infty$ the point process Π_t is replaced by Π and we can evaluate the probability. and complete the proof.

It is more difficult to come to a notion of ageing in an almost-sure sense, which is observable from a typical trajectory of the solution. Roughly speaking, given the state of the system at some time t, we may ask for the maximal time $R(t)$ such that the system is still in the same state at time $t + R(t)$. This 'residual lifetime function' – to borrow a terminology from renewal theory – hits zero whenever there is a change of state. To find a meaningful notion of the time scale in which we experience a change we would therefore ask for a characterisation of the upper envelopes of the residual lifetime function.

To make this plan concrete recall that $(X_t\colon t \geq 0)$ is the process of peaks of the solution. Define the *residual lifetime* function by

$$R(t) = \sup\big\{s \geq 0\colon X_t = X_{t+s}\big\},$$

for $t \geq 0$. Roughly speaking, $R(t)$ is the waiting time, at time t, until the next change of peak, see the schematic picture in Figure 3. We have shown in Theorem 5.1 that the law of $R(t)/t$ converges to the law given by the distribution function $1 - I$. In the following theorem, we describe the smallest asymptotic upper envelope for the process $(R(t)\colon t \geq 0)$.

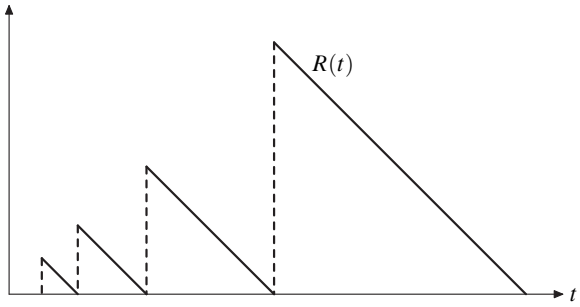


Figure 3. A schematic representation of the remaining lifetime function R.

Theorem 5.4 (Almost sure ageing, Theorem 1.2 in [27]). *For any nondecreasing function $h\colon (0,\infty) \to (0,\infty)$ we have, almost surely,*

$$\limsup_{t\uparrow\infty} \frac{R(t)}{th(t)} = \begin{cases} 0 & \text{if } \displaystyle\int_1^\infty \frac{\mathrm{d}t}{th(t)^d} < \infty, \\ \infty & \text{if } \displaystyle\int_1^\infty \frac{\mathrm{d}t}{th(t)^d} = \infty. \end{cases}$$

The proof of Theorem 5.4 is technically more involved, because we can no longer benefit from the point process approach and have to do significant parts of the argument from first principles. We consider events

$$P\left\{\frac{R(t)}{t} \geq \theta_t\right\} \approx P\{Z_t = Z_{t+t\theta_t}\},$$

for $\theta_t \uparrow \infty$. We significantly refine the argument leading to Theorem 5.1 and replace the convergence of $P\{Z_t = Z_{t+t\theta}\}$ by a moderate deviation statement: For $\theta_t \uparrow \infty$ not too fast we show that

$$P\{Z_t = Z_{t+t\theta_t}\} \sim C\, \theta_t^{-d},$$

for a suitable constant $C > 0$. Then, if $\varphi(t) = th(t)$, this allows us to show that, for any $\varepsilon > 0$, the series $\sum_n P\{R(e^n) \geq \varepsilon\varphi(e^n)\}$ converges if $\sum_n h(e^n)^{-d}$ converges, which is essentially equivalent to $\int h(t)^{-d}\,\mathrm{d}t/t < \infty$. By Borel–Cantelli we get that

$$\limsup_{n\to\infty} \frac{R(e^n)}{\varphi(e^n)} = 0,$$

which implies the upper bound in Theorem 5.4. The lower bound follows using a more delicate second moment estimate.

6 Conclusion

The aim of this project was to study the possible effects of a highly irregular potential on a diffusion on a d-dimensional lattice. By modeling the potential as a spatially

independent, identically distributed random field with polynomial tails we have seen that the diffusion shows interesting extreme behaviour, in particular

- the growth rate of the total mass is asymptotically *random*,
- the solution is asymptotically concentrated in a *single point* at most times,
- this point goes to infinity at *superlinear* speed,
- the solution is asymptotically concentrated in *two points* at all times,
- the system exhibits *ageing* behaviour.

In the proofs we combine a very fine analysis of the random walk paths contributing in the Feynman–Kac formula with extreme value theory for the random field.

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From exploration paths to mass excursions – variations on a theme of Ray and Knight

Etienne Pardoux* and Anton Wakolbinger**

1 Introduction

The two classical theorems of Ray and Knight (see e.g. [24], [32] or [33]) give beautiful connections between Brownian excursions (described by Itô's excursion measure) and excursions of Feller's branching diffusion.

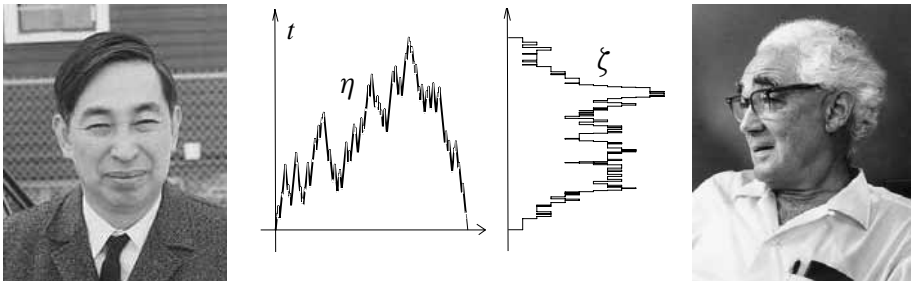

Figure 1. Itô meets Feller. Sketch of a Brownian excursion and the corresponding excursion of a Feller branching diffusion. (Photo of William Feller: courtesy of Mladen Vranic, Toronto.)

Here is an informal statement of the second Ray–Knight theorem: *The time which a (suitably stopped) reflected Brownian motion spends near level t* (and which is formally captured by its *local time* at *t*), *viewed as a process in t, is a Feller branching diffusion*. Let's go for the trees in the forest: The reflected Brownian motion is the concatenation of many *Brownian excursions*, and the random path of the Feller branching diffusion is a sum of many *Feller excursions* (we will come back to this in Section 4). And indeed, as adumbrated in Figure 1, the just described "Ray–Knight mapping" works also on these building blocks, and maps a Brownian excursion into a Feller excursion.

A nice way to understand the Ray–Knight mapping is to interpret the Brownian excursion as the *exploration path* of a tree, and the Feller excursion as *width profile* of the same tree. This interpretation, and the mapping from exploration excursions to width profiles (or *mass excursions*), is most easily conceived in a (pre-limit) situation of binary trees in continuous time. We will review this in Section 2. There, we will also point to a few historic landmarks and give some more hints to the literature.

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In Section 3 we will state a continuous-time version of the Harris representation of binary Galton–Watson trees in terms of continuous and piecewise linear exploration paths whose slopes change at constant rate.

In Section 4 we describe the result of a scaling limit. This takes the exploration paths to reflected Brownian motion (exploring a forest of continuum trees) and the rescaled mass processes to a Feller branching diffusion. With the right scaling the image of Itô's excursion measure under this mapping is the excursion measure of Feller's branching diffusion, which is an *excursion measure from an exit boundary* as defined by Pitman and Yor [30]. Poisson processes and subordinators will play a central role. Section 5 deals with subcritical branching by a Girsanov reweighting of both the exploration and the mass excursion measures.

In Sections 6–8 we give a brief synopsis of a few recent developments in the framework of "exploration and mass excursions". Intended symmetries in the presentation are captured by the following tableau (where FBD stands for Feller's branching diffusion):

Sections 4 and 5: Ray–Knight representation of FBD	Section 6: Trees of excursions of FBD
Section 8: Ray–Knight representation of FBD with logistic growth	Section 7: Trees of excursions of FBD with logistic growth

In Section 6 we focus on Bertoin's *trees of alleles in branching processes with rare neutral mutations*, with all mutations leading to ever new types. In the scaling limit studied in [6], the *tree of alleles* can be viewed as a rooted tree all of whose nodes have a countable out-degree. The root is labelled by a *subcritical* Feller branching diffusion, and all the other nodes are labelled by subcritical Feller excursions, where given that the label of the parent is a mass path $z = (z_t)$, the labels of its children are a Poisson population of mass excursions with intensity measure $A(z)\bar{Q}$, with $A(z) = \int_0^\infty z_t\, dt$ being the "size" of z and $\bar{Q}$ being the subcritical Feller excursion measure. As we will review in Section 6, the total size of the generations in the "tree of alleles" is then a (discrete time, continuum mass) branching process which can be represented as an iteration of independent copies of inverse Gaussian subordinators.

Without changing the mathematics of this model, one may think of a geographically instead of a genetically structured population and replace the concept of "mutation to an ever new type" by that of "migration to an ever new colony". Interesting extensions of this model have been considered. In [7], Bertoin allows for dependencies between the number of emigrant and "homebody" children, otherwise leaving the independence in the individual reproduction untouched. Another extension (which includes the model with local competition discussed in Section 7) is to replace the excursion measure $\bar{Q}$ of the subcritical Feller branching by the excursion measure Q of some other diffusion on $\mathbb{R}_+$, but with the same emigration mechanism as in the model described at the beginning of Section 6. This is the class of *Virgin Island models* studied by Hutzenthaler [14].

The last two sections feature *Feller's branching diffusion with logistic growth*, a process which has been studied in detail by Lambert [18]. In Section 7 we review the Virgin Island model in which the measure Q that governs the tree of colony sizes is the excursion measure of Feller's branching diffusion with logistic growth. In an individual-based interpretation, this process incorporates supercritical reproduction and pairwise fights between individuals within each colony.

At first sight, the Feller branching diffusion with logistic growth does not lend itself to a Ray–Knight representation, because the competition between individuals destroys the "branching property", i.e. the independence in the reproduction. (Other than in Section 7, we now focus on the situation within one colony.) In Section 8, however, we will provide such a representation, by introducing an order among the individuals and decreeing that the pairwise fights are always won by the individual "to the left". As we will see, this results in an exploration process which is a reflected Brownian motion with constant upward drift plus a downward drift which is proportional to the local time accumulated at the current level. The exploration path encodes a forest of countably many continuous trees in the same way as reflected Brownian motion does in the critical Feller branching case, with a sampling from the exploration time axis corresponding to a sampling from the leaves in the forest, see [23]. With the above-mentioned "left-right rule" for the individual fights, the excursions which come later in the exploration tend to be smaller – the trees to the right are "under attack from those to the left".

In this exposé our aim is to explain concepts and ideas on an intuitive rather than a thoroughly formal level. To this end we sometimes resort to a verbal description and refrain from giving full and rigorous proofs.

2 Harris paths and tree profiles

With a binary tree in continuous time one can associate (like in Figure 2) two *excursions from zero*. One is the *exploration excursion* η which arises by traversing the tree at a constant speed and recording the height as a function of the exploration time s. The other is the *mass excursion* ζ which gives the profile of the tree, i.e. the number of extant branches as a function of the real time t.

The idea to establish a correspondence between planar (rooted) trees and paths by traversing the vertices of the tree and recording the height (i.e. the distance of the root) as a function of the "exploration time" goes back to Theodore Harris ([13], cf. [28], ch. 6). Following Pitman and Winkel [29] we name such an exploration excursion a *Harris path*. Later we will also consider the concatenation of such excursions, which describe the exploration of a forest of trees (and is called Harris path as well). For the moment, let us consider one single tree.

The number ζ_t of branches extant in the tree at time t equals half the number of the level t-crossings of the Harris path η, which in turn equals the number of excursions of η above height t. Let us agree (for the moment) on a traversal speed 2. This results in slope ± 2 of the Harris path, and consequently half the number of its level t-crossings

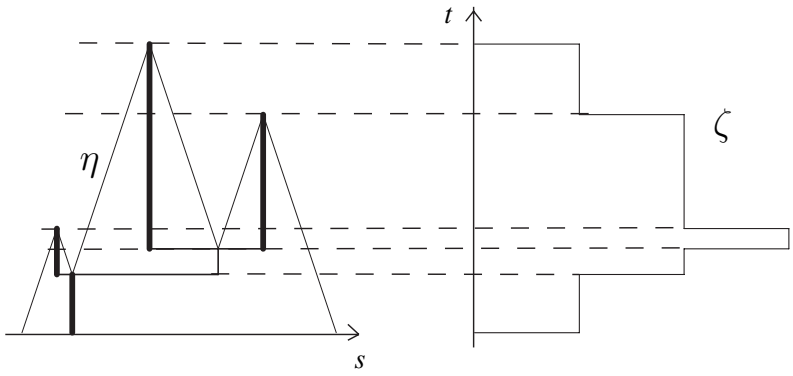

Figure 2. Left: A binary tree and its Harris path (exploration excursion) η. Right: The tree profile (mass excursion) ζ.

can be read off as

$$\zeta_t = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_0^\infty \mathbf{1}_{\{t < \eta_s < t+\varepsilon\}} ds. \tag{1}$$

With the chosen slope ± 2 of the Harris path, it is clear that the total branch length of the tree equals the total time that is needed to traverse the tree. In particular, the integrated mass excursion equals the length of the exploration excursion, i.e.

$$A(\zeta) := \int_0^\infty \zeta_t \, dt = \inf\{s > 0 : \eta(s) = 0\} =: R(\eta). \tag{2}$$

If the tree is random, say critical binary Galton–Watson with branching rate σ^2, then the durations of the successive periods of increase and decrease of the exploration turn out to be i.i.d. exponential with parameter $\sigma^2/2$, see Section 3.

In an (N^2, N)-scaling as described in Section 4, the concatenation of i.i.d. copies of rescaled exploration excursions η^N converges, as $N \to \infty$, to a reflected Brownian motion, and the sum of i.i.d. copies of rescaled mass excursions ζ^N converges to a Feller branching diffusion. Both limiting objects can be represented in terms of Poisson populations, with the intensity measures being Itô's excursion measure on one side and the excursion measure of Feller's branching diffusion (as described in [30]) on the other. In this way, "Itô meets Feller", as the two did in Princeton in 1954, two years after the appearance of Harris' paper [13] with its section on "walks and trees".

In 1963 Daniel Ray and Frank Knight published their papers [31] and [17] which contain the essence of what is now known as the two Ray–Knight theorems. The relation (1), which persists in the scaling limit and allows to read off the mass excursion as a local time process of the exploration excursion (see Section 4), is at the heart of this.

Further landmarks in exploring the connection between Feller branching processes and Brownian excursions are the work of Kawazu and Watanabe [16] and of Neveu

and Pitman [25]. In Aldous' 1991–93 trilogy [3], the *continuum random tree* shaped up as a central object. It arises as a limit of rescaled Galton–Watson trees and plays in the realm of random trees a role similar to that of Brownian motion in the classical invariance principle. New limit objects, called *Lévy trees*, appear as soon as heavy-tailed offspring distributions come into play. For the description and the analysis of these trees as well, exploration and "height" processes are an important tool. Yet another pioneering development has been Le Gall's *Random snake* [21], which, based on the idea of exploration processes, provides a representation of Dawson and Watanabe's *super-Brownian motion* (and other measure-valued branching processes, [8]) as a continuum-tree-indexed Markov motion. For this and further extensions, we refer to the monographs of Duquesne and Le Gall [10], Evans [11] and Pitman [28], and to the survey papers [22], [23] by Le Gall.

3 A discrete Ray–Knight theorem

In this section we state a version of the Ray–Knight theorem for Harris paths. The central observation is Lemma 3.1, which (in the critical case) traces back to [20]. Our proof, which can be easily adapted to a non-critical binary branching like that of Lemma 8.1 below, is similar to that of a more general result by Geiger and Kersting ([12], Theorem 2.1), who, however, use exploration paths with downward jumps. See also [29] and [4] for other variants of the proof of Lemma 3.1.

Consider a binary critical Galton–Watson tree in continuous time with branching rate (or variance parameter) σ^2, called $\mathrm{T}(\sigma^2)$ for short. Think of each branch having an $\mathrm{Exp}(\sigma^2/2)$-distributed lifetime and carrying a rate $\sigma^2/2$-Poisson process of birth time points. When the death clock rings, the branch terminates (in a leaf of the tree), when a birth clock rings, then a new branch, and hence a new independent subtree, starts, say, to the right of the mother branch.

The tree is traversed with constant speed 2 in the following "depth first search" manner: Start from the root and follow the leftmost branch up to its leaf, then turn and go down. Let $B_1 > B_2 > \cdots > B_K$ be the time points of births along the leftmost branch, written in descending order. If $K = 0$, that is if there are no birth points along the leftmost branch, then go down to height 0 and stop. Otherwise, turn at height B_1 and enter the branch born there, proceeding in the analogous way as before, now using the birth time points along that branch. When coming down to height B_1 again, proceed downwards to height B_2 if $K > 1$ (and then turn and enter the branch born at time B_2, and so on), otherwise go down to height 0 and stop there.

Lemma 3.1. *The exploration process of the tree* $\mathrm{T}(\sigma^2)$ *constructed in the just described way is in distribution equal to an excursion* E *from* 0 *of a process with continuous, piecewise linear paths with slopes* ± 2*, starting at height* 0 *with positive slope, changing slope at rate* σ^2*, and dying at its first return to* 0*.*

Proof. Whenever the exploration process moves upwards, it traverses, independently of its past, an $\mathrm{Exp}(\sigma^2/2)$-distributed height before changing slope. Now consider a

downward piece of the exploration process. The birth points along the branches of the tree form a Poisson process with intensity $\sigma^2/2$. The same is true for the yet unexplored birth points on the path between any point in the tree and the root, independently of the previous exploration. Hence, if the height of the current point is t, the distance travelled down from this point is distributed as $\min(T, t)$, where T is an $\mathrm{Exp}(\sigma^2/2)$-random variable. □

For an $\mathbb{R}_+$-valued path $h = (h_u, u \geq 0)$, we put

$$\Lambda_s(t, h) := \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \int_0^s \mathbf{1}_{\{t < h_u < t+\varepsilon\}} du \tag{3}$$

provided the right hand side exists, and define $\Lambda(t, h) := \Lambda_\infty(t, h)$.

In view of (1) and (3) we thus obtain from Lemma 3.1 the following

Corollary 3.2. *For a random excursion E as in Lemma 3.1, $\Lambda(\cdot, E)$ has the same distribution as the profile (or "mass excursion") of the random tree $\mathrm{T}(\sigma^2)$, and hence is a critical binary Galton–Watson process with branching rate σ^2 and one initial individual.*

4 Brownian scaling: Itô meets Feller

Now let us have a look at a scaling by N which, as $N \to \infty$, takes a sequence of Galton–Watson processes into Feller's branching diffusion. Time is speeded up by the factor N, mass is scaled down by the same factor N, and there are $\lfloor Nx \rfloor$ initial individuals instead of one, with x being a positive real number. As to the exploration paths, this results in a concatenation of $\lfloor Nx \rfloor$ exploration excursions. In view of (1) and (3), the downscaling of the mass is achieved by speeding up the exploration by a factor N, which results in slopes $\pm 2N$. Measured in real time, the rate of change of the slope is $\frac{\sigma^2}{2} N$, and measured in exploration time, it is $\sigma^2 N^2$.

Definition 4.1. For $N \in \mathbb{N}$ let H^N be a continuous, piecewise linear process with slopes $\pm 2N$, starting in 0 with positive slope, changing slope at rate $\sigma^2 N^2$ and reflected at 0. Moreover, for $x > 0$, let $H^{N,x}$ be the path H^N stopped at the time S_x^N when completing $\lfloor Nx \rfloor$ excursions from 0. In other words, S_x^N equals the smallest s for which $\Lambda_s(0, H^N) \geq \lfloor Nx \rfloor / N$.

Remark 4.2. Due to Lemma 3.1, $H^{N,x}$ is equal in distribution to the exploration path of a rescaled Galton–Watson forest consisting of $\lfloor xN \rfloor$ trees. Hence, analogous to Corollary 3.2, the "level counts" of the rescaled Harris path are equal in distribution to a rescaled Galton–Watson process, i.e.

$$(\Lambda(t, H^{N,x}))_{t \geq 0} \stackrel{d}{=} \left(\frac{1}{N} \Gamma_{tN}^{\lfloor Nx \rfloor} \right)_{t \geq 0}, \tag{4}$$

where $(\Gamma_t^k)_{t \geq 0}$ is a critical binary Galton–Watson process with branching rate σ^2 and k initial individuals.

The sequence of paths H^N as described in Definition 4.1 converges, as $N \to \infty$, in distribution to a reflected Brownian motion with variance parameter $4/\sigma^2$. (Note that the expected time between two consecutive changes of the slope of H^N is $\Delta_N := 1/(\sigma^2 N^2)$, and the variance of the height difference is $(2N)^2(1/((\sigma^2 N^2))^2) = (4/\sigma^2)\Delta_N$.) Although local times are *not* continuous functionals of the paths, it is possible to take the limit $N \to \infty$ in (4), see e.g. [4]. This is one road to the classical

Ray–Knight Theorem. *Let H be reflected Brownian motion with variance parameter $4/\sigma^2$. For $x \geq 0$ define*

$$S_x := \inf\{s > 0 : \Lambda_s(0, H) \geq x\} \tag{5}$$

and put $H^x := (H_s)_{0 \leq s \leq S_x}$ and $\Lambda(H^x) := (\Lambda_{S_x}(t, H))_{t \geq 0}$. Then

$$\Lambda(H^x) \stackrel{d}{=} Z^x. \tag{6}$$

Here, Z^x is a *critical Feller branching diffusion* with variance parameter σ^2, i.e. a weak solution of the SDE

$$dZ_t = \sigma\sqrt{Z_t}\, dW_t, \quad Z_0 = x, \tag{7}$$

with W a standard Brownian motion.

The quantity $\Lambda_s(t, H)$ gives one way to measure the time which the path H spends at level t up to time s. An alternative way to do this is via the *semimartingale local time* $L_s(t, H)$ (see [32], Chapter VI)). For unit variance ($4/\sigma^2 = 1$), $L_s(t, H) = \Lambda_s(t, H)$ a.s. ([32], Corollary VI.1.9). L and Λ obey the scalings $L_s(t, kH) = kL_s(t, H)$, $\Lambda_s(t, kH) = \frac{1}{k}\Lambda_s(t, H)$ for $k > 0$. Consequently, L and Λ are related via

$$L_s(t, H) = \tfrac{4}{\sigma^2}\Lambda_s(t, H) \quad \text{a.s.}, \tag{8}$$

which corresponds to the *occupation times formula*, see e.g. [32], Corollary VI.1.6.

Note that H can be represented as $H = \frac{2}{\sigma}|\beta|$, with β a standard Brownian motion. By Tanaka's formula, one has $|\beta_s| = B_s + L_s(0, \beta)$ for a standard Brownian motion B. Since $L_s(0, |\beta|) = 2L_s(0, \beta)$ and because of the scaling of $L_s(0, H)$ we obtain

$$H_s = \frac{2}{\sigma}B_s + \frac{1}{2}L_s(0, H). \tag{9}$$

Let n be Itô's excursion measure of Brownian motion, and n_+ its restriction to $\mathcal{E}_+$, the set of $[0, \infty)$-valued excursions. The intensity measure for the excursion representation of (9) on the $\Lambda_\cdot(0, H)$-axis is given by

$$\tilde{n} := \tfrac{2}{\sigma}n_+(\tfrac{2}{\sigma}\eta \in \cdot). \tag{10}$$

In other words: Let (ξ_i, η_i) be the points of a Poisson process on $\mathbb{R}_+ \times \mathcal{E}_+$ with intensity measure $dx \otimes \tilde{n}$ and write $\bigoplus_{\xi_i \leq x} \eta_i$ for the *concatenation* of all the excursions η_i with

$\xi_i \le x$, constructed as in [32], Proposition XII.2.5. Put $H^x := (H_s)_{0\le s\le S_x}$ with S_x defined in (5). Then

$$H^x \stackrel{d}{=} \bigoplus_{\xi_i \le x} \eta_i. \tag{11}$$

The prefactor $2/\sigma$ in (10) comes from the scaling relation $\Lambda_s(0, \frac{2}{\sigma}|\beta|) = \frac{\sigma}{2}\hat{a}\Lambda_s(0,|\beta|)$. Indeed, because of the relation $L_s(0,|\beta|) = 2L_s(0,\beta)$, the measure n_+ is the intensity measure for the excursion representation of reflected Brownian motion $|\beta|$ on the $L_\cdot(0,|\beta|)(= \Lambda_\cdot(0,|\beta|))$-axis.

Clearly, $\Lambda\big(\bigoplus_{\xi_i\le x}\eta_i\big) = \sum_{\xi_i\le x}\Lambda(\eta_i)$. Combining this with (11), we arrive at the following re-formulation of the Ray–Knight representation (6):

$$\sum_{\xi_i\le x}\Lambda(\eta_i) \stackrel{d}{=} Z^x \tag{12}$$

Let $\tilde{Q}$ be the image of $\tilde{n}$ under the mapping $\eta \mapsto \zeta := \Lambda(\eta)$, i.e.,

$$\tilde{Q} = \tilde{n}(\Lambda(\eta) \in \cdot). \tag{13}$$

Then, by the Poisson mapping theorem, $(\xi_i, \zeta_i) := (\xi_i, \Lambda(\eta_i))$ is a Poisson point process with intensity measure $dx \otimes \tilde{Q}$. Thus, (12) translates into

$$Z^x \stackrel{d}{=} \sum_{\xi_i\le x}\zeta_i, \quad x \ge 0, \tag{14}$$

which is a representation of Feller's branching diffusion in terms of a *path-valued subordinator* that decomposes Z^x with respect to the ancestral mass. In particular, (14) renders the so-called *branching property* of Feller's branching diffusion: $Z^{x+x'} \stackrel{d}{=} Z^x + Z^{x'}$, with Z^x and $Z^{x'}$ independent.

The measure $\tilde{Q}$ can be understood as the Lévy measure of the path-valued subordinator (14) (or also as the *canonical measure* of the infinitely divisible random measure $Z^x_t\,dt$). We claim that

$$\tilde{Q}(\cdot) = \lim_{x\to 0}\frac{1}{x}\mathbf{P}(Z^x \in (\cdot)), \tag{15}$$

which identifies $\tilde{Q}$ as the *excursion measure* of Feller's branching diffusion (7) in the sense of Pitman and Yor (see [30], Section 4, and [14], Section 9).

To see (15) it suffices to look at the random variables $\langle f, Z^x\rangle := \int_0^\infty f(t)Z^x_t\,dt$ for continuous functions $f : \mathbb{R}_+ \to \mathbb{R}_+$ with compact support that vanish on $[0,\varepsilon]$ for some $\varepsilon > 0$. Because $\tilde{Q}(\zeta_\varepsilon > 0) < \infty$, only a finite (Poisson) number of summands contribute to $\langle f, Z^x\rangle$. As $x \to 0$, the probability that more than one summand contributes is $o(x)$, hence $\mathbf{P}(\langle f, Z^x\rangle \in (\cdot)) = x\tilde{Q}(\langle f, Z^x\rangle \in (\cdot)) + o(x)$.

The (σ-finite) measure $\tilde{Q}$ is Markovian, having the semigroup of (7). Let us emphasize, however, that for the dynamics (7), other than in the classical Itô excursion theory, the point 0 is not regular but absorbing.

As a preparation for the next two sections we compute for the area under Feller's branching diffusion the decomposition that corresponds to the representation (14). In other words, we compute the Poisson representation of the infinitely divisible random variable $\int_0^\infty Z_t^x\,dt$, with Z^x being the solution of (7). Here, a crucial observation is the identity

$$R(\eta) = A(\zeta) \tag{16}$$

for $\zeta = \Lambda(\eta)$, with $R(\eta)$ being the length of the exploration excursion η and $A(\zeta)$ the area under the mass excursion ζ , cf. (2). This identity follows with the choice $f \equiv 1$ from the occupation times formula ([32], VI.1.6)

$$\int_0^{R(\eta)} f(\eta_s)ds = \int_0^\infty f(t)\Lambda_{R(\eta)}(t,\eta)dt.$$

We recall that the image of n under the mapping $\eta \mapsto R(\eta)$ is

$$\rho(da) := n(R(\eta) \in da) = \frac{1}{\sqrt{2\pi a^3}}da, \tag{17}$$

see [32], Proposition XII 2.8. This ρ is the Lévy measure of the *inverse Brownian local time at* 0, which is a $\frac{1}{2}$-stable subordinator. Using (14), (2) and (5) we obtain

$$A(Z^x) := \int_0^\infty Z_t^x\,dt \stackrel{d}{=} \sum_{\xi_i \le x} A(\zeta_i) = \sum_{\xi_i \le x} R(\eta_i) = S_x. \tag{18}$$

Hence $(A(Z^x))$ as well as (S_x) is a subordinator with Lévy measure

$$\tilde{Q}(A(\zeta) \in da) = \tilde{n}(R(\eta) \in da) = \tfrac{2}{\sigma}n_+(R(\eta) \in da) = \tfrac{1}{\sigma}\rho(da), \tag{19}$$

where we used (17) and the fact that $n_+ \circ R^{-1} = \frac{1}{2}n \circ R^{-1}$ in the last equality of (19).

Thus, due to Lévy's representation of Brownian local time as current maximum of a Brownian motion ([32], Theorem VI 2.3), the distribution of S_x equals that of the time at which a standard Brownian motion first hits the level x/σ (or equivalently, the time at which a Brownian motion with variance parameter σ^2 first hits the level x.)

5 Subcritical branching: reweighting the excursions

As a preparation for Section 6 we analyze the Ray–Knight representation of a *subcritical* Feller branching diffusion Z^x that satisfies

$$dZ_t = \sigma\sqrt{Z_t}\,dW_t - cZ_t\,dt, \quad Z_0 = x. \tag{20}$$

for a fixed $c > 0$.

Let us first discuss the dynamics of the exploration process. The subcriticality leads to a decrease of the birth rate, and hence to a downward drift in the exploration process.

To figure out what this drift is, let us revert to the (continuous time, discrete mass) picture described at the beginning of Section 4. There, the rate of birth points along the branches (in real time after speeding up by the factor N) was $\frac{\sigma^2}{2}N$, and now it is $\frac{\sigma^2}{2}N - c$. Due to the exploration speed $2N$, the rate (in exploration time) of change from a downwards to an upwards slope is thus $\sigma^2 N^2 - 2cN$. The rate from an upwards to a downwards slope remains unaffected and is $\sigma^2 N^2$. In the limit $N \to \infty$ this leads to the drift $-\frac{2c}{\sigma^2}\,ds$ and the quadratic variation $\frac{4}{\sigma^2}\,ds$, and to the exploration process being a reflected Brownian motion governed by the equation

$$H_s = \frac{2}{\sigma}\Big(B_s - \frac{c}{\sigma}s\Big) + \frac{1}{2}L_s(0,H). \tag{21}$$

The excursion measure $\bar{n}$ governing (21) is (10) multiplied by a Girsanov density, up to time $R(\eta)\wedge s$, $s>0$, is $\exp\big(-\int_0^{R(\eta)\wedge s}\frac{c}{\sigma}\,d\eta_r - \frac{1}{2}\int_0^{R(\eta)\wedge s}\big(\frac{c}{\sigma}\big)^2 dr\big)$. As $s\to\infty$, this converges to $g(R(\eta)) := \exp\big(-\frac{1}{2}\big(\frac{c}{\sigma}\big)^2 R(\eta)\big)$; hence

$$\frac{d\bar{n}}{d\tilde{n}}(\eta) = g(R(\eta)). \tag{22}$$

Because of (13), (16) and (22), the excursion measure $\bar{Q}$ of the c-subcritical Feller branching diffusion arises by reweighting that of the critical Feller branching diffusion with the Girsanov density $g(A(\zeta))$:

$$\frac{d\bar{Q}}{d\tilde{Q}}(\zeta) = g(A(\zeta)). \tag{23}$$

This can also be seen without recurring to the exploration excursions: the Girsanov density which introduces the c-subcriticality for a Feller branching diffusion is

$$\exp\Big(-\int_0^\infty \frac{cZ_t}{\sigma\sqrt{Z_t}}dW_t - \frac{1}{2}\int_0^\infty -\frac{(cZ_t)^2}{\sigma^2 Z_t}\,dt\Big),$$

which for an excursion $Z=\zeta$ equals $g(A(\zeta)) = \exp\big(-\frac{1}{2}\big(\frac{c}{\sigma}\big)^2 A(\zeta)\big)$.

To obtain the Lévy measure of the subordinator (S_x) given by (5) and (18), but now in the c-subcritical case, we have to multiply (19) by the Girsanov factor $g(a)$. This Lévy measure is thus given by

$$\nu(da) := g(a)\tfrac{1}{\sigma}\rho(da) = \exp\big(-\tfrac{1}{2}\big(\tfrac{c}{\sigma}\big)^2 a\big)\tfrac{1}{\sigma}\frac{1}{\sqrt{2\pi a^3}}da. \tag{24}$$

The distribution of S_x is explicit. Indeed, again due to Lévy's representation of local time, the distribution of S_x equals the distribution of the time at which a Brownian motion with variance parameter σ^2 and drift c first hits the level x. This distribution is known as the *inverse Gaussian* with parameters x/c and x^2/σ^2, and has density

$$\mathbf{P}(S_x \in da) = \frac{x}{\sqrt{2\pi\sigma^2 a^3}}\exp\Big(-\frac{(ca-x)^2}{2\sigma^2 a}\Big). \tag{25}$$

6 Bertoin's "Trees of alleles with rare mutations"

In the second paper of a recent trilogy [5], [6], [7] on trees of alleles and trees of colonies in branching processes, Jean Bertoin considers a critical Galton–Watson process in discrete generations with $\lfloor Nx \rfloor$ ancestors, offspring variance σ^2, and probability c/N that an individual at its birth acquires a new mutation never seen so far in the population, which it then inherits to all its descendants (see in particular Section 4 of [6]). The evolution is neutral in the sense that all the individuals, irrespective of their type, have the same reproduction law.

The situation is thus similar to the so called *infinite sites model* in population genetics, with the *type* or *allele* of an individual being the set of all mutations it carries. In this way one obtains a *tree of alleles*: the root consists of all individuals that descend from the ancestors without any mutation. Each child of the root consists of a mutant child χ of one of these non-mutant individuals, plus that part of χ's offspring that carries no additional mutation. Bertoin investigates the process of the total sizes of the alleles and shows that as $N \to \infty$ this process, when divided by N^2, converges to a *continuous state branching process with discrete generations and reproduction measure* ν given by (24). We give a brief intuitive explanation of this along the lines of the previous section.

With the Brownian scaling discussed at the beginning of Section 4, and with one of the two factors N taken for rescaling the mass and the other one for rescaling the time, the rescaled mass process of the non-mutant individuals converges to the c-subcritical Feller branching diffusion $Z^{(0)} := Z^x$ following (20). Write $A^{(0)} =: \int_0^\infty Z_t^{(0)}\, dt$ for the total non-mutant (or "wild-type") mass. The mass $cA^{(0)}$, which is lost from the non-mutants due to mutation, serves as ancestral mass for another c-subcritical Feller branching diffusion $Z^{(1)}$. In this way, one obtains inductively a sequence $Z^{(k)}$, $k = 1, 2, \dots$ of c-subcritical Feller branching diffusions, obeying (20) with $Z^{(k)}$, $W^{(k)}$ and $cA^{(k-1)} := c\int_0^\infty Z_t^{(k-1)}\, dt$ in place of Z, W and x, and with $Z^{(k)}$ independent of $(Z, Z^{(1)}, \dots, Z^{(k-1)})$, given $A^{(k-1)}$. The process $\mathbb{A} = (A^{(0)}, A^{(1)}, \dots)$ is an $\mathbb{R}_+$-valued Markov chain, with $A^{(k)}$ describing the sum of the sizes of the (countably many) k-th step mutant alleles.

In view of equation (18), $A^{(0)}$ has the same distribution as S_x, where $S = (S_\ell)_{\ell \geq 0}$ is a subordinator with Lévy measure ν defined in (24). Consequently the Markov chain $\mathbb{A}$ can be represented as an iteration of independent subordinators. For this, let $S^{(0)}, S^{(1)}, S^{(2)}, \dots$ be independent copies of S, and put $M_0 := S_x^{(0)}$,

$$M_1 := S^{(1)}_{cM_0}, \quad \dots, \quad M_k := S^{(k)}_{cM_{k-1}}, \quad \dots. \tag{26}$$

The process $\mathbb{A} = (A^{(0)}, A^{(1)}, \dots)$ (which describes the total generation sizes in the tree of alleles) then obeys

$$(A^{(0)}, A^{(1)}, \dots) \stackrel{d}{=} (M_0, M_1, \dots). \tag{27}$$

Thus, $\mathbb{A}$ is a continuous state branching process with discrete generations (a so-called *Jiřina process*).

Indeed, for each k, M_k is a sum of jumps of $S^{(k)}$, and for $k \geq 1$ each of these jumps "stems" from a jump of $S^{(k-1)}$. By forgetting the structure of M_0 (and thus decreeing that all the summands of M_1 stem from M_0), but keeping track of the genealogy the subordinator jumps in the later generations, one arrives at a tree whose nodes are labelled with the jump sizes, with M_0 at its root. This is what Bertoin calls the *tree indexed continuous state branching process* (*CSBP*) *with reproduction measure* ν.

As the main result of [6], Bertoin proves that in the regime described at the beginning of this section, the rescaled tree of alleles $N^{-2}\mathcal{A}^N$ converges in the sense of finite dimensional distributions to the just described tree indexed CSBP.

We also mention recent related work of Abraham and Delmas [1] in the framework of continuous state branching processes. Intuitively, the forest of non-mutant trees (which makes up the original allele) arises from a forest with a critical offspring dynamics by *pruning*, i.e. "cutting off" the mutant individuals together with their entire offspring. This procedure is iterated when passing from the k-th step mutants to the $(k+1)$-st step ones. In this sense, the individual genealogy that underlies this model fits into a general framework of *pruned trees*, see [2] and references therein.

There is also a geographic (instead of a genetic) interpretation of the tree of mass excursions: instead of types, one may think of colonies (or islands), with "mutation to an ever new type" becoming "emigration to an ever new island". It is this picture which Bertoin adopts in [7]. There, he also considers a situation in which a *bivariate subordinator* $(T(\ell), Y(\ell))_{\ell \geq 0}$ (instead of the pair $(S_\ell, S_{c\ell})_{\ell \geq 0}$) appears in an analogue of (26). The jumps of Y occur at the same points ℓ as those of T, the pair of jump sizes being governed by a Lévy measure on $\mathbb{R}_+ \times \mathbb{R}_+$. With an appropriate scaling, the bivariate subordinator allows to describe dependencies between the numbers of "homebody" and emigrant children in a large population limit, see Theorem 2 in [7]. With $(T^{(0)}, Y^{(0)}), (T^{(1)}, Y^{(1)}), \ldots$ being i.i.d. copies of (T, Y), the analogue of (26) and (27) becomes

$$A_x^{(0)} := T^{(0)}(x), \quad A_x^{(1)} := T^{(1)}(Y^{(0)}(x)), \quad A_x^{(2)} := T^{(2)}(Y^{(1)}(Y^{(0)}(x))), \ \ldots. \tag{28}$$

Let us write $R(x) := T^{(0)}(x) + T^{(1)}(Y^{(0)}(x)) + T^{(2)}(Y^{(1)}(Y^{(0)}(x))) + \cdots$. Both $T(\ell)_{\ell \geq 0}$ and $(R(\ell))_{\ell \geq 0}$ are subordinators, hence $T(\ell)$ and $R(\ell)$ are sums over countably many jumps. We denote the populations of jump sizes in $T(x)$ and in $R(x)$ by $\mathcal{J}_x$ and $\mathcal{C}_x$, noting that both $\mathcal{J} = (\mathcal{J}_\ell)_{\ell \geq 0}$ and $\mathcal{C} = (\mathcal{C}_\ell)_{\ell \geq 0}$ are measure-valued subordinators. A decomposition of $\mathcal{C}_x$ with respect to the "first generation colonies" gives

$$\mathcal{C}_x \stackrel{d}{=} \mathcal{J}_x + \widetilde{\mathcal{C}}_{Y(x)}, \tag{29}$$

with $(\widetilde{\mathcal{C}}_\ell)$ an independent copy of $(\mathcal{C}_\ell)$. This is a re-formulation of Bertoin's stochastic fixed point equation in [7], Theorem 1, which there is expressed as an integral equation involving the Lévy measures of (T, Y) and of $\mathcal{C}$.

In the next section we will discuss another extension of the "tree of alleles" model, again formulated in a geographic framework with emigration to ever new colonies. In

this model, the current population size in a colony will have an impact on the individual death rate. The population size in one colony, as a function of the ancestral mass x, is then no subordinator any more. Still, due to the "Virgin Island assumption", the tree of colonies will be described by an iteration of subordinators exactly as in (26), with the subordinators $S^{(1)}, S^{(2)}, \ldots$ figuring in (26) being independent copies of a subordinator. While this subordinator need not have a representation like (5), its Lévy measure still is the image of an excursion measure Q under the mapping $\zeta \mapsto A(\zeta)$, see formula (31) below.

7 Feller branching with logistic growth, and Virgin Islands

As an additional ingredient to the stochastic dynamics in (20) we now add a nonlinear drift. For simplicity we assume it to be *logistic*, thus considering

$$dZ_t = \sigma\sqrt{Z_t}\, dW_t + (\theta Z_t - \gamma Z_t^2)\, dt - cZ_t\, dt, \quad Z_0 = x. \tag{30}$$

In a population model, the additional drift terms $\theta Z_t\, dt$ and $-\gamma Z_t^2\, dt$ describe a supercritical reproduction and a killing due to pairwise fights; we will elaborate more on this in the next section. In a geographic picture, the drift term $-cZ_t\, dt$ results from *emigration*. The SDE (30) describes the evolution of the population size in the "mother colony", and the total mass that emigrates from the mother colony is $c\int_0^\infty Z_t dt =: cA^{(0)}$. The *Virgin Island assumption* is that each migration (of an infinitesimal mass $cZ_t\, dt$) is to a new colony, where $cZ_t\, dt$ becomes a potential ancestral mass.

Thus, $cA^{(0)} =: cM_0$ serves as the (random) time argument in a subordinator $\widetilde{S}$ with Lévy measure μ defined by

$$\mu(da) = Q(A(\zeta) \in da), \tag{31}$$

where the mass excursion measure Q is again defined by (15), but now with Z following (30) instead of (20). Proceeding inductively like in (26), we now arrive at a *tree of colonies*. This is the *Virgin Island model* studied by M. Hutzenthaler in [14], also for more general drift and diffusion coefficients than those in (30). Figure 3, adapted from [14], symbolizes a "tree of mass excursions" (embedded in time) which could either be a tree of alleles (as in the previous section) or a tree of colonies. In [14], the analogy between this time embedding and a (continuous-mass generalization of a) Crump–Mode–Jagers branching process is elaborated. In the Feller branching case, a similar construction has been carried out in [9] as a basis for a superprocess with dependent spatial motion and interactive immigration.

Let us emphasize again that for the logistic Feller branching (30) there is no subordinator representation as in (14), since the non-linear drift in (30) destroys the independence in the reproduction (and the infinite divisibility of Z_t). However, due to the Virgin Island assumption, which makes the evolution of the different colonies independent of each other, the tree of colony sizes still does have a representation in terms of an iteration of independent copies of a subordinator $\widetilde{S}$, and hence as a tree-indexed continuous state branching process as described after formula (27). In the case discussed

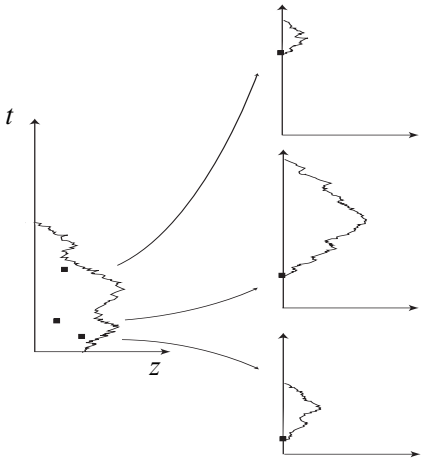

Figure 3. The root and three of its (countably many) children in a tree of excursions.

there (that is for $\theta = \gamma = 0$), the Lévy measure of these subordinators was given by (24). In the present case (with $\gamma > 0$) there is no explicit formula for the Lévy measure of the subordinators except the equality (31). However, there is still a handy criterion that allows to decide whether the total mass (summed over all colonies) in the Virgin Island model is finite a.s. This happens if and only if $\mathbf{E}\widetilde{S}_{ca_0} \leq a_0$ for all $a_0 \in \mathbb{R}_+$, or equivalently iff

$$c \int_0^\infty a\, \mu(da) \leq 1. \tag{32}$$

Because of (31), the first moment of μ is

$$\int_0^\infty a\, \mu(da) = \int_0^\infty a\, Q(A(\zeta) \in da) = \int_0^\infty dt \int_0^\infty y\, Q(\zeta_t \in dy), \tag{33}$$

with the last equality due to Fubini. Remarkably,

$$\int_0^\infty dt\, Q(\zeta_t \in dy) = m(y)\, dy, \tag{34}$$

where

$$m(y) = \frac{1}{\sigma^2 y/2} \exp\left(\int_0^y \frac{z(\theta - c - \gamma z)}{\sigma^2 z/2} dz \right) \tag{35}$$

is the *speed density* of (30) (in its adequate norming). Indeed, both sides of (34) are invariant measures for the semigroup of (30), and therefore must be proportional to each other. That they are in fact equal follows e.g. from Lemma 9.8 in [14]; our (34) is

equation (178) in [14]. Putting (33) – (35) together we see that (32) is equivalent to

$$c \int_0^\infty \exp\left((\theta - c)y - \gamma \tfrac{\sigma^2}{4} y^2\right) dy \leq 1, \tag{36}$$

which thus characterizes the a.s. finiteness of the total mass in the Virgin Island model obtained from (30).

It turns out that the Virgin Island model is most favorable for survival in the limit $t \to \infty$ when compared with models with the same local population dynamics (30) but a possibly different migration mechanism. To be specific, fix for $d \in \mathbb{N}$ probability weights m_k, $k \in \mathbb{Z}^d$, and consider the system of interacting diffusions

$$\begin{aligned} dZ_{k,t} = \sigma \sqrt{Z_{k,t}}\, dW_{k,t} + (\theta Z_{k,t} - \gamma Z_{k,t}^2)\, dt + c\Big(\sum_j m_{j-k} Z_{j,t} - Z_{k,t}\Big) dt, \\ Z_{k,0} = x\delta_{0k},\ k \in \mathbb{Z}^d, \end{aligned} \tag{37}$$

where W_k, $k \in \mathbb{Z}^d$, are independent standard Brownian motions. Using a self-duality of the solution of (37) and a comparison between (37) (now with a spatially homogeneous initial configuration) and a *mean field model*, it is shown ([15], Theorem 1, Theorem 3 and Corollary 4) that under the assumption (36) the total mass process $\sum_{k\in\mathbb{Z}^d} Z_{k,t}$ from (37) hits 0 in finite time a.s., irrespective of the choice of the weights m_k. In [14] a direct comparison of (37) with the corresponding Virgin Island model is announced also for more general diffusion and drift coefficients, in which case no self-duality would be available.

We conclude this section with a representation of the random variable $\int_0^\infty Z_t^x dt$, with Z^x being the solution of (30). This uses a time change introduced by Lambert in [18]. Consider the additive functional

$$A_t = \int_0^t Z_s^x ds,$$

and the associated time change

$$\alpha_t = \inf\{s > 0,\ A_t > s\}.$$

As noted in [18], the process $Y_t^x := Z_{\alpha_t}^x$ is an Ornstein–Uhlenbeck process, solving the SDE

$$dY_t^x = (\theta - c - \gamma Y_t^x)dt + \sigma dB_t, \quad Y_0^x = x,$$

with this identification is valid only for $0 \leq t \leq \tau_x$, where $\tau_x := \inf\{t > 0,\ Y_t^x = 0\}$. Let T_x be the extinction time of the logistic Feller process Z_t^x. We clearly have $\alpha_{\tau_x} = T_x$, and consequently

$$\tau_x = \int_0^\infty Z_t^x dt.$$

In the particular case $\gamma = \theta = 0$, this identity ties in with the remark at the end of Section 5.

8 A Ray–Knight representation of logistic Feller branching

As mentioned in the previous section, the Feller branching diffusion with logistic growth, which follows the SDE (30), has no subordinator representation as in (14), nor has it a Ray–Knight representation in terms of a concatenation of independent exploration excursions. This is due to the non-linear term on the r.h.s. of (30) that comes from the pairwise fights in which one of the two fighters is killed. However, by breaking the symmetry between the individuals we will manage to bring an exploration process and a Ray–Knight representation back into the picture.

To explain the strategy, we consider a "discrete mass - continuous time" approximation of (30) and its exploration process. As in Section 4, for $N \in \mathbb{N}$, the approximation will be given by the total mass $Z^{(N)}$ of a population of individuals, each of which has mass $1/N$. The initial mass is $Z_0^{(N)} = \lfloor Nx \rfloor / N$, and $Z^{(N)}$ follows a Markovian jump dynamics: from its current state k/N,

$$Z^{(N)} \text{ jumps to } \begin{cases} (k+1)/N \text{ at rate } kN\sigma^2/2 + k\theta, \\ (k-1)/N \text{ at rate } kN\sigma^2/2 + k(k-1)\gamma/N. \end{cases} \tag{38}$$

The quadratic death term $k(k-1)\gamma/N$ can be attributed to each of the $k(k-1)/2$ pairs fighting at rate 2γ, with each of the fights being lethal for one of the two individuals. The dynamics of the total mass will not be affected if we view the individuals alive at time t as being arranged "from left to right", and decree that each of the pairwise fights is won by the individual to the left. In this way we arrive at the "death rate due to fights" $2\gamma \mathcal{L}_i(t)/N$ for individual i, where $\mathcal{L}_i(t)$ denotes the number of contemporaneous individuals to the left of individual i at time t. In this way we grow a forest of $\lfloor Nx \rfloor$ trees, with all the individuals being under attack from the contemporaneans to their left. This forest is explored with speed $2N$ in the way as described in Section 3, leading to slopes $\pm 2N$ of the exploration path H^N. For an individual i living at real time t and being explored in an upward piece of H^N at exploration time s, the exploration process H^N experiences a rate of change from positive to negative slope which is increased by the pairwise fights. This additional rate of change from positive to negative slope is $2\gamma \mathcal{L}_i(t)/N$ in real time, and $4\gamma \mathcal{L}_i(t)$ in exploration time. In terms of the "local time" (3) this can be expressed as $4\gamma N \Lambda_s(H_s^N, H^N)$, since the number of contemporaneans to the left of the individual i is $\mathcal{L}_i(t) = N\Lambda_s(t, H^N)$. In the same way as we arrived at Lemma 3.1 in the case $\theta = \gamma = 0$, we can now identify the stochastic dynamics of $s \mapsto H_s^N$:

Lemma 8.1. *The exploration path $s \mapsto H_s^N$ obeys the following stochastic dynamics:*

- *At time $s = 0$, H^N starts at height 0 and with slope $2N$.*
- *When H^N moves upwards, its slope jumps from $2N$ to $-2N$ at rate $N^2\sigma^2 + 4\gamma N \Lambda_s(H_s^N, H^N)$.*
- *When H^N moves downwards, its slope jumps from $-2N$ to $2N$ at rate $N^2\sigma^2 + 2N\theta$.*
- *Whenever H^N reaches 0, its slope jumps from $-2N$ to $2N$, i.e. H^N is reflected at 0.*

Write

$$S_x^N = \inf\{s : \Lambda_s^N(0, H^N) \geq \lfloor Nx \rfloor / N\}. \tag{39}$$

for the first time at which H^N completes $\lfloor Nx \rfloor$ excursions. Just as we obtained from Lemma 3.1 the discrete Ray–Knight representation for a Galton–Watson process (Corollary 3.2), we obtain in the following Corollary of Lemma 8.1 a similar representation for the Galton–Watson process with logistic growth:

Corollary 8.2. *Let H^N be a stochastic process following the dynamics specified in Lemma 8.1. Then $t \mapsto \Lambda_{S_x^N}(t, H^N)$ follows the jump dynamics (38).*

In [19] we prove that the sequence of processes H^N converges, as $N \to \infty$, to the weak solution of

$$H_s = \frac{2}{\sigma} B_s + \frac{2\theta}{\sigma^2} s - \gamma \int_0^s L_r(H_r, H) dr + \frac{1}{2} L_s(0, H), \quad s \geq 0. \tag{40}$$

with B a standard Brownian motion and $L_s(t, H)$ the semimartingale local time of H, with L and Λ connected by (8). One ingredient in this proof is the following

Proposition 8.3 ([19]). *For $\sigma > 0$, $\theta, \gamma \geq 0$, the stochastic integral equation (40) has a unique weak solution. This solution is obtained by a Girsanov transform from a reflected Brownian motion with variance parameter $\sigma^2/4$.*

A main result of [19] is a Ray–Knight representation of Feller's branching diffusion with logistic growth in terms of a reflected Brownian motion H which experiences a constant positive drift plus a negative drift that is proportional to the local time spent by H so far at its current level:

Theorem 8.4. *Let H be the solution of (40), and for $x > 0$ let S_x be defined by (5). Then $(\Lambda_{S_x}(t, H))_{t \geq 0}$ is a Feller branching diffusion with logistic growth, i.e. a weak solution of (30) (with $c = 0$).*

The strategy in [19] to prove this theorem is to justify the passage to the limit $N \to \infty$ in Corollary 8.2. As a conclusion from this theorem, we obtain an analogue of the representation (14) for the logistic Feller process (30), but now as a path-valued Markovian jump process rather than a path-valued subordinator. To see this, let (ξ_i, η_i) be the point process of excursions on $\mathbb{R}_+ \times \mathcal{E}$, where $\mathcal{E}$ is the space of excursions from 0, and such that $(H_s)_{0 \leq s \leq S_x}$ is the concatenation of the excursions η_i with $\xi_i \leq x$. For $\eta \in \mathcal{E}$, let $\zeta(\eta) := \Lambda_{R(\eta)}(\cdot, \eta)$ be the image of η under the Ray–Knight mapping. Then another way to state Theorem 8.4 is that

$$\sum_{i : \xi_i \leq x} \zeta(\eta_i) \stackrel{d}{=} Z^x, \tag{41}$$

where Z^x solves (30) (with $c = 0$).

Again using the device that "those to the left win against those to the right" (which of course again is no dictum politicum) we can identify the transition probabilities of the path-valued Markov process $(Z^x)_{x \geq 0}$. Indeed, the following is readily checked:

Remark 8.5. For $x > 0$ let Z^x be a solution of (30) with $c = 0$. For a given path $z = (z_t)_{t\geq 0}$ and for $\varepsilon > 0$, let $X^\varepsilon(z)$ be a solution of

$$dX_t = \sigma\sqrt{X_t}\, dW_t^{(x,x+\varepsilon)} + \big((\theta - 2z_t\gamma)X_t - \gamma X_t^2\big)\, dt, \quad X_0 = \varepsilon, \tag{42}$$

where the standard Wiener process $W^{(x,x+\varepsilon)}$ is independent from the Wiener process W in (30). Then $Z^{x+\varepsilon} := Z^x + X^\varepsilon(Z^x)$ is a weak solution of

$$dZ_t = \sigma\sqrt{Z_t}\, dW_t^{(0,x+\varepsilon)} + \theta Z_t - \gamma Z_t^2 dt, \quad Z_0 = x + \varepsilon.$$

We conjecture that the Markov process $(Z^x)_{x\geq 0}$ follows a "jump kernel" Q^z that is given by Pitman and Yor's excursion measure of the diffusion process (42), i.e.

$$Q^z = \lim_{\varepsilon\to 0} \frac{1}{\varepsilon}\mathbf{P}(X^\varepsilon(z) \in \cdot).$$

With z as on the l.h.s. of (41), Q^z would then be the image under the Ray–Knight mapping $\eta \mapsto \zeta = \Lambda(\eta)$ of the conditional intensity kernel of the point process (ξ_i, η_i), given its restriction to $[0, x] \times \mathcal{E}_+$.

Note added in proof. Following a similar route as in [26] we were recently able to prove Theorem 8.4 also directly by a Girsanov argument, see [27]. We thank J. F. Le Gall for pointing us to [26].

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Gaussian approximation of functionals: Malliavin calculus and Stein's method

Gesine Reinert

1 Introduction

Over the last few years a very fruitful interplay between Malliavin calculus and Stein's method has been developed, yielding not only a new angle on limit theorems, but also new results, notably invariance theorems and a result on the universality of Wiener chaos. These results allow to derive bounds on distributional distances for fairly general uni- or multivariate real-valued functionals of random fields, and they include many well-studied normal approximations as special cases.

Below are a few examples to illustrate the range of objects which have been considered. These objects are often phrased in terms of symmetric real-valued functions f on $\mathbb{R}^d$, that is, $f(i_{\sigma(1)}, \ldots, i_{\sigma(d)}) = f(i_1, \ldots, i_d)$ for any permutation σ on $\{1, \ldots, d\}$ and any $(i_1, \ldots, i_d) \in \mathbb{R}^d$. Often we also assume that f vanishes on diagonals, that is, $f(i_1, \ldots, i_d) = 0$ whenever there exist $k \neq j$ such that $i_k = i_j$.

Example 1.1 (Multilinear homogeneous sums). Fix integers $N, d \geq 2$. Let $\mathbf{X} = \{X_i : i \geq 1\}$ be a collection of centered independent random variables; and let $f : \{1, \ldots, N\}^d \to \mathbb{R}$ be a symmetric function vanishing on diagonals. Then

$$Q_d(\mathbf{X}) = \sum_{1 \leq i_1, \ldots, i_d \leq N} f(i_1, \ldots, i_d) X_{i_1} \ldots X_{i_d}$$

is called the *multilinear homogeneous sum*, of order d, based on f and on the first N elements of $\mathbf{X}$. In Section 5 we shall give bounds to the standard normal distribution, in Wasserstein distance, for such sums.

Example 1.2 (Functionals of Rademacher sequences). Let $\mathbf{X} = \{X_n : n \geq 1\}$ be a *Rademacher sequence*, that is, a sequence of i.i.d. random variables with values in $\{-1, 1\}$ such that $\mathbb{P}(X_1 = 1) = \mathbb{P}(X_1 = -1) = 1/2$. Assume that $f_n : \mathbb{N}^n \to \mathbb{R}$ vanishes on diagonals, and put

$$Q(\mathbf{X}) = \sum_{n \geq 0} \sum_{i_1, \ldots, i_n} f_n(i_1, \ldots, i_n) X_{i_1} \ldots X_{i_n}.$$

We are interested in assessing how far away $Q(\mathbf{X})$ is from a normally distributed random variable. Note that here, in contrast to Example 1.1, the sum is potentially over an infinite number of summands. An easy example is the number of (weighted) d-runs in an infinite Bernoulli sequence; see [35]. As a variant it is possible to obtain similar results when replacing the Rademacher sequence by a sequence of compensated Poisson variables; see [41].

Example 1.3 (A functional of a Gaussian process). Let B be a centered Gaussian process with stationary increments such that $\int_{\mathbb{R}} |\rho(x)|dx < \infty$, where $\rho(u-v) := \mathbb{E}\big[(B_{u+1} - B_u)(B_{v+1} - B_v)\big]$. Let $f : \mathbb{R} \to \mathbb{R}$ be a non-constant function which is twice continuously differentiable, let $Z \sim \mathcal{N}(0,1)$ be a standard normal variable, assume that $\mathbb{E}|f(Z)| < \infty$ and $\mathbb{E}[f''(Z)^4] < \infty$. Fix $a < b$ in $\mathbb{R}$ and, for any $T > 0$, consider

$$F_T = \frac{1}{\sqrt{T}} \int_{aT}^{bT} \big(f(B_{u+1} - B_u) - \mathbb{E}[f(Z)]\big)du.$$

In Section 4 we shall assess its distributional distance to the standard normal.

Example 1.4 (Functions of functions of independent normals). An example which is considered in [10] is to let $\mathbf{X} = (X_1, \ldots, X_n)$, where each $X_i = u_i(Z)$, with Z standard normal, and u_i being a real-valued, smooth function, for each i. Let $g : \mathbb{R} \to \mathbb{R}$ be twice continuously differentiable and put $W = g(X)$. For example we could consider $W = \sum_{i \le j} a_{i,j} X_i X_j$; or $W = ReTr(f(A(X)))$, where $A(x)$ is a complex $n \times n$ matrix. Under a "symmetric interaction rule" on g, [10] derives a normal approximation for W, with bounds, using Stein's method.

Some applications where functionals of random fields play an important role include power and bipower variations of stochastic integrals as in [6] and [17], the correlation structure of Mexican needlets (which are a class of wavelet systems) and models for cosmological data analysis (see [23] and [26]); and the estimation of Hurst indices, see [55].

The common theme behind these examples and applications are possibly nonlinear functionals of independent random elements which admit a *chaos decomposition*, see (8), which looks like

$$F = \mathbb{E}(F) + \sum_{n \ge 1} n! \sum_{i_1 < i_2 < \cdots < i_n} f_n(i_1, \ldots, i_n) X_{i_1} \ldots X_{i_n}, \tag{1}$$

where the functions f_n are usually assumed to be symmetric and to vanish on diagonals. Heuristically, if the f_n's render the summands to be only "weakly" dependent, then the average should be approximately normally distributed under some conditions which should be related to those of the asymptotics of U-statistics; see for example [22] for the latter.

The main aims are not only to obtain normal asymptotics for functionals of the form (1), but also to give explicit bounds on distances (such as Wasserstein or Kolmogorov distance) to the normal distribution, as well as easy criteria for such bounds to tend to zero under the asymptotic regime under consideration. For the first aim, bounds on the distance, Stein's method has proven a powerful tool in many special cases of (1). For the second aim, the *influence function*, see (15), is a straightforward quantity in which to express the bounds.

The purpose of this paper is an expository overview, mainly based on the results in [30], [33], [34], and [35]. While detailed proofs are omitted, the main ideas for the

proofs are outlined, and special emphasis is put on the interplay between Malliavin calculus and Stein's method.

The paper is organised as follows. In Section 2 we briefly review Stein's method for normal approximation, and outline how in particular exchangeable pair couplings come into use. We shall see that Taylor expansions play a prominent role, and thus a differentiable structure is key for applying Stein's method for normal approximations. For infinite-dimensional objects, such a differentiable structure is provided by Malliavin calculus, and Section 3 provides a very brief introduction to the main ingredients for making the connection with Stein's method. In Section 4, it is shown how Stein's method and Malliavin calculus combine in various ways; a first application, to second-order Poincaré inequalities, is given. Section 5 details the universality theorem of Wiener chaos, where universality is for multilinear homogeneous sums, in the sense that the asymptotic normality of the sum does not depend on the precise underlying distribution of the random variables. Finally, Section 6 points out generalisations as well as open problems.

2 Stein's method for normal approximation

2.1 The main idea. In [52], Stein published a novel method for proving normal approximations with bounds on the distance; see also [53]. Here is just a brief overview; for more details see for example [15] or [16]. The method is based on the observation that

$$Z \sim \mathcal{N}(0,\sigma^2) \iff \mathbb{E}Zf(Z) = \sigma^2\mathbb{E}f'(Z) \text{ for all smooth functions } f. \tag{2}$$

Here and in the following, $\mathcal{N}(0,\sigma^2)$ denotes the mean zero variance σ^2 normal distribution. Also, smoothness means sufficiently often continuously differentiable; the precise conditions may vary throughout this paper.

The main idea of Stein's method for normal approximation is that for a random variable W with $\mathbb{E}W = 0$ and $\mathrm{Var}(W) = \sigma^2$, if

$$\sigma^2\mathbb{E}f'(W) - \mathbb{E}Wf(W)$$

is close to zero for many functions f, then because of (2), W should be close to $Z \sim \mathcal{N}(0,\sigma^2)$ in distribution.

To make use of this idea, given a test function h, we solve for $f = f_h$ in the so-called *Stein equation*

$$\sigma^2 f'(w) - wf(w) = h(w/\sigma) - \mathbb{E}h(Z). \tag{3}$$

Now we can evaluate the difference of expectations $\mathbb{E}h(W/\sigma) - \mathbb{E}h(Z)$ by the expectation of the left-hand side of (3), namely $\sigma^2\mathbb{E}f'(W) - \mathbb{E}Wf(W)$. We can bound the solutions of (3) in terms of the derivatives of h; for example we find $\| f'' \| \leq \frac{2}{\sigma^3} \| h' \|$, see [53], p. 25. Here $\| \cdot \|$ denotes the supremum norm.

2.2 A very basic example. Let $X, X_1, \ldots, X_n$ be i.i.d. mean zero random variables with $\mathrm{Var}(X) = \frac{1}{n}$, and put $W = \sum_{i=1}^n X_i$. Let $W_i = W - X_i = \sum_{j \neq i} X_j$. Then using Taylor expansion around X_i,

$$\begin{aligned} \mathbb{E}Wf(W) &= \sum_{i=1}^n \mathbb{E}X_i f(W) \\ &= \sum_{i=1}^n \mathbb{E}X_i f(W_i) + \sum_{i=1}^n \mathbb{E}X_i^2 f'(W_i) + R \\ &= \frac{1}{n}\sum_{i=1}^n \mathbb{E}f'(W_i) + R, \end{aligned} \tag{4}$$

where

$$R = \sum_{i=1}^n \mathbb{E}X_i\{f(W) - f(W_i) - (W - W_i)f'(W_i)\}.$$

So $\mathbb{E}f'(W) - \mathbb{E}Wf(W) = \frac{1}{n}\sum_{i=1}^n \mathbb{E}\{f'(W) - f'(W_i)\} + R$, and we can bound the remainder term R. Similarly using Taylor expansion again we can bound the difference $\frac{1}{n}\sum_{i=1}^n \mathbb{E}f'(W_i) - \mathbb{E}f'(W)$. The result is summarised in the following theorem, see for example [47], Theorem 2.1.

Theorem 2.1. *For any continuous, bounded real-valued function h with piecewise continuous, bounded first derivative, and for $Z \sim \mathcal{N}(0,1)$,*

$$|\mathbb{E}h(W) - \mathbb{E}h(Z)| \quad \leq \quad \|h'\|\Big(\frac{2}{\sqrt{n}} + \sum_{i=1}^n \mathbb{E}|X_i^3|\Big).$$

Thus Stein's method cannot only be used to prove approximations, but it gives an explicit bound on the distance to normal in terms of test functions.

While the i.i.d. case is very well covered by a range of techniques, Stein's method is particularly powerful in the presence of dependence. It is easy to see how local dependence would yield a slightly modified Taylor expansion in (4). To disentangle dependence, couplings are often used; here we use exchangeable pair couplings as an illustration. For an overview on couplings for normal approximations, see for example [47].

2.3 Exchangeable pair coupling. Let (W, W') be a pair of exchangeable random variables; assume $\mathbb{E}W = 0$ and $\mathbb{E}W^2 = 1$, and that there is a $0 < \lambda < 1$ such that the following *regression condition* holds:

$$\mathbb{E}(W'|W) = (1 - \lambda)W. \tag{5}$$

The regression condition (5) is natural in view of the fact that if (W, W') were bivariate standard normal with correlation ρ, then (5) would be satisfied with $\lambda = 1 - \rho$.

Example 2.2. Let us revisit the example from Subsection 2.2 of a sum of i.i.d. random variables, $X_1, \ldots, X_n$, with mean zero, variance $\frac{1}{n}$, and $W = \sum_{i=1}^n X_i$. To construct an exchangeable pair, pick an index I uniformly from $\{1, \ldots, n\}$. If $I = i$, we replace X_i by an independent copy X_i^*, and put

$$W' = W - X_I + X_I^*.$$

Then (W, W') is exchangeable, and

$$\mathbb{E}(W'|W) \quad = \quad W - \frac{1}{n}W + \mathbb{E}X_I^* = \left(1 - \frac{1}{n}\right)W.$$

Thus (5) is satisfied with $\lambda = \frac{1}{n}$.

Under the regression condition (5) it is easy to see that

$$\mathbb{E}Wf'(W) = \frac{1}{2\lambda}\mathbb{E}(W - W')(f'(W) - f'(W')).$$

Essentially Taylor expansion gives that, for any smooth $h\colon \mathbb{R} \to \mathbb{R}$

$$\begin{aligned}|\mathbb{E}\,h(W) - \mathbb{E}\,h(Z)| \quad \leq \quad & (\sup h - \inf h)\sqrt{\mathbb{E}\left(1 - \frac{1}{2\lambda}\mathbb{E}((W - W')^2|W)\right)^2} \\ & + \frac{1}{4\lambda}\|h'\|\mathbb{E}|W - W'|^3.\end{aligned}$$

In [49] the exchangeable pair coupling has been extended to a multivariate setting to

$$\mathbb{E}(W' - W|W) = -\Lambda W \tag{6}$$

for an invertible $d \times d$ matrix Λ. Both formulations (5) and (6) allow an additive error term R; see [49] and [50]. Examples where dependence is present and exchangeable pair couplings are straightforward include simple random sampling and some permutation statistics; see for example [53].

2.4 Stein's method for chi-square approximation. Stein's method has been generalised to many other distributions; foremost the Poisson distribution, see for example [2], [5], and [11], but also to the chi-square distribution, in [24] and [43], see [46] for an overview. In [24] the general case of Gamma distributions is studied, leading to the Stein equation for χ_p^2

$$xf'(x) + \frac{1}{2}(p - x)f(x) = h(x) - \chi_p^2 h, \tag{7}$$

with $\chi_p^2 h$ denoting the expectation of h under the χ_p^2 distribution. The role of this equation is similar to that of (3). [43] showed that if $h\colon \mathbb{R} \to \mathbb{R}$ is absolutely bounded,

$|h(x)| \leq ce^{ax}$ for some $c > 0, a \in \mathbb{R}$, and the first k derivatives of h are bounded, then the equation (7) has a solution $f = f_h$ such that, for $j = 0, \ldots, k$,

$$\| f^{(j)} \| \leq \frac{\sqrt{2\pi}}{\sqrt{p}} \| h^{(j)} \|$$

with $h^{(0)} = h$. While in what follows we shall concentrate on normal approximations, many of our results have analogous chi-square approximation results.

2.5 Ingredients for normal approximation via Stein's method. Stein's method for normal approximation being based on a differential equation, a main ingredient is a differential structure which allows for Taylor expansion. As we are interested in functionals of random fields, here we shall employ Malliavin calculus for this structure. Other choices could include Fréchet derivatives for stochastic processes [4], or Gâteaux derivatives for random measures [48].

The second ingredient for a successful approximation of Stein's method for normal approximation is the ability to make use of weak dependence. In the above example this could happen via exchangeable pairs or other coupling constructions. While coupling constructions are sometimes not straightforward to find, here we shall use the notion of an *influence function* to quantify weak dependence.

3 Ingredients from stochastic analysis

For a calculus which allows to treat possibly non-linear functionals of Gaussian processes on possibly infinite-dimensional spaces we employ Malliavin calculus, introduced by [25]. Versions for functionals of other stochastic processes are available, such as for Rademacher processes ([44], [45]), and for compensated Poisson processes (see for example [54]).

The three necessary concepts for our purposes are (isonormal Gaussian) processes, a chaos decomposition in terms of multiple integrals, and Malliavin operators. We shall explain these in turn. For further expository presentations see for example [28], [32] and [40].

3.1 Isonormal Gaussian processes. Let $\mathfrak{H}$ be a real separable Hilbert space with inner product $\langle \cdot, \cdot \rangle_{\mathfrak{H}}$, and for any $q \geqslant 1$ let $\mathfrak{H}^{\otimes q}$ be the q^{th} tensor product of $\mathfrak{H}$; similarly denote by $\mathfrak{H}^{\odot q}$ the associated q^{th} symmetric tensor product. We call $\mathbf{X} = \{X(h), h \in \mathfrak{H}\}$ an *isonormal Gaussian process* over $\mathfrak{H}$, defined on some probability space $(\Omega, \mathcal{F}, P)$, if it is a centered Gaussian family, whose covariance is $\mathbb{E}[X(h)X(g)] = \langle h, g \rangle_{\mathfrak{H}}$. We assume that $\mathcal{F}$ is generated by $\mathbf{X}$. We also say that $\mathbf{X}$ is a *centered Gaussian Hilbert space*, with respect to the inner product given by the covariance, isomorphic to $\mathfrak{H}$.

For example, the Wiener integral corresponds to $\mathfrak{H} = L^2([0,1], dx)$. In this case, $\mathbf{X} = (X_t, t \in [0,1])$ defined by $X_t = X(\mathbf{1}_{[0,t]})$ is (the space generated by) a standard Brownian motion. As another example, if $\mathfrak{H} = L^2(A, \mathcal{A}, d\mu)$, where $(A, \mathcal{A})$ is a

measurable space, then $\mathbf{X}$ is (the space generated by) a Gaussian measure over A. Isonormal Gaussian processes have been introduced by [19]; see also [22] for much more detail on Gaussian processes indexed by Hilbert spaces.

3.2 Chaos decomposition in terms of multiple integrals. To define the Wiener chaos we employ Hermite polynomials; we use as definition for the q^{th} Hermite polynomial

$$H_q(x) = (-1)^q e^{\frac{x^2}{2}} \frac{d^q}{dx^q}\big(e^{-\frac{x^2}{2}}\big),$$

with $H_0(x) = 1$. For every $q \geqslant 1$, the q^{th} *Wiener chaos* of X, denoted by $\mathcal{H}_q$, is the closed linear subspace of $L^2(\Omega, \mathcal{F}, P)$ generated by the random variables of the type $\{H_q(X(h)), h \in \mathfrak{H}, \|h\|_{\mathfrak{H}} = 1\}$. We put $\mathcal{H}_0 = \mathbb{R}$. For every $q \geqslant 1$, we introduce the mapping

$$I_q(h^{\otimes q}) = q! H_q(X(h)).$$

This mapping can be extended to a linear isometry between the symmetric tensor product $\mathfrak{H}^{\odot q}$ (equipped with the modified norm $\sqrt{q!}\,\|\cdot\|_{\mathfrak{H}^{\otimes q}}$) and the q^{th} Wiener chaos $\mathcal{H}_q$.

If $\mathfrak{H} = L^2(A, \mathcal{A}, d\mu)$, and $\mathbf{X}$ is (the space generated by) a Gaussian measure over A, where $(A, \mathcal{A})$ is a Polish space and μ is σ-finite and non-atomic, then the integral I_q corresponds to the Wiener–Itô integral and can be constructed as follows. For step functions of the type

$$\sum_{1 \leq i_1, \ldots, i_q \leq n} a_{i_1, \ldots, i_q} \mathbf{1}_{A_{i_1}}(x_1) \cdots \mathbf{1}_{A_{i_q}}(x_q)$$

with the $A_i's$ pairwise disjoint, and $a_{i_1, \ldots, i_q} = 0$ whenever $|\{i_1, \ldots, i_q\}| < q$, we define the (multiple) integral as

$$I_q(f) = \sum_{1 \leq i_1, \ldots, i_q \leq n} a_{i_1, \ldots, i_q} X(A_{i_1}) \cdots X(A_{i_q}).$$

Then we use that the set of such elementary functions is dense in $\mathfrak{H}^{\otimes q}$ to extend the notion of an integral for all $f \in L^2(\mu^q)$.

Note that $\mathbb{E} I_q(f) = 0$. To state further properties of the integral $I_q(f)$, let $\tilde{f}$ denote the canonical symmetrisation of f:

$$\tilde{f}(i_1, \ldots, i_q) = \frac{1}{q!} \sum_{\pi} f(i_{\pi(1)}, \ldots, i_{\pi(q)}).$$

Then the integral is symmetric in the sense that

$$I_q(f) = I_q(\tilde{f}).$$

Moreover, for every functional F of $\mathbf{X}$ which satisfies $\mathbb{E}[F(\mathbf{X})^2] < \infty$ there exists a unique sequence $\{f_q, q \geq 1\}$ with $f_q \in \mathfrak{H}^{\odot q}, q \geq 1$ such that

$$F = \mathbb{E}(F) + \sum_{q=1}^{\infty} I_q(f_q) = \sum_{q=0}^{\infty} I_q(f_q), \tag{8}$$

where we put $I_0(f_0) = \mathbb{E}(F)$. The series converges in $L^2(P)$. Equation (8) is called *chaos decomposition* of F.

3.3 Malliavin operators. Malliavin calculus, introduced in [25], originally for finding conditions under which solutions of stochastic differential equations have a density, is an infinite-dimensional calculus on spaces of functionals of (Gaussian) processes. Here we cannot give it justice, but instead concentrate on the operators needed for our purpose; see for example [39] for more detail on Malliavin calculus.

Let $\mathbf{X} = \{X(h), h \in \mathfrak{H}\}$ be an isonormal Gaussian process, defined on the probability space $(\Omega, \mathcal{F}, P)$. To clarify the domains of the Malliavin operators we define, for $k \geq 1$, the Hilbert spaces $L^2(\sigma(\mathbf{X}), P, \mathfrak{H}^{\otimes k})$ of $\mathfrak{H}^{\otimes k}$-valued functionals on $\mathbf{X}$, with scalar product $\langle F, G\rangle_{L^2(\sigma(\mathbf{X}),P,\mathfrak{H}^{\otimes k})} = \mathbb{E}\langle F, G\rangle_{\mathfrak{H}^{\otimes k}}$. We also introduce $S \subset L^2(\sigma(\mathbf{X}), P, \mathfrak{H})$ as the set of all cylindrical random variables of the form $F = f(X(\phi_1), \ldots, X(\phi_n))$, where $f : \mathbb{R}^n \to \mathbb{R}$ is infinitely differentiable with compact support, and $\phi_1, \ldots, \phi_n \in \mathfrak{H}$. For such $F \in S$ we define its *Malliavin derivative* $DF \in \mathfrak{H}$ with respect to $\mathbf{X}$ as

$$DF = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i}(X(\phi_1), \ldots, X(\phi_n))\phi_i.$$

In particular $DX(h) = h$ for every $h \in \mathfrak{H}$.

If $\mathfrak{H} = L^2(A, \mathcal{A}, \mu)$, where $(A, \mathcal{A})$ is a measurable space and μ has no atoms, and if $F = \sum_{q=0}^{\infty} I_q(f_q)$ satisfies $\mathbb{E}[F(\mathbf{X})^2] < \infty$, then a version of $DF = \{D_a F, a \in A\}$ is given by

$$D_a F = \sum_{q=1}^{\infty} q I_{q-1}(f_q(\cdot, a)).$$

In general, the k^{th} derivative $D^k F \in L^2(\sigma(\mathbf{X}), P, \mathfrak{H}^{\otimes k})$ is defined by iteration. The domain of the operator D^k in $L^2(\sigma(\mathbf{X}), P, \mathfrak{H}^{\otimes k})$, denoted by $\mathbb{D}^{k,2}$, is the closure of the set S with respect to the norm

$$\|F\|_{k,2}^2 = \mathbb{E}\left[F^2\right] + \sum_{i=1}^{k} \mathbb{E}\left(\|D^i F\|_{\mathfrak{H}^{\otimes i}}^2\right).$$

The chain rule. For $\phi\colon \mathbb{R}^m \to \mathbb{R}$ being a continuously differentiable function with bounded partial derivatives, and $F = (F_1, \ldots, F_m) \in \mathbb{D}^{1,2}$, we have

$$D\phi(F) = \sum_{j=1}^{m} \frac{\partial \phi}{\partial x_j}(F) DF_j. \tag{9}$$

We note that the assumptions on ϕ can be weakened to Lipschitz, if F has a law which is absolutely continuous on $\mathbb{R}^m$.

The chain rule (9) does not hold in the Rademacher nor in the Poisson case. But in both cases we can usefully bound

$$D\phi(F) - \sum_{j=1}^{m} \frac{\partial \phi}{\partial x_j}(F) DF_j;$$

see [35] and [41].

Skorohod integral and integration by parts. The *Skorohod integral* or *divergence operator* δ is the adjoint of the derivative $D\colon \mathbb{D}^{1,2} \to L^2(\sigma(\mathbf{X}), P, \mathfrak{H})$, and can be defined via the *integration by parts* formula

$$\mathbb{E}[F\delta(u)] = \mathbb{E}\langle DF, u\rangle_{\mathfrak{H}} \tag{10}$$

for $F \in \mathbb{D}^{1,2}$ and $u \in \operatorname{dom}(\delta)$. The domain $\operatorname{dom}(\delta)$ of δ is the set of all random elements in $u \in L^2(\sigma(\mathbf{X}), P, \mathfrak{H})$ such that for all $F \in \mathbb{D}^{1,2}$, we have $\mathbb{E}[\langle DF, u\rangle_{\mathfrak{H}}] \le c\mathbb{E}[F^2]^{\frac{1}{2}}$, where c is a constant depending on u but not on F.

If $\mathfrak{H} = L^2(A, \mathcal{A}, \mu)$, where $(A, \mathcal{A})$ is a measurable space and μ has no atoms, and if $F = \sum_{q=0}^{\infty} I_q(f_q)$ satisfies $\mathbb{E}[F(\mathbf{X})^2] < \infty$, and $u(z) = \sum_{q=0}^{\infty} I_q(f_q(\cdot, z))$, then

$$\delta(u) = \sum_{q=0}^{\infty} I_{q+1}(\tilde{f}_q).$$

The Ornstein–Uhlenbeck operator. If $F = \sum_{q=0}^{\infty} I_q(f_q) \in L^2(\sigma(\mathbf{X}), P, \mathfrak{H})$ with chaos decomposition (8) and $\mathbb{E}[F(\mathbf{X})^2] < \infty$, the *Ornstein–Uhlenbeck operator* is defined as

$$LF = -\sum_{q=1}^{\infty} q I_q(f_q),$$

provided that this series converges in $L^2(P)$. The crucial relation between the Ornstein–Uhlenbeck operator, the Malliavin derivative and the Skorohod integral is

$$\delta D = -L. \tag{11}$$

We note that the image of L is the set $\{F \in L^2(\sigma(\mathbf{X}), P, \mathfrak{H}) : \mathbb{E}[F] = 0\}$, and that $LF = L(F - \mathbb{E}[F])$. Hence we can define the (*pseudo*)-*inverse* L^{-1} such that for $F = \sum_{q=1}^{\infty} I_q(f_q) \in L^2(\sigma(\mathbf{X}), P, \mathfrak{H})$, we have

$$L^{-1}F = -\sum_{q=1}^{\infty} \frac{1}{q} I_q(f_q).$$

Moreover, L is the (infinitesimal) generator of the Ornstein–Uhlenbeck semigroup T_t, defined such that for $F = \sum_{q=0}^{\infty} I_q(f_q) \in L^2(\sigma(\mathbf{X}), P, \mathfrak{H})$, and $t \ge 0$,

$$T_t f = \sum_{q=0}^{\infty} e^{-qt} I_q(f_q).$$

Alternatively, we can use a representation via *Mehler's formula*: if $\mathbf{X}'$ is an independent copy of $\mathbf{X}$, then

$$T_t F = \mathbb{E}[F(e^{-t}a + \sqrt{1-e^{-2t}}\mathbf{X}')]\big|_{a=\mathbf{X}} \tag{12}$$

holds; see e.g. [39].

4 Combining Stein's method and Malliavin calculus

4.1 A basic result for the distance to normality. It is convenient to use Wasserstein distance in our context; but results are also available in Kolmogorov distance, and in total variation distance. Let U, Z be two generic real-valued random variables. The *Wasserstein distance* between the law of U and the law of Z is defined as

$$d_W(U,Z) = \sup_{f:\|f\|_{\mathrm{Lip}}\le 1} |\mathbb{E}[f(U)] - \mathbb{E}[f(Z)]|,$$

where $\|f\|_{\mathrm{Lip}} = \sup_{x\neq y} \frac{|f(x)-f(y)|}{\|x-y\|_{\mathrm{Euclid}}}$ is the Lipschitz norm. Here $\|\cdot\|_{\mathrm{Euclid}}$ is the usual Euclidean norm. The *Kolmogorov distance* between two $\mathbb{R}^d$-valued random elements $U = (U_1, \ldots, U_d)$ and $Z = (Z_1, \ldots, Z_d)$ is defined as

$$d_{\mathrm{Kol}}(U,Z) = \sup_{\mathbf{x}=(x_1,\ldots,x_d)\in\mathbb{R}^d} |\mathbb{P}(U_1 \le x_1, \ldots, U_d \le x_d) - \mathbb{P}(Z_1 \le x_1, \ldots, Z_d \le x_d)|.$$

The topologies induced by d_W and by d_{Kol}, on the class of all probability measures on $\mathbb{R}$, are strictly stronger than the topology of weak convergence.

Instead of starting with Lipschitz test functions, in view of Taylor's formula let $g\colon \mathbb{R} \to \mathbb{R}$ be continuously differentiable with bounded first derivative, and $F \in \mathbb{D}^{1,2}$ with $\mathbb{E}(F) = 0$. Then the following calculation shows how Stein's method and Malliavin calculus interact.

$$\begin{aligned}
\mathbb{E}[Fg(F)] &= \mathbb{E}[LL^{-1}Fg(F)] \\
&= \mathbb{E}[g(F)(-\delta(DL^{-1}F))] && \text{by (11)} \\
&= \mathbb{E}[g(F)\delta(-DL^{-1}F)] \\
&= \mathbb{E}[\langle Dg(F), -DL^{-1}F\rangle_{\mathfrak{H}}] && \text{by (10)} \\
&= \mathbb{E}[g'(F)\langle DF, -DL^{-1}F\rangle_{\mathfrak{H}}] && \text{by (9)}.
\end{aligned}$$

Comparing this calculation to $\mathbb{E}g'(F)$ as arising from (3), the following theorem by [31], Theorem 3.1, is now straightforward.

Theorem 4.1. *Let $Z \sim \mathcal{N}(0,1)$ and let $F \in \mathbb{D}^{1,2}$ be such that $\mathbb{E}(F) = 0$. Then*

$$d_W(F,Z) \le \mathbb{E}|1 - \langle DF, -DL^{-1}F\rangle_{\mathfrak{H}}|.$$

For Rademacher sequences, [35] show that from the lack of a chain rule like (9) arises an additional additive term in the bound, $\frac{20}{3}\mathbb{E}\big[\langle |DL^{-1}F|, |DF|^3\rangle_{\ell^2(\mathbb{N})}\big]$. In view of Theorem 5.3 this term turns out to be natural.

Other versions of this theorem are available; for multivariate normal approximation see [36], for chi-square approximations see [31] and [34], and for Poisson sequences see [41] and [42].

4.2 Connections with exchangeable pairs. We point out two connections with exchangeable pairs as in Subsection 2.3; firstly a connection between Malliavin operators and exchangeable pairs, and secondly a connection between exchangeable pairs and a Mehler-type formula.

Assume that $\mathbf{X} = (X_1, \dots, X_d)$ is a vector of finitely many components, and

$$F = F(\mathbf{X}) = \sum_{q=1}^{d} \sum_{1 \le i_1 < \cdots < i_q \le d} q! f_q(i_1, \dots, i_q) X_{i_1} \cdots X_{i_q} = \sum_{q=1}^{d} I_q(f_q)$$

with $\mathbb{E}(F) = 0$ and $\mathbb{E}(F^2) = 1$. For an exchangeable pair, pick an index $I \in \{1, 2, \dots, d\}$ at random so that $\mathbb{P}(I = i) = \frac{1}{d}$, independent of $X_1, \dots, X_d$, and if $I = i$ replace X_i by an independent copy X_i^* in all sums in the decomposition (13) which involve X_i. Call the resulting expression F'. Also denote the vector of variables with the exchanged component by $\mathbf{X}'$. Then (F, F') forms an exchangeable pair. Related to the multivariate regression condition (6), putting $\mathbf{W} = (I_1(f_1), \dots, I_d(f_d))$, we have that

$$\begin{aligned}
&\mathbb{E}[I_q'(f_q) - I_q(f_q)|\mathbf{W}] \\
&\quad = -\frac{1}{d} \sum_{i=1}^{d} \sum_{1 \le i_1 < \cdots < i_q \le d} \mathbf{1}_{\{i_1, \dots, i_q\}}(i)\ q! f_q(i_1, \dots, i_q) \mathbb{E}(X_{i_1} \cdots X_{i_q}|\mathbf{W}) \\
&\quad = -\frac{q}{d} I_q(f_q)
\end{aligned}$$

and we obtain

$$\mathbb{E}(F' - F|\mathbf{W}) = \frac{1}{d} LF = -\frac{1}{d} \delta DF. \tag{13}$$

In [35] this expression is used in a similar fashion as (5) to obtain a bound to the standard normal distribution.

Equation (13) also leads to a connection between Mehler-type representations (12) and exchangeable pairs. Take an independent copy $\mathbf{X}^* = \{X_1^*, X_2^*, \dots, X_d^*\}$ of $\mathbf{X} = (X_1, \dots, X_d)$, fix $t > 0$, and define $\mathbf{X}^t = \{X_1^t, X_2^t, \dots X_d^t\}$ as follows: independently, for every $k \ge 1$, $X_k^t = X_k$ with probability e^{-t} and $X_k^t = X_k^*$ with probability $1 - e^{-t}$ (for example $X_1^t = X_1$, $X_2^t = X_2^*, \dots, X_d^t = X_d$). Then formally, using (13) and that

$LF = \lim_{t\to 0} \frac{T_t F - F}{t}$,

$$\begin{aligned}\mathbb{E}[F(\mathbf{X}') - F(\mathbf{X})|\mathbf{W}] &= \frac{1}{d}\lim_{t\to 0}\frac{T_t F(\mathbf{X}) - F(\mathbf{X})}{t} \\ &= \frac{1}{d}\lim_{t\to 0}\frac{1}{t}[\mathbb{E}(F(\mathbf{X}^t)|\mathbf{X}) - F(\mathbf{X})].\end{aligned}$$

Thus our exchangeable pair for (13) can be viewed as the limit as $t \to 0$ of this construction. For further connections between Mehler-type expressions and Stein's method in a Gaussian setting see also [4], [10], and [31].

4.3 Application to Poincaré-type inequalities. In its most basic formulation, the *Gaussian Poincaré inequality* states that, for every differentiable function $f : \mathbb{R} \to \mathbb{R}$, and $Z \sim \mathcal{N}(0, 1)$

$$\mathrm{Var}[f(Z)] \leq \mathbb{E}[f'(Z)^2],$$

with equality if and only if f is affine. Thus, if the random variable $f'(Z)$ has small L^2-norm, then $f(Z)$ has small fluctuations. For extensions of this inequality to smooth functionals of multi-dimensional (and possibly infinite-dimensional) Gaussian fields, and to non-Gaussian probability distributions see for example [3], [8], [9], [12], [13], [14], and [21].

In our set-up, let $\mathfrak{H}$ be a separable real Hilbert space, and let $\mathbf{X}$ be an isonormal Gaussian process over $\mathfrak{H}$. Then in [33], Proposition 3.1, the following theorem is proved.

Theorem 4.2. *Fix $p \geqslant 2$ and let $F \in \mathbb{D}^{1,p}$ be such that $\mathbb{E}(F) = 0$.*

(1) *The following estimate holds:*

$$\mathbb{E}\left\|DL^{-1}F\right\|_{\mathfrak{H}}^p \leq \mathbb{E}\left\|DF\right\|_{\mathfrak{H}}^p.$$

(2) *If in addition $F \in \mathbb{D}^{2,p}$, then*

$$\mathbb{E}\left\|D^2L^{-1}F\right\|_{\mathrm{op}}^p \leq \frac{1}{2^p}\,\mathbb{E}\left\|D^2F\right\|_{\mathrm{op}}^p,$$

where $\left\|D^2F\right\|_{\mathrm{op}}$ indicates the operator norm of the random Hilbert–Schmidt operator

$$\mathfrak{H} \to \mathfrak{H}\colon\ f \mapsto \left\langle f, D^2F\right\rangle_{\mathfrak{H}}$$

(and similarly for $\|D^2L^{-1}F\|_{\mathrm{op}}$).

(3) *If p is an even integer, then*

$$\mathbb{E}\big(F^p\big) \leq (p-1)^{p/2}\,\mathbb{E}\big(\|DF\|_{\mathfrak{H}}^p\big).$$

The proofs for Item 1 and Item 2 are based on Mehler's formula (12); the argument can be sketched as follows. Assume that $\mathfrak{H} = \mathrm{L}^2(A, \mathcal{A}, \mu)$, with μ non-atomic. Let

X' indicate an independent copy of X. Assume that F has chaos decomposition (8). Then, with (12),

$$\begin{aligned} D_x L^{-1} F &= -\sum_{q\geqslant 1} I_{q-1}\left(f_q(X,x)\right) \\ &= \int_0^\infty e^{-t} T_t D_x F(X) dt \\ &= \int_0^\infty e^{-t}\, \mathbb{E}_{X'}\, D_x F\left(e^{-t}X + \sqrt{1-e^{-2t}}X'\right) dt \\ &= \mathbb{E}_Y\, \mathbb{E}_{X'}\, D_x F\left(e^{-Y}X + \sqrt{1-e^{-2Y}}X'\right), \end{aligned}$$

where $Y \sim \mathcal{E}(1)$ is an independent exponential random variable of mean 1. Here, if U is a random variable, then $\mathbb{E}_U$ denotes the expectation with respect to U. It follows that

$$\begin{aligned} \mathbb{E}\left\|DL^{-1}F\right\|_{\mathfrak{H}}^p &\leq \mathbb{E}_X\, \mathbb{E}_Y\, \mathbb{E}_{X'} \left\|DF\left(e^{-Y}X + \sqrt{1-e^{-2Y}}X'\right)\right\|_{\mathfrak{H}}^p \\ &= \mathbb{E}\left\|DF\right\|_{\mathfrak{H}}^p, \end{aligned}$$

where we used that $e^{-t}X' + \sqrt{1-e^{-2t}}X \overset{\text{law}}{=} X$ for any $t > 0$. The proof for Item 2 is very similar. To see how the proof for Item 3 works, note that

$$\begin{aligned} \mathbb{E}\left(F^{2k}\right) &= \mathbb{E}\left(LL^{-1}F \times F^{2k-1}\right) \\ &= -\mathbb{E}\left(\delta DL^{-1}F \times F^{2k-1}\right) && \text{by (11)} \\ &= (2k-1)\mathbb{E}\left(\langle DF, -DL^{-1}F\rangle_{\mathfrak{H}} F^{2k-2}\right) && \text{by (10) and (9).} \end{aligned}$$

Now apply Hölder's inequality, re-arrange and then apply the Cauchy–Schwarz inequality to obtain Item 3.

Example 4.3 (The Gaussian process example revisited). As in Example 1.3 assume that B is centered Gaussian, with stationary increments, such that $\int_{\mathbb{R}} |\rho(x)|dx < \infty$, where $\rho(u-v) := \mathbb{E}\big[(B_{u+1} - B_u)(B_{v+1} - B_v)\big]$. Let $Z \sim \mathcal{N}(0,1)$ and let $f : \mathbb{R} \to \mathbb{R}$ be a non-constant real function which is twice continuously differentiable and symmetric, such that $\mathbb{E}|f(Z)| < \infty$ and $\mathbb{E}[f''(Z)^4] < \infty$. Fix $a < b$ in $\mathbb{R}$ and, for any $T > 0$, put

$$F_T = \frac{1}{\sqrt{T}} \int_{aT}^{bT} \big(f(B_{u+1} - B_u) - \mathbb{E}\, f(Z)\big) du.$$

Let h be a real-valued Lipschitz function with Lipschitz constant 1. Then, as $T \to \infty$, Theorem 4.2 can be employed to show that

$$\left|\mathbb{E}\left[h\left(\frac{F_T}{\sqrt{\mathrm{Var}(F_T)}}\right)\right] - \mathbb{E}[h(Z)]\right| = O(T^{-1/4}),$$

see Theorem 6.1 in [33].

Essentially combining Theorem 4.1 with estimates from Theorem 4.2 gives the following second-order infinite-dimensional Poincaré inequality, see Theorem 1.1 in [33].

Theorem 4.4. *Let $F \in \mathbb{D}^{2,4}$ be such that $\mathbb{E}(F) = \mu$ and $\mathrm{Var}(F) = \sigma^2 > 0$. Let $Z \sim \mathcal{N}(\mu, \sigma^2)$. Then*

$$d_W(F, Z) \leq \frac{\sqrt{10}}{2\sigma^2} \mathbb{E}\big[\|D^2 F\|_{\mathrm{op}}^4\big]^{\frac{1}{4}} \times \mathbb{E}\big[\|DF\|_{\mathfrak{S}}^4\big]^{\frac{1}{4}}.$$

Theorem 4.4 is used in [33] to derive random contraction inequalities, which lead to new necessary and sufficient conditions which ensure that sequences of random variables belonging to a fixed Wiener chaos converge in distribution to a standard normal variable; a simplified version is as follows.

Theorem 4.5. *Fix $q \geq 2$, and let $F_n = I_q(f_n)$ be a sequence of multiple Wiener–Itô integrals such that $\mathbb{E}(F_n^2) \to 1$ as $n \to \infty$. Then, as $n \to \infty$.*

$$F_n \xrightarrow{\text{law}} \mathcal{N}(0,1) \iff \left\|D^2 F_n\right\|_{\mathrm{op}} \xrightarrow{L^4(\Omega)} 0.$$

In the next section we shall meet equivalent conditions for multilinear homogeneous sums to converge in distribution to a standard normal variable.

5 Universality of Wiener chaos

In this section we illustrate how Stein's method combined with Malliavin calculus leads to a universality statement of Wiener chaos. This section is based on [34]. The setting is that of multilinear homogeneous sums as in Example 1.1; recall that $\mathbf{X} = \{X_i : i \geq 1\}$ is a sequence of centered, independent random variables. Let $f : \{1, \ldots, N\}^d \to \mathbb{R}$ be a symmetric function, vanishing on diagonals, and consider the multilinear homogeneous sum

$$Q_d(\mathbf{X}) = Q_d(N, f, \mathbf{X}) \quad = \sum_{1 \leq i_1, \ldots, i_d \leq N} f(i_1, \ldots, i_d) X_{i_1} \ldots X_{i_d}. \tag{14}$$

Note that, for $d = 2$, $Q_d(\mathbf{X})$ is a quadratic form with no diagonal term; see for example [20] for normal approximations of such objects.

While $Q_d(\mathbf{X})$ is a sum of locally dependent random variables, the neighbourhoods of dependence are typically too large to make a Taylor expansion of the type (4) and hence a direct application of Stein's method feasible. Also to note that $Q_d(\mathbf{X})$ is a completely degenerate U-statistic, so standard results for normal approximation of non-degenerate U-statistics do not apply.

However, if $\mathbf{X} = \mathbf{G}$, where $\mathbf{G} = (G_i, i \geq 1)$ are i.i.d. standard normal, then $Q_d(\mathbf{G})$ is an element of the d^{th} Wiener chaos. Applying Theorem 4.1 to elements of the d^{th} Wiener chaos yields an easy to compute bound on the Wasserstein distance to the standard normal distribution, see Theorem 3.1 in [34], as follows.

Theorem 5.1. *Fix $d \geqslant 2$. Let $F = I_d(h)$, $h \in \mathfrak{H}^{\odot d}$, be an element of the d^{th} Gaussian Wiener chaos such that $\mathbb{E}(F^2) = 1$, and let $Z \sim \mathcal{N}(0,1)$. Then*

$$d_W(F,Z) \leq \sqrt{\frac{d-1}{3d}|\mathbb{E}(F^4) - 3|}.$$

We note that for $Z \sim \mathcal{N}(0,1)$ we have $\mathbb{E}[Z^4] = 3$.

5.1 The influence function. Following [27], for f as in (14) the *influence* of the variable i is defined as

$$\mathrm{Inf}_i(f) = \frac{1}{(d-1)!} \sum_{1 \leq i_2, \ldots, i_d \leq N} f^2(i, i_2, \ldots, i_d). \tag{15}$$

It roughly quantifies the contribution of X_i to the overall configuration of the homogeneous sum $Q_d(\mathbf{X})$. A similar notion was developed in [51].

Example 5.2 (2-runs). If W_n counts the number of 2-runs in n independent Bernoulli(p) trials $X_1, \ldots, X_n$, then we can write W_n as multilinear homogeneous sum with $d = 2$; standardising,

$$\frac{W_n}{\sqrt{\mathrm{Var}(W_n)}} = \sum_{1 \leq i_1, i_2 \leq N} f(i_1, i_2) X_{i_1} X_{i_2}$$

with

$$f(i_1, i_2) \quad = \quad \frac{1}{\sqrt{\mathrm{Var}(W_n)}} \frac{1}{2!} (\mathbf{1}(i_2 = i_1 + 1) + \mathbf{1}(i_1 = i_2 + 1)).$$

Then, using the torus convention,

$$\mathrm{Inf}_i(f) = \frac{1}{4\mathrm{Var}(W_n)} \sum_j (\mathbf{1}(i = j + 1) + \mathbf{1}(j = i + 1))^2 = \frac{1}{2\mathrm{Var}(W_n)}.$$

With p fixed, $\mathrm{Var}(W_n) \sim n$, see for example [49], and hence $\mathrm{Inf}_i(f) \sim n^{-1}$.

5.2 A bound on the distance to normal, and universality of Wiener chaos. The assumptions for our bound on the distance to the normal for a multilinear homogeneous sum (14), and for our universality result, are as follows. Assume that the underlying collection of independent, centered random variables $\mathbf{X} = (X_i, i \geq 1)$ satisfy that for all X_i we have that $\mathbb{E}(X_i^2) = 1$ and $\mathbb{E}(X_i^4) < \infty$. Fix $d \geqslant 2$, and let $\{N_n, f_n : n \geqslant 1\}$ be such that $N_n \to \infty$ as $n \to \infty$. Suppose that each $f_n \colon \{1, \ldots, N_n\}^d \to \mathbb{R}$ is symmetric and vanishes on diagonals. Assume that $Q_d(n, \mathbf{X}) = Q_d(N_n, f_n, \mathbf{X})$ satisfies $\mathbb{E}[Q_d(n, \mathbf{X})^2] = 1$ for all n.

Let $\mathbf{G} = (G_i, i \geq 1)$ be an i.i.d. centered standard Gaussian sequence. The following theorem from [34] gives a bound between the distance between $Q_d(n, \mathbf{X})$ and a standard normal variable, in terms of the influence function.

Theorem 5.3. *Let $h\colon \mathbb{R} \to \mathbb{R}$ have bounded derivatives up to order 3. Then there exists an explicit constant $C > 0$, such that*

$$|\mathbb{E}\, h(Q_d(n, \mathbf{X})) - \mathbb{E}\, h(Q_d(n, \mathbf{G}))| \leq C\left(\max_{1\leq i\leq N_n} \mathrm{Inf}_i(f_n) + \sqrt{\max_{1\leq i\leq N_n} \mathrm{Inf}_i(f_n)}\right),$$

$$|\mathbb{E}\, h(Q_d(n, \mathbf{G}) - \mathbb{E}\, h(Z)| \leq C\sqrt{|\mathbb{E}[Q_d(n, \mathbf{G})^4] - 3|}$$

and

$$|\mathbb{E}[Q_d(n, \mathbf{X})^4] - \mathbb{E}[Q_d(n, \mathbf{G})^4]| \leq C\left(\max_{1\leq i\leq N_n} \mathrm{Inf}_i(f_n) + \sqrt{\max_{1\leq i\leq N_n} \mathrm{Inf}_i(f_n)}\right).$$

The proof consists of bounding $|\mathbb{E}\, h(Q_d(n, \mathbf{X})) - \mathbb{E}\, h(Q_d(n, \mathbf{G}))|$ by applying Theorem 3.18 in [27], which gives a bound in terms of the influence function, using a generalisation of the Lindeberg invariance principle, and bounding $|\mathbb{E}\, h(Q_d(n, \mathbf{G}) - \mathbb{E}\, h(Z)|$ using Theorem 5.1.

Before we continue to universality, it should be pointed out that the above invariance principle is very related to the following qualitative limit theorem which was proved in [18], in the above setting and under slightly weaker assumptions.

Theorem 5.4. *If, as $n \to \infty$,*

(i) $\mathbb{E}[Q_d(n, \mathbf{X})^4] \to 3$, *and*

(ii) $(d-1)!\max_{1\leq i\leq N_n} \mathrm{Inf}_i(f_n) \to 0$,

then $Q_d(n, \mathbf{X})$ converges in law to a standard Gaussian random variable $Z \sim \mathcal{N}(0, 1)$.

Finally the main theorem from [34] shows the universality of Wiener chaos. By universality we mean the observation that most information about large random systems does not depend on the particular distribution of the components.

Theorem 5.5. *Fix integers $m \geqslant 1$ and $d_1, \ldots, d_m \geqslant 2$. For every $j = 1, \ldots, m$, let $\{(N_n^{(j)}, f_n^{(j)}) : n \geqslant 1\}$ be a sequence such that $\{N_n^{(j)} : n \geqslant 1\}$ is a sequence of integers going to infinity, and each function $f_n^{(j)}\colon \{1, \ldots, N_n^{(j)}\}^{d_j} \to \mathbb{R}$ is symmetric and vanishes on diagonals. Define $Q_{d_j}(N_n^{(j)}, f_n^{(j)}, \mathbf{G})$, $n \geqslant 1$, according to (14) and assume that, for every $j = 1, \ldots m$, the sequence $\mathbb{E}[Q_{d_j}(N_n^{(j)}, f_n^{(j)}, \mathbf{G})^2]$, $n \geqslant 1$, is bounded. Let V be a $m \times m$ non-negative symmetric matrix whose diagonal elements are different from zero, and let $\mathcal{N}_m(0, V)$ indicate a centered Gaussian vector with covariance V. Then, as $n \to \infty$, the following conditions* (1) *and* (2) *are equivalent.*

(1) *The vector $\{Q_{d_j}(N_n^{(j)}, f_n^{(j)}, \mathbf{G}) : j = 1, \ldots, m\}$ converges in law to $\mathcal{N}_m(0, V)$;*

(2) *for every sequence $\mathbf{X} = \{X_i : i \geqslant 1\}$ of independent centered random variables, with unit variance and such that $\sup_i \mathbb{E}|X_i|^3 < \infty$, the law of the vector $\{Q_{d_j}(N_n^{(j)}, f_n^{(j)}, \mathbf{X}) : j = 1, \ldots, m\}$ converges to the law of $\mathcal{N}_m(0, V)$ in the Kolmogorov distance.*

It is obvious that (2) implies (1). To see that the converse holds, fix $z \in \mathbb{R}$. We have

$$\begin{aligned}&\big|\mathbb{P}\big[Q_d(n,\mathbf{X}) \le z\big] - \mathbb{P}\big[Z \le z\big]\big| \\ &\quad \le \big|\mathbb{P}\big[Q_d(n,\mathbf{X}) \le z\big] - \mathbb{P}\big[Q_d(n,\mathbf{G}) \le z\big]\big| + \big|\mathbb{P}\big[Q_d(n,\mathbf{G}) \le z\big] - \mathbb{P}\big[Z \le z\big]\big| \\ &\quad =: \delta_n^{(a)}(z) + \delta_n^{(b)}(z).\end{aligned}$$

To show that $\delta_n^{(a)}(z) \to 0$ use Theorem 2.2 in [27]; to derive that $\delta_n^{(b)}(z) \to 0$ we employ Theorem 5.1.

6 Generalizations

Using similar tools as for normal approximations, chi-square approximations are also available; these are sometimes called *non-central limit theorems*; see for example [31] and [34]. In [31], [33], and [34], bounds on distributional distances are available not only for metrics based on smooth functions and Wasserstein distance, but also for other distances such as Kolmogorov distance, and total variation distance. These papers also contain generalisations to multivariate settings.

Recently these ideas have been applied to Wigner chaos in a free probability setting, yielding convergence criteria to the semicircular law, see [37]. In [29] the universality principle for Gaussian Wiener chaos is applied to prove multi-dimensional central limit theorems, and an almost-sure central limit theorem, for the spectral moments associated with random matrices with real-valued i.i.d. entries.

An application to finding the density of a random variable which is measurable and differentiable with respect to an isonormal Gaussian process is in [38], relating back to the original aims by [25]. In [1], the approach is applied to obtain partial differential equations for densities of multi-dimensional random variables.

We could think of other conceivable generalisations. As Stein's method does not require an ordered index set, the results should be generalizable, for example to statistics based on edges in random graphs. Also it should be straightforward to generalise the universality result for $N = \infty$. Another direction would be to generalise the results to approximations by a Gaussian process, or by a Gaussian random measure. Convergence to a Gaussian random measure via Stein's method has been set up in [48]. In [40] functionals of Gaussian random measures are considered, and [7] show an almost-sure CLT for multiple stochastic integrals. In [4] convergence to a Gaussian process has been studied via Stein's method, but not yet in connection with Malliavin calculus.

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Merging and stability for time inhomogeneous finite Markov chains

Laurent Saloff-Coste* and Jessica Zúñiga**

1 Introduction

As is apparent from most text books, the definition of a Markov process includes, in the most natural way, processes that are time inhomogeneous. Nevertheless, most modern references quickly restrict themselves to the time homogeneous case by assuming the existence of a time homogeneous transition function, a case for which there is a vast literature.

The goal of this paper is to point out some interesting problems concerning the quantitative study of time inhomogeneous Markov processes and, in particular, time inhomogeneous Markov chains on finite state spaces. Indeed, almost nothing is known about the quantitative behavior of time inhomogeneous chains. Even the simplest examples resist analysis. We describe some precise questions and examples, and a few results. They indicate the extent of our lack of understanding, illustrate the difficulties and, perhaps, point to some hope for progress.

We think the problems discussed below have an intrinsic mathematical interest (indeed, some of them appear quite hard to solve) and are very natural. Nevertheless, it is reasonable to ask whether or not time inhomogeneous chains are relevant in some applications. Most of the recent interest in Markov chains is related to Monte Carlo Markov Chain algorithms. In this context, one seeks a Markov chain with a given stationary distribution. Hence, time homogeneity is rather natural. See, e.g., [26]. Still, one of the popular algorithms of this sort, the Gibbs sampler, can be viewed as a time inhomogeneous chain (one that, despite huge amount of attention, is still resisting analysis). Time inhomogeneity also appears in the so-called simulated annealing algorithms. See [12] for a discussion that is close in spirit to the present work and for older references. However, certain special features of each of these two algorithms distinguish them from the more basic time inhomogeneous problems we want to discuss here. Namely, in the Gibbs sampler, each individual step is not ergodic (it involves only one coordinate) whereas, in the simulated annealing context, the time inhomogeneity vanishes asymptotically. Other interesting stochastic algorithms that present time inhomogeneity are discussed in [10].

In many applications of finite Markov chains, the kernel describes transitions between different classes in a population of interest. Assuming that these transition probabilities can be observed empirically, one application is to compute the stationary

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measure which describes the steady state of the system. Examples of this type include models for population migrations between countries, models for credit scores used to study the default risk of certain loan portfolios, etc. In such examples, it is natural to consider cases when the Markov kernel describing the evolution of the system depends on time in either a deterministic or a random manner. The reason for the time inhomogeneity may come, for example, from seasonal factors. Or it may model various external events that are independent of the state of the system. Even if one decides that time homogeneity is warranted, one may wish to study the possible effects of small but non-vanishing time dependent perturbations of the model. It seems rather important to understand whether or not such perturbations can drastically alter the behavior of the underlying model. This type of practical questions fit nicely with the theoretical problems discussed below.

A large class of natural examples of time inhomogeneous chains comes from time inhomogeneous random walks on groups. These are discussed in [2], [28]. A special case is the semi-random transpositions model discussed in [14], [21], [22], [28].

2 Merging and stability

This section introduces the two main properties we want to focus on: merging (in total variation or relative-sup) and stability. Given two Markov kernels K_1, K_2, we set

$$K_1K_2(x,y) = \sum_z K_1(x,z)K_2(z,y).$$

Given a sequence $(K_i)_1^\infty$ and $0 \le m \le n$, we set

$$K_{m,n} = K_{m+1} \dots K_n, \quad K_{m,m} = I.$$

2.1 Merging. Recall that an aperiodic irreducible Markov kernel K on a finite state space admits a unique invariant probability measure π. Further, for any starting measure μ_0 and any large time n, the distribution $\mu_n = \mu_0 K^n$ at time n is both essentially independent from the starting distribution μ_0 and well approximated by π.

Consider now the evolution of a system started according to an initial distribution μ_0 and driven by a sequence $(K_i)_1^\infty$ of Markov kernels so that, at time n, the distribution is $\mu_n = \mu_0 K_1 K_2 \dots K_n$. In [1], [4] such a sequence $(\mu_n)_1^\infty$ of probability measures is called a "set of absolute probabilities" but we will not use this terminology here. In many cases, for very large n, the distribution μ_n will be essentially independent of the initial distribution μ_0. Namely, if μ_0, μ_0' are two initial distributions and $\mu_n = \mu_0 K_1 \dots K_n$, $\mu_n' = \mu_0' K_1 \dots K_n$, then it will often be the case that

$$\lim_{n\to\infty} \|\mu_n - \mu_n'\|_{\mathrm{TV}} = 0.$$

We call this loss of memory property *merging* (total variation merging, to be more precise).

One may also want to know whether or not

$$\lim_{n\to\infty} \sup_x \left\{ \left| \frac{\mu'_n(x)}{\mu_n(x)} - 1 \right| \right\} = 0.$$

We call this later property relative-sup merging. Total variation merging is often discussed under the name of "weak ergodicity". See, e.g., [1], [4], [6], [15], [16], [18], [24]. We think "merging" is more appropriate.

If there is merging, then one may want to ask quantitative questions about the merging time. For any $\epsilon \in (0,1)$, we set

$$T_1(\epsilon) = \inf \{ n : \forall \mu_0, \mu'_0,\ \|\mu_n - \mu'_n\|_{\mathrm{TV}} \le \epsilon \} \tag{2.1}$$

and

$$T_\infty(\epsilon) = \inf \left\{ n : \forall \mu_0, \mu'_0,\ \left\| \frac{\mu'_n}{\mu_n} - 1 \right\|_\infty \le \epsilon \right\}. \tag{2.2}$$

The next definition introduces the collective notions of merging and merging time for a given set $\mathcal{Q}$ of Markov kernels.

Definition 2.1. Let $\mathcal{Q}$ be a set of Markov kernels on a finite state space. We say that $\mathcal{Q}$ is merging in total variation (resp. relative-sup) if any sequence $(K_i)_1^\infty$ of kernels in $\mathcal{Q}$ is merging in total variation (resp. relative-sup). We say that $\mathcal{Q}$ has total-variation (resp. relative-sup) ϵ-merging time at most $T(\epsilon)$ if the total variation (resp. relative-sup) ϵ-merging time (2.1) (resp. (2.2)) is bounded above by $T(\epsilon)$, for any sequence $(K_i)_1^\infty$ of kernels in $\mathcal{Q}$.

Let us emphasize that, from the view point of the present work, it is more natural to think in terms of properties shared by all sequences drawn from a set of kernels than in terms of properties of some particular sequence.

2.2 Stability. In the previous section, the notion of merging was introduced as a natural generalization of the loss of memory property in the time inhomogeneous context. The notion of *stability* introduced below is a generalization of the existence of a positive invariant distribution.

Definition 2.2. Fix $c \ge 1$. Given a Markov chain driven by a sequence of Markov kernels $(K_i)_1^\infty$, we say that a probability measure π is c-stable (for $(K_i)_1^\infty$) if there exists a positive measure μ_0 such that the sequence $\mu^n = \mu_0 K_{0,n}$ satisfies

$$c^{-1}\pi \le \mu_n \le c\pi.$$

When such a measure π exists, we say that $(K_i)_1^\infty$ is c-stable.

Example 2.3. Let K be an irreducible aperiodic kernel. Then the chain driven by K is 1-stable. Indeed, it admits a positive invariant measure π and $\pi K^n = \pi$. Further, for any probability measure μ_0 with $\|(\mu_0/\pi) - 1\|_\infty \le \epsilon$, the sequence $\mu_n = \mu_0 K^n$, $n = 1, 2, \ldots$, satisfies $(1-\epsilon)\pi \le \mu_n \le (1+\epsilon)\pi$. Indeed, in the space of signed measures, the linear map $\mu \mapsto \mu K$ is a contraction for the distance $d(\mu, \nu) = \|(\mu/\pi) - (\nu/\pi)\|_\infty$.

In the next definition, we consider the notion of c-stability for a family $\mathcal{Q}$ of Markov kernels on a fixed state space. This definition is of interest even in the case when $\mathcal{Q} = \{Q_1, Q_2\}$ is a pair.

Definition 2.4. Fix $c \geq 1$. Given a set $\mathcal{Q}$ of Markov kernels on a fixed state space, we say that a probability measure π is a c-stable measure for $\mathcal{Q}$ if there exists a positive measure μ_0 such that for any choice of sequence $(K_i)_1^\infty$ in $\mathcal{Q}$, the sequence $\mu_n = \mu_0 K_{0,n}$ satisfies

$$c^{-1}\pi \leq \mu_n \leq c\pi.$$

When such a measure π exists, we say that $\mathcal{Q}$ is c-stable.

Example 2.5. Assume the state space is a group G and let $\mathcal{Q}$ be the set of all Markov kernels Q such that $Q(zx, zy) = Q(x, y)$ for all $x, y, z \in G$. This set is 1-stable with 1-stable measure u, the uniform measure on G.

Example 2.6. On the two-point space, a finite set $\mathcal{Q}$ of Markov kernels is c-stable if and only if it contains no pairs $\{Q_1, Q_2\}$ with $Q_i = \begin{pmatrix} a_i & 1-a_i \\ 1-b_i & b_i \end{pmatrix}$ such that $Q_1 \neq Q_2$, $a_1 = 0, b_2 = 0$. This condition is clearly necessary. It is not immediately obvious that it is sufficient. See [29].

Remark 2.7. Consider the problem of deciding whether or not a pair $\mathcal{Q} = \{Q_1, Q_2\}$ of two irreducible ergodic Markov kernels with invariant measure π_1, π_2, respectively, is c-stable. This can be pictured by considering a rooted infinite binary tree with edges labeled Q_1 (= left) and Q_2 (= right) as in Figure 1. Obviously, any sequence $(K_i)_1^\infty$ with $K_i \in \mathcal{Q}$ corresponds uniquely to an end $\omega \in \Omega$ where Ω denotes the set of the ends the tree. Given an initial measure μ_0 (placed at the root), the measure $\mu_n^\omega = \mu_0 K_{0,n}$ is obtained by following ω from the root down to level n. Thus, for each choice of μ_0, we obtain a tree with vertices labeled with measures.

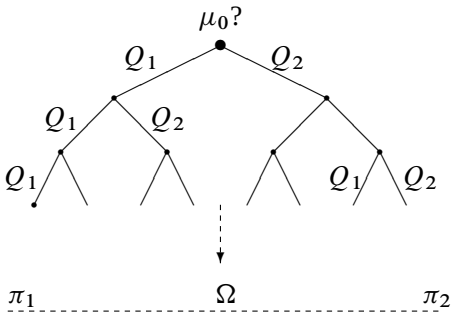

Figure 1. The Q_1, Q_2 tree.

The question of c-stability is the problem of finding an initial measure μ_0 which, in some sense, minimizes the variations among the μ_n^ω's. At the left-most and right-most ends ω_1, ω_2, we get $\mu_n^{\omega_i} \to \pi_i$. Note that, if Q_1, Q_2 share the same invariant measure

$\pi_1 = \pi_2 = \pi$, then the choice $\mu_0 = \pi$ yields a tree all of whose vertices are labeled by π. The existence of a c-stable measure μ_0 can be viewed as a weakening of this. The difficulty is that the existence of an invariant measure and thus the equality between π_1 and π_2 can be viewed as an algebraic property whereas there seems to be no algebraic tools to study c-stability.

2.3 Simple results and examples. We are interested in finding conditions on the individual kernels K_i of a sequence $(K_n)_1^\infty$ that imply merging. This is not obvious even if we consider the very special case when all the K_i's are drawn from a finite set of kernels $\mathcal{Q} = \{Q_0, \ldots, Q_m\}$ or even from a pair $\mathcal{Q} = \{Q_0, Q_1\}$.

- Suppose that Q_0, Q_1 are irreducible and aperiodic. Does it imply any sequence $(K_i)_1^\infty$ drawn from $\mathcal{Q} = \{Q_0, Q_1\}$ is merging?

The answer is no. Let π_0 be the invariant measure of Q_0 and let $Q_1 = Q_0^*$ be the adjoint of Q_0 on $\ell^2(\pi_0)$. If (Q_0, π_0) is not reversible (i.e., Q_0 is not self-adjoint on $\ell^2(\pi_0)$) then it is possible that $Q_0 Q_0^*$ is not irreducible. When $Q_0 Q_0^*$ is not irreducible, the sequence $K_i = Q_{i \bmod 2}$ is not merging.

- Suppose that Q_0, Q_1 are reversible, irreducible and aperiodic. Does it imply any sequence $(K_i)_1^\infty$ drawn from $\mathcal{Q} = \{Q_0, Q_1\}$ is merging in relative-sup?

The answer is no, even on the two point space! On the two point space, $\mathcal{Q} = \{Q_0, Q_1\}$ is merging in total variation as long as Q_0, Q_1 are irreducible aperiodic but relative sup merging fails for the irreducible aperiodic pairs of the type

$$Q_0 = \begin{pmatrix} 0 & 1 \\ 1-a & a \end{pmatrix}, \quad Q_1 = \begin{pmatrix} b & 1-b \\ 1 & 0 \end{pmatrix},$$

with $0 < a, b < 1$. See [29].

The following examples are instructive.

Example 2.8. On $S = \{1, \ldots, 5\}$ consider the reversible kernels Q_0, Q_1 corresponding to the graphs in Figure 2 (all edges have weight 1). Consider the sequence $K_i = Q_{i \bmod 2}$ so that $K_1 = Q_1, K_2 = Q_0, K_3 = Q_1, \ldots$. If, at an even time $n = 2\ell$, the chain is at states 2 or 5 then from that time on, the chain will be in $\{2, 5\}$ at even times and in $\{3, 4\}$ at odd times. In this example, the chain driven by $(K_i)_1^\infty$ is merging in total variation but is not merging in relative-sup.

Example 2.9. The kernels depicted in Figure 3 yield an example where total variation (hence, a fortiori, relative-sup) merging fails. In this example, the sequence $(K_i)_1^\infty$ with $K_i = Q_{i \bmod 2}$ fails to be merging in total variation because the chain will eventually end up oscillating either between 2 and 1, or between $\{4, 7\}$ and $\{5, 6\}$, with a preference for one or the other depending on the starting distribution μ_0.

Let us give two simple results concerning merging.

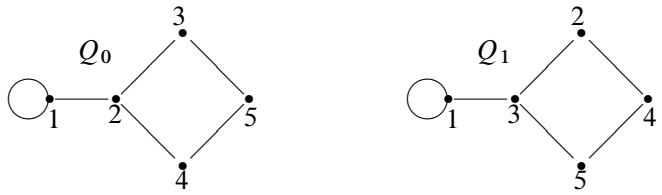

Figure 2. A five-point example.

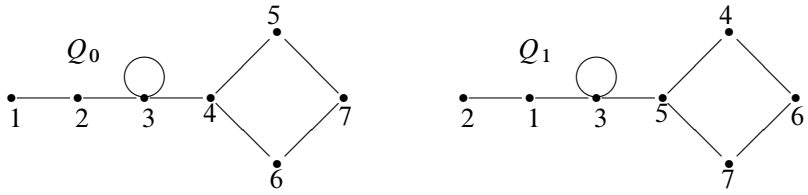

Figure 3. A seven-point example.

Proposition 2.10. *Assume that, for each i, there exists a state y_i and a real $\epsilon_i \in (0,1)$ such that*

$$\forall\, x, \quad K_i(x, y_i) \geq \epsilon_i.$$

If $\sum_i \epsilon_i = \infty$ then the sequence $(K_i)_1^\infty$ is merging in total variation. If, in addition, each K_i is irreducible then the sequence $(K_i)_1^\infty$ is also merging in relative-sup.

Proof. For total variation, this can be proved by a well-known Doeblin's coupling argument (see, e.g., [13], [29]) and irreducibility of the kernels is not needed. Of course, the mass might ultimately concentrate on a fraction of the state space.

Merging in relative-sup is a bit more subtle and irreducibility is needed for that conclusion to hold (even in the time homogeneous case). A proof using singular values can be found in [29]. □

Remark 2.11. Under the much stronger hypothesis $\forall\, x, y, \quad K_i(x, y) \geq \epsilon_i > 0$, one gets an immediate control of any sequence $\mu_n = \mu_0 K_{0,n}$, $n = 1, 2, \ldots$, in the form

$$\forall\, z, \quad \epsilon_n \leq \min_{x,y}\{K_n(x, y)\} \leq \mu_n(z) \leq \sup_{x,y}\{K_n(x, y)\} \leq 1 - (N-1)\epsilon_n$$

where N is the size of the state space.

Remark 2.12. The hypothesis $\exists\, y_i, \forall\, x, \; K_i(x, y_i) \geq \epsilon_i > 0$, is obviously too strong in many cases but it can often be applied to study a time inhomogeneous chain $(K_i)_1^\infty$ by grouping terms and considering the sequence $Q_i = K_{n_i, n_{i+1}}$ for an appropriately chosen increasing sequence n_i. In the simplest case, for a given sequence $(K_i)_1^\infty$, one seeks $\epsilon \in (0,1)$ and an integer m such that $K_{\ell m, \ell m+m}(x, y) \geq \epsilon$ for all x, y, ℓ. When such a lower bound holds, one concludes that (1) the chain is merging in total variation

and relative-sup and (2) there exists $c \in (0,1)$ such that for any starting measure μ_0 and n large enough, the measures $\mu_n = \mu_0 K_{0,n}$ satisfy $c \leq \mu_n(z) \leq 1-c$. However, this type of argument is bound to yield very poor quantitative results in most cases.

For the next result, recall that an adjacency matrix A is a matrix whose entries are either 0 or 1.

Proposition 2.13. *On a finite state space let $(K_i)_1^\infty$ be a sequence of Markov kernels. Assume that:*

(1) (Uniform irreducibility) *There exist ℓ, $\epsilon \in (0,1)$ and adjacency matrices $(A_i)_1^\infty$, such that, $\forall\, i,x,y$, $A_i^\ell(x,y) > 0$ and $K_i(x,y) \geq \epsilon A_i(x,y)$.*

(2) (Uniform laziness) *There exists $\eta \in (0,1)$ such that, $\forall\, i,x$, $K_i(x,x) \geq \eta$.*

Then the chain driven by $(K_i)_1^\infty$ is merging in total variation and relative-sup norm. Moreover, there exist n_0 and $c \in (0,1)$ such that for any starting distribution μ_0, all $n \geq n_0$ and all z, $\mu_n = \mu_0 K_{0,n}$ satisfies $\mu_n(z) \in (c, 1-c)$.

Proof. Let N be the size of the state space. Using (1)–(2), one can show (see [29]) that $K_{n,n+N}(x,y) \geq (\min\{\epsilon,\eta\})^{N-1}$. The desired result follows from Proposition 2.10 and Remark 2.12. □

Note that this argument can only give very poor quantitative results!

3 A short review of the literature

The largest body of literature concerning time inhomogeneous Markov processes come, perhaps, from the analysis of Partial Differential Equations where time dependent coefficients are allowed. The book [36] can serve as a basic reference. Unfortunately, it seems that the results developed in that context are local in nature and are not very relevant to the quantitative problems we are interested in. The literature on (finite) time inhomogeneous Markov chains can be organized under three basic headings: Weak ergodicity, asymptotic structure, and products of stochastic matrices. We now briefly review each of these directions.

3.1 Weak ergodicity. One of the earliest references concerning the asymptotic behavior of time inhomogeneous chains is a note of Emile Borel [2] where he discusses time inhomogeneous card shufflings. In the context of general time inhomogeneous chains on finite state spaces, *weak ergodicity*, which we call *total variation merging*, i.e., the tendency to forget the distant past, was introduced in [19] and is the main subject of [16]. See also [5] and the reference to the work of Doeblin given there. A sample of additional old and not so old references in this direction is [15], [18], [23], [24], [25], [32]. An historical review is given in [33]. The main tools developed in these references to prove weak ergodicity are the use of ergodic coefficients and couplings. A modern perspective, close in spirit to our interests, is in [10], [11], [13]. It may be

worth pointing out that, by design, ergodic coefficients mostly capture some asymptotic properties and are not well suited for quantitative results, even in the time homogeneous case.

3.2 Asymptotic structure. One of the basic results in the theory of time homogeneous finite Markov chains describes the decomposition of the state space into non-essential (or transient) states, essential classes and periodic subclasses. It turns out that, perhaps surprisingly, there exists a completely general version of this result for time inhomogeneous chains. This result is rather more subtle than its time homogeneous counterpart. Sonin [34], Theorem 1, calls it the Decomposition-Separation Theorem and reviews its history which starts with a paper of Kolmogorov [19], with further important contributions by Blackwell [1], Cohn [4] and Sonin [34].

Fix a sequence $(K_n)_1^\infty$ of Markov kernels on a finite state space Ω. The Decomposition-Separation Theorem yields a sequence $(\{S_n^k, k = 0, \dots c\})_{n=1}^\infty$ of partitions of Ω so that:

(a) With probability one, the trajectories of any Markov chain (X_n) driven by $(K_n)_1^\infty$ will, after a finite number of steps, enter one of the sequence $S^k = (S_n^k)_{n=1}^\infty$, $k = 1, \dots, c$, and stay there forever. Further, for each k,

$$\sum_{n=1}^{\infty} \mathbf{P}(X_n \in S_n^k; X_{n+1} \notin S_{n+1}^k) + \mathbf{P}(X_n \notin S_n^k; X_{n+1} \in S_{n+1}^k) < \infty.$$

(b) For each $k = 1, \dots, c$, and for any two Markov chains $(X_n^1)_1^\infty, (X_n^2)_1^\infty$ driven by $(K_n)_1^\infty$ such that $\lim_{n\to\infty} \mathbf{P}(X_n^i \in S_n^k) > 0$, and any sequence of states $x_n \in S_n^k$,

$$\lim_{n\to\infty} \frac{\mathbf{P}(X_n^1 = x_n | X_n^1 \in S_n^k)}{\mathbf{P}(X_n^2 = x_n | X_n^2 \in S_n^k)} = 1.$$

The sequence $(S_n^0)_1^\infty$ describes "non-essential states" and a chain is weakly ergodic (i.e., merging in total variation) if and only if $c = 1$, i.e., there is only one essential class. We refer the reader to [34] for a detailed discussion and connections with other problems.

The Decomposition-Separation Theorem can be illustrated (albeit, in a rather trivial way) using Example 2.9 of Figure 3 above. In this case, $\Omega = \{1, \dots, 7\}$. We consider the sequence of partitions (S_n^k), $k \in \{0, 1, 2\}$, where $S_{2n}^0 = \{1, 3, 5, 6\}$, $S_{2n+1}^0 = \{2, 3, 4, 7\}$, $S_{2n}^1 = \{2\}$, $S_{2n+1}^1 = \{1\}$ and $S_{2n}^2 = \{4, 7\}$, $S_{2n+1}^2 = \{5, 6\}$. Any chain driven by $Q_1, Q_0, Q_1, \dots$ will eventually end up staying either in S_n^1 or in S_n^2 forever.

The Decomposition-Separation Theorem is a very general result which holds without any hypothesis on the kernels K_n. We are instead interested in finding hypotheses, perhaps very restrictive ones, on the individual kernels K_n that translate into strong quantitative results concerning the merging property of the chain.

3.3 Products of stochastic matrices. There is a rather rich literature on the study of products of stochastic matrices. Recall that stochastic matrices are matrices with

non-negative entries and row sums equal to 1. This last assumption, which breaks the row/column symmetry, implies that there is significant differences between forward and backward products of stochastic matrices. Given a sequence K_i of stochastic matrices The forward products form the sequence

$$K^f_{0,n} = K_1 K_2 \dots K_n, \quad n = 1, \dots,$$

whereas the backward products form the sequence

$$K^b_{0,n} = K_n \dots K_2 K_1, \quad n = 1, \dots.$$

There is a crucial difference between these two sequences: The entries $K^f_{0,n}(x, y)$ do not have any general monotonicity properties but, for any y,

$$n \mapsto M(n, y) = \max_x \{K^b_{0,n}(x, y)\}$$

is monotone non-increasing and

$$n \mapsto m(n, y) = \min_x \{K^b_{0,n}(x, y)\}$$

is monotone non-decreasing. These properties are obvious consequences of the fact that the matrices K_i are stochastic matrices. Of course, both $\lim_{n\to\infty} M(n, y)$ and $\lim_{n\to\infty} m(n, y)$ exist for all y.

If, for some reason, we know that

$$\forall\, x, x', \quad \lim_{n\to\infty} \sum_y |K^b_{0,n}(x, y) - K^b_{0,n}(x', y)| = 0$$

then it follows that the backward products converge to a row-constant matrix Π, i.e.,

$$\forall\, x, x', y, \quad \Pi(x, y) = \lim_{n\to\infty} K^b_{0,n}(x, y), \quad \Pi(x, y) = \Pi(x', y).$$

The references [16], [19], [23], [25], [35], [38] form a sample of old and recent works dealing with this observation.

Changing viewpoint and notation somewhat, consider all finite products of matrices drawn from a set $\mathcal{Q}$ of $N \times N$ stochastic matrices. For $\omega = (\dots, K_{i-1}, K_i, K_{i+1}, \dots) \in \mathcal{Q}^{\mathbb{Z}}$ a doubly infinite sequence of matrices and $m \le n \in \mathbb{Z}$, set

$$K^\omega_{m,n} = K_{m+1} \dots K_n \quad (K_{m,m} = I).$$

A stochastic matrix is called (SIA) if its products converge to a constant row matrix. Here, (SIA) stands for stochastic, irreducible and aperiodic although "irreducible" really means that the matrix has a unique recurrent class (transient states are allowed so that the constant row limit matrix may have some 0 columns). A central result in this area (e.g., [35], [38]) is that, if $\mathcal{Q}$ is finite and all finite products of matrices in $\mathcal{Q}$ are (SIA) then, for any doubly infinite sequence $\omega \in \mathcal{Q}^{\mathbb{Z}}$,

$$\lim_{n-m\to\infty} \sum_y |K^\omega_{m,n}(x, y) - K^\omega_{m,n}(x', y)| = 0 \tag{3.1}$$

and

$$\lim_{m\to-\infty} K^{\omega}_{m,n} = \Pi^{\omega}_{n} \tag{3.2}$$

where Π^{ω}_{n} is a row-constant matrix. Let π^{ω}_{n} be the probability measure corresponding to the rows of row-constant matrix Π^{ω}_{n}. Observe that (3.1) and (3.2) imply

$$\lim_{n\to\infty} \sum_{y} |K^{\omega}_{0,n}(x,y) - \pi^{\omega}_{n}(y)| = 0.$$

The following proposition establishes some relations between these considerations, total variation merging and stability.

Proposition 3.1. *Let $\mathcal{Q}$ be a set of $N \times N$ stochastic matrices. Assume that $\mathcal{Q}$ is merging (in total variation) and c-stable w.r.t. a positive measure π. Then*

(1) *Any finite product P of matrices in $\mathcal{Q}$ is irreducible aperiodic and its unique positive invariant measure π_P satisfies $c^{-1}\pi \le \pi_P \le c\pi$.*

(2) *For any $\omega \in \mathcal{Q}^{\mathbb{Z}}$ and any $n \in \mathbb{Z}$, π^{ω}_{n} satisfies $c^{-1}\pi \le \pi^{\omega}_{n} \le c\pi$, i.e., any limit row π' of backward products of matrices in $\mathcal{Q}$ satisfies $c^{-1}\pi \le \pi' \le c\pi$.*

Proof. (1) As $\mathcal{Q}$ is c-stable w.r.t. π, there exists a positive measure μ_0 such that for any finite product P of matrices in $\mathcal{Q}$ and any n, $c^{-1}\pi \le \mu_0 P^n \le c\pi$. Since $\mathcal{Q}$ is merging, we must have $\lim_{n\to\infty} P^n = \Pi_P$ with Π_P having constant rows, call them π_P. This implies $c^{-1}\pi \le \pi_P \le c\pi$. Since π is positive, π_P must be positive and $\lim_{n\to\infty} P^n = \Pi_P$ implies that P is irreducible aperiodic. We note that (1) is, in fact, a sufficient condition for stability. See [29], Proposition 4.9. Under the hypothesis that $\mathcal{Q}$ is merging, (1) is thus a necessary and sufficient condition for c-stability.

(2) Fix $\omega \in \mathcal{Q}^{\mathbb{Z}}$. By hypothesis, on the one hand, there exists a positive probability measure μ_0 such that $c^{-1}\pi \le \mu_0 K^{\omega}_{m,n} \le c\pi$. On the other hand, merging imply that $\lim_{m\to-\infty} K^{\omega}_{m,n} = \Pi^{\omega}_{n}$ and thus, $\lim_{m\to-\infty} \mu_0 K^{\omega}_{m,n} = \pi^{\omega}_{n}$. The desired result follows. □

3.4 Product of random stochastic matrices. For pointers to the literature on products of random stochastic matrices and Markov chains in a random environment, see, e.g., [3], [6], [27], [37] and the references therein. We end this section with short comments regarding the simplest case of products of random stochastic matrices, i.e., the case where the matrices K_i form an i.i.d sequence of stochastic matrices. The backward and forward products $K^{b}_{0,n} = K_n \dots K_1$, $K^{f}_{0,n} = K_1 \dots K_n$ become random variables taking values in the set of all $N \times N$ stochastic matrices. Although these two sequences of random variables have very different behavior as n varies, $K^{b}_{0,n}$ and $K^{f}_{0,n}$ have the same law. Takahashi [37] proves that if

$$\forall\, x, x', \quad \lim_{n\to\infty} \sum_{y} |K^{f}_{0,n}(x,y) - K^{f}_{0,n}(x',y)| = 0 \quad \text{almost surely}$$

then $K_{0,n}^f$ converges in law and the limit law is that of the limit random variable $\lim_{n\to\infty} K_{0,n}^b$. Rosenblatt [27] applies the theory of random walks on semigroups to show that the Cesaro sums $n^{-1}\sum_1^n K_{0,j}^f(x,y)$ always converge to a constant almost surely. The articles [3], [6] discuss similar results under more general hypotheses on the nature of the random sequence $(K_i)_1^\infty$. Unfortunately, these interesting results concerning random environments do not shed much light on the quantitative questions emphasized here.

4 Quantitative results and examples

Informally, the question we want to focus on is the following. Let (K,π) be an irreducible aperiodic Markov kernel and its stationary probability measure. Let $(K_i)_1^\infty$ be a sequence of Markov kernels so that, for each i, K_i is a perturbation of K with invariant measure π_i that is a perturbation of π (what "perturbation" means here is left open on purpose). For an initial distribution μ_0, consider the associated sequence of measures defined by $\mu_n = \mu_0 K_1 \dots K_n$, $n = 1, 2, \dots$.

Problem 4.1. (1) Does total variation merging hold?

(2) Does relative-sup merging hold?

(3) Does there exists $c \geq 1$ such that, for n large enough,

$$\forall\, x, \quad c^{-1} \leq \frac{\mu_n(x)}{\pi(x)} \leq c?$$

Obviously, these questions call for quantitative results describing the merging times, the constant c and the "large" time n in terms of bounds on the allowed perturbations.

To understand what is meant by quantitative results, it is easier to consider a family of problems depending on a parameter representing the size and complexity of the problem. So, one starts with a family (Ω_N, K_N, π_N) of ergodic Markov kernels depending on the parameter N whose mixing time sequence $(T_1(N,\epsilon))_1^\infty$ (say, in total variation) is understood. Then, for each N, we consider perturbations $(K_{N,i})_{i=1}^\infty$ of K_N with stationary measure $\pi_{N,i}$ close to π_N and ask if the merging time of $(K_{N,i})_{i=1}^\infty$ can be controlled in terms of $T_1(N,\epsilon)$.

Problem 4.2. Let $\Omega_N = \{0,\dots,N\}$. Let $\mathcal{Q}_N$ be the set of all birth and death chains Q on V_N with $Q(x,x+\epsilon) \in [1/4, 3/4]$ for all $x, x+\epsilon \in V_N$, $\epsilon \in \{-1,0,1\}$ and with reversible measure π satisfying $1/4 \leq (N+1)\pi(x) \leq 4$, $x \in V_N$.

(1) Prove or disprove that there exists a constant A independent of N such that $\mathcal{Q}_N$ has total variation ϵ-merging time at most $AN^2(1+\log_+ 1/\epsilon)$.

(2) Prove or disprove that there exists a constant A independent of N such that $\mathcal{Q}_N$ has relative-sup ϵ-merging time at most $AN^2(1+\log_+ 1/\epsilon)$.

(3) Prove or disprove that there exist constants $A, C \geq 1$, such that, for any N and any sequence $(K_i)_1^\infty \in \mathcal{Q}_N$, we have

$$\forall\, x, y \in \Omega_N,\ \forall\, n \geq AN^2,\ \ \frac{1}{C(N+1)} \leq K_{0,n}(x,y) \leq \frac{C}{N+1}.$$

Here the time homogeneous model is the birth and death chain K_N with constant rates $p = q = r = 1/3$ and $\pi_N = 1/(N+1)$, so that $K_N(x,y) = 0$ unless $|x-y| \leq 1$, $K(0,0) = K(N,N) = 2/3$ and $K(x,x) = K(x,x\pm 1) = 1/3$ otherwise. Of course, it is well known that $T_1(K_N,\epsilon) \simeq T_\infty(K_N,\epsilon) \simeq N^2(1+\log_+(1/\epsilon))$ for small $\epsilon > 0$. Problem 1.2 asks whether or not these mixing/merging times are stable under suitable time inhomogeneous perturbations of K_N and whether or not the limiting behavior stays comparable to that of the model chain. To the best of our knowledge the answer is not known and this innocent looking problem should be taken seriously.

There appears to be only a small number of papers that attempt to prove quantitative results for time inhomogeneous chains. These include [11], [13], [14], [21], [22] and the authors' works [28], [29], [30], [31]. The works [14], [21], [22], [28] treat only examples of time inhomogeneous chains that admit an invariant measure. Technically, this is a very specific hypothesis and, indeed, these works show that many of the well developed techniques that have been used to study time homogeneous chains can be successfully applied under this hypothesis.

4.1 Singular values. A typical qualitative result about finite Markov chains is that an irreducible aperiodic chain is ergodic. We do not know of any quantitative versions of this statement. Let K be an irreducible aperiodic Markov kernel with stationary measure π so that $\mu_n = \mu_0 K^n \to \pi$ as n tends to infinity, for any starting distribution μ_0.

If (K,π) is reversible (i.e., $\pi(x)K(x,y) = \pi(y)K(y,x)$) and if β denotes the second largest absolute value of the eigenvalues of K acting on $\ell^2(\pi)$ then $\beta < 1$ and

$$2\|\mu_n - \pi\|_{\mathrm{TV}} \leq \|\mu_0/\pi\|_2 \beta^n \tag{4.1}$$

where $\|\mu_0/\pi\|_2$ is the norm of $f_0 = \mu_0/\pi$ in $\ell^2(\pi)$. This can be considered as a quantitative result although it involves the perhaps unknown reversible measure π.

If (K,π) is not reversible, the inequality still holds with β being the second largest singular value of K on $\ell^2(\pi)$ (i.e., the square root of the second largest eigenvalue of KK^* where K^* is the adjoint of K on $\ell^2(\pi)$). However, it is then possible that $\beta = 1$, in which case the inequality fails to capture the qualitative ergodicity of the chain.

Inequality (4.1) has an elegant generalization to the time inhomogeneous setting. Let $(K_i)_1^\infty$ be a sequence of irreducible Markov kernels (on a finite state space). Fix a positive probability measure μ_0 (by positive we mean here that $\mu_0(x) > 0$ for all x) and set

$$\mu_n = \mu_0 K_{0,n}.$$

In the time inhomogeneous setting, we want to compare this sequence of measures $(\mu_n)_1^\infty$ to the sequence of measures $(K_{0,n}(x,\cdot))_1^\infty$ describing the distribution at time n of the chain started at an arbitrary point x.

To state the result, for each i, consider K_i as a linear operator acting from $\ell^2(\mu_i)$ to $\ell^2(\mu_{i-1})$. One easily checks that this operator is a contraction. Its singular values are the square roots of the eigenvalues of the operator $P_i = K_i^* K_i : \ell^2(\mu_i) \to \ell^2(\mu_i)$ where $K_i^* : \ell^2(\mu_{i-1}) \to \ell^2(\mu_i)$ is the adjoint operator which is a Markov operator with kernel

$$K_i^*(x, y) = \frac{K_i(y, x)\mu_{i-1}(y)}{\mu_i(x)}.$$

We let

$$\sigma_i = \sigma(K_i, \mu_i, \mu_{i-1})$$

be the second largest singular value of $K_i : \ell^2(\mu_i) \to \ell^2(\mu_{i-1})$. It is the square root of the second largest eigenvalue of the Markov kernel

$$P_i(x, y) = \frac{1}{\mu_i(x)} \sum_z K_i(z, x) K_i(z, y) \mu_{i-1}(z). \tag{4.2}$$

Theorem 4.3. *With the notation introduced above, we have*

$$\|K_{0,n}(x, \cdot) - \mu_n\|_{\mathrm{TV}} \le \mu_0(x)^{-1/2} \prod_1^n \sigma_i$$

and

$$\left| \frac{K_{0,n}(x, y)}{\mu_n(y)} - 1 \right| \le [\mu_0(x)\mu_n(y)]^{-1/2} \prod_1^n \sigma_i$$

For the proof, see [11], [29]. The proofs given in [11] and [29] are rather different in spirit, with [11] avoiding the explicit use of singular values. Introducing singular values allows for further refinements and is useful for practical estimates. See [28], [29]. When coupled with the hypothesis of c-stability, the above result becomes a powerful and very applicable tool. See, e.g., [29], Theorem 4.11, and the examples treated in [29], [30]. Unfortunately, proving c-stability is not an easy task.

A good example of application of Theorem 4.3 is the following result taken from [29]. We refer the reader to [29] for the proof.

Theorem 4.4. *Fix $1 < a < A < \infty$. Let $\mathcal{Q}_N(a, A)$ be the set of all constant rate birth an death chains on $\{0, \dots, N\}$ with parameters p, q, r satisfying $p/q \in [a, A]$. The set $\mathcal{Q}_N(a, A)$ is merging in relative-sup with relative-sup ϵ-merging time bounded above by*

$$T_\infty(\epsilon) \le C(a, A)(N + \log_+ 1/\epsilon).$$

In contrast, note that the set $\mathcal{Q} = \{Q_1, Q_2\}$ where Q_i is the p_i, q_i constant rate birth and death chain on $\{0, \dots, N\}$ and $p_1 = q_2$, $q_1 = p_2$ cannot be merging faster than N^2 because the product $K = Q_1 Q_2$ is, essentially, a simple random walk on a circle with almost uniform invariant measure. See [29], Example 2.17.

It may be illuminating to point out that Theorem 4.3 is of some interest even in the time homogeneous case. Suppose K is irreducible aperiodic kernel with stationary measure π and second largest singular value σ on $\ell^2(\pi)$. Then we have

$$\left|\frac{K^n(x,y)}{\pi(y)} - 1\right| \le [\pi(x)\pi(y)]^{-1/2}\sigma^n. \tag{4.3}$$

One difficulty attached to this estimate is that both $[\pi(x)\pi(y)]^{-1/2}$ and σ depends on the perhaps unknown stationary measure π.

Consider instead an initial measure $\mu_0 > 0$ and set $\mu_n = \mu_0 K^n$. Then we also have

$$\left|\frac{K^n(x,y)}{\mu_n(y)} - 1\right| \le [\mu_0(x)\mu_n(y)]^{-1/2} \prod_1^n \sigma_i \tag{4.4}$$

where σ_i is the second largest singular value of $K\colon \ell^2(\mu_i) \to \ell^2(\mu_{i-1})$. In particular, setting $\mu_0^* = \min_x\{\mu_0(x)\}$,

$$\left|\frac{\pi(y)}{\mu_n(y)} - 1\right| \le [\mu_0^*\mu_n(y)]^{-1/2} \prod_1^n \sigma_i. \tag{4.5}$$

The estimates (4.4)–(4.5) have the disadvantage that each σ_i depends on μ_0 through μ_{i-1} and μ_i. They have the advantage that they do not depend in any direct way of π. From a computational viewpoint, they offer a dynamical estimate of the error in the approximation of π by μ_n.

4.2 An example where stability fails. In this section, we present a simple example that indicates why stability is a difficult property to study from a quantitative viewpoint. Let $\Omega_N = \{0, 1, \dots, N\}$, $N = 2n + 1$. Fix $p, q, r \ge 0$ with $p + q + r = 1$, $p \ne q$, and $\eta_1 \in [0, 1)$. Consider the Markov kernels Q_1 given by

$$\begin{aligned}
Q_1(2x, 2x+1) &= p, \quad x = 0, \dots, n,\\
Q_1(2x, 2x-1) &= q, \quad x = 1, \dots, n,\\
Q_1(2x-1, 2x) &= q, \quad x = 1, \dots, n,\\
Q_1(2x+1, 2x) &= p, \quad x = 0, \dots, n-1,\\
Q_1(x, x) &= r, \quad x = 1, \dots, 2n,
\end{aligned}$$

and

$$Q_1(0,0) = q + r, \quad Q_1(N,N) = \eta_1, \quad Q_1(N, N-1) = 1 - \eta_1.$$

This chain has reversible measure π_1 given by

$$\pi_1(0) = \cdots = \pi_1(N-1) = (1-\eta_1)p^{-1}\pi_1(N) = \frac{(1-\eta_1)p^{-1}}{N(1-\eta_1)p^{-1} + 1}.$$

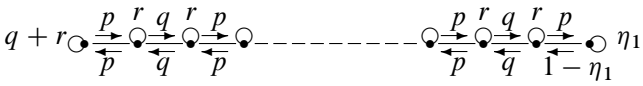

Figure 4. The chain with kernel Q_1.

Next, we let Q_2 be the kernel obtained by exchanging the roles of p and q and replacing η_1 by $\eta_2 \in [0,1)$. Obviously, this kernel has reversible measure π_2 given by

$$\pi_2(0) = \cdots = \pi_2(N-1) = (1-\eta_2)q^{-1}\pi_2(N) = \frac{(1-\eta_2)q^{-1}}{N(1-\eta_2)q^{-1}+1}.$$

As long as p, q are bounded away from 0 and 1 and η_1, η_2 are bounded away from 1 these kernels Q_1, Q_2 can be viewed as perturbations of the simple random walk on a stick (with loops at the ends). Their respective invariant measures are close to uniform. In fact, they are uniform if $\eta_1 = q + r$, $\eta_2 = p + r$.

It is clear that, even if $r\eta_1\eta_2 = 0$, for any sequence $(K_i)_1^\infty$ with $K_i \in \{Q_1, Q_2\}$ we have

$$\min_{x,y\in\Omega_N} \{K_{m,m+2N+1}(x,y)\} \geq (\min\{p,q\})^{2N+1} > 0.$$

Hence, if we let $\mu_0 = u$ be the uniform measure and set $\mu_n = \mu_0 K_{0,n}$ then there exists a constant $c = c(p,q,N) \in (1,\infty)$ such that

$$\forall\, n, \quad c^{-1} \leq \mu_n(x) \leq c.$$

Further, it follows that any such sequence $(K_i)_1^\infty$ is merging in total variation and in relative-sup.

Nevertheless, we are going to show that the stability property fails at the quantitative level as N tends to infinity. For this purpose, we compute the kernel of $K = Q_1Q_2$. To understand K, it is useful to imagine that the elements of $\{0,\ldots,N\}$ arranged on a circle with the even points in the upper half of the circle and the odd points on the lower half of the circle. The only points on the horizontal diameter of the circle are 0 and N.

The kernel K is given by the formulae:

$$\begin{aligned}
K(2x,2x+2) = p^2,\ K(2x+2,2x) = q^2, &\qquad x = 0,\ldots n-2,\\
K(2x+1,2x+3) = q^2,\ K(2x+3,2x+1) = p^2, &\qquad x = 0,\ldots,n-2,\\
K(0,0) = 2pq + r,\ \ K(x,x) = 2pq + r^2, &\qquad x = 1,\ldots,N-2,\\
K(x,x+1) = K(x+1,x) = r(p+q) &\qquad x = 1,\ldots,N-2,\\
K(0,1) = q^2 + r(1-r),\ K(1,0) = p^2 + r(1-r),&\\
K(N-1,N) = p\eta_2 + rq,&\\
K(N,N-1) = (1-\eta_2)\eta_1 + (1-\eta_1)r,&\\
K(N-2,N) = q^2,\ K(N,N-2) = (1-\eta_1)p,&
\end{aligned}$$

$$K(N-1,N-1) = p(q+1-\eta_2) + r^2,$$
$$K(N,N) = \eta_1\eta_2 + (1-\eta_1)q.$$

The following special cases are of interest.

(i) $r = 0, \eta_1 = q, \eta_2 = p$. In this case $\pi_1 = \pi_2$ is uniform and K is the kernel of a nearest-neighbors random walk on the circle with transition probabilities p^2, q^2 and holding $2pq$. Of course, this chain admits the uniform measure as invariant measure.

(ii) $r = 0, \eta_1 = \eta_2 = 0$. In this case, K is essentially the kernel of a $p' = p^2, q' = q^2, r' = 2pq$ birth and death chain. More precisely, after writing $x_0 = N, x_1 = N-2, \ldots, x_{n-1} = 1, x_n = 0, x_{n+1} = 2, \ldots, x_{N-1} = N-3, x_N = N-1$, we have

$$K(x_i, x_{i+1}) = p^2, \quad K(x_i, x_{i-1}) = q^2, \quad K(x_i, x_i) = 2pq$$

except for $K(x_0, x_1) = p$, $K(x_0, x_0) = q$, $K(x_N, x_N) = p + pq$. This chain has invariant measure

$$\pi(x_i) = \pi(x_0)p^{-1}(p/q)^{2i}, \quad i = 1, \ldots, N.$$

Using the same notation as in (ii) above, we can compute the invariant measure π of K when $r = 0$ for arbitrary values of η_1, η_2. Indeed, π must satisfy the following equations:

$$\begin{aligned}
\pi(x_i) &= 2pq\pi(x_i) + p^2\pi(x_{i-1}) + q^2\pi_i(x_{i+1}), \quad i = 2, \ldots, N-1,\\
\pi(x_1) &= 2pq\pi(x_1) + (1-\eta_1)p\pi(x_0) + q^2\pi(x_2),\\
\pi(x_0) &= (\eta_1\eta_2 + (1-\eta_1)q)\pi(x_0) + q^2\pi(x_1) + p\eta_2\pi(x_N),\\
\pi(x_N) &= p(q+1-\eta_2)\pi(x_N) + (1-\eta_2)\eta_1\pi(x_0) + p^2\pi(x_{N-1}).
\end{aligned}$$

Because of the first equation, we set $\pi(x_i) = \alpha + \beta(p/q)^{2i}$ for $i = 1, \ldots, N$. This gives

$$\begin{aligned}
(1-\eta_1)p\pi(x_0) &= (\beta+\alpha)p^2,\\
(p - \eta_1(\eta_2 - q))\pi(x_0) &= q^2(\alpha + \beta(p/q)^2) + p\eta_2(\alpha + \beta(p/q)^{2N}),\\
(1-\eta_2)\eta_1\pi(x_0) &= \alpha(q^2 + p(\eta_2 - p)) + p\eta_2\beta(p/q)^{2N}.
\end{aligned}$$

Since the equations of the system $\pi = \pi K$ are not independent, the three equations above are not either. Indeed, subtracting the last equation from the second yields the first. So the previous system is equivalent to

$$\begin{aligned}
(1-\eta_1)p^{-1}\pi(x_0) &= \beta + \alpha,\\
(1-\eta_2)\eta_1\pi(x_0) &= \alpha(q^2 + p(\eta_2 - p)) + p\eta_2\beta(p/q)^{2N}.
\end{aligned}$$

Hence, recalling that $q^2 - p^2 = q - p$ since $p + q = 1$,

$$\beta = \frac{(1-\eta_1)(q/p) - (1-\eta_2)}{q - p + p\eta_2(1-(p/q)^{2N})}\pi(x_0)$$

and

$$\alpha = \frac{(1-\eta_2)\eta_1 - (1-\eta_1)\eta_2(p/q)^{2N}}{q - p + p\eta_2(1-(p/q)^{2N})}\pi(x_0).$$

When $\eta_1 = \eta_2 = 0$ (resp. $\eta_1 = q, \eta_2 = p$), we recover $\alpha = 0$, $\beta = p^{-1}\pi(x_0)$ (resp. $\alpha = \pi(x_0)$, $\beta = 0$).

The denominator $q - p + p\eta_2(1-(p/q)^{2N})$ is positive or negative depending on whether $q > p$ or $q < p$. By inspection of these formulae, one easily proves the following facts (the notation x_i refers to the relabelling of the state space introduced in (ii) above).

- Assume that $q > p$, $r = 0$. For any fixed $\eta_1 > 0$, there is a constant $c = c(p, q, \eta_1, \eta_2) \in (1, \infty)$ such that, for all large enough N, we have

  $$\forall\, x, \quad c^{-1} \le (N+1)\pi(x) \le c.$$

  If $\eta_1 = 0$ then there is a constant $c = c(p, q, \eta_2) \in (1, \infty)$ such that, for all large enough N, we have

  $$\forall\, x_i, \quad c^{-1} \le (q/p)^{2i}\pi(x_i) \le c.$$

- Assume that $q < p$, $r = 0$. For any fixed $\eta_2 > 0$, there is a constant $c = c(p, q, \eta_1, \eta_2) \in (1, \infty)$ such that, for all large enough N, we have

  $$\forall\, x, \quad c^{-1} \le (N+1)\pi(x) \le c.$$

  If $\eta_2 = 0$ then there is a constant $c = c(p, q, \eta_1) \in (1, \infty)$ such that, for all large enough N, we have

  $$\forall\, x_i, \quad c^{-1} \le (q/p)^{2(i-N)}\pi(x_i) \le c.$$

On the one hand, when $r = \eta_1 = \eta_2 = 0$ and $0 < p \ne q < 1$ are fixed, there are no constants c independent of N for which the set $\mathcal{Q} = \{Q_1, Q_2\}$ is c-stable. One can even take p_N, q_N so that $p_N/q_N = 1 + aN^{-\alpha} + o(N^{-1})$ as N tends to infinity with $a > 0$ and $0 < \alpha < 1$. Then Q_1 and Q_2 are asymptotically equal but there are no constants c independent of N for which $\mathcal{Q} = \{Q_1, Q_2\}$ is c-stable.

On the other hand, when $0 < p, q, r < 1$, $\eta_1 = q + r$ and $\eta_2 = p + r$, the uniform measure is invariant for both kernels and $\mathcal{Q}$ is 1-stable.

It seems likely that for fixed η_1, η_2, r, p, q with $0 < p, q < 1$ and either $r > 0$ or $\eta_1\eta_2 > 0$ the set $\mathcal{Q}$ is c-stable but we do not know how to prove that.

5 Time dependent edge weights

In this section, we consider a family of graphs $\mathcal{G}_N = (\Omega_N, E_N)$. These graphs are non-oriented with no multiple edges (edges are pairs of vertices $e = \{x, y\}$ or singletons $e = \{x\}$). We assume connectedness. We let $d(x)$ be the degree of x, i.e., $d(x) = \#\{e \in E : e \ni x\}$ and set

$$\delta(x) = \frac{d(x)}{\sum_x d(x)}.$$

For simplicity, we assume that these graphs have bounded degree, i.e.,

$$\forall\, N, \quad \forall\, x \in \Omega_N, \quad d(x) \le D,$$

uniformly in N. A simple example is the lazy stick of length $(N+1)$ as in Problem 4.2 and Figure 5.

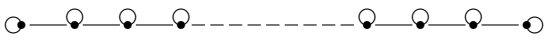

Figure 5. The lazy stick.

5.1 Adapted kernels. For any choice of positive weights $\mathbf{w} = (w_e)_{e\in E}$ on $\mathcal{G}_n$, we obtain a reversible Markov kernel $K(\mathbf{w})$ with support on pairs (x, y) such that $\{x, y\} \in E$, in which case

$$K(\mathbf{w})(x, y) = \frac{w_{\{x,y\}}}{\sum_{e\ni x} w_e}.$$

The reversible measure is

$$\pi(\mathbf{w})(x) = c(\mathbf{w})^{-1} \sum_{e\ni x} w_e, \quad c(\mathbf{w}) = \sum_x \sum_{e\ni x} w_e.$$

For instance, picking $\mathbf{w} = \mathbf{1}$, i.e., $w_e = 1$ for all $e \in E$, we obtain the kernel $K_{\text{sr}}(x, y) = K(\mathbf{1})(x, y) = 1_E(\{x, y\})/d(x)$ of the simple random walk on the given graph. The reversible measure for K_{sr} is $\pi(\mathbf{1}) = \delta$.

Set

$$R(\mathbf{w}) = \max\left\{w_e/w_{e'} : e, e' \in E\right\}.$$

Observe that $R(\mathbf{w}) \le b$ implies

$$\forall\, x, \quad b^{-1}\delta(x) \le \pi(\mathbf{w})(x) \le b\delta(x). \tag{5.1}$$

For instance, to prove the upper bound, let $w_0 = \min\{w_e\}$ and write

$$\pi(\mathbf{w})(x) = c(\mathbf{w})^{-1} \sum_{e\ni x} w_e \le \frac{1}{\sum_x d(x)} \sum_{e\ni x} \frac{w_e}{w_0} \le b\delta(x).$$

The proof of the lower bound is similar. Further, we also have

$$\forall\, x, y, \quad (Db)^{-1}\pi(\mathbf{w})(y) \le \pi(\mathbf{w})(x) \le Db\pi(\mathbf{w})(y). \tag{5.2}$$

Indeed, $\sum_{e\ni x} w_e \le Dbw_0 \le Db\sum_{e\ni y} w_e$.

For any N and $b > 1$, set

$$\mathcal{Q}(\mathcal{G}_N, b) = \{K(\mathbf{w}) : R(\mathbf{w}) \le b\}.$$

For any N, $b > 1$ and fixed probability measure π on Ω_N, set

$$\mathcal{Q}(\mathcal{G}_N, b, \pi) = \{K(\mathbf{w}) : R(\mathbf{w}) \le b,\ \pi(\mathbf{w}) = \pi\}.$$

The set of weight $\mathcal{Q}(\mathcal{G}_N, b, \pi)$ may well be empty. However, we can use the Metropolis algorithm construction to prove the following lemma.

Lemma 5.1. *Assume that $\{x\} \in E$ for all x (i.e, the graphs $\mathcal{G}_N$ have a loop at each vertex) and that $a^{-1} \le \pi(x)/\delta(x) \le a$. Then the set $\mathcal{Q}(\mathcal{G}_N, a^2(b^3 + bD), \pi)$ is non-empty for any $b \ge 1$. It contains a continuum of kernels $K(\mathbf{w})$ for any $b > 1$.*

Proof. Starting from any weight $\mathbf{v}$ with $R(\mathbf{v}) \le b$, we define a new weight $\mathbf{w}$ by setting

$$\forall\, \{x, y\} \in E, x \ne y, \quad w_{\{x,y\}} = v_{\{x,y\}} \min\left\{\frac{\pi(x)}{\pi(\mathbf{v})(x)}, \frac{\pi(y)}{\pi(\mathbf{v})(y)}\right\}$$

and

$$w_{\{x\}} = c(\mathbf{v})\pi(x) - \sum_{y\ne x} v_{\{x,y\}} \min\left\{\frac{\pi(x)}{\pi(\mathbf{v})(x)}, \frac{\pi(y)}{\pi(\mathbf{v})(y)}\right\}.$$

It is clear that $\pi(\mathbf{w}) = \pi$ (Indeed, $K(\mathbf{w})$ is the kernel of the Metropolis algorithm chain for π with proposal based on $K(\mathbf{v})$). Further, since

$$\sum_{y\ne x} v_{\{x,y\}} \min\left\{\frac{\pi(x)}{\pi(\mathbf{v})(x)}, \frac{\pi(y)}{\pi(\mathbf{v})(y)}\right\} \le \pi(x)\left(c(\mathbf{v}) - \frac{v_{\{x\}}}{\pi(\mathbf{v})(x)}\right),$$

we have

$$\frac{\pi(x)v_{\{x\}}}{\pi(\mathbf{v})(x)} \le w_{\{x\}} \le c(\mathbf{v})\pi(x).$$

Now, since $a^{-1}\delta(x) \le \pi(x) \le a\delta(x)$ and $\mathbf{v} \in \mathcal{Q}(\mathcal{G}_N, b)$, we obtain

$$\forall\, x \ne y, x' \ne y', \quad \frac{w_{\{x,y\}}}{w_{\{x',y'\}}} \le b^3a^2.$$

and

$$\forall\, \{x, y\} \in E, x', \quad \max\left\{\frac{w_{\{x,y\}}}{w_{\{x'\}}}, \frac{w_{\{x'\}}}{w_{\{x,y\}}}\right\} \le a^2bD.$$

Hence $R(\mathbf{w}) \le a^2(b^3 + bD)$ and $K(\mathbf{w}) \in \mathcal{Q}(\mathcal{G}_N, a^2(b^3 + bD), \pi)$ as desired. □

5.2 Time homogeneous results. For each N, let σ_N be the second singular value of $(K_{\mathrm{sr}}, \delta)$, i.e., the second largest eigenvalue in absolute value of the simple random walk on $\mathcal{G}_N$. For instance, for the "lazy stick" of Figure 5, $1-\sigma_N$ is of order $1/N^2$. For any $\mathbf{w}$, let $\sigma(\mathbf{w})$ be the second largest singular value of $(K(\mathbf{w}), \pi(\mathbf{w}))$. The following lemma concerns the time homogeneous chains associated with kernels in $\mathcal{Q}(\mathcal{G}_N, b)$.

Proposition 5.2. *For any $b \geq 1$ and any $K(\mathbf{w}) \in \mathcal{Q}(\mathcal{G}_N, b)$,*

$$b^{-2}(1-\sigma_N) \leq 1-\sigma(\mathbf{w}).$$

In particular, uniformly over $w \in \mathcal{Q}(\mathcal{G}_N, b)$,

$$\left| \frac{K(\mathbf{w})^n(x,y)}{\pi(\mathbf{w})(y)} - 1 \right| \leq b d_*^{-1} \Delta_N (1-b^{-2}(1-\sigma_N))^n, \tag{5.3}$$

with $\Delta_N = \sum_x d(x)$, $d_* = \min_x\{d(x)\}$.

Proof. This is based on the basic comparison techniques of [7]. In the present case, it is best to compare the lowest and second largest eigenvalues of K_{sr}, call them β_- and β_1, respectively, with the same quantities $\beta_-(\mathbf{w})$ and $\beta_1(\mathbf{w})$ relative to $K(\mathbf{w})$. The relation with the singular value $\sigma(\mathbf{w})$ is given by $\sigma(\mathbf{w}) = \max\{-\beta_-(\mathbf{w}), \beta_1(\mathbf{w})\}$. For comparison purpose, one uses the Dirichlet forms (recall that edges here are (non-oriented) pairs $\{x, y\}$)

$$\mathcal{E}_{\mathbf{w}}(f,f) = \frac{1}{c(\mathbf{w})} \sum_{e=\{x,y\}} |f(x)-f(y)|^2 w_e$$

and

$$\mathcal{E}_{\mathrm{sr}}(f,f) = \mathcal{E}_{\mathbf{1}}(f,f) = \frac{1}{\Delta_N} \sum_{e=\{x,y\}} |f(x)-f(y)|^2.$$

Clearly, for any f,

$$\mathcal{E}_{\mathrm{sr}}(f,f) \leq \frac{c(\mathbf{w})b}{\Delta_N} \mathcal{E}_{\mathbf{w}}(f,f), \quad \mathrm{Var}_{\pi(\mathbf{w})}(f) \leq \frac{\Delta_N b}{c(\mathbf{w})} \mathrm{Var}_{\delta}(f). \tag{5.4}$$

This yields $1-\beta_1 \leq b^2(1-\beta_1(\mathbf{w}))$. A similar argument using (the sum here is over all x, y with $\{x, y\} \in E$, which explains the $\frac{1}{2}$ factor)

$$\mathcal{F}_{\mathbf{w}}(f,f) = \frac{1}{2c(\mathbf{w})} \sum_{x,y:\{x,y\}\in E} |f(x)+f(y)|^2 w_{\{x,y\}}$$

yields $1+\beta_- \leq b^2(1+\beta_-(\mathbf{w}))$. This gives the desired result. □

Example 5.3. For our present purpose, call "(d,ϵ)-expander family" any infinite family of regular graphs $\mathcal{G}_N$ of fixed degree d, with $|\Omega_N| = \#\Omega_N$ tending to infinity with N and satisfying $\sigma_N \leq 1-\epsilon$. See [17], [20] for various related definitions and discussions of particular examples. Proposition 5.2 shows that for any $K(\mathbf{w}) \in \mathcal{Q}(\mathcal{G}_N, b)$, we have

$$\left| \frac{K(\mathbf{w})^n(x,y)}{\pi(\mathbf{w})(y)} - 1 \right| \leq b|\Omega_N|(1-\epsilon/b^2)^n,$$

Let us point out that, beside singular values , there are further related techniques that yield complementary results. They include the use of Nash and logarithmic Sobolev inequalities (modified or not). See [8], [9], [28], [30]. For instance, to show that on the "lazy stick" $\mathcal{G}_N$ of Figure 5, any chains with kernel in $\mathcal{Q}(\mathcal{G}_N, b)$ converges to stationarity in order N^2, one uses the Nash inequality technique of [8].

5.3 Time inhomogeneous chains. A fundamental question about time inhomogeneous Markov chains is whether or not a result similar to (5.3) holds true for time inhomogeneous chains with kernels in $\mathcal{Q}_N(\mathcal{G}_N, b)$. Little is known about this.

Fix $b > 1$. Let $(K_i)_1^\infty$ be a sequence of Markov kernels in $\mathcal{Q}(\mathcal{G}_N, b)$ and $K_{m,n}$ be the associated iterated kernel. Recall that the property "$\sigma_N < 1$" is equivalent to the irreducibility and aperiodicity of K_{sr}. Because all the kernels in $\mathcal{Q}(\mathcal{G}_N, b)$ are (uniformly) adapted to the graph structure $\mathcal{G}_N$, there exists $\ell = \ell(N, b)$ and $\epsilon = \epsilon(N, b) > 0$ such that, for all n, $K_{n,n+\ell}(x, y) \geq \epsilon$. As explained in Section 2.3, this implies relative-sup merging for any such time inhomogeneous chain. However, this result is purely qualitative. No acceptable quantitative result can be obtain by such an argument.

Problem 5.4. Fix reals $D, b > 1$. Prove or disprove that there exists a constant A such that for any family $\mathcal{G}_N$ with maximal degree at most D, any sequence $(K_i)_1^\infty$ with $K_i \in \mathcal{Q}(\mathcal{G}_N, b)$, any initial distributions μ_0, μ_0' and any $\epsilon > 0$, if

$$n \geq A(1 - \sigma_N)^{-1}(\log |\Omega_N| + \log_+(1/\epsilon))$$

then $\mu_n = \mu_0 K_{0,n}$ and $\mu_n' = \mu_0' K_{0,n}$ satisfy

$$\max_{x \in \Omega_N} \left\{ \left| \frac{\mu_n'(x)}{\mu_n(x)} - 1 \right| \right\} \leq \epsilon.$$

This is an open problem, even for the "lazy stick" of Figure 5. It seems rather unclear whether one should except a positive answer or not.

Next, we consider another question, quite interesting but, a priori, of a different nature. Recall that, given $\mathcal{G}_N$, δ denotes the normalized reversible measure of K_{sr}.

Problem 5.5. Fix reals $D, b > 1$. Prove or disprove that there exists a constant $A \geq 1$ such that for any family $\mathcal{G}_N$ with maximal degree at most D, any sequence $(K_i)_1^\infty$with $K_i \in \mathcal{Q}(\mathcal{G}_N, b)$ and any initial distributions μ_0, if

$$n \geq A(1 - \sigma_N)^{-1}(\log |\Omega_N|)$$

then $\mu_n = \mu_0 K_{0,n}$ satisfies

$$\forall\, x \in \Omega_N, \quad A^{-1} \leq \frac{\mu_n(x)}{\delta(x)} \leq A.$$

In words, a positive solution to Problem 5.4 yields the relative-sup merging in time of order at most $A(1-\sigma_N)^{-1}\log|\Omega_N|$, uniformly for any time inhomogeneous chain with kernels in $\mathcal{Q}(\mathcal{G}_N, b)$ whereas a positive solution to Problem 5.5 would indicate that, after a time of order at most $A(1-\sigma_N)^{-1}\log|\Omega_N|$, uniformly for any time inhomogeneous chain with kernels in $\mathcal{Q}(\mathcal{G}_N, b)$ and for any initial distribution μ_0, the measure $\mu_n = \mu_0 K_{0,n}$ is comparable to δ. In fact, because of the uniform way in which Problem 5.5 is formulated, a positive answer implies that the measure δ is A-stable for $\mathcal{Q}(\mathcal{G}_N, b)$.

At this writing, the best evidence for a positive answer to these problems is contained in the following two partial results. The first result concerns sequences whose kernels share the same invariant distribution. For the proof, see [28].

Theorem 5.6. *Fix reals $D, b > 1$ and measures π_N on Ω_N. Assume that $\mathcal{G}_N$ has maximal degree at most D and that $\mathcal{Q}(\mathcal{G}_N, b, \pi_N)$ is non-empty. Under these circumstances, there is a constant $A = A(D, b)$ such that for any $\epsilon > 0$, any sequence $(K_i)_1^\infty$ with $K_i \in \mathcal{Q}(\mathcal{G}_N, b, \pi_N)$ and any pair μ_0, μ_0' of initial distributions, if*

$$n \geq A(1-\sigma_N)^{-1}(\log|\Omega_n| + \log_+(1/\epsilon))$$

then $\mu_n = \mu_0 K_{0,n}$ and $\mu_n' = \mu_0' K_{0,n}$ satisfy

$$\max_{x\in\Omega_N}\left\{\left|\frac{\mu_n'(x)}{\mu_n(x)} - 1\right|\right\} \leq \epsilon.$$

Note the hypothesis that $\mathcal{Q}(\mathcal{G}_N, b, \pi_N)$ is non-empty implies that $b^{-1} \leq \pi_N/\delta \leq b$. The second result assumes c-stability. For the proof, see [30].

Theorem 5.7. *Fix reals $D, b, c > 1$. Assume that $\mathcal{G}_N$ has maximal degree at most D. Let $(K_i)_1^\infty$ be a sequence of kernels on Ω_N with $K_i \in \mathcal{Q}(\mathcal{G}_N, b)$. Assume that the distribution δ on Ω_N is c-stable for $(K_i)_1^\infty$. Then there exists a constant $A = A(D, b, c)$ such that for any $\epsilon > 0$ and pair μ_0, μ_0' of initial distributions, if*

$$n \geq A(1-\sigma_N)^{-1}(\log|\Omega_n| + \log_+(1/\epsilon))$$

then $\mu_n = \mu_0 K_{0,n}$ and $\mu_n' = \mu_0' K_{0,n}$ satisfy

$$\max_{x\in\Omega_N}\left\{\left|\frac{\mu_n'(x)}{\mu_n(x)} - 1\right|\right\} \leq \epsilon.$$

Theorem 5.6 can be viewed as a special case of Theorem 5.7. Indeed, if $\mathcal{Q}(\mathcal{G}_N, b, \pi_N)$ is not empty then we must have $b^{-1}\delta \leq \pi_N \leq b^1\delta$ so that δ is a b-stable measure for any sequence of kernels in $\mathcal{Q}(\mathcal{G}_N, b, \pi_N)$. By Lemma 5.1, it is not difficult to produce examples where Theorem 5.6 applies. Finding examples of application of Theorem 5.7 (where the K_i's do not all share the same invariant distribution) is a difficult problem.

Under the stability hypothesis of Theorem 5.7, methods such as Nash inequalities and logarithmic Sobolev inequality can also be applied. See [30].

Remark 5.8. Consider the kernels Q_1, Q_2 of Section 4.2, with fixed p, q, r, η_1, η_2 with $r = \eta_1 = \eta_2 = 0$ and $0 < p \neq q < 1$. The kernels Q_1, Q_2 are adapted to the graph structure of Figure 6. We proved in Section 4.2 that stability fails for

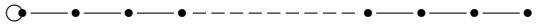

Figure 6. The underlying graph for the kernels Q_1, Q_2 of Section 4.2.

$\mathcal{Q} = \{Q_1, Q_2\}$. Even on the "lazy stick" of Figure 5, we do not understand whether stability holds or not. An interesting example of stability on the lazy stick is proved in [29]. This example involves perturbations that are localized at the ends of the stick. Further examples are discussed in [31].

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Some mathematical aspects of market impact modeling

Alexander Schied* and Alla Slynko

1 Introduction

Market impact risk is a specific kind of liquidity risk. It describes the risk of not being able to execute a trade at the currently quoted price because this trade feeds back in an unfavorable manner on the underlying price. Spectacular cases in which market impact risk played an important role were the debacle of Metallgesellschaft in 1993, the LTCM crisis in 1998, or the unwinding of Jérôme Kerviel's portfolio by Societé Générale in 2008. But market risk can also be significant in much smaller trades, and it belongs to the daily business of many financial institutions. The basic observation is that the liquidity costs of large trades can be reduced significantly by splitting the large trade into a sequence of smaller trades, sometimes called child orders, which are then spread out over a certain time interval. In recent years, there has been a strong trend toward the application of electronic trading algorithms to compute the size and schedule of the child orders. These algorithms are typically based on a market impact model, that is, on a stochastic model for asset prices that takes into account the feedback effects of trading strategies.

While standard financial market models assume that asset prices are given exogenously, and thus result in a predominantly linear theory, market impact models allow trading strategies to feed back on asset prices, which results in a predominantly nonlinear theory. This makes market impact modeling a fascinating and rewarding research subject from a mathematical point of view. Moreover, market impact models are often used in practical applications and it would be desirable to gain a better understanding of their behavior and their stability. From an economic perspective, market impact is one of the basic mechanisms responsible for price formation, and so its analysis might contribute to new insights on how financial markets function.

One of the earliest market impact model classes that has so far been proposed, and which has also been widely used in the financial industry, is based on the discrete-time model by Bertsimas & Lo [9] and Almgren & Chriss [6], [7] and its continuous-time variant by Almgren [5]. We will call these models *first-generation market impact models* in the sequel. They distinguish between the following two impact components. The first component is temporary and only affects the individual trade that has also triggered it. The second component is permanent and affects all current and future trades equally. The unaffected price process is driven by the actions of noise traders and therefore usually assumed to be a martingale.

The distinction between temporary and permanent price impact is reasonable as long as the time between the individual child orders is sufficiently long. On a finer

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time scale, one will realize that price impact is in fact not temporary but transient. That is, a child order creates some immediate price impact that subsequently decays over a certain, but often short, time span. That is, price impact is only temporary and at least a part of it disappears, often within just a few minutes. This resilience effect has been well established in several empirical studies on market microstructure; see Bouchaud [12] and Hasbrouck [31] for two recent surveys with comprehensive lists of references. Note that this decay of price impact is ultimately responsible for the fact that liquidity costs can be reduced when splitting up large orders into smaller child orders. The increase in trading frequency in modern electronic trading systems has thus led to a development of a *second generation of market impact models*. In these models, the decay of price impact is modeled explicitly. Among the first models of this type are the model by Bouchaud, Gefen, Potters & Wyart [13] and the limit order book model by Obizhaeva & Wang [37]. The former was extended and studied by Gatheral [25], the latter by Alfonsi, Fruth & Schied [1], [2], Alfonsi & Schied [3], Alfonsi, Schied & Slynko [4], Gatheral, Schied & Slynko [27], [28], and Predoiu, Shaikhet & Shreve [38].

There are also other approaches in the literature for modeling the market impact of a large trader; we refer to [8], [19], [29], [39] and the references therein.

In this paper, we will first survey some results on the first-generation market impact model by Almgren & Chriss [6], [7] and by Almgren [5]. Here we will focus on the mathematical problem of finding optimal strategies for executing a given order over a specified time horizon. We will see that this problem leads to a stochastic control problem with fuel constraint. In presenting the mathematics of this problem we will follow Schied & Schöneborn [40], Schied, Schöneborn & Tehranchi [41], and Schöneborn [42]. In the second part of this paper, we will focus on the effects created by the transience of price impact. To this end, we will consider a linear, second generation model with general resilience. We will focus in particular on possible model irregularities and the relations to potential theory. This second part is based on [4] and on [28].

2 A first-generation market impact model

In this section, we consider the analysis of the optimal order execution problem for the continuous-time version of the market impact model proposed in [5], [6], [7], [9]. In the first subsection, we introduce the model and consider the problem of maximizing the expectation or a mean-variance functional of the revenues. In the subsequent subsection, we discuss the problem of maximizing the expected utility of revenues.

2.1 The approach by Almgren and Chriss. In the Almgren–Chriss market impact model it is assumed that the number of shares in the trader's portfolio is described by an absolutely continuous trajectory $t \mapsto X_t$. Given this trading trajectory, the price at which transactions occur is

$$S_t = S_t^0 + \eta \dot{X}_t + \gamma(X_t - X_0),$$

where η and γ are constants and S_t^0 is the unaffected stock price process. The term $\eta \dot{X}_t$ corresponds to the *temporary* or *instantaneous impact* of trading $\dot{X}_t\, dt$ shares at time t and only affects this current order. The term $\gamma(X_t - X_0)$ corresponds to the *permanent price impact* that has been accumulated by all transactions until time t. The unaffected stock price is taken as a Bachelier model,

$$S_t^0 = S_0 + \sigma W_t,$$

where W is a standard Brownian motion. At first sight, it might seem to be a shortcoming of this model that it allows for negative values of the unaffected price process. In reality, however, even very large asset positions are typically liquidated within a few days or hours. Hence negative prices occur only with negligible probability.

Let us now consider a *trade execution strategy* in which an initial long or short position of x_0 shares is liquidated by time T. The asset position of the trader, $X = (X_t)_{0\le t\le T}$, thus satisfies the boundary condition $X_0 = x_0$ and $X_T = 0$. In such a strategy, $-\dot{X}_t\, dt$ shares are sold at price S_t at each time t. Thus, the *revenues* arising from the strategy $X = (X_t)_{0\le t\le T}$ are

$$\begin{aligned}\mathcal{R}(X) &:= \int_0^T S_t(-\dot{X}_t)\, dt \\ &= -\int_0^T S_t^0 \dot{X}_t\, dt - \eta \int_0^T \dot{X}_t^2\, dt - \gamma \int_0^T X_t \dot{X}_t\, dt - \gamma x_0^2 \\ &= x_0 S_0 + \int_0^T X_t\, dS_t^0 - \eta \int_0^T \dot{X}_t^2\, dt - \frac{\gamma}{2} x_0^2.\end{aligned}$$

The *optimal trade execution problem* consists in maximizing a certain objective function, which may involve revenues and additional risk terms, over the class of admissible trading strategies X with side conditions $X_0 = x_0$ and $X_T = 0$. The easiest case corresponds to maximizing the expected revenues,

$$\mathbb{E}[\,\mathcal{R}(X)\,] = x_0 S_0 - \frac{\gamma}{2} x_0^2 - \eta\, \mathbb{E}\Big[\int_0^T \dot{X}_t^2\, dt\Big].$$

In this case, which was first considered in [9] in a discrete-time setting, a simple application of Jensen's inequality shows that the unique optimal strategy X^* is characterized by having the constant trading rate

$$\dot{X}_t^* = -\frac{x_0}{T},$$

regardless of the choice of the unaffected price process. When, as is usually assumed in practice, time is parameterized in volume time, such a constant trading rate corresponds to a VWAP strategy, where VWAP stands for volume-weighted average price.

Almgren & Chriss [6], [7] were the first to point out that executing orders late in the trading interval $[0, T]$ incurs volatility risk. They therefore suggested to maximize a mean-variance functional of the form

$$\mathbb{E}[\,\mathcal{R}(X)\,] - \frac{\alpha}{2}\mathrm{var}\,(\mathcal{R}(X)), \tag{1}$$

where α is a risk-aversion parameter. For *deterministic* strategies X, the mean-variance functional (1) becomes

$$x_0 S_0 - \frac{\gamma}{2} x_0^2 - \int_0^T \left(\frac{\alpha}{2} \sigma^2 X_t^2 + \eta \dot{X}_t^2 \right) dt.$$

Mean-variance maximization over deterministic strategies is thus equivalent to minimizing the action-type functional $\int_0^T L(X_t, \dot{X}_t)\, dt$ where the Lagrangian L is given by $L(x, p) = \frac{\alpha}{2}\sigma^2 x^2 + \eta p^2$. Calculus of variations easily yields

$$X_t^* = x_0 \frac{\sinh \kappa (T - t)}{\sinh \kappa T}, \quad \text{with } \kappa = \sqrt{\frac{\alpha \sigma^2}{2\eta}}, \tag{2}$$

as the unique minimizer under the side conditions $X_0 = x_0$ and $X_T = 0$. When strategies are not assumed to be deterministic, mean-variance optimization is more involved. The main difficulty stems from the fact that the mean-variance functional is not time consistent so that techniques from stochastic optimal control cannot be applied directly. We refer to Lorenz & Almgren [34] and Forsyth [23]. Due to these complications, it can make sense to consider alternative optimization criteria than mean-variance optimization. In the next section we will investigate the maximization of the expected utility of revenues. Another risk criterion was recently suggested by Gatheral & Schied [26].

2.2 Maximization of the expected utility of revenues. From an economic point of view it is quite natural to consider the maximization of the expected utility, $\mathbb{E}[\, u(\mathcal{R}(X))\,]$, where $u\colon \mathbb{R} \to \mathbb{R}$ is an increasing and strictly concave utility function (see, e.g., Chapter 2 in Föllmer & Schied [22]). This problem formulation has also the advantage that it can be approached by stochastic optimal control. To see how this works, let us parameterize our strategies $X = (X_t)_{0 \le t \le T}$ by $\xi_t := -\dot{X}_t$. We then write

$$X_t^\xi := x_0 - \int_0^t \xi_s\, ds, \quad 0 \le t \le T. \tag{3}$$

More precisely, we introduce the class $\mathcal{X}(x_0, T)$ of all progressively measurable processes $(\xi_t)_{0 \le t \le T}$ such that $\int_0^T \xi_t^2\, dt < \infty$, $\int_0^T \xi_t\, dt = x_0$, and $X_t^\xi(\omega)$ defined by (3) is bounded uniformly in t and ω by a constant that may depend on ξ. We next introduce the controlled diffusion process

$$R_t^\xi := R_0 + \sigma \int_0^t X_s^\xi\, dB_s - \eta \int_0^t \xi_s^2\, ds, \quad 0 \le t \le T.$$

The problem of maximizing the expected utility of revenues is then mathematically equivalent to maximizing $\mathbb{E}[u(R_T^\xi)]$ over $\xi \in \mathcal{X}(x_0, T)$. Note that this is not an entirely standard control problem because that the class $\mathcal{X}(x_0, T)$ of admissible controls depends on the state variables x_0 and T. Problems of this type are sometimes called finite-fuel control problems.

To derive heuristically the Hamilton–Jacobi–Bellman (HJB) equation for this problem, let

$$v(T, x_0, R_0) := \sup_{\xi \in \mathcal{X}(x_0, T)} \mathbb{E}[\, u(R_T^\xi)\,]$$

denote the corresponding value function. We would expect that for any $\xi \in \mathcal{X}(x_0, T)$ the process

$$V_t^\xi := v(T - t, X_t^\xi, R_t^\xi)$$

is a supermartingale, and that it is a true martingale for an optimal strategy ξ. Itô's formula yields

$$dV_t^\xi = \sigma v_R X_t^\xi \, dB_t - \Big(v_t - \frac{1}{2}\sigma^2 (X_t^\xi)^2 v_{RR} + \eta \xi_t^2 v_R + \xi_t v_X\Big)\, dt.$$

We thus expect that v should solve the partial differential equation (PDE)

$$v_t = \frac{1}{2}\sigma^2 X^2 v_{RR} - \inf_{\xi \in \mathbb{R}} \big(\eta \xi^2 v_R + \xi v_X\big). \tag{4}$$

This equation, however, does not yet take into account the fuel constraint on strategies. This fuel constraint enters the problem through the initial condition satisfied by v:

$$\lim_{T \downarrow 0} v(T, x_0, R_0) = \begin{cases} u(R_0) & \text{when } x_0 = 0, \\ -\infty & \text{otherwise.} \end{cases} \tag{5}$$

The intuition for the singular part of this initial condition is the following. When there is no time left ($T = 0$) for liquidating a nonzero asset position ($x_0 \neq 0$), then the liquidation task has not been fulfilled, and this case should receive a penalty.

We have the following result from [41]:

Theorem 2.1 ([41]). *For $u(x) = -e^{-\alpha x}$ and $\kappa = \sqrt{\frac{\alpha\sigma^2}{2\eta}}$, the value function is*

$$v(T, x_0, R_0) = -\exp\big[-\alpha R_0 + x_0^2 \eta \alpha \kappa \cdot \coth(\kappa T)\big], \tag{6}$$

and the unique maximizing strategy ξ^* is given by the deterministic function

$$\xi_t^* = x_0 \kappa \frac{\cosh(\kappa(T - t))}{\sinh(\kappa T)}.$$

Remark 2.2. (a) One can check easily that the function in (6) solves indeed the singular initial value problem (4), (5).

(b) Note that the optimal strategy X^{ξ^*} coincides with the mean-variance optimal strategy (2). This is clear as soon as one knows that the optimal strategy is deterministic, because for a deterministic strategy the revenues are normally distributed, and so the expected exponential utility is an exponential of the mean-variance functional (1).

(c) The fact that optimal strategies for exponential utility functions are deterministic is not limited to the Almgren–Chriss model. It is also true for more general second-generation market impact models; see [41].

For utility functions other than the exponential utility function, the existence of classical solutions to the singular initial value problem (4), (5) is open. But the problem can be simplified by allowing for an infinite time horizon. To set up the corresponding problem, let $\mathcal{X}$ denote the class of all progressively measurable processes ξ such that $\int_0^t \xi_s^2\,ds < \infty$ for all $t \geq 0$ and such that $X_t^\xi(\omega)$ is bounded uniformly in t and ω by a constant that may depend on ξ. Let $\mathcal{X}_0$ be the subclass of all $\xi \in \mathcal{X}$ for which R_t^ξ converges to a limit R_∞^ξ as $t \uparrow \infty$. Then one possible problem formulation is to maximize the expected utility $\mathbb{E}[\,u(R_\infty^\xi)\,]$ over $\xi \in \mathcal{X}_0$. The corresponding value function is denoted by

$$v_0(x_0, R_0) := \sup_{\xi \in \mathcal{X}_0} \mathbb{E}[\,u(R_\infty^\xi)\,]. \tag{7}$$

Alternatively, we can consider the value function

$$v_1(x_0, R_0) := \sup_{\xi \in \mathcal{X}} \lim_{t \uparrow \infty} \mathbb{E}[\,u(R_t^\xi)\,]. \tag{8}$$

The existence of the limit in (8) follows from Jensen's inequality and the fact that R_t^ξ satisfies the supermartingale inequality $\mathbb{E}[\,R_t^\xi \mid \mathcal{F}_s\,] \leq R_s^\xi$ for $s \leq t$ (even though it may fail to be a supermartingale due to the possible lack of integrability). Neither in (7) nor in (8) do we need to require that strategies $\xi \in \mathcal{X}$ liquidate the asset position x_0 in the sense that $X_t^\xi \to 0$ as $t \uparrow \infty$. Intuitively, this is due to the fact that expected utility discourages the possession of positions in an asset whose price process follows a martingale, so that we can expect that every optimal strategy will automatically satisfy $X_t^\xi \to 0$. This will indeed come out of our analysis.

In both cases, (7) and (8), the corresponding value function should become independent of time, and one can expect that it solves the PDE

$$0 = \frac{1}{2}\sigma^2 X^2 v_{RR} - \inf_{\xi \in \mathbb{R}} \big(\eta \xi^2 v_R + \xi v_X\big). \tag{9}$$

The initial condition (5) becomes

$$v(0, R_0) = u(R_0). \tag{10}$$

It thus seems that the variable x_0 can take over the role of "time" for the problem (9), (10). The reduced form of (9), however, is

$$v_X^2 = -2\eta\sigma^2 X^2 v_R \cdot v_{RR},$$

which is a fully nonlinear equation in *all* derivatives of v and hence not solvable in a straightforward manner.

The ordinary approach to solving stochastic control problems by means of PDEs is to obtain first a solution of the PDE in question and then to define a Markovian control

policy as the optimizer of the nonlinear term in the HJB equation. In our case, this Markovian control policy would be

$$\widehat{\xi}(x_0, R_0) = \arg\min_{\xi} \left\{\eta\xi^2 v_R(x_0, R_0) + \xi v_X(x_0, R_0)\right\} = -\frac{v_X(x_0, R_0)}{2\eta v_R(x_0, R_0)}, \quad (11)$$

when v is a sufficiently smooth solution. The optimality of the resulting strategy will then have to be shown by a verification argument.

In our case, however, the existence of smooth solutions to the problem (9), (10) is unclear. We therefore proceed, as it were, by *reversing* the above steps. The idea is to determine first the Markovian policy $\widehat{\xi}$ by means of another PDE and then use $\widehat{\xi}$ to define a function v as the solution of the linear transport equation

$$v_X + 2\eta\widehat{\xi} v_R = 0,$$

which is equivalent to (11). Due to degeneracies in our equations, we actually need to modify this idea through working with the following transformed function:

$$\widetilde{\xi}(Y, R_0) := \frac{\widehat{\xi}(\sqrt{Y}, R_0)}{\sqrt{Y}}. \quad (12)$$

Assuming that v is a sufficiently smooth solution of (9), (10) one computes that $\widetilde{\xi}$, when defined through (12) and (11), should solve the following nonlinear parabolic initial value problem:

$$\begin{cases} \widetilde{\xi}_Y = \dfrac{\sigma^2}{4\widetilde{\xi}}\widetilde{\xi}_{RR} - \dfrac{3}{2}\eta\widetilde{\xi}\cdot\widetilde{\xi}_R, \\ \\ \widetilde{\xi}(0, R) = \sqrt{\dfrac{\sigma^2 A(R)}{2\eta}}, \end{cases} \quad (13)$$

where $A(R) = -u''(R)/u'(R)$ denotes the coefficient of absolute risk aversion of our utility function. The following result is taken from [40].

Theorem 2.3 ([40]). *Suppose that u belongs to C^6 and that its absolute risk aversion satisfies $A_{\min} \le A(R) \le A_{\max}$ for two constants $0 < A_{\min} \le A_{\max} < \infty$. Then:*

(a) *The initial value problem (13) admits unique classical solution $\widetilde{\xi} \in C^{2,4}$ s.th.*

$$\sqrt{\frac{\sigma^2 A_{\min}}{2\eta}} \le \widetilde{\xi}(Y, R) \le \sqrt{\frac{\sigma^2 A_{\max}}{2\eta}}.$$

(b) *The transport equation*

$$\begin{cases} \widetilde{v}_Y = -\eta\widetilde{\xi}\widetilde{v}_R, \\ \widetilde{v}(0, R) = u(R), \end{cases}$$

admits a unique $C^{2,4}$-solution $\widetilde{v}$.

(c) *The function* $v(x_0, R) := \widetilde{v}(x_0^2, R_0)$ *is a classical* $C^{2,4}$*-solution of the HJB equation* (9), (10), *and* $\widehat{\xi}$ *defined by* $\widehat{\xi}(x_0, R_0) := x_0\widetilde{\xi}(x_0^2, R)$ *satisfies* (11).

(d) *The function* v *is equal to both value functions* v_0 *and* v_1 *defined in* (7) *and* (8). *Moreover, the a.s. unique optimal control policy* $\xi^* \in \mathcal{X}$ *for both optimization problems is given in feedback form by*

$$\xi_t^* = \widehat{\xi}(X_t^{\xi^*}, R_t^{\xi^*}) = -\frac{v_X}{2\eta v_R}(X_t^{\xi^*}, R_t^{\xi^*}). \tag{14}$$

It belongs to $\mathcal{X}_0$, *and we have*

$$v(x_0, R_0) = \lim_{t\to\infty} \mathbb{E}[\,u(R_t^{\xi^*})\,] = \mathbb{E}[\,u(R_\infty^{\xi^*})\,].$$

The preceding theorem implies the following corollary.

Corollary 2.4 ([40]). *If* $u(R) = -e^{-\alpha R}$, *then*

$$X_t^{\xi^*} = X_0 \exp(-\kappa t).$$

Proof. When u is of exponential type the corresponding absolute risk aversion satisfies $A(R) = \alpha$ for all R. Hence we can take $A_{\min} = A_{\max} = \alpha$ in (1) and obtain $\widehat{\xi}(x_0, R_0) = x_0\kappa$, which gives the result via (14). □

So we find again that, in the case of exponential utility, optimal strategies are deterministic. The next theorem shows that the general principle behind this result is that optimal strategies inherit the monotonicity properties of the absolute risk aversion of u.

Theorem 2.5 ([40]). *Let* u^1 *and* u^0 *be two utility functions satisfying the assumptions of Theorem* 2.3. *When the corresponding respective coefficients of risk aversion satisfy* $A^1 \geq A^0$ *then the respective optimal strategies inherit this monotonicity relation, i.e.,* $\widehat{\xi}^1 \geq \widehat{\xi}^0$.

Idea of proof. The function $g := \widetilde{\xi}^1 - \widetilde{\xi}^0$ solves

$$g_Y = \frac{1}{2}ag_{RR} + bg_R + Vg,$$

where

$$a = \frac{\sigma^2}{2\widetilde{\xi}^0}, \quad b = -\frac{3}{2}\eta\widetilde{\xi}^1, \quad \text{and} \quad V = -\frac{\sigma^2\widetilde{\xi}^1_{RR}}{4\widetilde{\xi}^0\widetilde{\xi}^1} - \frac{3}{2}\eta\widetilde{\xi}^0_R.$$

The boundary condition of g is

$$g(0, R) = \sqrt{\frac{\sigma^2 A^1(R)}{2\eta}} - \sqrt{\frac{\sigma^2 A^0(R)}{2\eta}} \geq 0.$$

Therefore the maximum principle or a Feynman–Kac argument together with appropriate localization give the result; see [40] for details. □

Corollary 2.6 ([40]). *The optimal strategy* $\widehat{\xi}(X, R)$ *is nondecreasing* (*nonincreasing*) *in* R *iff* $A(R)$ *is nondecreasing* (*nonincreasing*).

Proof. When $A(R)$ is nondecreasing, consider the utility functions $u^0(R) := u(R)$ and $u^1(R) := u(R+\delta)$, where $\delta > 0$ is fixed. Thus, the result follows from Theorem 2.5. □

It is possible to derive further qualitative properties of optimal strategies. For instance, it is fairly surprising that $\widehat{\xi}$ is not necessarily nonincreasing as a function of η or nondecreasing as a function of the initial portfolio x_0. We refer to [40] for details.

Additional surprising features and interesting mathematical problems arise when one considers an extended market model with d risky assets. In this case, the "time" parameter X becomes a vector in $\mathbb{R}^d$, and so the value function satisfies a "parabolic" PDE with a d-dimensional "time" parameter. We refer to Chapter 5 in Schöneborn [42] for a detailed analysis of this multi-asset situation and for many other interesting results.

Another important generalization of our setting is the extension to the case of several large traders who are competing in a single market. Such extensions were first considered by Brunnermeier & Pedersen [14] and Carlin, Lobo & Viswanathan [16]. Schöneborn & Schied [43] show that the qualitative behavior of the competitors of a large seller depends crucially on the ratio γ/η of the permanent and temporary price impact components. When this ratio is large, the market has a *plastic* behavior with respect to price impact since the permanent impact component dominates. When the ratio is small, the market behavior can be qualified as *elastic*. Schöneborn & Schied [43] show in particular that competitors tend to engage in *predatory trading* in plastic market environments. That is, the competitors shorten the asset when prices are still high and buy back when the seller has depressed asset prices just before completing the order execution. This behavior is "predatory", because it increases the seller's execution costs. In elastic markets, on the other hand, competitors tend to act as liquidity providers by building up long positions, buy shares offered by the seller, and thus alleviate the seller's execution costs. All these results assume a perfect information structure. A model with imperfect information is developed in Moallemi, Park & van Roy [35].

3 Second-generation market impact models

In this section we present results from [4] and [28]. In the first subsection we discuss the discrete-time model of [4], which builds on earlier models [13], [37], [1], [2], [3], [25]. In Subsection 3.2 we will analyze the continuous-time extension of this model in [28] and in particular highlight its connections with potential theory. Throughout this section, we will focus on second-generation market impact models with *linear* impact. Models with *nonlinear* impact are considered in [13], [2], [3], [25]. See [27] for a discussion of the relations between these models.

3.1 Transient price impact in discrete time. The results in this section are taken from [4], and we refer to this paper for all details and proofs. Let us first introduce the following market impact model for a trader who can move asset prices. As long as this trader is not active, asset prices are determined by the actions of the other market participants and are described by a process S_t^0, $t \geq 0$, which is assumed to be a rightcontinuous martingale on a given filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t), \mathbb{P})$ for which $\mathcal{F}_0$ is $\mathbb{P}$-trivial. (S_t^0) will again be called the *unaffected price process*. A *strategy* $\boldsymbol{\xi}$ consists of a sequence $\xi_{t_0}, \xi_{t_1}, \ldots, \xi_{t_N}$ of trades by which this trader purchases or liquidates a portfolio of a given number of shares. We thus assume that

$$\sum_{n=0}^{N} \xi_{t_n} = x_0,$$

where $x_0 > 0$ corresponds to a buy program and $x_0 < 0$ corresponds to a sell program. A strategy with $x_0 = 0$ is called a *round trip*.

The order ξ_{t_n} is placed at time t_n, where t_n belongs to a given set $\mathbb{T} := \{t_0, t_1, \ldots, t_N\}$ of trading times such that $0 \leq t_0 < t_1 < \cdots < t_N < \infty$. We assume moreover that each ξ_{t_n} is bounded from below and measurable with respect to $\mathcal{F}_{t_n}$. The set of all such strategies is denoted by $\Xi(x_0, \mathbb{T})$. Both x_0 and $\mathbb{T}$ will be allowed to vary in the sequel.

When the strategy $\boldsymbol{\xi} = (\xi_{t_0}, \xi_{t_1}, \ldots, \xi_{t_N})$ is applied, the price at time t is defined as

$$S_t = S_t^0 + \sum_{t_n < t} \xi_{t_n} G(t - t_n),$$

where $G\colon [0, \infty) \to [0, \infty)$ is a bounded function, the *resilience function*. Thus, $\xi_{t_n} G(0)$ denotes the immediate price impact of the order ξ_{t_n}. After a time span Δt, this initial impact decays[1] to $\xi_{t_n} G(\Delta t)$. This description of market impact thus comprises the following three types of price impact, the *instantaneous impact* $\xi_{t_n}(G(0) - G(0+))$, the *permanent impact* $\xi_{t_n} G(\infty)$, where $G(\infty) := \lim_{t \uparrow \infty} G(t)$, and the *transient impact* $\xi_{t_n}(G(0+) - G(\infty))$.

Let us now define the expected execution costs of a strategy $\boldsymbol{\xi} \in \Xi(x_0, \mathbb{T})$. When the trade ξ_{t_n} is executed, the price is moved from S_{t_n} to $S_{t_n+} = S_{t_n} + \xi_{t_n} G(0)$. Intuitively, this linear price impact corresponds to a constant supply curve for which $G(0)^{-1}\, dy$ buy or sell orders are available at each price y, with y ranging from S_{t_n} to S_{t_n+}, as shown in Figure 1. The trade ξ_{t_n} is thus carried out at the following average cost:

$$c(\xi_{t_n}) = \int_{S_{t_n}}^{S_{t_n+}} y\, G(0)^{-1}\, dy = \frac{1}{2G(0)} \big(S_{t_n+}^2 - S_{t_n}^2\big).$$

This quantity is positive for buy orders $\xi_{t_n} > 0$ and negative for sell orders $\xi_{t_n} < 0$ (at least as long as prices stay positive). It can thus also be regarded as *the cost of the trade* ξ_{t_n}. The *expected execution costs* of the strategy $\boldsymbol{\xi} = (\xi_{t_0}, \xi_{t_1}, \ldots, \xi_{t_N})$ are now

[1] The economic intuition is that $G(t)$ should be a nonincreasing function of t. For the mathematical problem formulation, however, such a restriction is not necessary.

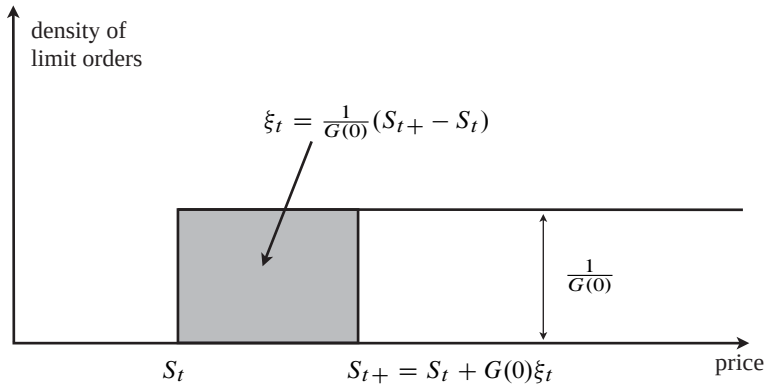

Figure 1. For a supply curve with a constant density $\frac{1}{G(0)}$ of limit sell orders, the price is shifted from S_t to $S_{t+} = S_t + G(0)\xi_t$ when a market buy order of size $\xi_t > 0$ is executed.

defined as the expected cumulative costs of all trades in this strategy, i.e.,

$$\mathbb{E}\Big[\sum_{n=0}^{N} c(\xi_{t_n})\Big] = \frac{1}{2G(0)}\mathbb{E}\Big[\sum_{n=0}^{N}\big(S_{t_n+}^2 - S_{t_n}^2\big)\Big].$$

Using the martingale property of S^0, one easily checks that the expected execution costs of a strategy $\boldsymbol{\xi} = (\xi_{t_0}, \xi_{t_1}, \ldots, \xi_{t_N}) \in \Xi(x_0, \mathbb{T})$ are given by

$$\mathbb{E}\Big[\sum_{n=0}^{N} c(\xi_{t_n})\Big] = x_0 S_0^0 + \mathbb{E}[\,C_{\mathbb{T}}(\boldsymbol{\xi})\,],$$

where $C_{\mathbb{T}}$ is the quadratic form defined as

$$C_{\mathbb{T}}(\boldsymbol{y}) := \frac{1}{2}\sum_{i,j=0}^{N} y_i y_j G(|t_i - t_j|), \quad \boldsymbol{y} = (y_0, \ldots, y_N) \in \mathbb{R}^{N+1}.$$

This result has the following significance. Suppose that $\boldsymbol{y}^* \in \mathbb{R}^{N+1}$ minimizes $C_{\mathbb{T}}(\boldsymbol{y})$ in the class of $\boldsymbol{y} \in \mathbb{R}^{N+1}$ with $\boldsymbol{y}^\top \mathbf{1} = x_0$, where $\mathbf{1} = (1, \ldots, 1) \in \mathbb{R}^{N+1}$. Then the deterministic strategy $\boldsymbol{\xi}^* := \boldsymbol{y}^*$ minimizes the expected trade execution costs over all strategies in $\Xi(x_0, \mathbb{T})$. Clearly, such a minimizer $\boldsymbol{y}^*$ exists as soon as $C_{\mathbb{T}}(\boldsymbol{y}) \geq 0$ for all $\boldsymbol{y}$. But the situation in which $C_{\mathbb{T}}(\boldsymbol{y}) \geq 0$ holds for all $\boldsymbol{y}$ and $\mathbb{T}$ is well known. It is tantamount to requiring that the function $G(|\cdot|)$ is *positive definite* in the sense of Bochner [11]. When even $C_{\mathbb{T}}(\boldsymbol{y}) > 0$ for all $\mathbb{T}$ and $\boldsymbol{y} \neq \mathbf{0}$, then G we will say that G is *strictly positive definite*.

Bochner's celebrated theorem characterizes precisely those functions G that are positive definite within the class of continuous functions: A continuous function G is

positive definite if and only if the function $x \to G(|x|)$ is the Fourier transform of a positive finite Borel measure μ on $\mathbb{R}$, i.e.,

$$G(|x|) = \int e^{ixz}\,\mu(dz), \quad x \in \mathbb{R}.$$

It is not difficult to show that G is even strictly positive definite as soon as the support of μ is not discrete.

The following result gives a sufficient criterion when a function G is strictly positive definite. Its weak form asserting that every nonincreasing convex function $G \geq 0$ is positive definite can be derived from the results by Carathéodory [15], Toeplitz [44], and Young [45], but was re-discovered many times.

Proposition 3.1. *If the resilience function G is convex, nonincreasing and nonconstant, then it is strictly positive definite.*

Remark 3.2. An important question concerns the viability of a market impact model. For a standard asset pricing model, viability can be characterized in terms of the absence of arbitrage opportunities, which is essentially equivalent to the existence of an equivalent martingale measure. In a market impact model, the existence of such small-investor arbitrage is usually guaranteed by assuming martingale dynamics for the unaffected stock price process S^0. Huberman & Stanzl [32], however, were among the first to point out that there can be additional irregularities for large investors. They identified in particular the so-called *price manipulation strategies*. These are round trips (i.e., admissible strategies with $x_0 = 0$) with strictly negative execution costs. When suitable rescaled and repeated, such price manipulation strategies can lead to a weak form of arbitrage. Moreover, they can prevent the existence of optimal execution strategies. For these reasons, models that admit price manipulation should be deemed as non-viable. We will see later that it is not sufficient just to exclude price manipulation. There can be other types of irregularities as well. ◇

Let us consider a few examples of strictly positive definite resilience functions and have a look at the corresponding optimal strategies.

Example 3.3 (Exponential resilience). Exponential resilience corresponds to the choice of the resilience function $G(t) = e^{-\rho t}$ with $\rho > 0$ G is clearly strictly positive definite. In fact, the optimal strategy $\boldsymbol{\xi}^*$ is explicitly known for an arbitrary time grid $\mathbb{T}$; see [1]. Figure 2 shows the optimal strategy for various values of N. When $N \uparrow \infty$, the strategies with equidistant time grids converge to a continuous-time strategy with two identical block trades at the beginning and end of trading and a continuous VWAP (Volume-Weighted Average Price) strategy in between, as shown in Example 3.15 below. ◇

Example 3.4. The resilience function

$$G(t) = \frac{e(e - \cos t)}{1 + e^2 - 2e\cos t}$$

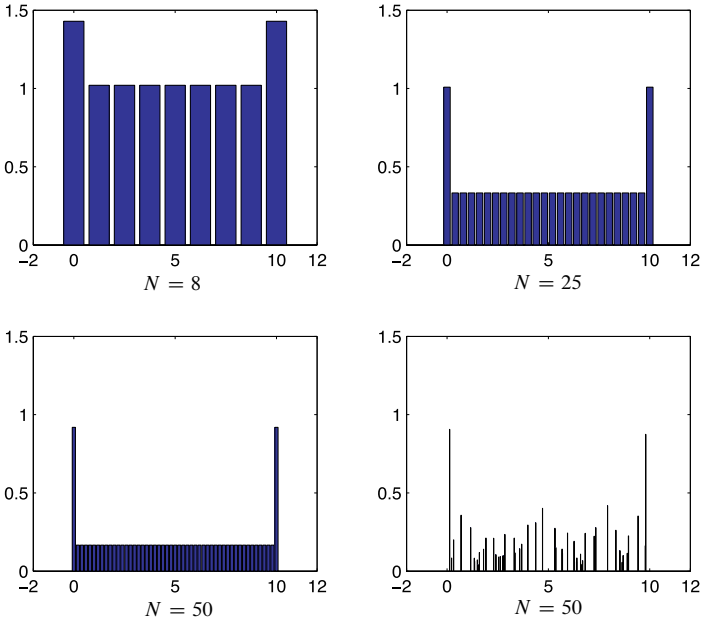

Figure 2. Optimal strategies for exponential resilience $G(t) = e^{-t}$. Horizontal axes correspond to time, vertical axes to trade size. We chose $x_0 = 10$, $T = 10$, the equidistant time grid, $t_i = iT/N$, for $N = 8,\ 25,\ 50$, and randomly spaced trading times for $N = 50$.

is positive definite as the Fourier transform of purely discrete measure

$$\mu = \frac{1}{2}\sum_{k=0}^{\infty} e^{-k}(\delta_k + \delta_{-k}).$$

Corresponding optimal trading strategies are given in Figure 3. ◇

Example 3.5 (Permanent price impact). The constant resilience function $G(t) \equiv 1$ is positive definite as the Fourier transform of the measure $\mu = \delta_0$. In this case, every strategy $\boldsymbol{\xi}$ in $\Xi(x_0, \mathbb{T})$ is optimal and satisfies $\mathcal{C}(\boldsymbol{\xi}) = x_0 S_0 + \frac{1}{2}x_0^2$. ◇

Example 3.6 (Capped linear resilience). The linear resilience function $G(t) = (1 - \rho t)^+$ is strictly positive definite for $\rho > 0$. For $\rho \leq 1/T$ the optimal strategy is independent of the underlying time grid: it consists of two symmetric trades of size $x_0/2$ at $t = 0$ and $t = T$, all other trades are zero. The case when $\rho > 1/T$ with $\rho = k/T$ where $k \in \mathbb{N}$ divides N and an equidistant grid of $N + 1$ trading dates, the optimal strategy consists of $k + 1$ equidistant trades of equal size; see [4], Proposition 7. ◇

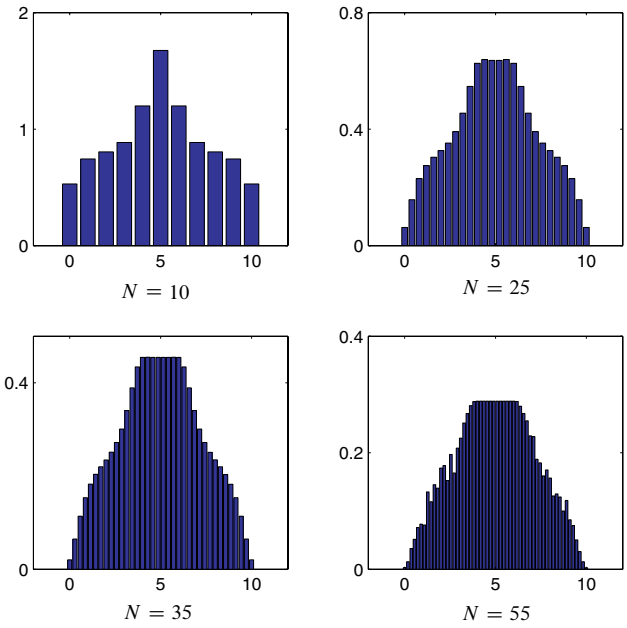

Figure 3. Optimal strategies for the resilience function $G(t) = \frac{e(e-\cos t)}{1+e^2-2e\cos t}$. Horizontal axes correspond to time, vertical axes to trade size. We chose $x_0 = 10$, $T = 10$, and the equidistant time grid, $t_i = iT/N$, for $N = 10, 25, 35, 55$.

Example 3.7 (Power-law resilience). Several empirical studies have found that market impact decays with a power law function of the form $G(t) = \eta(1+\lambda t)^{-\gamma}$ for some $\eta, \gamma, \lambda > 0$. For instance, [13] find a value of $\gamma \approx 0.4$. See also [25] for additional arguments and references. By Proposition 3.1, G is strictly positive definite for all values of $\eta, \gamma, \lambda > 0$. As can be seen in Figure 4 the corresponding optimal strategies behave in a very regular manner, even for randomly chosen trading times. ◇

Example 3.7 shows that optimal strategies are well-behaved when we take, for instance, the resilience function

$$G(t) = \frac{1}{(1+t)^2}.$$

The picture can change dramatically, however, when taking a slightly different definition of power-law decay as in the next example.

Example 3.8 (Alternative definition of power-law resilience). The resilience function

$$G(t) = \frac{1}{1+t^2}.$$

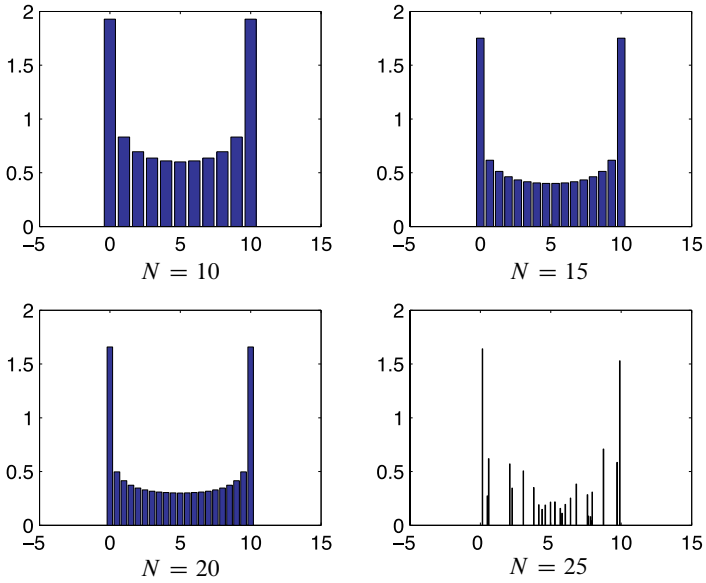

Figure 4. Optimal strategies for power-law resilience $G(t) = (1+t)^{-0.4}$ and various values of N. Horizontal axes correspond to time, vertical axes to trade size. We chose $x_0 = 10$, $T = 10$, and the equidistant time grid, $t_i = iT/N$, for $N = 10, 15, 20$. For $N = 25$ we use randomly chosen trading times.

is the Fourier transform of the measure $\mu(dx) = \frac{1}{2}e^{-|x|}dx$ and thus strictly positive definite. Figure 5 shows, however, that the optimal strategies oscillate stronger and stronger between positive and negative trades as the time grid becomes finer and finer. For $N = 120$, several individual child orders are of the order 20.000, while the total order size is just $x_0 = 10$. ◇

Also the next example shows that the phenomenon of alternating trade signs in the optimal strategy can actually become quite dramatic.

Example 3.9 (Gaussian resilience). The Gaussian resilience function $G(t) = e^{-t^2}$ is, modulo constants, its own Fourier transform. Hence it is strictly positive definite. Figure 6 shows, however, that for increasing N the optimal strategy starts oscillating stronger and stronger between positive and negative trades. ◇

The strong oscillations found in the preceding two examples must be regarded as model irregularities, and market impact models that admit such an alternation between sell and buy trades cannot be regarded as viable and need to be excluded. It shows moreover that there can be irregularities in market impact models even when there are no price manipulation strategies in the sense explained in Remark 3.2, because both

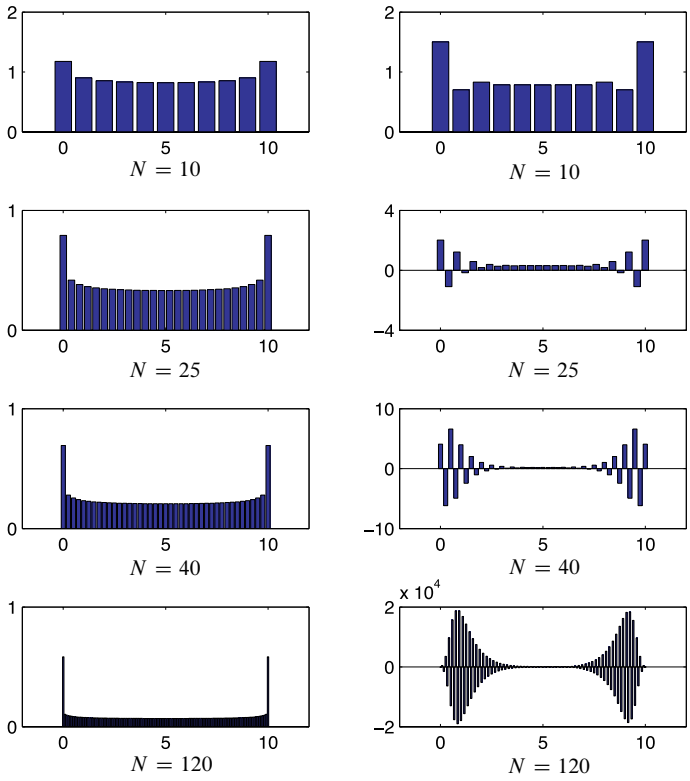

Figure 5. Optimal strategies for the resilience functions $G(t) = 1/(1+t)^2$ (left column) and $G(t) = 1/(1+t^2)$ (right column), with equidistant trading dates. Horizontal axes correspond to time, vertical axes to trade size. We chose $x_0 = 10$, $T = 10$, and the equidistant time grid, $t_i = iT/N$, for $N = 10,\ 25,\ 40,\ 120$. Note the dramatic increase of the size of individual trades as N becomes larger, in case of resilience function $G(t) = 1/(1+t^2)$.

resilience functions $G(t) := \frac{1}{1+t^2}$ and $G(t) = e^{-t^2}$ are strictly positive definite. The oscillations observed in Examples 3.8 and 3.9 thus motivate the following definition.

Definition 3.10 ([4]). A market impact model admits *transaction-triggered price manipulation* if the expected trade execution costs of a sell (buy) program can be decreased by intermediate buy (sell) trades. More precisely, in our setting, the model admits transaction-triggered price manipulation if there exists $x_0 \neq 0$, a time grid $\mathbb{T}$, and a vector $\boldsymbol{z} \in \mathbb{R}^{N+1}$, such that $\boldsymbol{z}^\top \mathbf{1} = x_0$ and

$$C_{\mathbb{T}}(\boldsymbol{z}) < \min\{C_{\mathbb{T}}(\boldsymbol{y}) \mid \boldsymbol{y}^\top \mathbf{1} = x_0 \text{ and all components of } \boldsymbol{y} \text{ have the same sign}\}.$$

It is not difficult to show that the absence of transaction-triggered price manipulation implies the absence of price manipulation strategies

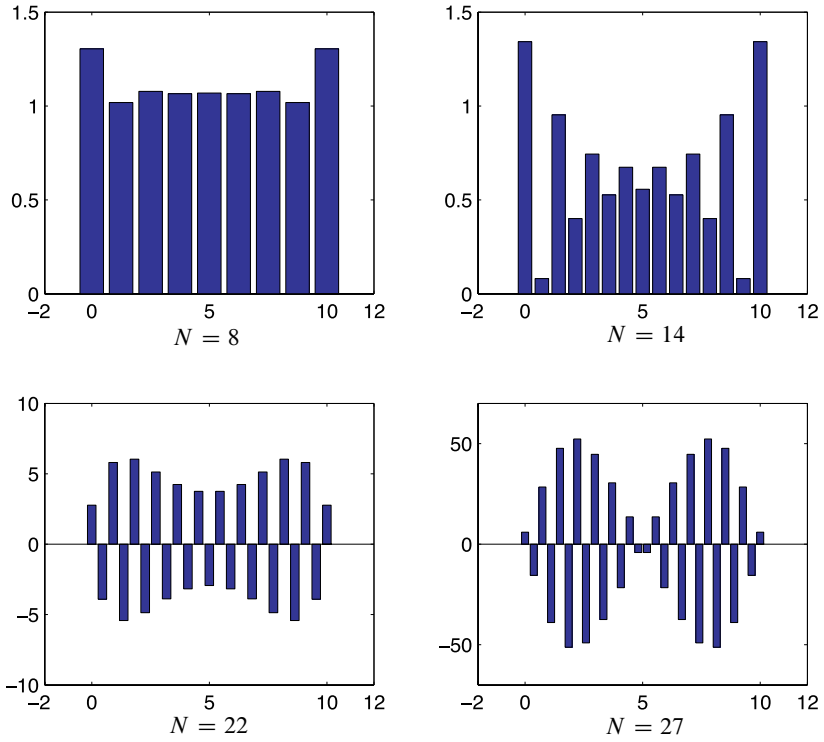

Figure 6. Optimal strategies for Gaussian resilience $G(t) = e^{-t^2}$. Horizontal axes correspond to time, vertical axes to trade size. We chose $x_0 = 10$, $T = 10$, and the equidistant time grid, $t_i = iT/N$, for $N = 8, 14, 22, 27$.

Our goal is now to formulate conditions on a positive definite resilience function that guarantee that all components of an optimal strategy $\boldsymbol{y}^*$ have the same sign. It is interesting to note that this problem is closely related to the *positive portfolio problem*, which consists in characterizing the absence of short sales in a Markowitz portfolio. This is a well-known problem in finance and aims at guaranteeing the nonnegativity of the minimizer in the following problem:

$$\text{minimize } \boldsymbol{y}^\top M\boldsymbol{y} - \boldsymbol{m}^\top \boldsymbol{y} \text{ under the constraint that } \boldsymbol{y}^\top \mathbf{1} = x_0, \tag{15}$$

where M is a covariance matrix of assets and $\boldsymbol{m}$ is the vector of (expected) returns. The positive portfolio problem has received considerable attention in finance but only relatively few results have been obtained to date; see Green [30], Nielsen [36], Best & Grauer [10], and the references therein. In our situation, $M_{ij} = G(|t_i - t_j|)$ is a covariance matrix as soon as G is positive definite, and so our problem of minimizing

$C_{\mathbb{T}}(y)$ with constraint $y^\top \mathbf{1} = x_0$ is a special case of (15). The following result can therefore also be understood as a contribution to the positive portfolio problem.

Theorem 3.11 ([4]). *For a convex, nonincreasing, and nonconstant resilience function G there are no transaction-triggered price manipulation strategies. If G is even strictly convex, then all trades in an optimal trade execution strategy are strictly positive for a buy program and strictly negative for a sell program.*

There is also the following partial converse to the preceding theorem. It applies in particular to strictly positive definite resilience functions that are strictly concave in a neighborhood of zero such as

$$\begin{aligned} G_0(t) &= e^{-t^2}, \quad G_1(t) := \frac{1}{1+t^2}, \\ G_2(t) &:= 2\frac{1-\cos \rho t}{t^2}, \quad \text{or} \quad G_3(t) := 1 + \frac{\sin \rho t}{t}. \end{aligned} \tag{16}$$

Proposition 3.12 ([4]). *Suppose that G is strictly positive definite and nonincreasing and*

$$\text{there are } s,\, t > 0,\, s \neq t, \text{ such that} \quad G(0) - G(s) < G(t) - G(t+s).$$

Then the model admits transaction-triggered price manipulation strategies.

3.2 Transient price impact in continuous time. Based on the paper [28], to which we refer for all details and proofs, we now extend the model of Section 3.1 to continuous time. To this end, we assume again that (S^0_t) is a rightcontinuous martingale defined on a given filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t), \mathbb{P})$ satisfying the usual conditions. We also assume that $\mathcal{F}_0$ is $\mathbb{P}$-trivial. A strategy will now be a stochastic process $X = (X_t)$ that describes the number of shares held by the trader at each time $t \geq 0$. It will be called an *admissible strategy* if

- the function $t \to X_t$ is leftcontinuous and adapted;
- the function $t \to X_t$ has finite and $\mathbb{P}$-a.s. bounded total variation;
- there exists $T > 0$ such that $X_t = 0$ $\mathbb{P}$-a.s. for all $t \geq T$.

When the admissible strategy X is applied, the price at time t is defined by

$$S_t = S^0_t + \int_{\{s<t\}} G(t-s)\, dX_s,$$

where $G\colon (0,\infty) \to [0,\infty)$ is a measurable function, the resilience function introduced in previous sections. We assume first that

$$G \text{ is bounded and } G(0) := \lim_{t \downarrow 0} G(t) \text{ exists.} \tag{17}$$

The assumption (17) will be relaxed later so as to include *weakly singular* resilience functions such as $G(t) = t^{-\gamma}$ for $0 < \gamma < 1$.

Following and extending the discussion presented in Section 3.1, one can deduce that the expected costs of an admissible strategy X are given by

$$-X_0 S_0^0 + \frac{1}{2}\mathbb{E}[\mathcal{C}(X)], \tag{18}$$

where

$$\mathcal{C}(X) := \iint G(|t-s|)\, dX_s\, dX_t.$$

As before, price manipulation in the sense of [32] can be excluded as soon as $\mathcal{C}(X) \geq 0$ for all admissible strategies. This latter property can be characterized by the following straightforward extension of Bochner's theorem.

Proposition 3.13 ([28]). *For a continuous resilience function satisfying assumption* (17)*, we have* $\mathcal{C}(X) \geq 0$ *for all admissible strategies* X *if and only if* $G(|\cdot|)$ *can be represented as the Fourier transform of a positive finite Borel measure* μ *on* $\mathbb{R}$*, i.e.,* $G(|x|) = \int e^{ixz}\, \mu(dz)$*. If, in addition, the support of* μ *is not discrete, then* $\mathcal{C}(X) > 0$ *for every nonzero admissible strategy* X*.*

Let us turn to the optimal trade execution problem, which consists in minimizing the expected costs for strategies liquidating a given long or short position of x_0 shares within a given time frame. It is clear that this problem is not well-defined as soon as the model admits price manipulation strategies. We will therefore assume from now on that the resilience function G is positive definite. In contrast to the discrete-time case, however, this requirement alone will not be sufficient to guarantee the existence of optimal strategies; see Theorem 3.18 below. It follows from (18) that every admissible strategy that minimizes the expected execution costs must have sample paths in the set of minimizers of $\mathcal{C}(\cdot)$ within the class

$$\mathcal{X}(x_0, \mathbb{T}) := \big\{X \,\big|\, \text{deterministic strategy with } X_0 = x_0 \text{ and support in } \mathbb{T}\big\}.$$

It is hence enough to study the minimization of $\mathcal{C}(\cdot)$ over the deterministic strategies in $\mathcal{X}(x_0, \mathbb{T})$. In particular, there will be at most one optimal strategy when G is strictly positive definite.

Our first result is a classical first-order condition characterizing optimal strategies as measure-valued solutions to generalized Fredholm integral equations of the first kind.

Proposition 3.14 ([28]). *Suppose that* G *is positive definite. Then* $X^* \in \mathcal{X}(x_0, \mathbb{T})$ *minimizes* $\mathcal{C}(\cdot)$ *over* $\mathcal{X}(x_0, \mathbb{T})$ *if and only if there is a constant* $\lambda \in \mathbb{R}$ *such that* X^* *solves the generalized Fredholm integral equation*

$$\int G(|t-s|)\, dX_s^* = \lambda \quad \text{for all } t \in \mathbb{T}. \tag{19}$$

In this case $\mathcal{C}(X^*) = \lambda x_0$*. In particular,* λ *must be nonzero as soon as* G *is strictly positive definite and* $x_0 \neq 0$*.*

To illustrate the application of Proposition 3.14 let us discuss the following examples.

Example 3.15 (Exponential resilience). Consider the case of exponential resilience, $G(t) = e^{-\rho t}$. We have seen above that the function G is strictly positive definite. The unique optimal trade execution strategy in $\mathcal{X}(x_0, [0, T])$ is given by

$$dX_s^* = \frac{-x_0}{\rho T + 2}\big(\delta_0(ds) + \rho\, ds + \delta_T(ds)\big).$$

This result was obtained in [37] using optimal control techniques, but it can also be proved very easily by simply checking that X^* solves the generalized Fredholm integral equation in Proposition 3.14; see [28]. ◇

Example 3.16 (Capped linear resilience). As in Example 3.6, we consider the resilience function $G(t) = (1 - \rho t)^+$ for some $\rho > 0$ and $\mathbb{T} = [0, T]$. For $\rho \le 1/T$, it is easy to verify that the strategy X^* that consists of two equal block trades of size $-x_0/2$ at $t = 0$ and $t = T$ and no trading in between satisfies the generalized Fredholm equation (19) and hence is the unique optimal strategy. Similarly, when $\rho = N/T$ for some $N \in \mathbb{N}$, then one shows that there is a unique optimal strategy X^*, which consists of $N + 1$ equidistant equal block trades of size $-x_0/(N + 1)$ at times $t_k := kT/N$, $k = 0, 1, \ldots, N$. Also in the general case, the unique optimal strategy corresponds to a purely discrete measure which can be given in explicit form; see [28] for details. An illustration is given in Figure 7. ◇

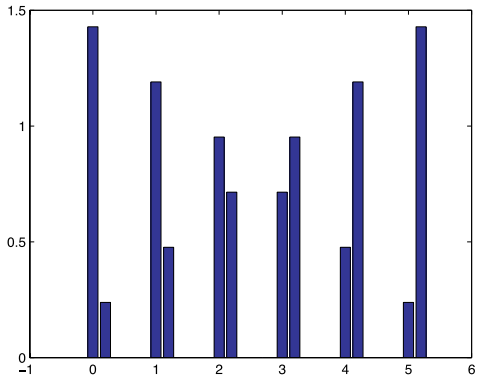

Figure 7. Optimal strategy for the capped linear resilience $G(t) = (1 - t)^+$, with $x_0 = -10$, $T = 5.15$ and $N = 5$. Horizontal axes correspond to time, vertical axes to trade size.

We now turn to the question of existence or nonexistence of optimal strategies.

Example 3.17 (Gaussian resilience). Let us consider the Gaussian resilience function $G(t) = e^{-t^2}$ and set $\mathbb{T} = [0, T]$. Clearly, G is strictly positive definite. Nevertheless,

it was already observed in Example 3.9 that for this resilience function optimal execution strategies in discrete time show dramatic oscillations when the grid of trading times becomes more refined. This divergence of the discrete-time optimal strategies is reflected by the fact that in continuous time optimal execution strategies exist only for the trivial case $x_0 = 0$. To prove this, suppose by the way of contradiction that $X^* \in \mathcal{X}(x_0, \mathbb{T})$ is an optimal strategy, with $x_0 \neq 0$. Then it would be a solution of the Fredholm integral equation (19) for some $\lambda \neq 0$. Let us consider the function $h(t) := \int_{[0,T]} e^{-(t-s)^2}\, dX_s^*$ for $t \in \mathbb{R}$. It is not hard to show that $h(t)$ is analytic in t. Hence, h cannot be equal to λ on $[0, T]$ unless it is constant on the entire real line. But this contradicts the fact that $h(t) \to 0$ as $|t| \to \infty$. Therefore X^* cannot exist. $\diamond$

Here is a general criterion that extends the argument given in the preceding example. It applies in particular to the resilience functions listed in (16).

Theorem 3.18 ([28]). *Suppose that $G(|\cdot|)$ can be represented as the Fourier transform of a finite positive Borel measure μ for which*

$$\int e^{\varepsilon x}\, \mu(dx) < \infty \quad \text{for some } \varepsilon > 0.$$

Suppose furthermore that the support of μ is not discrete. Then there are no optimal strategies in $\mathcal{X}(x_0, \mathbb{T})$ when $x_0 \neq 0$ and $\mathbb{T}$ is not discrete.

Now let us state our main result on existence, uniqueness and monotonicity of optimal strategies for the case of resilience functions satisfying the assumption (17).

Theorem 3.19 ([28]). *Let G be a nonconstant nonincreasing convex resilience function satisfying assumption (17). Then there exists a unique optimal strategy X^* within each class $\mathcal{X}(x_0, \mathbb{T})$, for given x_0 and $\mathbb{T}$. Moreover, X_t^* is a monotone function of t. That is, there is no transaction-triggered price manipulation in the considered market impact model.*

The preceding result is based on and extends Theorem 3.11. The idea behind it is to use a discrete-time approximation by means of a sequence of discrete sets $\mathbb{T}_1 \subset \mathbb{T}_2 \subset \cdots \subset \mathbb{T}$. On each set $\mathbb{T}_n$ we can apply Theorem 3.11 and obtain a unique optimal strategy X^n, which is a monotone step function. The measures $\frac{-1}{x_0} dX^n$ are probability measures on the compact set $\mathbb{T}$ and hence a subsequence converges weakly to a probability measure on $\mathbb{T}$, which in turn corresponds to a strategy X^* in $\mathcal{X}(x_0, \mathbb{T})$. One finally checks that X^* is optimal.

Next, let us relax the assumption (17) and allow the resilience function G to have a (weak) singularity at $t = 0$. More precisely, let us assume that

$$\begin{aligned} G\colon (0,\infty) \to [0,\infty) \quad & \text{is nonconstant, nonincreasing, convex,} \\ & \text{and satisfies } \int_0^1 G(t)\, dt < \infty. \end{aligned} \tag{20}$$

Under assumption (20), the earlier definition of the price at time t as

$$S_t = S_t^0 + \int_{\{s<t\}} G(t-s)\, dX_s \tag{21}$$

is no longer possible for every admissible strategy X. In particular, X must be continuous for (21) to make sense when $G(0+) = +\infty$. We therefore call an admissible strategy X *G-admissible* when its the total variation process $|X|$ satisfies

$$\iint G(|t-s|)\, d|X|_s\, d|X|_t < \infty.$$

We denote by $\mathcal{X}_G(x_0, \mathbb{T})$ the class of all G-admissible strategies in $\mathcal{X}(x_0, \mathbb{T})$. For $X \in \mathcal{X}_G(x_0, \mathbb{T})$ we define as before

$$\mathcal{C}(X) := \iint G(|t-s|)\, dX_s\, dX_t.$$

We have the following result.

Proposition 3.20 ([28]). *Let G be a resilience functions satisfying* (20)*. Then there exists a nonnegative Radon measure μ on $\mathbb{R}$ such that*

$$\mathcal{C}(X) = \int |\hat{X}(z)|^2\, \mu(dz), \tag{22}$$

where $\hat{X}(z) = \int e^{itz}\, dX_t$ for any G-admissible X.

Idea of proof. We first note that there exists a nonnegative Radon measure η such that G can be written as

$$G(t) = G(\infty-) + \int_{(0,\infty)} (y-t)^+\, \eta(dy).$$

Then one defines the function

$$\varphi(x) := \frac{1}{\pi} \int_{(0,\infty)} \frac{1-\cos xy}{x^2}\, \eta(dy)$$

and checks that (22) holds for

$$\mu(dx) = G(\infty-)\delta_0(dx) + \varphi(x)\, dx. \qquad \square$$

Let us now consider the existence of optimal strategies in $\mathcal{X}_G(x_0, \mathbb{T})$. A first observation is that optimal strategies will not exist if, for instance, $\mathbb{T}$ is a discrete set, because then $\mathcal{X}_G(x_0, \mathbb{T})$ is empty unless G is bounded. Otherwise, we have the following extension of Theorem 3.19.

Theorem 3.21 ([28]). *Suppose that assumption* (20) *holds and that the set $\mathcal{X}_G(x_0, \mathbb{T})$ is not empty. Then there exists a unique optimal strategy X^* in $\mathcal{X}_G(x_0, \mathbb{T})$. Moreover, X_t^* is a monotone function of t, and so there is no transaction-triggered price manipulation.*

The proof of the preceding theorem relies on approximating the weakly singular resilience function by bounded convex resilience functions G_n. To these functions we then apply Theorem 3.19 and use a similar convergence argument as sketched subsequently to Theorem 3.19.

Definition 3.22. A set $A \subset \mathbb{R}$ will be called *exceptional* when there exists a Borel set $B \supset A$ that is a nullset for every positive finite Borel measure ν on $\mathbb{R}$ for which $\iint G(|t-s|)\,\nu(ds)\,\nu(dt) < \infty$. We will say that a property holds *quasi everywhere* when it holds outside an exceptional set.

With this terminology, which is borrowed from potential theory, we can now investigate in which sense we can still define a price process via (21).

Proposition 3.23 ([28]). *For any G-admissible strategy X, $\int_{\{s<t\}} G(t-s)\,dX_s$, and hence the price process S_t in (21), is finite for quasi every $t \geq 0$.*

Now we state a variant of Proposition 3.14, which holds under assumption (20).

Proposition 3.24 ([28]). *A strategy $X^* \in \mathcal{X}_G(x_0, \mathbb{T})$ is optimal if and only if there is a constant λ such that X^* solves the generalized Fredholm integral equation*

$$\int G(|t-s|)\,dX_s^* = \lambda \quad \text{for quasi every } t \in \mathbb{T}.$$

Moreover, λ must be nonzero as soon as $x_0 \neq 0$.

Already in Definition 3.22 it became apparent that there is a close relation between classical potential theory and our theory of market impact. This relation stems from the fact that our cost functional $\mathcal{C}(\cdot)$ is just equal to the *Cartan energy* of a measure μ, namely to

$$E(\mu) := \iint G(|t-s|)\,\mu(ds)\,\mu(dt).$$

Here we assume that μ belongs to the set $\mathcal{M}(G, \mathbb{T})$ of all signed Borel measures with support in the compact set $\mathbb{T}$ and whose total variation $|\mu|$ satisfies

$$\iint G(|t-s|)\;|\mu|\,(ds)\;|\mu|\,(dt) < \infty.$$

Clearly, every μ in $\mathcal{M}(G, \mathbb{T})$ can be identified with a unique strategy within the class $\mathcal{X}_G(-\mu(\mathbb{T}), \mathbb{T})$. We also introduce the following three sets of measures: the set $\mathcal{M}^+(G, \mathbb{T})$ of all *positive* Borel measures in $\mathcal{M}(G, \mathbb{T})$; the set $\mathcal{M}_1(G, \mathbb{T})$ of all measures μ in $\mathcal{M}(G, \mathbb{T})$ with $\mu(\mathbb{T}) = 1$; the set $\mathcal{M}_1^+(G, \mathbb{T}) = \mathcal{M}^+(G, \mathbb{T}) \cap \mathcal{M}_1(G, \mathbb{T})$.

One of the goals of potential theory consists in finding and characterizing a *capacitary distribution* for a given compact $\mathbb{T}$. This is simply a minimizer μ^* of the energy $E(\mu)$ within the class $\mathcal{M}_1^+(G, \mathbb{T})$; see, e.g., Cartan [17], [18], Choquet [20], Fuglede [24], and Landkof [33]. Note that here the minimization is constrained to positive measures from the beginning. Usually the existence of μ^* is proved by a Cartan-type

theorem that asserts the completeness of the set $\mathcal{M}^+(G,\mathbb{T})$ with respect to the norm $\|\mu\| := \sqrt{E(\mu)}$; see, e.g., [33], Chapter I, § 4.

The results on market impact models as stated in this section compare as follows to these older results on capacitary distributions in the special case when G is as in (20). First, Theorems 3.19 and 3.21 present a new method to show the existence and uniqueness of capacitary distribution for all convex nonincreasing functions $G \geq 0$ without using a Cartan-type theorem. Second, in our method, the capacitary distribution is not obtained as a minimizer within the class $\mathcal{M}_1^+(G,\mathbb{T})$, but within the larger class of *signed* measures $\mathcal{M}_1(G,\mathbb{T})$. As a consequence, the capacitary distribution μ^* is the solution of an unconstrained optimization problem. This allows its characterization in terms of the simple first order condition

$$G_{\mu^*}(t) = 1 \quad \text{quasi everywhere on } \mathbb{T},$$

where

$$G_\mu(t) := \int G(|t-s|)\,\mu(ds).$$

Constrained optimization over positive measures, however, only leads to the "Kuhn–Tucker-type" conditions

$$\begin{aligned} G_{\mu^*}(t) &\geq 1 \quad \text{quasi everywhere on } \mathbb{T},\\ G_{\mu^*}(t) &= 1 \quad \mu^*\text{-a.e. on } \mathbb{T}; \end{aligned}$$

see, e.g., Donogue [21], p. 302.

The *capacity* of a compact set $\mathbb{T} \subset [0,\infty)$ is usually defined by one of the following two alternatives:

$$\mathrm{Cap}\,(\mathbb{T}) = \left(\inf_{\mu \in \mathcal{M}_1^+(G,\mathbb{T})} \iint G(|t-s|)\,\mu(ds)\,\mu(dt) \right)^{-1}$$

or

$$\overline{\mathrm{Cap}}\,(\mathbb{T}) = \sup\{\mu(\mathbb{T}) \mid \mu \in \mathcal{M}^+(G,\mathbb{T}),\ G_\mu \leq 1 \text{ quasi everywhere on } \mathbb{T}\}.$$

Our results yield a simple proof of the following result.

Proposition 3.25. *Let the function G satisfy (20). Then*

$$\mathrm{Cap}\,(\mathbb{T}) = \overline{\mathrm{Cap}}\,(\mathbb{T}).$$

for all compact sets $\mathbb{T} \subset [0,\infty)$.

Proof. We start with proving the inequality "$\leq$". Let μ^* be a minimizer of the energy functional $E(\mu)$ in $\mathcal{M}_1^+(G,\mathbb{T})$. Then, by Theorem 3.21, μ^* is also a minimizer in $\mathcal{M}_1(G,\mathbb{T})$ and so

$$G_{\mu^*}(t) = \lambda \text{ quasi everywhere on } \mathbb{T} \text{ for some } \lambda \in \mathbb{R}$$

by Proposition 3.24. Therefore $\mathrm{Cap}\,(\mathbb{T}) = \frac{1}{\lambda}$. On the other hand, the measure $\frac{1}{\lambda}\,\mu^*$ satisfies $G_{\frac{1}{\lambda}\mu^*} \leq 1$ quasi everywhere on $\mathbb{T}$ and this implies that

$$\overline{\mathrm{Cap}}\,(\mathbb{T}) \geq \frac{1}{\lambda}\,\mu^*(\mathbb{T}) = \frac{1}{\lambda} = \mathrm{Cap}\,(\mathbb{T}).$$

Now we prove the inequality " $\geq$". To this end suppose that the measure $\mu \in \mathcal{M}^+(G,\mathbb{T})$ is such that $G_\mu \leq 1$ quasi everywhere on $\mathbb{T}$. Then, for $c := \mu(\mathbb{T})$, the measure $\widehat{\mu} := \frac{1}{c}\mu$ is in $\mathcal{M}_1^+(G,\mathbb{T})$ and so

$$\iint G(|t-s|)\,\widehat{\mu}(ds)\,\widehat{\mu}(dt) = \int G_{\widehat{\mu}}(t)\,\widehat{\mu}(dt) \leq \frac{1}{c}.$$

Hence

$$\begin{aligned}\frac{1}{\mathrm{Cap}\,(\mathbb{T})} &= \inf_{\nu\in\mathcal{M}_1^+(G,\mathbb{T})} \iint G(|t-s|)\,\nu(ds)\,\nu(dt)\\ &\leq \iint G(|t-s|)\,\widehat{\mu}(ds)\,\widehat{\mu}(dt) \leq \frac{1}{c},\end{aligned}$$

i.e., $c \leq \mathrm{Cap}\,(\mathbb{T})$. Taking the supremum over μ gives the result. □

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The self-avoiding walk: A brief survey

Gordon Slade*

1 Self-avoiding walks

This article provides an overview of the critical behaviour of the self-avoiding walk model on $\mathbb{Z}^d$, and in particular discusses how this behaviour differs as the dimension d is varied. The books [29], [40] are general references for the model. Our emphasis will be on dimensions $d = 4$ and $d \geq 5$, where results have been obtained using the renormalisation group and the lace expansion, respectively.

An n-step self-avoiding walk from $x \in \mathbb{Z}^d$ to $y \in \mathbb{Z}^d$ is a map $\omega\colon \{0, 1, \ldots, n\} \to \mathbb{Z}^d$ with: $\omega(0) = x$, $\omega(n) = y$, $|\omega(i+1) - \omega(i)| = 1$ (Euclidean norm), and $\omega(i) \neq \omega(j)$ for all $i \neq j$. The last of these conditions is what makes the walk self-avoiding, and the second last restricts our attention to walks taking nearest-neighbour steps.

Let $d \geq 1$. Let $\mathcal{S}_n(x)$ be the set of n-step self-avoiding walks on $\mathbb{Z}^d$ from 0 to x. Let $\mathcal{S}_n = \cup_{x\in\mathbb{Z}^d} \mathcal{S}_n(x)$. Let $c_n(x) = |\mathcal{S}_n(x)|$, and let $c_n = \sum_{x\in\mathbb{Z}^d} c_n(x) = |\mathcal{S}_n|$. We declare all walks in $\mathcal{S}_n$ to be equally likely: each has probability c_n^{-1}. See Figure 1. We write $\mathbb{E}_n$ for expectation with respect to this uniform measure on $\mathcal{S}_n$.

What it is not:

• It is not the so-called "true" or "myopic" self-avoiding walk, i.e., the stochastic process which at each step looks at its neighbours and chooses uniformly from those visited least often in the past — the two models have different critical behaviour (see [28], [50] for recent progress on the "true" self-avoiding walk).
• It is by no means Markovian.
• It is not a stochastic process: the uniform measures on $\mathcal{S}_n$ do not form a consistent family.

2 Motivations

There are several motivations for studying the self-avoiding walk.

It provides an interesting and difficult problem in enumerative combinatorics: the determination of the probability of a walk in $\mathcal{S}_n$ requires the determination of c_n. It is also a challenging problem in probability, one that has proved resistant to the standard methods that have been successful for stochastic processes.

In addition, it is a fundamental example in the theory of critical phenomena in equilibrium statistical mechanics, and in particular is formally the $N \to 0$ limit of the N-vector model [15]. Finally, it is the standard model in polymer science of long chain

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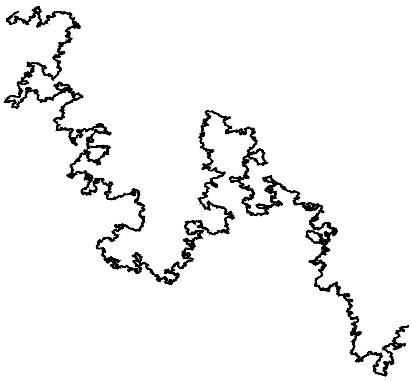


Figure 1. A random self-avoiding walk on $\mathbb{Z}^2$ with 10^6 steps. Illustration by T. Kennedy.

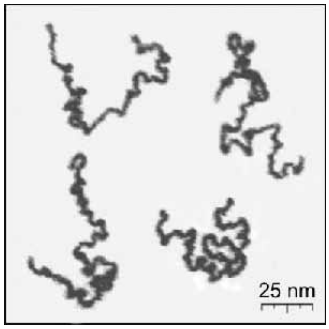


Figure 2. Appearance of real linear polymer chains as recorded using an atomic force microscope on surface under liquid medium. Chain contour length is ≈204 nm; thickness is ≈0.4 nm. [47]

polymers, with the self-avoidance condition modelling the excluded volume effect [14]. Figure 2 shows some 2-dimensional physical linear polymers, which may be compared with Figure 1.

3 Basic questions

Three basic questions are to determine the behaviour of:

- c_n = number of n-step self-avoiding walks,
- $\mathbb{E}_n|\omega(n)|^2 = \frac{1}{c_n}\sum_{\omega\in\mathcal{S}_n}|\omega(n)|^2$ = mean-square displacement,
- the scaling limit, i.e., find ν and X such that $n^{-\nu}\omega(\lfloor nt\rfloor) \Rightarrow X(t)$.

The inequality $c_{n+m} \le c_n c_m$ follows from the fact that the right-hand side counts the number of ways that an m-step self-avoiding walk can be concatenated onto the

end of an n-step self-avoiding walk, and such concatenations produce all $(n+m)$-step self-avoiding walks as well as contributions where the two pieces intersect each other. A consequence of this is that the *connective constant* $\mu = \lim_{n\to\infty} c_n^{1/n}$ exists, with $c_n \geq \mu^n$ for all n (see [40], Lemma 1.2.2, for the elementary proof). Since the d^n n-step walks that take steps only in the positive coordinate directions must be self-avoiding, we have $\mu \geq d$. And since the set of n-step walks without immediate reversals has cardinality $(2d)(2d-1)^{n-1}$ and contains all n-step self-avoiding walks, we have $\mu \leq 2d-1$. Several authors have considered the problem of tightening these bounds. For example, for $d = 2$ it is known that $\mu \in [2.625\,622,\ 2.679\,193]$ [33], [46] and the non-rigorous estimate[1] $\mu = 2.638\,158\,530\,31(3)$ was obtained in [31].

Another basic question is to determine the behaviour of the two-point function $G_z(x) = \sum_{n=0}^{\infty} c_n(x) z^n$, when z equals the radius of convergence $z_c = \mu^{-1}$ (see Corollary 3.2.6 in [40] for a proof that $z_c = \mu^{-1}$ for all x). There is now a strong body of evidence in favour of the predicted asymptotic behaviours:

$$c_n \sim A\mu^n n^{\gamma-1}, \quad \mathbb{E}_n|\omega(n)|^2 \sim Dn^{2\nu}, \quad G_{z_c}(x) \sim c|x|^{-(d-2+\eta)}, \tag{3.1}$$

with *universal* critical exponents γ, ν, η obeying Fisher's relation $\gamma = (2-\eta)\nu$. The exponents are written as in (3.1) to conform with a larger narrative in the theory of critical phenomena. For $d = 4$, logarithmic corrections are predicted: a factor $(\log n)^{1/4}$ should be inserted on the right-hand sides of the formulas for c_n and $\mathbb{E}_n|\omega(n)|^2$ (but no logarithmic correction to the leading behaviour of $G_{z_c}(x)$). A prediction of universality is the statement that the critical exponents depend only on the dimension d and not on fine details of how the model is defined. For example, the exponents are predicted to be the same for self-avoiding walks on the square, triangular and hexagonal lattices in two dimensions. This will not be the case for the connective constant or the amplitudes A, D, c, and for this reason the critical exponents have greater importance.

In the remainder of this paper, we discuss what has been proved concerning (3.1), dimension by dimension.

4 Dimension $d = 1$

At first glance it appears that for $d = 1$ the problem is trivial: $c_n = 2$ and $|\omega(n)| = n$ for all n, so $\gamma = \nu = 1$, and the walk moves ballistically left or right with speed 1.

However, the 1-dimensional problem is interesting for *weakly* self-avoiding walk. Let $g > 0$, let P_n be the uniform measure on *all* n-step nearest-neighbour walks $S = (S_0, S_1, \ldots, S_n)$ (with or without intersections), and let

$$Q_n(S) = \frac{1}{Z_n} \exp\Big[-g \sum_{i,j=0, i\neq j}^{n} \delta_{S_i,S_j}\Big] P_n(S),$$

where Z_n is a normalisation constant.

[1] The notation $\mu = 2.638\,158\,530\,31(3)$ is an abbreviation, common in the literature, for $\mu = 2.638\,158\,530\,31 \pm 0.000\,000\,000\,03$.

Theorem 4.1 ([17], [36]). *For every $g \in (0,\infty)$ there exist $\theta(g) \in (0,1)$ and $\sigma(g) \in (0,\infty)$ such that*

$$\lim_{n\to\infty} Q_n\left(\frac{|S_n| - \theta n}{\sigma\sqrt{n}} \le C\right) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{C} e^{-x^2/2} dx.$$

Note the ballistic behaviour for all $g > 0$: weakly self-avoiding walk is in the universality class of strictly self-avoiding walk. In particular, $\nu = 1$, in contrast to $\nu = \frac{1}{2}$ for $g = 0$. For any $g > 0$, no matter how small, the 1-dimensional weakly self-avoiding walk behaves in the same manner as the strictly self-avoiding walk, which corresponds to $g = \infty$. This is predicted to be the case in all dimensions.

The proof of Theorem 4.1 is based on large deviation methods. For a different approach based on the lace expansion, see [25]. The natural conjecture that $g \mapsto \theta(g)$ is (strictly) increasing remains unproved. For reviews of the case $d = 1$, see [26], [27].

5 Dimension $d = 2$

It was predicted by Nienhuis [44] that $\gamma = \frac{43}{32}$ and $\nu = \frac{3}{4}$ for $d = 2$. According to Fisher's relation, this gives $\eta = \frac{5}{24}$. This prediction has been verified by extensive Monte Carlo experiments (see, e.g., [39]), and by exact enumeration plus series analysis. For the latter, c_n is determined exactly for $n = 1, 2, \ldots, N$ and the partial sequence is analysed to determine its asymptotic behaviour. The *finite lattice method* is remarkable for $d = 2$, where c_n is known for all $n \le 71$ [32]; in particular,

$$c_{71} = 4\,190\,893\,020\,903\,935\,054\,619\,120\,005\,916 \approx 4.2 \times 10^{30}.$$

Concerning critical exponents and the scaling limit, a major breakthrough occurred in 2004 with the following result which connects self-avoiding walks and the Schramm–Loewner evolution (SLE).

Theorem 5.1 ([37], loosely stated). *If the scaling limit of the 2-dimensional self-avoiding walk exists and has a certain conformal invariance property, then the scaling limit must be* $\mathrm{SLE}_{8/3}$.

Moreover, known properties of $\mathrm{SLE}_{8/3}$ lead to calculations that rederive the values $\gamma = \frac{43}{32}$, $\nu = \frac{3}{4}$, assuming that $\mathrm{SLE}_{8/3}$ is indeed the scaling limit [37]. The above theorem is a breakthrough because it identifies the stochastic process $\mathrm{SLE}_{8/3}$ as the candidate scaling limit. However, the theorem makes a conditional statement, and the existence of the scaling limit (and therefore also its conformal invariance) remains as a difficult open problem. Numerical verifications that $\mathrm{SLE}_{8/3}$ is the scaling limit were performed in [34].

Current results fall soberingly short of existence of the scaling limit and critical exponents for $d = 2$. In fact, for $d = 2, 3, 4$ the best rigorous bounds on c_n are

$$\mu^n \le c_n \le \begin{cases} \mu^n e^{Cn^{1/2}} & (d=2), \\ \mu^n e^{Cn^{2/(d+2)}\log n} & (d=3,4). \end{cases}$$

The lower bound comes for free from $c_{n+m} \le c_n c_m$, and the upper bounds were proved in [19], [35]. Worse, for $d = 2, 3, 4$, neither of the inequalities $C^{-1}n \le \mathbb{E}_n|\omega(n)|^2 \le Cn^{2-\epsilon}$ (for some $C, \epsilon > 0$) has been proved. Thus, there is no proof that the self-avoiding walk moves away from its starting point at least as rapidly as simple random walk, nor sub-ballistically, even though it is preposterous that these bounds would not hold.

6 Dimension $d = 3$

For $d = 3$, there are no rigorous results for critical exponents. An early prediction for the values of ν, referred to as the Flory values [14], was $\nu = \frac{3}{d+2}$ for $1 \le d \le 4$. This does give the correct answer for $d = 1, 2, 4$, but it is not quite accurate for $d = 3$. The Flory argument is very remote from a rigorous mathematical proof.

For $d = 3$, there are three methods to compute the exponents. Field theory computations in theoretical physics [18] combine the $N \to 0$ limit for the N-vector model with an expansion in $\epsilon = 4 - d$ about dimension $d = 4$, with $\epsilon = 1$. Monte Carlo studies now work with walks of length 33,000,000 [12], using the pivot algorithm [41], [30]. Finally, exact enumeration plus series analysis has been used; currently the most extensive enumerations in dimensions $d \ge 3$ use the lace expansion [13], and for $d = 3$ walks have been enumerated to length $n = 30$, with the result $c_{30} = 270\,569\,905\,525\,454\,674\,614$. The exact enumeration estimates for $d = 3$ are $\mu = 4.684043(12)$, $\gamma = 1.1568(8)$, $\nu = 0.5876(5)$ [13]. Monte Carlo estimates are consistent with these values: $\gamma = 1.1575(6)$ [11] and $\nu = 0.587597(7)$ [12].

7 Dimension $d = 4$

7.1 The upper critical dimension. A prediction going back to [1] is that for $d = 4$,

$$c_n \sim A\mu^n (\log n)^{1/4}, \quad \mathbb{E}|\omega(n)|^2 \sim Dn(\log n)^{1/4}. \tag{7.1}$$

Correspondingly, when the 4-dimensional self-avoiding walk is rescaled by the factor $(Dn)^{-1/2}(\log n)^{-1/8}$, the scaling limit is predicted to be Brownian motion. The logarithmic corrections in (7.1) are typical of behaviour at the *upper critical dimension*, which is $d = 4$ for the self-avoiding walk. As discussed in Section 8 below, self-avoiding walks behave like simple random walks in dimensions greater than 4.

A quick way to guess that 4 is the upper critical dimension is to recall that the ranges of two independent Brownian motions do not intersect each other if and only if $d \ge 4$, a fact intimately related to the 2-dimensional nature of Brownian paths. Consequently, one might guess that conditioning a simple random walk not to intersect itself might have no noticeable effect on the scaling limit when $d \ge 4$.

7.2 Continuous-time weakly self-avoiding walk. Let X be the continuous-time simple random walk on $\mathbb{Z}^d$ with Exp(1) holding times and right-continuous sample paths.

In other words, the walk takes its nearest neighbour steps at the events of a rate-1 Poisson process. Let $\mathbb{E}_x$ denote expectation for this process started at $X(0) = x$. The local time at x up to time T is given by

$$t_{x,T} = \int_0^T \mathbb{1}_{X(s)=x}\, ds,$$

and the amount of self-intersection experienced by X up to time T is measured by

$$\int_0^T ds_1 \int_0^T ds_2 \mathbb{1}_{X(s_1)=X(s_2)} = \sum_{x\in\mathbb{Z}^d} t_{x,T}^2.$$

Let $g > 0$ and $x \in \mathbb{Z}^d$. The continuous-time weakly self-avoiding walk two-point function is defined by

$$G_{g,\lambda}(x) = \int_0^\infty \mathbb{E}_0(e^{-g\sum_{z\in\mathbb{Z}^d} t_{z,T}^2} \mathbb{1}_{X(T)=x}) e^{-\lambda T}\, dT,$$

where λ is a parameter (possibly negative) which is chosen in such a way that the integral converges. A subadditivity argument shows that there exists a *critical value* $\lambda_c = \lambda_c(g)$ such that $\sum_{x\in\mathbb{Z}^d} G_{g,\lambda}(x) < \infty$ if and only if $\lambda > \lambda_c$. The following theorem shows that the asymptotic behaviour of the critical two-point function has the same $|x|^{2-d}$ decay as simple random walk, i.e., $\eta = 0$, in all dimensions greater than *or equal to* 4, when g is small. In particular, there is no logarithmic correction at leading order when $d = 4$.

Theorem 7.1 ([8], [9]). *Let $d \geq 4$. There exists $\bar{g} > 0$ such that for each $g \in (0, \bar{g})$ there exists $c_g > 0$ such that as $|x| \to \infty$,*

$$G_{g,\lambda_c(g)}(x) = \frac{c_g}{|x|^{d-2}} (1 + o(1)).$$

The proof of Theorem 7.1 is based on a rigorous renormalisation method [8], [9] (see also [2]), discussed further below.

7.3 Hierarchical lattice and walk. Theorem 7.1 has precursors for the weakly self-avoiding walk on a 4-dimensional *hierarchical lattice*. The hierarchical lattice is a replacement of $\mathbb{Z}^d$ by a recursive structure which is well-suited to the renormalisation group, and which has a long tradition of use for development of renormalisation group methodology.

The hierarchical lattice $\mathbb{H}_{d,L}$ ia a countable group which depends on two integer parameters $L \geq 2$ and $d \geq 1$. It is defined to be the direct sum of infinitely many copies of the additive group $\mathbb{Z}_n = \{0, 1, \ldots, n-1\}$ with $n = L^d$. A vertex in the hierarchical lattice has the form $x = (\ldots, x_3, x_2, x_1)$ with each $x_i \in \mathbb{Z}_n$ and with all but finitely many entries equal to 0. For $x \in \mathbb{H}_{d,L}$, let

$$|x| = \begin{cases} 0 & \text{if all entries of } x \text{ are } 0, \\ L^N & \text{if } x_N \neq 0 \text{ and } x_i = 0 \text{ for all } i > N. \end{cases}$$

A metric (in fact an ultra-metric) on $\mathbb{H}_{d,L}$ is then defined by

$$\rho(x, y) = |x - y|.$$

To visualise the hierarchical lattice, an example of the vertices of a finite piece of the d-dimensional hierarchical lattice with parameters $L = 2$ and $d = 2$ is depicted in Figure 3. Vertices are arranged in nested blocks of cardinality L^{dj} where j is the block level.

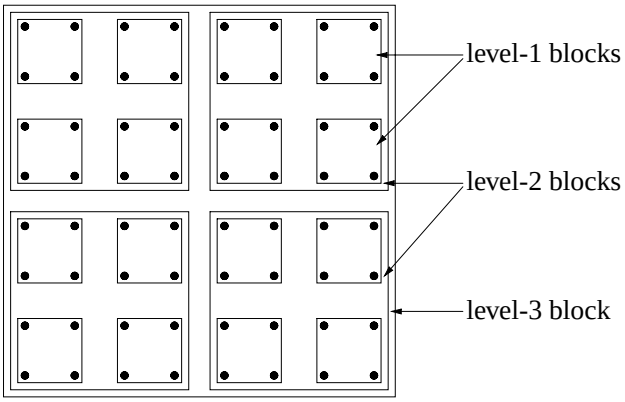


Figure 3. Vertices of the hierarchical lattice with $L = 2$, $d = 2$.

Every pair of vertices is joined by a bond, with the bonds labelled according to their level as depicted in Figure 4. The level $\ell(x, y)$ of a bond $\{x, y\}$ is defined to be the level of the smallest block that contains both x and y. The metric ρ on the hierarchical lattice is then given in terms of the level by

$$\rho(x, y) = L^{\ell(x,y)}.$$

There is more structure present in Figure 3 than actually exists within the hierarchical lattice. In particular, all vertices within a single level-1 block are distance L from each other, and their arrangement in a square in the figure has no relevance for the metric. With this in mind, the arrangement of the vertices as in Figure 3 serves to emphasise the difference between the hierarchical lattice and the Euclidean lattice $\mathbb{Z}^d$.

We now define a random walk on $\mathbb{H}_{d,L}$, in which the probability $P(x, y)$ of a jump from x to y in a single step is given by

$$P(x, y) = \text{const}\, \rho(x, y)^{-(d+2)}.$$

We consider both the discrete-time random walk, in which steps are taken at times $1, 2, 3, \ldots$, and also the continuous-time random walk in which steps are taken according to a rate-1 Poisson process. For the continuous-time process, the random walk Green

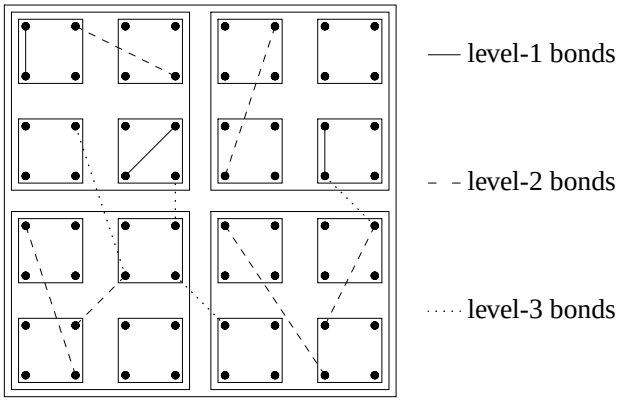


Figure 4. Bonds of the hierarchical lattice with $L = 2$, $d = 2$.

function is defined to be

$$G(x, y) = \int_0^\infty dT\, \mathbb{E}_x(\mathbb{1}_{X(T)=y}),$$

where $\mathbb{E}_x$ denotes expectation for the process X started at x. It is shown in [3] that for $d > 2$

$$G(x, y) = \text{const}\frac{1}{\rho(x, y)^{d-2}} \quad \text{if } x \neq y, \tag{7.2}$$

and in this sense the random walk on the hierarchical lattice behaves like a d-dimensional random walk.

The continuous-time weakly self-avoiding walk is defined as in Section 7.2, namely we modify the probability of a continuous-time random walk X on $\mathbb{H}_{d,L}$ by a factor $\exp[-g\sum_x t_{x,T}(X)^2]$. The prediction is that for all $g > 0$ and all $L \geq 2$ the weakly self-avoiding walk (with continuous or discrete time) on $\mathbb{H}_{d,L}$ has the same critical behaviour as the strictly self-avoiding on $\mathbb{Z}^d$ (at least for $d > 2$ where (7.2) holds). This has been exemplified for $d = 4$ in the series of papers [3], [5], [6], where, in particular, the following theorem is obtained. There are some details omitted here that are required for a precise statement, and we content ourselves with a loose statement that captures the main message from [5].

Theorem 7.2 ([5], loosely stated). *Fix $L \geq 2$. For the continuous-time weakly self-avoiding walk on the 4-dimensional hierarchical lattice $\mathbb{H}_{4,L}$, if $g \in (0, g_0)$ with g_0 sufficiently small, then there is a constant $c = c(g, L)$ such that*

$$\mathbb{E}^T_{0,g}|\omega(T)| \approx cT^{1/2}(\log T)^{1/8}\left[1 + \frac{\log\log T}{32\log T} + O\left(\frac{1}{\log T}\right)\right],$$

where the expectation on the left-hand side is that of weakly self-avoiding walk started at 0 and up to time T, and where the symbol $\approx$ requires an appropriate interpretation; see [5], *p.* 525, *for the details of this interpretation.*

It is also shown in [3] that $\eta = 0$ in the setting of Theorem 7.2. Very recently, related results for the critical two-point function and the susceptibility have been obtained in [21] for the *discrete-time* weakly self-avoiding walk on $\mathbb{H}_{4,L}$ with g sufficiently small and L sufficiently large. These results produce the predicted logarithmic correction for the susceptibility, closely related to (7.1).

The proofs of all these results for the 4-dimensional hierarchical lattice are based on renormalisation group methods, but the approach of [3], [5], [6] is very different from that of [21]. The approach of [21] is based on a direct analysis of the self-avoiding paths themselves. In contrast, the approach of [3], [5], [6], as well as the proof of Theorem 7.1, are based on a functional integral representation for the two-point function with no direct path analysis.

7.4 Functional integral representation. The point of departure of the proofs of Theorems 7.1–7.2, and more generally of the analysis in [3], [5], [6], [8], [9], [16], [43], is a functional integral representation for self-avoiding walks. Such representations have their roots in [45], [42], [38], [3] and recently have been summarised and extended in [7]. We now describe the representation for the continuous-time weakly self-avoiding walk on $\mathbb{Z}^4$.

In fact, the representation is valid for weakly self-avoiding walk on any finite set Λ, and an extension to $\mathbb{Z}^4$ requires a finite volume approximation followed by an infinite volume limit; the latter is not discussed here. For the present discussion, let Λ be an finite box in $\mathbb{Z}^d$, of cardinality M, and with periodic boundary conditions. Let Δ denote the lattice Laplacian on Λ. Let X be the continuous-time Markov process on Λ with generator Δ, and let $\mathbb{E}_x$ denote the expectation for this process started from $x \in \Lambda$. We define the weakly self-avoiding walk two-point function on Λ by

$$G_{x,y}^{\mathrm{wsaw},\Lambda} = \int_0^\infty \mathbb{E}_x\Big(e^{-g\sum_{z\in\Lambda} t_{z,T}^2}\mathbb{1}_{X(T)=y}\Big)e^{-\lambda T}\,dT,$$

where $g > 0$ and where $\lambda \in \mathbb{R}$ is chosen so that the integral converges.

Given $\varphi\colon \Lambda \to \mathbb{C}$, we write $\psi_x = \frac{1}{\sqrt{2\pi i}}d\varphi_x$, where $d\varphi_x$ denotes the differential and we fix any particular choice of the square root. For $x \in \Lambda$, we define

$$\tau_x = \varphi_x\bar{\varphi}_x + \psi_x \wedge \bar{\psi}_x,$$

where the wedge product is the usual anti-commuting product of differential forms, $\bar{\varphi}_x$ denotes the complex conjugate of φ_x, and $\bar{\psi}_x = \frac{1}{\sqrt{2\pi i}}d\bar{\varphi}_x$. Forms are always multiplied using the wedge product, and we drop the wedge from the notation in what follows. We also define

$$S = \sum_{x,y\in\Lambda}(-\Delta_{x,y})\varphi_x\bar{\varphi}_y + \sum_{x,y\in\Lambda}(-\Delta_{x,y})\psi_x\bar{\psi}_y.$$

The integral representation for $G_{x,y}^{\mathrm{wsaw},\Lambda}$ is

$$G_{x,y}^{\mathrm{wsaw},\Lambda} = \int e^{-S}e^{-\sum_{x\in\Lambda}(g\tau_x^2+\lambda\tau_x)}\bar{\varphi}_x\varphi_y, \tag{7.3}$$

where the integral is defined by the following procedure.

First, the integrand, which involves functions of differential forms, is defined by its formal power series about its degree-zero part. For example, with the abbreviated notation $S = -\varphi\Delta\bar{\varphi} - \psi\Delta\bar{\psi}$, the expansion of e^{-S} is

$$e^{-S} = e^{\varphi\Delta\bar{\varphi}+\psi\Delta\bar{\psi}} = e^{\varphi\Delta\bar{\varphi}} \sum_{N=1}^{|\Lambda|} \frac{1}{N!} \left(\psi\Delta\bar{\psi}\right)^N ,$$

where the sum is a *finite* sum due to the anti-commutativity of the wedge product. Second, in the expansion of the integrand, we keep only terms with one factor $d\varphi_x$ and one $d\bar{\varphi}_x$ for each $x \in \Lambda$, and discard the rest. Then we write $\varphi_x = u_x + iv_x$, $\bar{\varphi}_x = u_x - iv_x$ and similarly for the differentials, use the anti-commutativity of the wedge product to rearrange the differentials to $\prod_{x\in\Lambda} du_x dv_x$, and finally perform the resulting Lebesgue integral over $\mathbb{R}^{2|\Lambda|}$. For further discussion and a proof of (7.3), see [7].

The approach of [3], [5], [6], [8], [9] to the weakly self-avoiding walk is to study the integral on the right-hand side of (7.3), and simply to forget about the walks themselves. The differential form $e^{-S}e^{-V(\Lambda)}$, where $V(\Lambda) = \sum_{x\in\Lambda}(g\tau_x^2 + \lambda\tau_x)$, has a property called *supersymmetry* (see [7] for a discussion of this in our context). In physics, roughly speaking, this corresponds to symmetry under an interchange of bosons and fermions. Supersymmetry has interesting consequences. For example, a general theorem (see [6], [7]) implies that

$$\int e^{-S}e^{-V(\Lambda)} = 1. \tag{7.4}$$

We redefine S as $S = \varphi(\epsilon I - \Delta)\bar{\varphi} - \psi(\epsilon I - \Delta)\bar{\psi}$ for some (small) choice of $\epsilon > 0$, where I denotes the $|\Lambda| \times |\Lambda|$ identity matrix. This can be regarded an adjustment of the parameter λ. Then, given a form F, we write

$$\mathbb{E}_C F = \int e^{-S} F,$$

where $C = (\epsilon I - \Delta)^{-1}$. By (7.4), $\mathbb{E}_C 1 = 1$. We regard $\mathbb{E}_C$ as a mixed bosonic-fermionic Gaussian expectation, with covariance C. The operation $\mathbb{E}_C$ has much in common with standard Gaussian integration, and for this reason we write $\mathbb{E}$ for expectation, but this is not ordinary probability theory and the expectations are actually Grassmannian integrals.

7.5 The renormalisation group map. The renormalisation group approach of [8], [9] (and of several other authors as well) is based on a finite-range decomposition of the covariance $C = (\epsilon I - \Delta)^{-1}$, due to [4]. Fix a large integer L and suppose that $|\Lambda| = L^{Nd}$. Using the results of [4], it is possible to write

$$C = \sum_{j=1}^{N} C_j$$

where the C_j's are positive semi-definite operators with the important finite-range property

$$C_j(x,y) = 0 \quad \text{if } |x-y| \geq L^j.$$

The C_j's also have a certain self-similarity property, and obey the estimates

$$\sup_{x,y} \sup_{|\alpha|\leq\alpha_0} \left|\nabla_x^\alpha \nabla_y^\alpha C_j(x,y)\right| \leq \text{const} L^{-(j-1)(2+2|\alpha|)}$$

for given α_0 and for $j < N$, with a j-independent constant. This decomposition induces a field decomposition

$$\varphi = \sum_{j=1}^N \zeta_j, \quad d\varphi = \sum_{j=1}^N d\zeta_j,$$

and allows the expectation to be performed iteratively:

$$\mathbb{E}_C = \mathbb{E}_{C_N} \circ \cdots \circ \mathbb{E}_{C_2} \circ \mathbb{E}_{C_1},$$

where $\mathbb{E}_{C_j}$ integrates out the scale-j fields $\zeta_j, \bar{\zeta}_j, d\zeta_j, d\bar{\zeta}_j$. Under $\mathbb{E}_j$, the scale-j fields are uncorrelated when separated by distance greater than L^j, in contrast to the long-range correlations of the full expectation $\mathbb{E}_C$.

In what follows, we discuss the approach of [9] towards a direct evaluation of the integral $\int e^{-S} e^{-V(\Lambda)}$. In fact, as already pointed out above, it is a consequence of supersymmetry that this integral is equal to 1, so direct evaluation is not necessary. However, the method described below extends also to evaluate the integral in (7.3), and it is easier to discuss the method now in the simpler setting without the factor $\bar{\varphi}_x \varphi_y$ in the integrand.

We write $(\phi, d\phi) = (\varphi, \bar{\varphi}, d\varphi, d\bar{\varphi})$ and $(\xi, d\xi) = (\zeta, \bar{\zeta}, d\zeta, d\bar{\zeta})$. We set $\phi_j = \sum_{i=j+1}^N \xi_i$, with $\phi_0 = \phi$, $\phi_N = 0$; this gives

$$\phi_j = \phi_{j+1} + \xi_{j+1}.$$

Let $Z_0 = Z_0(\phi, d\phi) = e^{-V(\Lambda)}$, let

$$\begin{aligned} Z_1(\phi_1, d\phi_1) &= \mathbb{E}_{C_1} Z_0(\phi_1 + \xi_1, d\phi_1 + d\xi_1), \\ Z_2(\phi_2, d\phi_2) &= \mathbb{E}_{C_2} Z_1(\phi_2 + \xi_2, d\phi_2 + d\xi_2) = \mathbb{E}_{C_2} \mathbb{E}_{C_1} Z_0, \end{aligned}$$

and, in general, let

$$Z_j(\phi_j, d\phi_j) = \mathbb{E}_{C_j} \cdots \mathbb{E}_{C_1} Z_0(\phi, d\phi).$$

Our goal now is to compute directly

$$Z_N = \mathbb{E}_C Z_0 = \mathbb{E}_C e^{-V(\Lambda)}.$$

This leads us to study the *renormalisation group map* $Z_j \mapsto Z_{j+1}$ given by

$$Z_{j+1}(\phi_{j+1}, d\phi_{j+1}) = \mathbb{E}_{C_{j+1}} Z_j(\phi_{j+1} + \xi_{j+1}, d\phi_{j+1} + d\xi_{j+1}).$$

The finite-range property of C_j, together with our choice of side length L^N for Λ, leads naturally to the consideration of Λ as being paved by blocks of side L^j. Let $\mathcal{P}_j$ denote the set of finite unions of such blocks. Given forms F, G defined on $\mathcal{P}_j$, we define the product

$$(F \circ G)(\Lambda) = \sum_{X \in \mathcal{P}_j} F(X)G(\Lambda \setminus X).$$

For $X \in \mathcal{P}_0$, let

$$I_0(X) = e^{-V(X)}, \quad K_0(X) = \mathbb{1}_{X=\varnothing}.$$

Then we can write

$$Z_0 = I_0(\Lambda) = (I_0 \circ K_0)(\Lambda).$$

The method of [9] consists in the determination of an inductive parametrisation

$$Z_j = (I_j \circ K_j)(\Lambda), \qquad Z_{j+1} = \mathbb{E}_{C_{j+1}} Z_j = (I_{j+1} \circ K_{j+1})(\Lambda),$$

with each I_j parametrised in turn by a polynomial V_j evaluated at $\phi_j, d\phi_j$, given by

$$V_{j,x} = g_j \tau_x^2 + \lambda_j \tau_x + z_j \tau_{\Delta,x},$$

with

$$\tau_{\Delta,x} = \varphi_x(-\Delta\bar{\varphi})_x + (-\Delta\varphi)_x\bar{\varphi}_x + \frac{1}{2\pi i} d\varphi_x(-\Delta d\bar{\varphi})_x + \frac{1}{2\pi i}(-\Delta d\varphi)_x d\bar{\varphi}_x.$$

The term K_j accumulates error terms. The map $I_j \mapsto I_{j+1}$ is thus given by the *flow of the coupling constants* $(g_j, \lambda_j, z_j) \mapsto (g_{j+1}, \lambda_{j+1}, z_{j+1})$, and hence the renormalisation group map becomes the dynamical system

$$(g_j, \lambda_j, z_j, K_j) \mapsto (g_{j+1}, \lambda_{j+1}, z_{j+1}, K_{j+1}).$$

At the critical point, this dynamical system is driven to zero, and this permits the asymptotic computation of the two-point function. Details are given in [9].

8 Dimensions $d \geq 5$

8.1 Results. The following theorem shows that above the upper critical dimension the self-avoiding walk behaves like simple random walk, in the sense that $\gamma = 1$, $\nu = \frac{1}{2}$, $\eta = 0$, and the scaling limit is Brownian motion.

Theorem 8.1 ([22], [23]). *For $d \geq 5$, there are positive constants A, D, c, ϵ such that*

$$c_n = A\mu^n[1 + O(n^{-\epsilon})],$$
$$\mathbb{E}_n|\omega(n)|^2 = Dn[1 + O(n^{-\epsilon})],$$

and the rescaled self-avoiding walk converges weakly to Brownian motion:

$$\frac{\omega(\lfloor nt \rfloor)}{\sqrt{Dn}} \implies B_t.$$

Also [20], *as* $|x| \to \infty$,

$$G_{z_c}(x) = c|x|^{-(d-2)}[1 + O(|x|^{-\epsilon})].$$

The proofs of these results are based on the lace expansion, a technique that was introduced by Brydges and Spencer [10] to study the weakly self-avoiding walk in dimensions $d > 4$. Since 1985, the method has been highly developed and extended to several other models: percolation ($d > 6$), oriented percolation ($d + 1 > 4 + 1$), contact process ($d > 4$), lattice trees and lattice animals ($d > 8$), and the Ising model ($d > 4$). For a review and references, see [49].

The lace expansion requires a small parameter for its convergence. For the nearest-neighbour model in dimensions $d \geq 5$, the small parameter is proportional to $(d-4)^{-1}$, which is not very small when $d = 5$. Because of this, the proof of Theorem 8.1 is computer assisted. The weakly self-avoiding walk has an intrinsic small parameter g, and it is therefore easier to analyse than the strictly self-avoiding walk. Another option for the introduction of a small parameter is to consider the *spread-out* strictly self-avoiding walk, which takes steps within a box of side length L centred at its current position; this model also can be more easily analysed by taking L large to provide a small parameter L^{-1}.

The spread-out model can be generalised to have non-uniform step weights. For example, given $\alpha > 0$, and an n-step self-avoiding walk ω on $\mathbb{Z}^d$ taking *arbitrary* steps, we define the weight

$$W(\omega) = \prod_{i=1}^{n} \frac{1}{(L^{-1}|\omega(i-1) - \omega(i)| \wedge 1)^{d+\alpha}},$$

and consider the probability distribution on self-avoiding walks that corresponds to this weight. The following theorem, which is proved using the lace expansion, shows how the upper critical dimension changes once $\alpha \leq 2$ and the step weights have infinite variance.

Theorem 8.2 ([24]). *Let* $\alpha > 0$ *and*

$$f_\alpha(n) = a_\alpha \begin{cases} n^{-1/(\alpha \wedge 2)} & \alpha \neq 2, \\ (n \log n)^{-1/2} & \alpha = 2, \end{cases}$$

for a suitably chosen (explicit) constant a_α. *For* $d > 2(\alpha \wedge 2)$ *and for* L *sufficiently large, the process* $X_n(t) = f_\alpha(n)\omega(\lfloor nt \rfloor)$ *converges in distribution to an* α*-stable Lévy process if* $\alpha < 2$ *and to Brownian motion if* $\alpha \geq 2$.

In [43], the weakly self-avoiding walk with long-range steps characterised by $\alpha = \frac{3+\epsilon}{2}$, with small $\epsilon > 0$, is studied in dimension 3, which is *below* the upper critical dimension $3+\epsilon$. The main result is the control of the renormalisation group trajectory, a first step towards the computation of the asymptotics for the critical two-point function below the upper critical dimension. This is a rigorous version, for the weakly self-avoiding walk, of the expansion in $\epsilon = 4 - d$ discussed in [51]. The work of [43] is based on the functional integral representation outlined in Section 7.4.

8.2 The lace expansion. The original formulation of the lace expansion in [10] made use of a particular class of ordered graphs which Brydges and Spencer called "laces." Later it was realised that the same expansion can be obtained by repeated use of inclusion-exclusion [48]. We now sketch the inclusion-exclusion approach very briefly; further details can be found in [40] or [49].

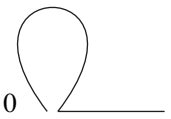
The lace expansion identifies a function $\pi_m(x)$ such that for $n \geq 1$,

$$c_n(x) = \sum_{y \in \mathbb{Z}^d} c_1(y) c_{n-1}(x-y) + \sum_{m=2}^{n} \sum_{y \in \mathbb{Z}^d} \pi_m(y) c_{n-m}(x-y). \tag{8.1}$$

In fact, it is possible to see that (8.1) *defines* $\pi_m(x)$, but the expansion will produce a useful expression for $\pi_m(x)$. We begin with the identity

$$c_n(x) = \sum_{y \in \mathbb{Z}^d} c_1(y) c_{n-1}(x-y) - R_n^{(1)}(x),$$

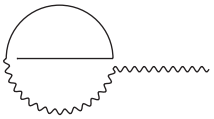
where $R_n^{(1)}(x)$ counts the number of terms which are included on the first term of the right-hand side but excluded on the left, namely the number of n-step walks which start at 0, end at x, and are self-avoiding except for an obligatory single return to 0. This is denoted schematically by

$R_n^{(1)}(x) = 0$  $x.$

If we relax and subsequently account for the constraint that the loop in the above diagram avoid the vertices in the "tail," then we are led to

$$R_n^{(1)}(x) = \sum_{m=2}^{n} u_m c_{n-m}(x) - R_n^{(2)}(x),$$

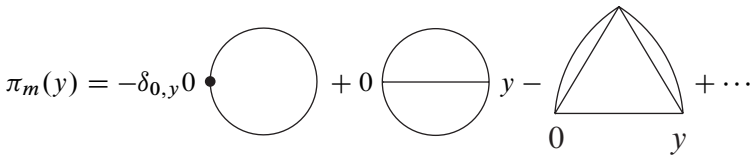
where u_m is the number of m-step self-avoiding returns, and

$R_n^{(2)}(x) = 0$  $x.$

In the above diagram, the proper line represents a self-avoiding return, while the wavy line represents a self-avoiding walk from 0 to x constrained to intersect the proper line. Repetition of the inclusion-exclusion process leads to

$$c_n(x) = \sum_{y \in \mathbb{Z}^d} c_1(y) c_{n-1}(x-y) + \sum_{m=2}^{n} \sum_{y \in \mathbb{Z}^d} \pi_m(y) c_{n-m}(x-y)$$

with



and where there are specific rules for which lines may intersect which in the diagrams on the right-hand side. These rules can be conveniently accounted for using the concept of lace.

We put (8.1) into a generating function to obtain

$$G_z(x) = \sum_{n=0}^{\infty} c_n(x) z^n = \delta_{0,x} + z \sum_{y \in \mathbb{Z}^d} c_1(y) G_z(x-y) + \sum_{y \in \mathbb{Z}^d} \Pi_z(y) G_z(x-y), \tag{8.2}$$

with

$$\Pi_z(y) = \sum_{m=2}^{\infty} \pi_m(y) z^m.$$

For $k \in [-\pi, \pi]^d$, let $\hat{f}(k) = \sum_x f(x) e^{ik \cdot x}$ denote the Fourier transform of an absolutely summable function f on $\mathbb{Z}^d$. From (8.2), we obtain

$$\hat{G}_z(k) = \frac{1}{1 - z\hat{c}_1(k) - \hat{\Pi}_z(k)}.$$

Note that setting $\hat{\Pi}_z(k)$ equal to zero yields the Fourier transform of the two-point function of simple random walk, and hence $\hat{\Pi}_z(k)$ encapsulates the self-avoidance.

8.3 One idea from the proof of Theorem 8.1. Let $\hat{F}_z(k) = 1/\hat{G}_z(k)$. By definition, $\hat{G}_z(0) = \sum_{n=0}^{\infty} c_n z^n$. Since $\lim_{n\to\infty} c_n^{1/n} = \mu = z_c^{-1}$, $\hat{G}_z(0)$ has radius of convergence z_c, and since $c_n \geq \mu^n$, $\hat{F}_{z_c}(0) = 0$. Suppose that it is possible to perform a joint Taylor expansion of $\hat{F}$ in k and z about the points $k = 0$ and $z = z_c$. The linear term in k vanishes by symmetry, so that

$$\hat{F}_z(k) = \hat{F}_z(k) - \hat{F}_{z_c}(0) \approx a|k|^2 + b\Big(1 - \frac{z}{z_c}\Big), \quad \text{for } k \approx 0,\ z \approx z_c^-,$$

with $a = \frac{1}{2d} \nabla_k^2 \hat{F}_{z_c}(0)$ and $b = -z_c \partial_z \hat{F}_{z_c}(0)$. We assume now that a and b are finite, although it is an important part of the proof to establish this, and it is not expected to be true when $d \leq 4$. Then

$$\hat{G}_z(k) \approx \frac{1}{a|k|^2 + b(1 - \frac{z}{z_c})}, \quad \text{for } k \approx 0,\ z \approx z_c^-, \tag{8.3}$$

which is essentially the corresponding generating function for simple random walk.

For this to work, it is necessary in particular that $z_c \partial_z \hat{\Pi}_{z_c}(k)$ be finite. The leading term in this derivative, due to the first term $\sum_{m=2}^{\infty} u_m z^m$ in the diagrammatic expansion for $\hat{\Pi}_z(k)$, is $\sum_{m=2}^{\infty} m u_m z_c^m$. By considering the factor m to be the number of ways to choose a nonzero vertex on a self-avoiding return, and by relaxing the constraint that the two parts of this return (separated by the chosen vertex) avoid each other, we find that this contribution is bounded above by

$$\sum_{m=2}^{\infty} m u_m z_c^m \le \sum_{x \in \mathbb{Z}^d} G_{z_c}(x)^2 = \int_{[-\pi,\pi]^d} \hat{G}_{z_c}(k)^2 \frac{d^d k}{(2\pi)^d}, \tag{8.4}$$

where the equality follows from Parseval's relation. A reason to be hopeful that this might lead to a finite upper bound is that if we insert the simple random walk behaviour on the right-hand side of (8.3) into (8.4) then we obtain

$$\int_{[-\pi,\pi]^d} \hat{G}_{z_c}(k)^2 \frac{d^d k}{(2\pi)^d} \approx \int_{[-\pi,\pi]^d} \frac{1}{|k|^4} \frac{d^d k}{(2\pi)^d} < \infty \quad \text{for } d > 4.$$

Here we have assumed what it is that we are trying to prove, but the proof finds a way to exploit this kind of self-consistent argument. For the details, we refer to [22], [23], or, in the much simpler setting of the spread-out model, to [49].

9 Conclusions

Our current understanding of the critical behaviour of the self-avoiding walk can be summarised as follows:

- $d = 1$: ballistic behaviour is trivial for the nearest-neighbour strictly self-avoiding walk, but is interesting for the weakly self-avoiding walk.
- $d = 2$: *if* the scaling limit can be proven to exist and to be conformally invariant *then* the scaling limit is $\mathrm{SLE}_{8/3}$, $\mathrm{SLE}_{8/3}$ explains the values $\gamma = \frac{43}{32}$ and $\nu = \frac{3}{4}$, currently there is no proof that the scaling limit exists.
- $d = 3$: numerically $\gamma \approx 1.16$ and $\nu \approx 0.588$, there are no rigorous results, and there is no idea how to describe the scaling limit as a stochastic process.
- $d = 4$: renormalisation group methods have proved that $\eta = 0$ for continuous-time weakly self-avoiding walk; on a 4-dimensional hierarchical lattice $\gamma = 1$ and $\nu = \frac{1}{2}$, both with log corrections, and $\eta = 0$.
- $d \ge 5$: the problem is solved using the lace expansion, $\gamma = 1$, $\nu = \frac{1}{2}$, $\eta = 0$, and the scaling limit is Brownian motion.

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L^p-independence of growth bounds of Feynman–Kac semigroups

Masayoshi Takeda*

1 Introduction

A. Beurling and J. Deny [6], [7] initiated the theory of Dirichlet forms. Using potential theory of Dirichlet forms, M. Fukushima [23] succeeded in the construction of symmetric Hunt processes associated with Dirichlet forms. Since then, the theory of Dirichlet forms has been developed by many persons as a useful tool for analyzing symmetric Markov processes (see e.g. [8], [24], [29], [30]). The theory of Dirichlet forms is an L^2-theory, which is one reason why the theory is suitable for treating singular Markov processes. On the other hand, the theory of Markov processes is, in a sense, an L^1-theory. To bridge this gap, we study here the L^p-independence of growth bounds of Markov semigroups, more generally, of generalized Feynman–Kac (Schrödinger) semigroups. The L^p-independence enables us to control L^∞-properties of the symmetric Markov process; in fact, we can state, in terms of the bottom of L^2-spectrum, a necessary and sufficient condition for the integrability of Feynman–Kac functionals ([36]) and for the stability of Gaussian two-sided estimates of Schrödinger heat kernels ([37]).

For the proof of the L^p-independence, we apply arguments in the Donsker–Varadhan large deviation theory. The large deviation principle for a symmetric Markov process is governed by its Dirichlet form, namely, the rate function is identified with its Dirichlet form. Hence we can expect that the L^p-independence is fulfilled for symmetric Markov processes satisfying the large deviation principle. This is our key idea throughout this paper.

Let X be a locally compact separable metric space and m a positive Radon measure on X with full support. Let $\mathbb{M} = (X_t, \mathbb{P}_x, \zeta)$ be an irreducible m-symmetric Markov process on X with strong Feller property. Here ζ is the lifetime of $\mathbb{M}$. We further assume that $\mathbb{M}$ is in Class (I) or Class (II) (Definition 2.1, Definition 2.2 in Section 2). Let μ be a signed smooth Radon measure on X in Class $\mathcal{K}_\infty$ (Definition 3.1) and F a symmetric function on $X \times X$ in Class $\mathcal{A}_2$ (Definition 3.2). We define the additive functional $A_t(\mu + F)$ by

$$A_t(\mu + F) = A_t(\mu) + A_t(F) = A_t(\mu) + \sum_{0<s\le t} F(X_{s-}, X_s).$$

Here $A_t(\mu)$ is the continuous additive functional with Revuz correspondence to μ (see (2.3) below). The second term $A_t(F)$ is a purely discontinuous additive functional

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which varies when the Markov process X_t jumps on the support of F. The additive functional $A_t(\mu + F)$ is quite general. In fact, it is known from a result of Motoo that if an additive functional is purely discontinuous and quasi-left-continuous, then it is of the form $A_t(F)$ (S. Watanabe [46]).

We denote by $(N(x, dy), H_t)$ the Lévy system of $\mathbb{M}$. We define the generalized Feynman–Kac semigroup $\{p_t^{\mu+F}\}_{t>0}$ by

$$p_t^{\mu+F} f(x) = \mathbb{E}_x[\exp(A_t(\mu + F)) f(X_t)],$$

and the Schrödinger type operator formally by

$$\mathcal{H}^{\mu+F} f = \mathcal{L} f + \mu f + \mu_H \mathbf{F} f,$$
$$\mu_H \mathbf{F} f = \left(\int_X \left(e^{F(x,y)} - 1 \right) f(y) N(x, dy) \right) \mu_H(dx),$$

where $\mathcal{L}$ is the generator of $\mathbb{M}$ and μ_H the Revuz measure of H_t. We then see that the semigroup $\{p_t^{\mu+F}\}_{t>0}$ is the one generated by $\mathcal{H}^{\mu+F}$, $p_t^{\mu+F} = \exp(t\mathcal{H}^{\mu+F})$.

We define the L^p-growth bound of $\{p_t^{\mu+F}\}_{t>0}$ by

$$\lambda_p(\mu + F) = -\lim_{t\to\infty} \frac{1}{t} \log \| p_t^{\mu+F} \|_{p,p}, \quad 1 \le p \le \infty,$$

where $\|\cdot\|_{p,p}$ is the operator norm from $L^p(X; m)$ to $L^p(X; m)$. The L^p-independence of the growth bounds of $\{p_t^{\mu+F}\}_{t>0}$ means that

$$\lambda_p(\mu + F) = \lambda_2(\mu + F), \quad 1 \le p \le \infty.$$

We now state our main theorem.

Theorem 1.1 ([39], [44]). *Let μ be a measure in the class $\mathcal{K}_\infty$ and F a function in the class $\mathcal{A}_2$.*

(i) *Assume that $\mathbb{M}$ is in Class* (I). *Then $\lambda_p(\mu + F)$ is independent of p.*

(ii) *Assume that $\mathbb{M}$ is in Class* (II). *Then $\lambda_p(\mu + F)$ is independent of p if and only if $\lambda_2(\mu + F) \le 0$.*

Takeda [39] proved Theorem 1.1 (i) for Feynman–Kac semigroups with local potential $A_t(\mu)$; the facts in [39] can be easily extended to $\{p_t^{\mu+F}\}_{t>0}$. Takeda [38] proved Theorem 1.1 (ii) for Feynman–Kac semigroups with local potential, and Takeda and Tawara [40] extended it to non-local Schrödinger operators whose principal part is the fractional Laplacian, $(1/2)(-\Delta)^{\alpha/2}$, and Tawara [44] further extended it to generalized operators treated in this paper. Theorem 1.1 (ii) says that the L^p-independence for a symmetric Markov process in Class (II) is completely determined by the L^2-growth bound. Recently, G. De Leva, D. Kim and K. Kuwae [18] extend our main results to Feynman–Kac semigroups generated by continuous additive functionals of zero energy.

As mentioned above, the idea for the proof of Theorem 1.1 lies in the Donsker–Varadhan theory, the large deviation theory for occupation distributions. We denote by

$(\mathcal{E}, \mathcal{F})$ the regular Dirichlet form generated by the symmetric Markov process $\mathbb{M}$. We then see that the semigroup $\{p_t^{\mu+F}\}_{t>0}$ generates the bilinear form $\mathcal{E}^{\mu+F}$:

$$\mathcal{E}^{\mu+F}(u,u) = \mathcal{E}(u,u) - \Big(\int_X u^2 d\mu + \int_{X\times X} u(x)u(y)F_1(x,y)N(x,dy)\mu_H(dx) \Big), \quad u \in \mathcal{F},$$

where

$$F_1(x,y) = e^{F(x,y)} - 1 \tag{1.1}$$

([47], Theorem 4.1). Let $\mathcal{P}(X)$ be the set of probability measures on X equipped with the weak topology. We define the function $I_{\mathcal{E}^{\mu+F}}$ on $\mathcal{P}(X)$ by

$$I_{\mathcal{E}^{\mu+F}}(\nu) = \begin{cases} \mathcal{E}^{\mu+F}(\sqrt{f}, \sqrt{f}) & \text{if } \nu = f \cdot m,\ \sqrt{f} \in \mathcal{F}, \\ \infty & \text{otherwise.} \end{cases} \tag{1.2}$$

For $\omega \in \Omega$ with $0 < t < \zeta(\omega)$, we define the occupation distribution $L_t(\omega) \in \mathcal{P}(X)$ by

$$L_t(\omega)(A) = \frac{1}{t}\int_0^t 1_A(X_s(\omega))ds,$$

where 1_A is the indicator function of the Borel set $A \subset X$. We then have the next theorem:

Theorem 1.2. *Assume that $\mathbb{M}$ is in Class* (I). *Let μ be a measure in $\mathcal{K}_\infty$ and F a function in $\mathcal{A}_2$.*

(i) *For each open set $G \subset \mathcal{P}(X)$,*

$$\liminf_{t\to\infty} \frac{1}{t}\log \mathbb{E}_x\big[e^{A_t(\mu+F)}; L_t \in G, t < \zeta\big] \geq -\inf_{\nu\in G} I_{\mathcal{E}^{\mu+F}}(\nu).$$

(ii) *For each closed set $K \subset \mathcal{P}(X)$,*

$$\limsup_{t\to\infty} \frac{1}{t}\log \sup_{x\in X} \mathbb{E}_x\big[e^{A_t(\mu+F)}; L_t \in K, t < \zeta\big] \leq -\inf_{\nu\in K} I_{\mathcal{E}^{\mu+F}}(\nu).$$

Theorem 1.2 was proven in [39] and [44]. Applying Theorem 1.2 to $G = K = \mathcal{P}(X)$, we see that

$$\begin{aligned} \lim_{t\to\infty} \frac{1}{t}\log \sup_{x\in X} \mathbb{E}_x\big[e^{A_t(\mu+F)}; t < \zeta\big] &= -\inf_{\nu\in\mathcal{P}(X)} I_{\mathcal{E}^{\mu+F}}(\nu) \\ &= -\inf\Big\{\mathcal{E}^{\mu+F}(u,u) : u \in \mathcal{F}, \int_X u^2 dm = 1\Big\}. \end{aligned} \tag{1.3}$$

The equation (1.3) leads us to Theorem 1.1 (i). Indeed, noting that

$$\sup_{x\in X}\mathbb{E}_x\big[e^{A_t(\mu+F)};t<\zeta\big]=\sup_{x\in X}p_t^{\mu+F}1(x)=\|p_t^{\mu+F}\|_{\infty,\infty}$$

and by the spectral theorem

$$\lambda_2(\mu+F)=\inf\left\{\mathcal{E}^{\mu+F}(u,u):u\in\mathcal{F},\ \int_X u^2dm=1\right\},\tag{1.4}$$

we have $\lambda_\infty(\mu+F)=\lambda_2(\mu+F)$ by (1.3), which implies that $\lambda_p(\mu+F)$ is independent of p by the Riesz–Thorin interpolation theorem ([17], 1.1.5).

The method for the proof of Theorem 1.1 (ii) is different from that of Theorem 1.1 (i): we first note that if the state space X is compact, only the Feller property is necessary for the proof of the upper bound. We thus extend the Markov process $\mathbb{M}$ to the one-point compactification X_∞ by making the infinity ∞ a trap, and derive the upper bound for this extended Markov process. Then the rate function becomes a function on the set of probability measures on X_∞ not on X; in this way, the adjoined point ∞ makes a contribution to the rate function. We show that the infimum of the rate function on the set of probability measures on X_∞ is equal to the infimum of the original rate function on the set of probability measures on X if and only if the L^2-spectral bound is non-positive. Consequently we obtain a necessary and sufficient condition for the L^p-independence. The idea of considering the contribution to the rate function from ∞ is due to A. Budhiraja and P. Dupuis [9], where a large deviation principle of occupation distributions was proved for Markov processes without stability property. H. Kaise and S. J. Sheu [26] studied the asymptotic of Feynman–Kac functionals by using this idea.

The Gärtner–Ellis theorem is well known as a useful approach to the proof of large deviation principles. A prerequisite condition for applying the Gärtner–Ellis theorem is the existence of a logarithmic moment generating function (Section 2.3 in [19]). We would like to emphasize that the L^p-independence of growth bounds of $\{p_t^{\mu+F}\}_{t>0}$ implies the existence of a logarithmic moment generating function of $A_t(\mu+F)$. As an application of this fact, we established in [42] the large deviation principle for purely discontinuous AFs of symmetric stable processes (Theorem 5.8).

Varadhan [45] gave an abstract formulation for the large deviation principle. Theorem 1.2 (i) and (ii) are slightly different from the lower estimate and the upper estimate in his formulation; at least, since the rate function $I_{\mathcal{E}^{\mu+F}}$ is the Schrödinger form, it is not always non-negative. Moreover, even if $\mu+F$ equals zero, we can not regard Theorem 1.2 as a large deviation from invariant measure because the Markov process is not supposed to be conservative. For this reason, we treat the normalized probability measure $Q_{x,t}$ on $\mathcal{P}(X)$ defined by

$$Q_{x,t}(B)=\frac{\mathbb{E}_x[e^{A_t(\mu+F)};L_t\in B,t<\zeta]}{\mathbb{E}_x[e^{A_t(\mu+F)};t<\zeta]},\quad B\in\mathcal{B}(\mathcal{P}(X)).\tag{1.5}$$

We show in Section 6 that if the symmetric Markov process $\mathbb{M}$ is in Class (I), then the family of probability measures $\{Q_{x,t}\}_{t>0}$ satisfies the large deviation principle with the

rate function $J(\nu) := I_{\mathcal{E}^{\mu+F}}(\nu) - \lambda_2(\mu + F)$, $\nu \in \mathcal{P}(X)$, as $t \to \infty$ in Varadhan's formulation (Theorem 6.3). In other words, $\{Q_{x,t}\}_{t>0}$ obeys the *full* large deviation principle with the *good* rate function $J(\nu)$. In addition, we see that there exists a unique normalized ground state ϕ_0 of the operator $\mathcal{H}^{\mu+F}$ and $\phi_0^2 \cdot m$ is a unique probability measure for which $J(\nu) = 0$. On account of these facts, we can regard Theorem 1.2 as a large deviation from the ground state of the generalized Schrödinger operator (Corollary 6.4).

2 Dirichlet Forms and symmetric Markov processes

In this section we briefly review the theory of Dirichlet forms, symmetric Markov processes and Feynman–Kac semigroups. Let X be a locally compact separable metric space and X_∞ the one-point compactification of X with adjoined point ∞. Let m be a positive Radon measure on X with full support. Let $\mathbb{M} = (\Omega, \mathcal{M}, \mathcal{M}_t, \theta_t, X_t, \mathbb{P}_x, \zeta)$ be an m-symmetric Markov process on X. Here, $\{\mathcal{M}_t\}$ is the minimal (augmented) admissible filtration, $\{\theta_t\}_{t\geq 0}$ is the shift operator satisfying $X_s(\theta_t) = X_{s+t}$ identically for $s, t \geq 0$, and ζ is the lifetime of $\mathbb{M}$, $\zeta = \inf\{t > 0 : X_t = \infty\}$. Let $\{p_t\}_{t>0}$ and $\{G_\beta\}_{\beta>0}$ be the semigroup and the resolvent of $\mathbb{M}$: for a bounded Borel function f on X

$$p_t f(x) = \mathbb{E}_x[f(X_t); t < \zeta], \quad G_\beta f(x) = \int_0^\infty e^{-\beta t} p_t f(x) dt.$$

Throughout this paper, we make two assumptions on $\mathbb{M}$.

Assumption I (Irreducibility). If a Borel set A is p_t-invariant, i.e.,

$$p_t(1_A f)(x) = 1_A p_t f(x), \quad m\text{-a.e. for } \forall t > 0, \ \forall f \in L^2(X; m) \cap \mathcal{B}_b(X),$$

then A satisfies either $m(A) = 0$ or $m(X \setminus A) = 0$. Here $\mathcal{B}_b(X)$ is the space of bounded Borel functions on X.

Assumption II (Strong Feller property). For each $t > 0$, $p_t(\mathcal{B}_b(X)) \subset C_b(X)$, where $C_b(X)$ is the space of bounded continuous functions on X.

Remark 2.1 (Absolute continuity condition). We see from Assumption II that the semigroup $\{p_t\}_{t>0}$ admits an integral kernel $\{p(t, x, y)\}_{t>0}$ with respect to the measure m,

$$p_t f(x) = \int_X p(t, x, y) f(y) dm(y).$$

We introduce two classes of symmetric Markov processes.

Definition 2.1. A symmetric Markov process $\mathbb{M}$ is said to be in *Class* (I), if for any $\epsilon > 0$, there exists a compact set $K \subset X$ such that

$$\sup_{x\in X} G_1 1_{K^c}(x) \leq \epsilon, \tag{2.1}$$

Here 1_{K^c} is the indicator function of the complement of K.

Remark 2.2. (i) If $G_1 1 \in C_\infty(X)$, then (2.1) is fulfilled. In this case, the Markov process $\mathbb{M}$ is explosive.

(ii) If $m(X) < \infty$ and $\|G_1\|_{1,\infty} < \infty$, then (2.1) is fulfilled because $\|G_1 1_{K^c}\|_\infty \leq \|G_1\|_{1,\infty} m(K^c)$. Here $\|\ \|_{1,\infty}$ is the operator norm from $L^1(X;m)$ to $L^\infty(X;m)$.

(iii) Let us consider one-dimensional diffusion processes on an interval (r_1, r_2). The boundary point r_i is classified into four classes: *regular boundary, exit boundary, entrance boundary, and natural boundary*. (a) If r_2 is a regular or exit boundary, then $\lim_{x\to r_2} G_1 1(x) = 0$. (b) If r_2 is an entrance boundary, then

$$\lim_{r\to r_2} \sup_{x\in(r_1,r_2)} G_1 1_{(r,r_2)}(x) = 0$$

(cf. [25], Section 5.11). As a result, if no boundaries are natural, then (2.1) is satisfied.

(iv) We introduce in Definition 3.1 the class $\mathcal{K}_{\infty,1}$ of 1-Green tight measures. The condition (2.1) says that the basic measure m is 1-Green tight.

Definition 2.2. A symmetric Markov process $\mathbb{M}$ is said to be in *Class* (II), if its semigroup $\{p_t\}_{t\geq 0}$ is conservative, $p_t 1 = 1$, and if it satisfies $p_t(C_\infty(X)) \subset C_\infty(X)$. Here $C_\infty(X)$ is the space of continuous functions on X vanishing at the infinity.

Remark 2.3. Suppose that $\mathbb{M}$ is in Class (II). We then see from Proposition 3.4 below that for any compact set K, $\lim_{x\to\infty} p_t 1_{K^c}(x) = 1$, and so $\sup_{x\in X} G_1 1_{K^c}(x) = 1$. Therefore, there exists no intersection of Class (I) and Class (II). For a one-dimensional diffusion process, if both boundaries are natural, then (2.1) is fulfilled.

Let $\{G_\beta(x,y)\}_{\beta\geq 0}$ be the resolvent kernel defined by

$$G_\beta(x,y) = \int_0^\infty e^{-\beta t} p(t,x,y)dt, \quad \beta \geq 0.$$

If the Markov process $\mathbb{M}$ is transient, then $G_0(x,y) < \infty$ $x \neq y$. In this case, we simply write $G(x,y)$ for $G_0(x,y)$ and call it the *Green function*. By [24], Lemma 4.2.4, the density $G_\beta(x,y)$ is assumed to be a non-negative Borel function such that $G_\beta(x,y)$ is symmetric and β-excessive in x and in y.

By the right continuity of sample paths of $\mathbb{M}$, $\{p_t\}_{t>0}$ can be extended to an $L^2(X;m)$-strongly continuous contraction semigroup, $\{T_t\}_{t>0}$ ([24], Lemma 1.4.3). The *Dirichlet form* $(\mathcal{E}, \mathcal{F})$ generated by $\mathbb{M}$ is defined by

$$\begin{cases} \mathcal{F} = \{u \in L^2(X;m) : \lim_{t\to 0} \frac{1}{t}(u - T_t u, u)_m < \infty\}, \\ \mathcal{E}(u,v) = \lim_{t\to 0} \frac{1}{t}(u - T_t u, v)_m, \quad u, v \in \mathcal{F}, \end{cases} \tag{2.2}$$

where $(u,v)_m$ is the inner product on $L^2(X;m)$. The Dirichlet form $(\mathcal{E}, \mathcal{F})$ is said to be *regular* if $\mathcal{F} \cap C_0(X)$ is dense in $\mathcal{F}$ with respect to the $\mathcal{E}_1$-norm and dense in $C_0(X)$ with respect to the uniform norm. Here $C_0(X)$ is the space of continuous functions on X with compact support and $\mathcal{E}_1(u,u) = \mathcal{E}(u,u) + (u,u)_m$. It follows from Assumption II that $(\mathcal{E}, \mathcal{F})$ becomes regular.

We define the (1-)*capacity* Cap associated with the Dirichlet form $(\mathcal{E}, \mathcal{F})$ as follows: for an open set $O \subset X$,

$$\mathrm{Cap}(O) = \inf\{\mathcal{E}_1(u,u) : u \in \mathcal{F}, u \geq 1,\ m\text{-a.e. on } O\}$$

and for a Borel set $A \subset X$,

$$\mathrm{Cap}(A) = \inf\{\mathrm{Cap}(O) : O \text{ is open, } O \supset A\}.$$

Let A be a subset of X. A statement depending on $x \in A$ is said to hold q.e. on A if there exists a set $N \subset A$ of zero capacity such that the statement is true for every $x \in A \setminus N$. "q.e." is an abbreviation of "quasi-everywhere". A real valued function u defined q.e. on X is said to be *quasi continuous* if for any $\epsilon > 0$ there exists an open set $G \subset X$ such that $\mathrm{Cap}(G) < \epsilon$ and $u|_{X\setminus G}$ is finite and continuous. Here, $u|_{X\setminus G}$ denotes the restriction of u to $X \setminus G$. Each function u in $\mathcal{F}$ admits a quasi-continuous version $\tilde{u}$, that is, $u = \tilde{u}$ m-a.e. In the sequel, we always assume that every function $u \in \mathcal{F}$ is represented by its quasi-continuous version.

A stochastic process $\{A_t\}_{t\geq 0}$ is said to be an *additive functional* (AF in abbreviation) if the following conditions hold:

(i) $A_t(\cdot)$ is $\mathcal{M}_t$-measurable for all $t \geq 0$.

(ii) There exists a set $\Lambda \in \mathcal{M}_\infty = \sigma(\cup_{t\geq 0}\mathcal{M}_t)$ such that $\mathbb{P}_x(\Lambda) = 1$, for all $x \in X$, $\theta_t\Lambda \subset \Lambda$ for all $t > 0$, and for each $\omega \in \Lambda$, $A_\cdot(\omega)$ is a function satisfying: $A_0 = 0$, $A_t(\omega) < \infty$ for $t < \zeta(\omega)$, $A_t(\omega) = A_\zeta(\omega)$ for $t \geq \zeta$, and $A_{t+s}(\omega) = A_t(\omega) + A_s(\theta_t\omega)$ for $s, t \geq 0$.

If an AF $\{A_t\}_{t\geq 0}$ is positive and continuous with respect to t for each $\omega \in \Lambda$, the AF is called a *positive continuous additive functional* (PCAF in abbreviation). Under the absolute continuity condition, "quasi everywhere" statements are strengthened to "everywhere" ones. Moreover, we can defined notions without exceptional set, for example, *smooth measures in the strict sense* or *positive continuous additive functional in the strict sense* (cf. Section 5.1 in [24]). Here we only treat the notions in the strict sense and omit the phrase "in the strict sense".

We denote S_{00} the set of positive Borel measures μ such that $\mu(X) < \infty$ and $G_1\mu(x)(= \int_X G_1(x,y)\mu(dy))$ is uniformly bounded in $x \in X$. A positive Borel measure μ on X is said to be *smooth* if there exists a sequence $\{E_n\}_{n=1}^\infty$ of Borel sets increasing to X such that $1_{E_n} \cdot \mu \in S_{00}$ for each n and

$$\mathbb{P}_x\big(\lim_{n\to\infty} \sigma_{X\setminus E_n} \geq \zeta\big) = 1, \quad \forall x \in X, \tag{5.1.28}$$

where $\sigma_{X\setminus E_n}$ is the first hitting time of $X \setminus E_n$. We denote by S_1 the totality of smooth measures. By Theorem 5.1.4 in [24], there exists a one-to-one correspondence (*Revuz correspondence*) between smooth measures and PCAFs as follows: for each smooth measure μ, there exists a unique PCAF $\{A_t\}_{t\geq 0}$ such that for any $f \in \mathcal{B}_+(X)$ and γ-excessive function h ($\gamma \geq 0$), $e^{-\gamma t}p_t h \leq h$,

$$\lim_{t\to 0} \frac{1}{t}\mathbb{E}_{h\cdot m}\Big[\int_0^t f(X_s)dA_s\Big] = \int_X f(x)h(x)\mu(dx). \tag{2.3}$$

Here, $\mathbb{E}_{h\cdot m}[\cdot] = \int_X \mathbb{E}_x[\cdot]h(x)m(dx)$. We denote by $A_t(\mu)$ the PCAF of the smooth measure μ. For a signed smooth measure $\mu = \mu^+ - \mu^-$, we define $A_t(\mu) = A_t(\mu^+) - A_t(\mu^-)$.

Let N be a kernel on $(X_\infty, \mathcal{B}(X_\infty))$ such that $N(x, \{x\}) = 0$ for any $x \in X$ and H_t a PCAF of $\mathbb{M}$. The pair (N, H_t) is said to be the *Lévy system* of $\mathbb{M}$ if for any bounded measurable function F on $(X_\infty \times X_\infty)$ vanishing on the diagonal set $\triangle = \{(x, x) : x \in X_\infty\}$, it holds that

$$\mathbb{E}_x\Big[\sum_{0<s\le t} F(X_{s-}, X_s)\Big] = \mathbb{E}_x\Big[\int_0^t \int_{X_\infty} F(X_s, y)N(X_s, dy)dH_s\Big], \tag{2.4}$$

where $X_{t-} = \lim_{s\uparrow t} X_s$. For the existence of the Lévy system, see Benveniste and Jacod [5]. We remark that

$$A_t(F) - \int_0^t \int_{X_\infty} F(X_s, y)N(X_s, dy)dH_s$$

is a martingale additive functional.

The regular Dirichlet form $(\mathcal{E}, \mathcal{F})$ is expressed by

$$\mathcal{E}(u, v) = \mathcal{E}^{(c)}(u, v) + \int_{X\times X\setminus\triangle} (u(x) - u(y))(v(x) - v(y))J(dx, dy) + \int_X u(x)v(x)k(dx)$$

(Beurling–Deny formula, [24], Theorem 3.2.1). The first term $\mathcal{E}^{(c)}$ is called *local part* of $(\mathcal{E}, \mathcal{F})$. $\mathcal{E}^{(c)}$ is a symmetric Dirichlet form satisfying the *strong local property*, that is, $\mathcal{E}^{(c)}(u, v) = 0$ for $u, v \in \mathcal{F} \cap C_0(X)$ such that u is constant on $\mathrm{Supp}[v]$. In addition, there exists uniquely a positive Radon measure $\mu^c_{\langle u\rangle}$, $u \in \mathcal{F}$, satisfying

$$\mathcal{E}^{(c)}(u, u) = \frac{1}{2}\mu^c_{\langle u\rangle}(X).$$

If we introduce a bounded signed measure $\mu^c_{\langle u,v\rangle}$, $u, v \in \mathcal{F}$, by

$$\mu^c_{\langle u,v\rangle} = \frac{1}{2}\big(\mu^c_{\langle u+v\rangle} - \mu^c_{\langle u\rangle} - \mu^c_{\langle v\rangle}\big),$$

then

$$\mathcal{E}^{(c)}(u, v) = \frac{1}{2}\mu^c_{\langle u,v\rangle}(X).$$

The second term is called the *jumping part* of $(\mathcal{E}, \mathcal{F})$. J is a symmetric positive Radon measure on the product space $X \times X$ off the diagonal set and called *jumping measure*. Using the Lévy system of $\mathbb{M}$, we have the following expression:

$$J(dx, dy) = \frac{1}{2}N(x, dy)\mu_H(dx),$$

where μ_H is the Revuz measure of the PCAF $\{H_t\}_{t\geq 0}$ of the Lévy system. The last term is called the *killing part*. k is a Radon measure on X and called *killing measure*. Moreover, it is expressed as

$$k(dx) = N(x,\infty)\mu_H(dx).$$

3 Generalized Feynman–Kac semigroups

In this section we introduce classes of local and non-local potentials. For a signed Borel measure μ we denote its total variation by $|\mu|$. Following Chen [11], [12], we define classes of local and non-local potentials.

Definition 3.1 (Kato measure, Green tight measure).

(a) A signed Borel measure μ is said to be the *Kato measure* (in notation, $\mu \in \mathcal{K}$) if $|\mu| \in S_1$ and

$$\lim_{t\to 0} \sup_{x\in X} \mathbb{E}_x[A_t(|\mu|)] = 0.$$

(b) A measure $\mu \in \mathcal{K}$ is said to be the β-*Green tight measure* (in notation, $\mu \in \mathcal{K}_{\infty,\beta}$) if for any $\epsilon > 0$ there exist a compact subset K and a positive constant $\delta > 0$ such that

$$\sup_{x\in X} \int_{K^c} G_\beta(x,y)|\mu|(dy) \leq \epsilon,$$

and for any Borel set $B \subset K$ with $|\mu|(B) < \delta$,

$$\sup_{x\in X} \int_{B} G_\beta(x,y)|\mu|(dy) < \epsilon.$$

For a positive measure μ on X, denote

$$G_\beta\mu(x) = \int_X G_\beta(x,y)\mu(dy).$$

We note that for any $\beta > 0$, $\mathcal{K}_{\infty,\beta} = \mathcal{K}_{\infty,1}$. Indeed, for a positive measure μ on X, let $\mu_{K^c}(\cdot) = \mu(K^c \cap \cdot)$. Since by the resolvent equation

$$G_\beta\mu_{K^c} = G_\gamma\mu_{K^c} + (\gamma-\beta)G_\beta G_\gamma\mu_{K^c}, \quad 0 < \beta < \gamma,$$

we have

$$\|G_\beta\mu_{K^c}\|_\infty \leq \|G_\gamma\mu_{K^c}\|_\infty + \frac{\gamma-\beta}{\beta}\|G_\gamma\mu_{K^c}\|_\infty = \frac{\gamma}{\beta}\|G_\gamma\mu_{K^c}\|_\infty.$$

We simply write $\mathcal{K}_\infty$ for $\mathcal{K}_{\infty,1}$ and call a measure in $\mathcal{K}_\infty$ a 1-*Green tight measure*. Moreover, if the Markov process is transient, a measure $\mu \in \mathcal{K}_{\infty,0}$ is called a *Green tight measure*. We remark that $\mathcal{K}_{\infty,0} \subset \mathcal{K}_\infty \subset \mathcal{K}$ ([11]).

We now provide an inequality proved in P. Stollmann and J. Voigt [32].

Theorem 3.1. *Let $\mu \in \mathcal{K}$. Then for each $\beta \geq 0$,*

$$\int_X u^2(x)\mu(dx) \leq \|G_\beta \mu\|_\infty \cdot \mathcal{E}_\beta(u,u), \quad u \in \mathcal{F}, \tag{3.1}$$

where $\mathcal{E}_\beta(u,u) = \mathcal{E}(u,u) + \beta(u,u)_m$.

Definition 3.2. Let F be a bounded measurable function on $X \times X$ vanishing on the diagonal set.

(a) F is said to be in the class $\mathcal{J}$ (resp. $\mathcal{J}_\infty$, $\mathcal{J}_{\infty,0}$) if

$$\mu_{|F|}(dx) := \Big(\int_X |F(x,y)| N(x,dy) \Big) \mu_H(dx) \in \mathcal{K} \text{ (resp. } \mathcal{K}_\infty, \mathcal{K}_{\infty,0}).$$

(b) F is said to be in the class $\mathcal{A}_\infty$ if for any $\epsilon > 0$ there exist a compact subset K and a positive constant $\delta > 0$ such that for all measurable set $B \subset K$ with $\mu_{|F|}(B) < \delta$,

$$\sup_{(x,w)\in X\times X} \int_{((K\setminus B)\times(K\setminus B))^c} \frac{G_1(x,y)|F(y,z)|G_1(z,w)}{G_1(x,w)} N(y,dz)\mu_H(dy) \leq \epsilon.$$

If F satisfies the above inequality for $G(x,y)$, we say that F belongs to the class $\mathcal{A}_{\infty,0}$.

(c) F is said to be in the class $\mathcal{A}_2$ if $F \in \mathcal{A}_\infty$ and if the measure $\mu_{|F|}$ satisfies that for any $\epsilon > 0$ there exist a compact subset K and a positive constant $\delta > 0$ such that for all measurable set $B \subset K$ with $\mu_{|F|}(B) < \delta$,

$$\sup_{(x,z)\in X\times X} \int_{K^c \cup B} \frac{G_1(x,y)G_1(y,z)}{G_1(x,z)} \mu_{|F|}(dy) \leq \epsilon.$$

The class $\mathcal{A}_{2,0}$ is defined in the same way as $\mathcal{A}_{\infty,0}$.

In the sequel we assume that F is symmetric, $F(x,y) = F(y,x)$. We write $\mu + F \in \mathcal{K}_\infty + \mathcal{A}_2$ if $\mu \in \mathcal{K}_\infty$ and $F \in \mathcal{A}_2$. For $\mu + F \in \mathcal{K}_\infty + \mathcal{A}_2$, we define the symmetric Dirichlet form $(\mathcal{E}_F, \mathcal{F})$ by

$$\begin{aligned}\mathcal{E}_F(u,u) &= \mathcal{E}^{(c)}(u,u) \\ &\quad + \int_{X\times X} (u(x)-u(y))^2 e^{F(x,y)} J(dx,dy) + \int_X u(x)^2 k(dx).\end{aligned}$$

We set

$$F_1 = e^F - 1. \tag{3.2}$$

We easily see from the boundedness of F that the function F_1 also belongs to Class $\mathcal{A}_2$. We now define another bilinear form $\mathcal{E}^{\mu+F}$ by

$$\begin{aligned}\mathcal{E}^{\mu+F}(u,u) &= \mathcal{E}_F(u,u) - \Big(\int_X u^2 d\mu + \int_X u^2 d\mu_{F_1} \Big) \\ &= \mathcal{E}(u,u) - \Big(\int_X u^2 d\mu \\ &\qquad + \int_{X\times X} u(x)u(y)F_1(x,y)N(x,dy)\mu_H(dx) \Big), \quad u \in \mathcal{F}.\end{aligned}$$

From Albeverio and Ma [2] (Theorem 4.1) and [3] (Proposition 3.3) we see that $(\mathcal{E}^{\mu+F}, \mathcal{F})$ is a lower semi-bounded closed symmetric form. Denote by $\mathcal{L}$, $\mathcal{L}^F$ and $\mathcal{H}^{\mu+F}$ the self-adjoint operators associated with $(\mathcal{E}, \mathcal{F})$, $(\mathcal{E}_F, \mathcal{F})$ and $(\mathcal{E}^{\mu+F}, \mathcal{F})$ respectively. Then $\mathcal{L}^F$ and $\mathcal{H}^{\mu+F}$ are formally written by

$$\mathcal{L}^F f = \mathcal{L} f + \left(\int_X (f(y) - f(x)) F_1(x, y) N(x, dy) \right) \mu_H(dx)$$

and

$$\mathcal{H}^{\mu+F} f = \mathcal{L} f + \mu_H \mathbf{F} f + \mu f = \mathcal{L}^F f + \mu_H V^F f + \mu f,$$

where

$$\mu_H \mathbf{F} f = \left(\int_X f(y) F_1(x, y) N(x, dy) \right) \mu_H(dx),$$
$$\mu_H V^F f = \left(\int_X F_1(x, y) N(x, dy) \right) f(x) \mu_H(dx).$$

Let $\{p_t^{\mu+F}\}_{t>0}$ be the L^2-semigroup generated by $\mathcal{H}^{\mu+F}$: $p_t^{\mu+F} = \exp(t\mathcal{H}^{\mu+F})$. Then it was shown in Ying [48], Chen–Song [14] that the semigroup $\{p_t^{\mu+F}\}_{t>0}$ is expressed by

$$p_t^{\mu+F} f(x) = \mathbb{E}_x[\exp(A_t(\mu + F)) f(X_t)],$$

where $A_t(\mu + F) = A_t(\mu) + \sum_{0<s\le t} F(X_{s-}, X_s)$.

Next two theorems on the generalized Feynman–Kac semigroups $\{p_t^{\mu+F}\}_{t>0}$ follows from Albeverio, Blanchard and Ma [1], Theorem 4.1, and Chung [15], Theorem 2, respectively.

Theorem 3.2. *Let $\mu + F \in \mathcal{K}_\infty + \mathcal{J}_\infty$. There exist constants c and $\kappa(\mu + F)$ such that*

$$\| p_t^{\mu+F} \|_{p,p} \le c e^{\kappa(\mu+F)t}, \quad 1 \le p \le \infty,\ t > 0.$$

Here, $\| \cdot \|_{p,p}$ means the operator norm from $L^p(X; m)$ to $L^p(X; m)$.

Theorem 3.3. *Suppose that a symmetric Markov process $\mathbb{M}$ is in Class* (II)*. Then for $\mu + F \in \mathcal{K}_\infty + \mathcal{J}_\infty$, $p_t^{\mu+F}(C_\infty(X)) \subset C_\infty(X)$ and $p_t^{\mu+F}(\mathcal{B}_b(X)) \subset C_b(X)$.*

Tawara [43] proved the next proposition which is an extension of Proposition 3.1 in Azencott [4]. For a Borel set A, let σ_A be the *first hitting time* of A, $\sigma_A = \inf\{t > 0 : X_t \in A\}$.

Proposition 3.4. *A symmetric Markov process $\mathbb{M}$ in Class* (II) *possesses the following properties:*

(a) *For $\beta > 0$ and $f \in C_\infty(X)$,*

$$\lim_{x\to\infty} G_\beta f(x) = 0.$$

(b) *For $t > 0$ and a compact set K,*

$$\lim_{x\to\infty} \mathbb{P}_x(\sigma_K \le t) = 0.$$

(c) *For $\beta > 0$ and a compact set K,*

$$\lim_{x\to\infty} \mathbb{E}_x[e^{-\beta\sigma_K}] = 0.$$

We see from Proposition 3.4 that for a symmetric Markov process $\mathbb{M}$ in Class (II),

$$p_t^{\mu+F}(C_u(X)) \subset C_u(X), \quad \lim_{x\to\infty} p_t^{\mu+F} f(x) = \lim_{x\to\infty} f(x), \tag{3.3}$$

where $C_u(X)$ is the space of uniformly continuous bounded functions on X such that $\lim_{x\to\infty} f(x)$ exists. The property (3.3) is crucial to study the rate function defined in Section 4.

4 Donsker–Varadhan type large deviation principle

For a symmetric Markov process, its Dirichlet form governs the Donsker–Varadhan large deviation principle, that is, the rate function is identified with the Dirichlet form. Therefore, we can expect that if the symmetric Markov process obeys the large deviation principle, then the L^2-theory is more dominant. In this section, we extend Donsker–Varadhan type large deviations to symmetric Markov processes with Feynman–Kac functional. In this case the rate function is not identified with a Dirichlet form but a Schrödinger form.

Let $\mu \in \mathcal{K}_\infty$ and $F \in \mathcal{A}_2$. We define the function $I_{\mathcal{E}^{\mu+F}}$ on $\mathcal{P}(X)$ by

$$I_{\mathcal{E}^{\mu+F}}(\nu) = \begin{cases} \mathcal{E}^{\mu+F}(\sqrt{f}, \sqrt{f}) & \text{if } \nu = f \cdot m,\ \sqrt{f} \in \mathcal{F}, \\ \infty & \text{otherwise.} \end{cases}$$

Let $L_t \in \mathcal{P}(X)$ be the *normalized occupation distribution*, that is, for $0 < t < \zeta$,

$$L_t(A) = \frac{1}{t}\int_0^t 1_A(X_s)ds, \quad A \in \mathcal{B}(X). \tag{4.1}$$

We then have the lower bound estimate.

Theorem 4.1 ([27], Theorem 4.1). *For each open set $G \subset \mathcal{P}(X)$,*

$$\liminf_{t\to\infty} \frac{1}{t} \log \mathbb{E}_x\left[\exp(A_t(\mu + F)); L_t \in G, t < \zeta\right] \ge -\inf_{\nu\in G} I_{\mathcal{E}^{\mu+F}}(\nu). \tag{4.2}$$

We obtain the next theorem by the same argument as in [39].

Theorem 4.2. *Assume that a symmetric Markov process* $\mathbb{M}$ *is in Class* (I). *Then for each closed set* $K \subset \mathcal{P}(X)$,

$$\limsup_{t\to\infty} \frac{1}{t} \log \sup_{x\in X} \mathbb{E}_x \left[\exp(A_t(\mu+F)); L_t \in K, t < \zeta\right] \leq -\inf_{\nu\in K} I_{\mathcal{E}^{\mu+F}}(\nu).$$

We will show in Section 6 that the infimum of $I_{\mathcal{E}^{\mu+F}}(\nu)$ is attained at the normalized ground state of the generalized Schrödinger operator $\mathcal{H}^{\mu+F}$. In this sense, Theorem 4.1 and Theorem 4.2 is regarded as a large deviation principle form not the invariant measure but the ground state. The essential idea of the proof of Theorem 4.1 and Theorem 4.2 lies in Donsker–Varadhan [20]; however, since $A_t(\mu+F)$ is not a function of L_t, we need to extend Donsker–Varadhan's argument to Markov processes with Feynman–Kac functional.

A key to the proof of Theorem 4.1 is the fact that any irreducible symmetric Markov process can be transformed to a symmetric ergodic process by a certain supermartingale multiplicative functional ([13]). A one-dimensional absorbing Brownian motion can be transformed to a symmetric ergodic diffusion by a drift transform. Using this fact, they proved in Donsker–Varadhan [20] the lower estimate for the one-dimensional Brownian motion. To prove the ergodicity, they used the Feller test, while we apply an ergodic theorem in the Dirichlet form theory.

A key to the proof of Theorem 4.2 is the definition of a suitable *I-function*. More precisely, define $\kappa(\mu+F)$ by

$$\kappa(\mu+F) = \lim_{t\to\infty} \frac{1}{t} \log \| p_t^{\mu+F} \|_{\infty,\infty}.$$

We see from Theorem 3.2 that $\kappa(\mu+F)$ is finite. For $\alpha > \kappa(\mu+F)$, the resolvent $G_\alpha^{\mu+F}$ is defined by

$$G_\alpha^{\mu+F} f(x) = \mathbb{E}_x\left[\int_0^\infty e^{-\alpha t + A_t(\mu+F)} f(X_t) dt\right], \quad f \in \mathcal{B}_b(X).$$

We set

$$\mathcal{D}_+(\mathcal{H}^{\mu+F}) = \left\{G_\alpha^{\mu+F} f : \alpha > \kappa(\mu+F), f \in L^2(X;m) \cap C_b(X), \right.$$
$$\left. f \geq 0 \text{ and } f \not\equiv 0\right\}.$$

Each function $\phi = G_\alpha^{\mu+F} f \in \mathcal{D}_+(\mathcal{H}^{\mu+F})$ is strictly positive because $\mathbb{P}_x(\sigma_O < \zeta) > 0$ for any $x \in X$ by Assumption I. Here O is a non-empty open set $\{x \in X : f(x) > 0\}$. We define the generator $\mathcal{H}^{\mu+F}$ by

$$\mathcal{H}^{\mu+F} u = \alpha u - f, \quad u = G_\alpha^{\mu+F} f \in \mathcal{D}_+(\mathcal{H}^{\mu+F}).$$

Suppose that $\mu + F \in \mathcal{K}_\infty + \mathcal{A}_2$ is *gaugeable*, that is,

$$\sup_{x\in X} \mathbb{E}_x\left[e^{A_\zeta(\mu+F)}\right] < \infty$$

and let $h(x) = \mathbb{E}_x\left[\exp\left(A_\zeta(\mu+F)\right)\right]$. The function $h(x)$ is strictly positive, $h(x) \geq c > 0$. Indeed, it follows from Proposition 2.2 in [11] and the definition of $\mathcal{J}_\infty$ that for $\mu \in \mathcal{K}_\infty$ and $F \in \mathcal{J}_\infty$, $\sup_{x\in E} \mathbb{E}_x(A_\zeta^{\mu+F}) < \infty$. Hence, by Jensen's inequality,

$$\inf_{x\in X} \mathbb{E}_x(\exp(A_\zeta^{\mu+F})) > 0.$$

After consideration of the Feynman–Kac functional, we define the modified I-function by

$$I_{\mu+F}(\nu) = -\inf_{\substack{\phi\in\mathcal{D}_+(\mathcal{H}^{\mu+F})\\ \epsilon>0}} \int_X \frac{\mathcal{H}^{\mu+F}\phi}{\phi+\epsilon h} d\nu, \quad \nu \in \mathcal{P}. \tag{4.3}$$

We need to add strictly positive functions ϵh, because the function $\mathcal{H}^{\mu+F}\phi/\phi$ is not always in $C_b(X)$. Since $\mathcal{P}(X)$ is equipped with the weak topology, it is crucial for the proof of Theorem 4.2 that the function $\frac{\mathcal{H}^{\mu+F}\phi}{\phi+\epsilon h}$ belongs to $C_b(X)$; in fact, we show the upper bound with this modified I-function $I_{\mu+F}$. The function h is said to be a *gauge function* and a necessary and sufficient condition for the measure $\mu + F$ being gaugeable is known (cf. [12]). An important remark on the proof of Theorem 4.1 and Theorem 4.2 is that we have only to prove these theorems for the β-subprocess of $\mathbb{M}$, the killed process by $\exp(-\beta t)$, $\beta > 0$. Owing to this, we may assume that $\mathbb{M}$ is transient. In addition, we may assume that $\mu + F$ is gaugeable because every Green-tight measure becomes gaugeable with respect to the β-subprocess of $\mathbb{M}$ for a large enough β([12], Theorem 3.4). The β-subprocess is a useful tool of studying Markov processes. It is worth to point out that this tool becomes available by extending the large deviation to symmetric Markov processes with finite lifetime.

The next proposition says that this modified I-function can be identified with the Schrödinger form.

Proposition 4.3. *It holds that for $\nu \in \mathcal{P}(X)$,*

$$I_{\mu+F}(\nu) = I_{\mathcal{E}^{\mu+F}}(\nu).$$

In [34] we proved Theorem 4.1 for symmetric Markov processes without Feynman–Kac functional. We there used the identity function 1 for the gauge function h in order to define the I-function. Note that the identity function is excessive for the Markov semigroup generated by $\mathcal{L}$ and the gauge function h is excessive for the Schrödinger semigroup generated by $\mathcal{H}^{\mu+F}$. Hence we can regard the function $I_{\mu+F}$ as an extension of the I-function in [34]. In [35] we proved the upper bound (ii) for each compact set of $\mathcal{P}$ without assuming (2.1). We did not need to add ϵh in (4.3) because the Markov process was supposed to be conservative and the I-function was defined by taking the infimum over uniformly positive functions in a domain of $\mathcal{H}^{\mu+F}$. We would like to emphasize that the function $I_{\mu+F}$ is independent of h if the function h is uniformly positive and bounded, that is, $I_{\mu+F}$ is identical to the Schrödinger form (1.2).

When the Markov process $\mathbb{M}$ be in Class (II), Theorem 4.2 does not hold generally. We thus first extend the Markov process $\mathbb{M}$ and the I-function; we define the transition

density $\bar{p}_t(x, dy)$ on $(X_\infty, \mathcal{B}(X_\infty))$: for $E \in \mathcal{B}(X_\infty)$,

$$\bar{p}_t(x, E) = \begin{cases} p_t(x, E \setminus \{\infty\}), & x \in X, \\ \delta_\infty(E), & x = \infty. \end{cases}$$

Let $\bar{\mathbb{M}}$ be the Markov process on X_∞ with transition probability $\bar{p}_t(x, dy)$, that is, an extension of $\mathbb{M}$ with ∞ being a trap. Furthermore, for $\mu + F \in \mathcal{K}_\infty + \mathcal{A}_2$, let the semigroup $\{\bar{p}_t^{\mu+F}\}_{t>0}$ and the resolvent $\{\bar{G}_\alpha^{\mu+F}\}_{\alpha>\kappa(\mu+F)}$ of $\bar{\mathbb{M}}$:

$$\bar{p}_t^{\mu+F} f(x) = \bar{\mathbb{E}}_x[\exp(A_t(\mu + F)) f(X_t)],$$
$$\bar{G}_\alpha^{\mu+F} f(x) = \int_0^\infty e^{-\alpha t} \bar{p}_t^{\mu+F} f(x) dt, \quad f \in \mathcal{B}_b(X_\infty).$$

Here, $\kappa(\mu + F)$ is the constant in Theorem 3.2. Then $\bar{G}_\alpha^{\mu+F} f(x) = G_\alpha^{\mu+F} f(x)$ for $x \in X$ and $\bar{G}_\alpha^{\mu+F} f(\infty) = f(\infty)/\alpha$. Set

$$\mathcal{D}_{++}(\bar{\mathcal{H}}^{\mu+F}) = \{\phi = \bar{G}_\alpha^{\mu+F} g : \alpha > \kappa(\mu + F), g \in C(X_\infty) \text{ with } g > 0\}.$$

We see that for $\phi = \bar{G}_\alpha^{\mu+F} g \in \mathcal{D}_{++}(\bar{\mathcal{H}}^{\mu+F})$, $\lim_{x\to\infty} \phi(x) = g(\infty)/\alpha$ by (3.3). Let us define the function $\bar{I}_{\mu+F}$ on $\mathcal{P}(X_\infty)$, the set of probability measures on X_∞, by

$$\bar{I}_{\mu+F}(\nu) = -\inf_{\phi \in \mathcal{D}_{++}(\bar{\mathcal{H}}^{\mu+F})} \int_{X_\infty} \frac{\bar{\mathcal{H}}^{\mu+F}\phi}{\phi} d\nu,$$

where $\bar{\mathcal{H}}^{\mu+F}\phi = \alpha \bar{G}_\alpha^{\mu+F} g - g$ for $\phi = \bar{G}_\alpha^{\mu+F} g \in \mathcal{D}_{++}(\bar{\mathcal{H}}^{\mu+F})$.

Note that $\bar{\mathbb{M}}$ has the Feller property, while it has no longer the strong Feller property. In the proof of the large deviation upper bound for a Markov process with compact state space, we need only the Feller property. Hence we have

Theorem 4.4 (Kim [27], Remark 4.1). *For each closed set $K \subset \mathcal{P}(X_\infty)$,*

$$\limsup_{t\to\infty} \frac{1}{t} \log \sup_{x\in X} \mathbb{E}_x [\exp(A_t(\mu + F)); L_t \in K] \le -\inf_{\nu\in K} \bar{I}_{\mu+F}(\nu). \tag{4.4}$$

5 L^p-independence of growth bounds

When the symmetric Markov process $\mathbb{M}$ is in Class (I), we have the next theorem by applying Theorem 4.1 and Theorem 4.3 to $G = K = \mathcal{P}(X)$.

Theorem 5.1. *If $\mathbb{M}$ is in Class* (I)*, then $\lambda_p(\mu + F)$ is independent of p.*

In the remainder of this section, we assume that $\mathbb{M}$ is in Class (II). We note that the rate function $\bar{I}_{\mu+F}$ in Theorem 4.4 is defined on the space of probability measures on X_∞ not on X. In this sense the adjoined point ∞ makes a contribution to the rate function. We see that

$$\bar{I}_{\mu+F}(\delta_\infty) = 0, \tag{5.1}$$

because $\bar{\mathcal{H}}^{\mu+F}\phi(\infty) = \alpha\phi(\infty) - g(\infty) = g(\infty) - g(\infty) = 0$ for any $\phi \in \mathcal{D}_{++}(\bar{\mathcal{H}}^{\mu+F})$. $\mathcal{P}(X_\infty) \setminus \{\delta_\infty\}$ and $(0,1] \times \mathcal{P}(X)$ are in one-to-one correspondence through the map

$$\nu \in \mathcal{P}(X_\infty) \setminus \{\delta_\infty\} \mapsto (\nu(X), \hat{\nu}(\cdot) = \nu(\cdot)/\nu(X)) \in (0,1] \times \mathcal{P}(X). \tag{5.2}$$

Lemma 5.2. *For $\nu \in \mathcal{P}(X_\infty) \setminus \{\delta_\infty\}$,*

$$\bar{I}_{\mu+F}(\nu) = I_{\mu+F}(\nu) = \nu(X) \cdot I_{\mathcal{E}^{\mu+F}}(\hat{\nu}).$$

Proof. For $\phi = \bar{G}_\alpha^{\mu+F} g \in \mathcal{D}_{++}(\bar{\mathcal{H}}^{\mu+F})$, $\bar{\mathcal{H}}^{\mu+F}\phi(\infty) = 0$ and $\bar{\mathcal{H}}^{\mu+F}\phi(x) = \mathcal{H}^{\mu+F}\phi(x)$ for $x \in X$. Hence for $\nu \in \mathcal{P}(X_\infty)$,

$$\begin{aligned}
\bar{I}_{\mu+F}(\nu) &= -\inf_{\phi \in \mathcal{D}_{++}(\bar{\mathcal{H}}^{\mu+F})} \int_{X_\infty} \frac{\bar{\mathcal{H}}^{\mu+F}\phi}{\phi} d\nu \\
&= -\inf_{\phi \in \mathcal{D}_{++}(\mathcal{H}^{\mu+F})} \int_X \frac{\mathcal{H}^{\mu+F}\phi}{\phi} d\nu \\
&= -\inf_{\phi \in \mathcal{D}_{++}(\mathcal{H}^{\mu+F})} \nu(X) \int_X \frac{\mathcal{H}^{\mu+F}\phi}{\phi} d\hat{\nu} \\
&= \nu(X) \cdot I_{\mathcal{E}^{\mu+F}}(\hat{\nu}).
\end{aligned}$$

□

We have the next equality through the one-to-one map (5.2):

$$\inf_{\nu \in \mathcal{P}(X_\infty) \setminus \{\delta_\infty\}} \bar{I}_{\mu+F}(\nu) = \inf_{0<\theta\le 1, \nu \in \mathcal{P}(X)} (\theta \cdot I_{\mathcal{E}^{\mu+F}}(\nu)).$$

In addition, noting that $\bar{I}_{\mu+F}(\delta_\infty) = 0$, we have the next corollary.

Corollary 5.3.

$$\inf_{\nu \in \mathcal{P}(X_\infty)} \bar{I}_{\mu+F}(\nu) = \inf_{0 \le \theta \le 1} \big(\theta \inf_{\nu \in \mathcal{P}(X)} I_{\mathcal{E}^{\mu+F}}(\nu)\big). \tag{5.3}$$

Let us denote by $\| p_t^{\mu+F} \|_{p,p}$ the operator norm of $p_t^{\mu+F}$ from $L^p(X;m)$ to $L^p(X;m)$ and define

$$\lambda_p(\mu+F) = -\lim_{t\to\infty} \frac{1}{t} \log \| p_t^{\mu+F} \|_{p,p}, \quad 1 \le p \le \infty.$$

We then have:

Corollary 5.4. *For $\mu + F \in \mathcal{K}_\infty + \mathcal{A}_2$,*

$$\lambda_\infty(\mu+F) \ge \inf_{0 \le \theta \le 1} \big(\theta \inf_{\nu \in \mathcal{P}(X)} I_{\mathcal{E}^{\mu+F}}(\nu)\big) = \inf_{0 \le \theta \le 1} (\theta \lambda_2(\mu+F)). \tag{5.4}$$

Noting that if $\lambda_2(\mu+F) \le 0$, then $\inf_{0\le\theta\le1}(\theta\lambda_2(\mu+F)) = \lambda_2(\mu+F)$, we have:

Corollary 5.5. *If* $\lambda_2(\mu + F) \le 0$, *then*

$$\lambda_\infty(\mu + F) \ge \lambda_2(\mu + F).$$

The inequality, $\lambda_2(\mu + F) \ge \lambda_\infty(\mu + F)$, generally holds. Indeed,

$$\begin{aligned} p_t^{\mu+F} f(x) &= \mathbb{E}_x[\exp(A_t(\mu + F)) f(X_t)] \\ &\le (\mathbb{E}_x[\exp(A_t(\mu + F)) f^2(X_t)])^{1/2} \cdot (\mathbb{E}_x[\exp(A_t(\mu + F))])^{1/2} \end{aligned}$$

and

$$\|p_t^{\mu+F} f\|_2^2 \le \|p_t^{\mu+F}(f^2)\|_1 \sup_{x\in X} \mathbb{E}_x[\exp(A_t(\mu + F))].$$

By the symmetry and the positivity of $p_t^{\mu+F}$,

$$\|p_t^{\mu+F}(f^2)\|_1 = \int_X f(x)^2 (p_t^{\mu+F} 1(x)) m(dx) \le \|f\|_2^2 \cdot \|p_t^{\mu+F}\|_{\infty,\infty}.$$

Hence we have $\|p_t^{\mu+F}\|_{2,2} \le \|p_t^{\mu+F}\|_{\infty,\infty}$, and thus $\lambda_2(\mu + F) \ge \lambda_\infty(\mu + F)$. Moreover, by the Riesz–Thorin interpolation theorem,

$$\|p_t^{\mu+F}\|_{2,2} \le \|p_t^{\mu+F}\|_{p,p} \le \|p_t^{\mu+F}\|_{\infty,\infty}, \quad 1 \le p \le \infty.$$

Therefore, we can conclude that

$$\lambda_2(\mu + F) \le 0 \implies \lambda_p(\mu + F) = \lambda_2(\mu + F), \quad 1 \le p \le \infty. \tag{5.5}$$

We see that if $\lambda_2(\mu + F) > 0$, then $\lambda_\infty(\mu + F) = 0$. Indeed, if $\lambda_2(\mu + F) > 0$, then by Corollary 5.4

$$\lambda_\infty(\mu + F) \ge \inf_{0\le\theta\le 1} \theta \inf_{\nu\in\mathcal{P}(X)} I_{\mathcal{E}^{\mu+F}}(\nu) = \inf_{0\le\theta\le 1} \theta(\lambda_2(\mu + F)) = 0.$$

On the other hand, it follows from (3.3) that $\lim_{x\to\infty} p_t^{\mu+F} 1(x) = 1$. Therefore, $\|p_t^{\mu+F}\|_{\infty,\infty} \ge 1$, which implies that $\lambda_\infty(\mu + F) \le 0$.

Theorem 5.6. *Assume that* $\mathbb{M}$ *is in Class* (II). *Let* $\mu + F \in \mathcal{K}_\infty + \mathcal{A}_2$. *Then* $\lambda_2(\mu + F) = \lambda_p(\mu + F)$ *for all* $1 \le p \le \infty$ *if and only if* $\lambda_2(\mu + F) \le 0$. *In particular, if* $\lambda_2(\mu + F) > 0$, *then* $\lambda_\infty(\mu + F) = 0$.

Example 5.1 (Brownian motion on $\mathbb{H}^d$). We consider the Brownian motion on the hyperbolic space $\mathbb{H}^d$ ($d \ge 2$), the diffusion process generated by the Laplace–Beltrami operator $(1/2)\Delta$. The corresponding Dirichlet form $(\mathcal{E}, \mathcal{F})$ is as follows:

$$\begin{cases} \mathcal{E}(u,u) = \dfrac{1}{2}\displaystyle\int_{\mathbb{H}^d} (\nabla u, \nabla v)\, dm, \quad u,\ v \in \mathcal{F}, \\ \mathcal{F} = \text{the closure of } C_0^\infty(\mathbb{H}^d) \text{ with respect to } \mathcal{E} + (\ ,\ )_m, \end{cases}$$

where m is the Riemannian volume.

The Brownian motion is in Class (II). Hence $\lambda_\infty = 0$, while

$$\lambda_2 = \inf\{\mathcal{E}(u,u) \mid u \in \mathcal{F}, \|u\|_2 = 1\} = \frac{1}{2}\left(\frac{d-1}{2}\right)^2.$$

Hence the L^p-independence does not hold; However, by adding a Kato measure $\mu \in \mathcal{A}_2$ with $\lambda_2(\mu) \leq 0$, the L^p-independence is recovered. In fact, we consider $\mathcal{H}^\mu = 1/2\Delta + \delta_r$, where δ_r is the surface measure of the sphere centred the origin with radius r.

(a) $d = 2$:

(i) $0 \leq r < r_0 \implies \lambda_\infty(\delta_r) = 0, \ \lambda_2(\delta_r) > 0.$

(ii) $r \geq r_0 > 0 \implies \lambda_p(\delta_r) = \lambda_2(\delta_r), \ 1 \leq p \leq \infty.$

Here r_0 is a unique solution of

$$(e^r - e^{-r}) \log\left(\frac{e^r+1}{e^r-1}\right) = 1.$$

(b) $d \geq 3$:

$$\lambda_\infty(\delta_r) = 0, \quad \lambda_2(\delta_r) > 0, \quad r \geq 0.$$

Corollary 5.7. *Suppose that $\mathbb{M}$ is transient. If $\lambda_2(0) = 0$, then the growth bound of the Feynman–Kac semigroup $\{p_t^{\mu+F}\}_{t>0}$ is L^p-independent for any $\mu + F \in \mathcal{K}_{\infty,0} + \mathcal{A}_{2,0}$.*

Proof. The boundedness of F implies that there exists a constant C' such that $\mathcal{E}_F(u,u) \leq C'\mathcal{E}(u,u)$ for all $u \in \mathcal{F}$. Consequently, we have

$$\begin{aligned}\mathcal{E}^{\mu+F}(u,u) &= \mathcal{E}_F(u,u) - \left(\int_X u^2 d\mu_{F_1} + \int_X u^2 d\mu\right) \\ &\leq C'\mathcal{E}(u,u) - \left(\int_X u^2 d\mu_{F_1} + \int_X u^2 d\mu\right).\end{aligned}$$

Hence, in order to show that $\lambda_2(\mu + F) \leq 0$, it is enough to prove that $\lambda_2(\mu) \leq 0$ for any $\mu \in \mathcal{K}_{\infty,0}$. To this end, we have only to prove that for any positive $\mu \in \mathcal{K}_{\infty,0}$,

$$\lambda_2(\mu) = \inf\left\{\mathcal{E}(u,u) + \int_X u^2 d\mu : u \in \mathcal{F}, \int_X u^2 dm = 1\right\} = 0.$$

Noting that by Theorem 3.1

$$\lambda_2(\mu) \leq \left(\mathcal{E}(u,u) + \int_X u^2 d\mu\right) \leq (1 + \|G\mu\|_\infty)\mathcal{E}(u,u), \quad u \in \mathcal{F},$$

we have the desired claim. □

For a compact set $K \subset X$, define the subspace $\mathcal{F}_{K^c}$ of $\mathcal{F}$ by

$$\mathcal{F}_{K^c} = \{u \in \mathcal{F} : u = 0, \text{ q.e. on } K\}.$$

We then see that $(\mathcal{E}, \mathcal{F}_{K^c})$ is regarded as a regular Dirichlet form on $L^2(K^c; m)$ by identifying the space $L^2_{K^c}(X; m) = \{u \in L^2(X; m) : u = 0, m\text{-a.e. on } K\}$ with $L^2(K^c; m)$, The Dirichlet form $(\mathcal{E}, \mathcal{F}_{K^c})$ is said to be *the part of the Dirichlet form* $(\mathcal{E}, \mathcal{F})$ on the open set K^c. Denote by $\mathcal{L}_K$ the self-adjoint operator associated with $(\mathcal{E}, \mathcal{F}_{K^c})$.

Remark 5.1. Let $\sigma(\mathcal{L}_K)$ be the spectrum of $\mathcal{L}_K$. Assume that for any compact set K,

$$\inf \sigma(\mathcal{L}_K) = 0. \tag{5.6}$$

Then, Corollary 5.7 holds without the transience condition. Indeed, for $\mu \in \mathcal{K}_\infty$,

$$\begin{aligned}\lambda_2(\mu) &= \inf\left\{\mathcal{E}(u,u) + \int_X u^2 d\mu : u \in \mathcal{F},\ \int_X u^2 dm = 1\right\} \\ &\le \inf\left\{\mathcal{E}(u,u) + \int_X u^2 d\mu : u \in \mathcal{F}_{K^c},\ \int_X u^2 dm = 1\right\}.\end{aligned}$$

By assumption (5.6) and Theorem 3.1, the right-hand side is dominated by $\|G_1 \mu_{K^c}\|_\infty$ ($\mu_{K^c}(\cdot) = \mu(K^c \cap \cdot)$), and $\|G_1 \mu_{K^c}\|_\infty$ tends to zero as $K \uparrow X$. We see that the assumption (5.6) is fulfilled for spatially homogeneous symmetric Lévy processes.

The uniform upper bound in Theorem 4.2 is crucial for the proof of L^p-independence, and so is the condition (2.1). As stated in Remark 2.2 (iii), we see that a one-dimensional diffusion process satisfies (2.1), if no boundaries are natural in Feller's boundary classification. As a result, the L^p-independence holds if no boundaries are natural. We see by exactly the same argument as in [39] that if one of the boundary points is natural, then the L^p-independence holds if and only if the L^2-growth bound is non-positive. For example, consider the one-dimensional diffusion process with generator $(1/2)\Delta + k \cdot d/dx$ on $(-\infty, \infty)$. Here k is a constant. Then both boundaries are natural and $\lambda_2(0)$ equals $k^2/2$, while $\lambda_\infty(0) = 0$ because of the conservativeness. Consequently, Theorem 4.2 does not hold when K are the whole space $\mathcal{P}$. This example was given in [22]. Next consider the Ornstein–Uhlenbeck process, the diffusion process generated by $(1/2)\Delta - x \cdot d/dx$ on $(-\infty, \infty)$. Then both boundaries are natural and $\lambda_2(0)$ and $\lambda_\infty(0)$ are zero, consequently the L^p-independence follows. We would like to remark that the uniform upper bound (ii) does not hold true, while the locally uniform upper bound was shown in [22]. In this sense, we can say that the L^p-independence of the Ornstein–Uhlenbeck operator holds for the reason that $\lambda_2(0) = 0$.

Let $\mathbb{M} = (\mathbb{P}_x, X_t)$ be a symmetric Lévy process with Lévy exponent ψ:

$$\mathbb{E}_x\left(\exp(i(\xi, X_t)\right) = \exp(-t\psi(\xi)).$$

Assume that

$$\int_{\mathbb{R}^d} e^{-t\psi(\xi)} d\xi < \infty, \quad \forall t > 0, \tag{5.7}$$

We can show that the assumption (5.7) implies the strong Feller property and $\lambda_2(0)$ equals 0. Hence, $\lambda_2(\mu + F) \le 0$ for any $\mu \in \mathcal{K}_\infty + \mathcal{A}_2$ and the L^p-independence of $\lambda_p(\mu + F)$ follows.

If the Lévy measure J of $\mathbb{M}$ is *exponentially localized*, that is, there exists a positive constant δ such that

$$\int_{|x|>1} e^{\delta|x|} J(dx) < \infty, \tag{5.8}$$

we can prove in the same way as in [35] that for μ in the class $\mathcal{K}$, $\lambda_p(\mu)$ is independent of p. For example, the Lévy measure of the *relativistic Schrödinger process*, the symmetric Lévy process generated by $\sqrt{-\Delta + m^2} - m$, $m > 0$, satisfies (5.8) (Carmona, Master and Simon [10]). On the other hand, the Lévy measure of the symmetric α-stable process on $\mathbb{R}^d$ is $\left(K(d,\alpha)/|x|^{d+\alpha}\right) dx$, and is not exponentially localized, though its Lévy exponent satisfies (5.7). This is the reason why we need to restrict the class of potentials to $\mathcal{K}_\infty + \mathcal{A}_2$.

As a useful approach in proving the large deviation principle, the Gärtner–Ellis theorem is well known ([19], Section 2.3). To apply the Gärtner–Ellis theorem, we shall show first that the limit

$$C(\theta) := \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}_x \left[\exp(\theta A_t(\mu + F))\right], \quad \theta \in \mathbb{R}^1 \tag{5.9}$$

exists ([19], Assumption 2.3.2). We call the limit the *logarithmic moment generating function* of $A_t(\mu + F)$. The existence of the limit (5.9) follows from the L^p-independence proved in this section. Indeed,

$$\begin{aligned} -\lambda_2(\theta(\mu + F)) &\le \limsup_{t\to\infty} \frac{1}{t} \log \mathbb{E}_x \left[\exp(\theta A_t(\mu + F))\right] \\ &\le \limsup_{t\to\infty} \frac{1}{t} \log \sup_{x\in\mathbb{R}^d} \mathbb{E}_x \left[\exp(\theta A_t(\mu + F))\right] \\ &= -\lambda_\infty(\theta(\mu + F)) = -\lambda_2(\theta(\mu + F)). \end{aligned}$$

We thus see that $-\lambda_2(\theta(\mu + F))$ is the logarithmic moment generating function of $A_t(\mu + F)$.

Let $I(\lambda)$ be the Fenchel–Legendre transform of $C(\theta) := -\lambda_2(\theta(\mu + F))$:

$$I(\lambda) = \sup_{\theta\in\mathbb{R}} \{\lambda\theta - C(\theta)\}, \quad \lambda \in \mathbb{R}.$$

If the function $C(\theta)$ is *essentially smooth*, in particular, differentiable on $\mathbb{R}$, we can establish the large deviation principle $A_t(\mu + F)/t$ with the rate function $I(\lambda)$ by applying the Gärtner–Ellis theorem. For example, we have:

Theorem 5.8 ([42]). *Let $\mathbb{P}_x$ be a symmetric α-stable process on $\mathbb{R}^d$ and assume that $d \le 2\alpha$. Then for a positive function $F \in \mathcal{A}_2$, $A_t(F)/t$ obeys the large deviation principle with the rate function $I(\lambda)$:*

(i) *For each closed set $K \in \mathbb{R}$,*

$$\limsup_{t\to\infty} \frac{1}{t} \log \mathbb{P}_x\left(\frac{A_t(F)}{t} \in K\right) \le -\inf_{\lambda\in K} I(\lambda).$$

(ii) *For each open set* $G \subset \mathbb{R}$,

$$\liminf_{t\to\infty} \frac{1}{t} \log \mathbb{P}_x\left(\frac{A_t(F)}{t} \in G\right) \geq -\inf_{\lambda\in G} I(\lambda).$$

6 A large deviation principle for normalized Markov processes

Varadhan [45] gave an abstract formulation for the large deviation principle. Theorem 4.1 and Theorem 4.2 are slightly different from the lower estimate and the upper estimate in his formulation. We show in this section that if the symmetric Markov process $\mathbb{M}$ is in Class (I), the normalized process obeys the large deviation principle in Varadhan's formulation. According to this modification, Theorem 4.1 and Theorem 4.2 can be regarded as a large deviation from the ground state of the generalized Schrödinger operator, that is, the minimizer in the right-hand side of (1.4).

We show the existence of the ground state. Let $\{u_n\}_{n=1}^{\infty} \subset \mathcal{F}$ be a minimizing sequence in (1.4), that is, $\|u_n\|_2 = 1$ and $\lambda_2(\mu + F) = \lim_{n\to\infty} \mathcal{E}^{\mu+F}(u_n, u_n)$. Put $\mu' = |\mu| + |\mu_{F_1}|$. Then $\mu' \in \mathcal{K}_\infty$ and by Theorem 3.1

$$\int_X u_n^2 d\mu' \leq \|G_\alpha \mu'\|_\infty \left(\mathcal{E}(u_n, u_n) + \alpha\right).$$

Since $\mathcal{E}(u_n, u_n) \leq c\mathcal{E}_F(u_n, u_n)$, we have

$$\begin{aligned}
\mathcal{E}^{\mu+F}(u_n, u_n) &\geq \mathcal{E}_F(u_n, u_n) - \|G_\alpha \mu'\|_\infty (\mathcal{E}(u_n, u_n) + \alpha) \\
&\geq \frac{1}{c}\mathcal{E}(u_n, u_n) - \|G_\alpha \mu'\|_\infty \left(\mathcal{E}(u_n, u_n) + \alpha\right) \\
&= \left(\frac{1 - c\|G_\alpha \mu'\|_\infty}{c}\right)\mathcal{E}(u_n, u_n) - \alpha\|G_\alpha \mu'\|_\infty.
\end{aligned}$$

Choosing α so large that $1 - c\|G_\alpha \mu'\|_\infty > 0$, we have

$$\mathcal{E}(u_n, u_n) \leq \frac{c}{1 - c\|G_\alpha \mu'\|_\infty} \left(\mathcal{E}^{\mu+F}(u_n, u_n) + \alpha\|G_\alpha \mu'\|_\infty\right),$$

and thus $\sup_n \mathcal{E}(u_n, u_n) < \infty$. Hence we see from (2.1) and (3.1) that for any $\epsilon > 0$ there exists a compact set K such that

$$\sup_n \int_{K^c} u_n^2 \cdot dm \leq \|G_1 I_{K^c}\|_\infty \cdot \left(\sup_n \mathcal{E}(u_n, u_n) + 1\right) < \epsilon,$$

which implies the tightness of $\{u_n^2 m\}_{n=1}^{\infty}$ in $\mathcal{P}(X)$. Hence there exists a subsequence $\{u_{n_k}^2 m\}_{k=1}^{\infty}$ such that $u_{n_k}^2 m$ converges weakly to a probability measure ν. Since the function $I_{\mathcal{E}^{\mu+F}}$ is lower semi-continuous by Proposition 4.3,

$$I_{\mathcal{E}^{\mu+F}}(\nu) \leq \liminf_{k\to\infty} I_{\mathcal{E}^{\mu+F}}(u_{n_k}^2 m) = \liminf_{k\to\infty} \mathcal{E}^{\mu+F}(u_{n_k}, u_{n_k}) < \infty.$$

Therefore, using Proposition 4.3 again, we see that ν is expressed by $\nu = \phi_0^2 m$, $\phi_0 \in \mathcal{F}$. The function ϕ_0 is just the ground state, $\lambda_2(\mu + F) = \mathcal{E}^{\mu+F}(\phi_0, \phi_0)$. The

uniqueness of the ground state follows from Assumption (I) (see Proposition 1.4.3 in [17]). Therefore we have:

Proposition 6.1 ([41]). *Assume that* $\mathbb{M}$ *is in Class* (I). *Then there exists a unique ground state* ϕ_0 *of* $\mathcal{H}^{\mu+F}$ *in* $\mathcal{F}$.

In the proof of the existence of the ground state, we usually use the $\mathcal{E}_1^{\mu+F}$-weak compactness of $\{u_n\}_{n=1}^{\infty}$ in $\mathcal{F}$ and the lower semi-continuity of $\mathcal{E}^{\mu+F}$ with respect to the $\mathcal{E}_1^{\mu+F}$-weak topology (e.g. [28]). On the other hand, we here use the tightness of $\{u_n^2 m\}_{n=1}^{\infty} \subset \mathcal{P}(X)$ and the lower semi-continuity of the function $I^{\mu+F}$ with respect to the weak topology in $\mathcal{P}(X)$. To this end, the identification of the I-function with the Schrödinger form plays a crucial role.

Define the probability measure $Q_{x,t}$ on $\mathcal{P}(X)$ by

$$Q_{x,t}(B) = \frac{\mathbb{E}_x[e^{A_t(\mu+F)}; L_t \in B, t < \zeta]}{\mathbb{E}_x[e^{A_t(\mu+F)}; t < \zeta]}, \ B \in \mathcal{B}(\mathcal{P}(X)). \tag{6.1}$$

Here L_t is the occupation distribution defined as in (4.1). Define the function J on $\mathcal{P}(X)$ by

$$J(\nu) = I_{\mathcal{E}^{\mu+F}}(\nu) - \lambda_2(\mu + F). \tag{6.2}$$

We see from Lemma 6.2 below that the function J possesses the properties as a rate function in the large deviation principle.

Lemma 6.2. *The function* J *satisfies the following:*
(i) $0 \le J(\nu) \le \infty$.
(ii) J *is lower semicontinuous.*
(iii) *For each* $l < \infty$, *the set* $\{\nu \in \mathcal{P}(X) : J(\nu) \le l\}$ *is compact.*
(iv) $J(\phi_0^2 \cdot m) = 0$ *and* $J(\nu) > 0$ *for* $\nu \ne \phi_0^2 \cdot m$.

Remark 6.1. Let $(\mathcal{E}^{\phi_0}, \mathcal{F}^{\phi_0})$ the bilinear form on $L^2(X; \phi_0^2 m)$ defined by

$$\begin{cases} \mathcal{E}^{\phi_0}(u, v) = \mathcal{E}^{\mu+F}(u\phi_0, u\phi_0) - \lambda_2(\mu + F), \\ \mathcal{F}^{\phi_0} = \{u \in L^2(X; \phi_0^2 m) : u\phi_0 \in \mathcal{F}\}. \end{cases}$$

We then see that $(\mathcal{E}^{\phi_0}, \mathcal{F}^{\phi_0})$ is a Dirichlet form and $\mathcal{E}^{\phi_0}$ is expressed by

$$\mathcal{E}^{\phi_0}(u, v) = \int_X \phi_0^2 d\mu^c_{\langle u,v\rangle} + \int_{X\times X\setminus\Delta} (u(x)-u(y))(v(x)-v(y))\phi_0(x)\phi_0(y)J(dx, dy)$$

([13]). Moreover, we see that

$$J(\nu) = I_{\mathcal{E}^{\phi_0}}(\nu), \tag{6.3}$$

where $I_{\mathcal{E}^{\phi_0}}$ is defined by

$$I_{\mathcal{E}^{\phi_0}}(\nu) = \begin{cases} \mathcal{E}^{\phi_0}(\sqrt{f}, \sqrt{f}) & \text{if } \nu = f \cdot \phi_0^2 m, \ \sqrt{f} \in \mathcal{F}^{\phi_0}, \\ \infty & \text{otherwise.} \end{cases} \tag{6.4}$$

We have the next large deviation principle ([41]):

Theorem 6.3. ([41]) *Let $\mathbb{M}$ be a symmetric Markov process in Class* (I). *Let μ be a measure in $\mathcal{K}_\infty$ and F a function in $\mathcal{A}_2$. Define by* (6.1) *the family $\{Q_{x,t}\}_{t>0}$ of probability measures on $\mathcal{P}(X)$. Then $\{Q_{x,t}\}_{t>0}$ obeys the large deviation principle with rate function J*:

(i) *For each open set $G \subset \mathcal{P}(X)$,*

$$\liminf_{t\to\infty} \frac{1}{t} \log Q_{x,t}(G) \geq -\inf_{\nu\in G} J(\nu).$$

(ii) *For each closed set $K \subset \mathcal{P}(X)$,*

$$\limsup_{t\to\infty} \frac{1}{t} \log Q_{x,t}(K) \leq -\inf_{\nu\in K} J(\nu).$$

Corollary 6.4. *The measure $Q_{x,t}$ weakly converges to $\delta_{\phi_0^2\cdot m}$ as $t \to \infty$.*

Proof. If a closed set K does not contain $\phi_0^2 \cdot m$, then it follows by Lemma 6.2 (iv) that $\inf_{x\in K} J(x) > 0$. Hence Theorem 6.3 (ii) says that $\lim_{t\to\infty} Q_{x,t}(K) = 0$ and $\lim_{t\to\infty} Q_{x,t}(K^c) = 1$. For a constant $\delta > 0$ and a bounded continuous function f on $\mathcal{P}(X)$, define the closed set $K \subset \mathcal{P}(X)$ by $K = \{\nu \in \mathcal{P}(X) : |f(\nu) - f(\phi_0^2\cdot m)| \geq \delta\}$. Then we have

$$\begin{aligned}
&\left| \int_{\mathcal{P}(X)} f(\nu) Q_{x,t}(d\nu) - f(\phi_0^2 \cdot m) \right| \\
&\quad \leq \int_{\mathcal{P}(X)} |f(\nu) - f(\phi_0^2 \cdot m)| Q_{x,t}(d\nu) \\
&\quad = \int_K |f(\nu) - f(\phi_0^2 \cdot m)| Q_{x,t}(d\nu) + \int_{K^c} |f(\nu) - f(\phi_0^2 \cdot m)| Q_{x,t}(d\nu) \\
&\quad \leq 2\|f\|_\infty Q_{x,t}(K) + \delta Q_{x,t}(K^c) \to \delta
\end{aligned}$$

as $t \to \infty$. Since δ is arbitrary, the proof of the corollary is complete. □

On account of Corollary 6.4, we can regard Theorem 6.3 as a large deviation from the ground state.

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Some recent progress on functional inequalities and applications

Feng-Yu Wang*

1 Introduction

Let $\mathbb{H}$ be a separable Hilbert space and $(L, \mathscr{D}(L))$ a negatively definite self-adjoint operator on $\mathbb{H}$ generating a contraction C_0-semigroup P_t. Let $(\mathscr{E}, \mathscr{D}(\mathscr{E}))$ be the associated quadric form. We have $\mathscr{E}(f,g) = -\langle f, Lg\rangle$ for $f, g \in \mathscr{D}(L)$. It is well known that $\|P_t\| \le \mathrm{e}^{-t/C}$ if and only if the Poincaré inequality

$$\|f\|^2 \le C\mathscr{E}(f,f), \quad f \in \mathscr{D}(\mathscr{E}),$$

holds. This inequality is also equivalent to $\inf \sigma(-L) \ge 1/C$, where $\sigma(\cdot)$ stands for the spectrum of a linear operator.

We shall introduce a Poincaré type inequality to describe the essential spectrum of L (Section 2), then apply to Dirichlet forms to cover some earlier results (Section 3). The Poincaré type inequality is also equivalent to the exponential decay of P_t in the tail norm (Section 4). In Section 5 we shall use the super Poincaré inequality for diffusions to investigate Talagrand type transportation-cost inequalities with super cost functions. Finally, we focus on functional inequalities on manifolds with unbounded below curvature (Section 6) and manifolds with non-convex boundary (Section 7). For applications of functional inequalities to isoperimetric/cost inequalities, we refer to [2], [7], [8], [10], [11], [14], [16] and references therein.

2 Poincaré type inequality on Hilbert spaces

Let $(L, \mathscr{D}(L))$ be a negative definite self-adjoint operator on a separable Hilbert space $\mathbb{H}$, and let $(\mathscr{E}, \mathscr{D}(\mathscr{E}))$ be the associate quadratic from. For $B \subset \mathbb{H}$, let

$$\|f\|_{B^*} = \sup\{|\langle f, g\rangle| : g \in B\}, \quad f \in \mathbb{H}.$$

We shall use the following Poincaré type inequality to study the essential spectrum of L:

$$\|f\|^2 \le r\mathscr{E}(f,f) + \beta(r)\|f\|_{B^*}^2, \quad r > r_0,\ f \in \mathscr{D}(\mathscr{E}), \tag{2.1}$$

where $r_0 \ge 0$ is a constant and $\beta : (r_0, \infty) \to (0, \infty)$ is a (decreasing) function.

Let $\sigma_{\mathrm{ess}}(L)$ be the essential spectrum of L, which consists of limit points in the spectrum $\sigma(L)$ and isolated eigenvalues of L with infinite multiplicity. The following Weyl's criterion on the essential spectrum is very useful in our study.

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Theorem 2.1 (Weyl's criterion). *$\lambda \in \sigma_{\rm ess}(L)$ if and only if there exists an orthonormal sequence $\{f_n\}_{n\geq 1}$ in $\mathbb{H}$ such that*

$$\|Lf_n - \lambda f_n\| \leq \frac{1}{n}, \quad n \geq 1.$$

The following result is due to [30], which provides a correspondence between upper bound of the essential spectrum for $-L$ and the Poincaré type inequality (2.1).

Theorem 2.2. *Let $r_0 \geq 0$. Then the following statements are equivalent:*

(1) $\sigma_{\rm ess}(-L) \subset [r_0^{-1}, \infty)$.

(2) *There exist a compact set $B \subset \mathbb{H}$ and a function $\beta\colon (r_0, \infty) \to (0, \infty)$ such that (2.1) holds.*

(3) *There exist $t > 0$ and $B \subset \mathbb{H}$ such that $P_t B$ is relatively compact and (2.1) holds for some $\beta\colon (r_0, \infty) \to (0, \infty)$.*

Proof. Since P_t sends compact sets into compact sets, it is obvious that (2) implies (3).

(1) $\Longrightarrow$ (2). Let $r > r_0$, we have $[0, r^{-1}] \cap \sigma_{\rm ess}(-L) = \emptyset$. So, the spectrum of $-L$ in $[0, r^{-1}]$ consists of finitely many eigenvalues including multiplicities. Let

$$\lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{n_r}$$

be all eigenvalues of $-L$ in $[0, r^{-1}]$ counting multiplicities, and $\{f_i\}_{0\leq i\leq n_r}$ the corresponding unit eigenvectors. For any $f \in \mathscr{D}(\mathscr{E})$, consider the orthogonal decomposition

$$f = f' + f'', \quad f' = \sum_{i=0}^{n_r} \langle f, f_i\rangle f_i.$$

Let $\{E_\lambda\}_{\lambda\geq 0}$ be the spectral family of $-L$. Then, by spectral representation

$$\begin{aligned}\mathscr{E}(f, f) &= \int_0^\infty \lambda \mathrm{d}E_\lambda(f, f)\\ &\geq \int_{r^{-1}}^\infty \lambda \mathrm{d}E_\lambda(f, f)\\ &\geq r^{-1}\int_{r^{-1}}^\infty \mathrm{d}E_\lambda(f, f)\\ &= r^{-1}\|f''\|^2.\end{aligned}$$

So,

$$\|f\|^2 = \|f'\|^2 + \|f''\|^2 \leq r\mathscr{E}(f, f) + \sum_{i=0}^{n_r} \langle f_i, f\rangle^2. \tag{2.2}$$

Since the spectrum of $-L$ is discrete in $[0, r_0^{-1})$, let

$$\lambda_0 \leq \lambda_1 \leq \cdots$$

be all eigenvalues including multiplicities, and $\{f_i\}$ the corresponding unit eigenvectors. Let

$$B = \{0, (n+1)^{-1} f_n : n \geq 0\}.$$

Then B is compact and

$$\sum_{i=0}^{n_r} \langle f, f_i\rangle^2 \leq (1+n_r)^3 \sup_{g\in B} |\langle f, g\rangle|^2 = (n_r+1)^3 \|f\|_{B^*}^2.$$

Combining this with (2.2), we prove (2.1) for $\beta(r) = (1+n_r)^3$.

(3) $\Longrightarrow$ (1). We need the following lemma.

Lemma 2.3. *Let $\{f_n\}$ be an orthonormal sequence. Then $\lim_{n\to\infty} \|f_n\|_{B^*} = 0$ holds for any relatively compact set B.*

Let $P_t B$ be relatively compact and let (2.1) hold. We intend to prove that for any $\lambda \in \sigma_{\text{ess}}(-L)$, one has $\lambda \geq r_0^{-1}$. By Weyl's criterion, there exists an orthonormal sequence $\{f_n\}$ such that $\|Lf_n + \lambda f_n\| \leq \frac{1}{n}, n \geq 1$. So,

$$\frac{\mathrm{d}}{\mathrm{d}s}\|P_s f_n\|^2 = 2\langle P_s L f_n, P_s f_n\rangle = -2\lambda \|P_s f_n\|^2 + \varepsilon_n(s),$$

where $|\varepsilon_n(s)| \leq 2n^{-1}$. Thus,

$$\begin{aligned}\|P_t f_n\|^2 - \mathrm{e}^{-2\lambda t} &= \int_0^t \frac{\mathrm{d}}{\mathrm{d}s}\{\|P_s f_n\|^2 \mathrm{e}^{-2\lambda(t-s)}\}\mathrm{d}s \\ &= \int_0^t \varepsilon_n(s)\mathrm{e}^{-2\lambda(t-s)}\mathrm{d}s.\end{aligned}$$

This implies

$$\lim_{n\to 0} \|P_t f_n\|^2 = \mathrm{e}^{-2\lambda t}. \tag{2.3}$$

Now, by (2.1) and noting that $\|P_t f\|_{B^*} = \|f\|_{(P_t B)^*}$, we obtain

$$\begin{aligned}\|P_t f_n\|^2 &\leq -r\langle P_t f_n, P_t L f_n\rangle + \beta(r)\|P_t f_n\|_{B^*}^2 \\ &\leq r\lambda\|P_t f_n\|^2 + \frac{r}{n} + \beta(r)\|f_n\|_{(P_t B)^*}^2, \quad r > r_0.\end{aligned}$$

By Lemma 2.3 and (2.3), letting $n \to \infty$ in the above inequality, we arrive at

$$\mathrm{e}^{-2\lambda t} \leq r\lambda \mathrm{e}^{-2\lambda t} + 0, \quad r > r_0.$$

Thus, $\lambda \geq r_0^{-1}$. □

Recall that a linear operator on a Banach space is called compact, if it sends bounded sets into relatively compact sets. Let $P_t = \mathrm{e}^{tL}$. It is well known that P_t is compact for some/all $t > 0$ if and only if $\sigma_{\text{ess}}(L) = \emptyset$.

Theorem 2.4. *The following statements are equivalent to each other:*

(1) $\sigma_{\rm ess}(L) = \emptyset$.

(2) (2.1) *holds for* $r_0 = 0$, *some compact set* B *and some* $\beta: (0,\infty) \to (0,\infty)$.

(3) *There exists* $t > 0$ *and* B *such that* $P_t B$ *is relatively compact and* (2.1) *holds for* $r_0 = 0$ *and some* $\beta: (0,\infty) \to (0,\infty)$.

(4) P_t *is compact for some* $t > 0$.

(5) P_t *is compact for all* $t > 0$.

3 Poincaré type inequality for Dirichlet forms

Consider $\mathbb{H} = L^2(\mu)$ for a σ-finite complete measure space $(E, \mathcal{F}, \mu)$. Let $(\mathcal{E}, \mathcal{D}(\mathcal{E}))$ be a symmetric Dirichlet form in $L^2(\mu)$. We shall study (2.1) for

$$B = B_\phi := \{g : |g| \le \phi\},$$

where $\phi > 0$ is a fixed function in $L^2(\mu)$. In this case

$$\|f\|_{B^*} = \sup_{|g|\le\phi} |\mu(gf)| = \mu(\phi|f|).$$

In particular, if μ is finite we may take $\phi = 1$ such that $\mu(\phi|f|) = \|f\|_1$. The following result is taken from [28] with a simpler proof.

Theorem 3.1. *Let* $r_0 \ge 0$. *If* $\sigma_{\rm ess}(-L) \subset [r_0^{-1}, \infty)$, *then for any* $\phi \in L^2(\mu)$ *with* $\phi > 0$ μ*-a.e. there exists* $\beta: (r_0,\infty) \to (0,\infty)$ *such that*

$$\mu(f^2) \le r\mathcal{E}(f,f) + \beta(r)\mu(\phi|f|)^2, \quad r > r_0, f \in \mathcal{D}(\mathcal{E}). \tag{3.1}$$

Proof. By Theorem 2.2, there is a compact set $B \subset L^2(\mu)$ and a function $\tilde\beta: (r_0,\infty) \to (0,\infty)$ such that

$$\mu(f^2) \le r\mathcal{E}(f,f) + \tilde\beta(r)\|f\|_{B^*}^2, \quad r > r_0, f \in \mathcal{D}(\mathcal{E}). \tag{3.2}$$

For any $g \in B$ and $f \in \mathcal{D}(\mathcal{E})$, we have

$$\begin{aligned}\mu(|fg|) &\le R\mu(\phi|f|) + \mu(|fg|1_{\{|g|>R\phi\}}) \\ &\le R\mu(\phi|f|) + \sqrt{\mu(f^2)\varepsilon(R)}, \quad R > 0,\end{aligned}$$

where

$$\varepsilon(R) := \sup_{g\in B} \mu(g^2 1_{\{|g|>R\phi\}}), \quad R > 0.$$

Then

$$\|f\|_{B^*}^2 \le 2R^2\mu(\phi|f|)^2 + 2\varepsilon(R)\mu(f^2).$$

Combining this with (3.2) we obtain

$$\mu(f^2) \le s\mathcal{E}(f,f) + 2\tilde{\beta}(s)R^2\mu(\phi|f|)^2 + 2\tilde{\beta}(s)\varepsilon(R)\mu(f^2), \quad s > r_0.$$

If $\lim_{R\to\infty}\varepsilon(R) = 0$, then for any $r > r_0$ the set

$$A_r := \{(s,R) \in (r_0, r)\times(0,\infty) :\ s \le r(1-2\tilde{\beta}(s)\varepsilon(R))\} \ne \emptyset.$$

By the above inequality, for $(s,R) \in A_r$ we have

$$\begin{aligned}\mu(f^2) &\le \frac{s}{1-2\tilde{\beta}(s)\varepsilon(R)}\mathcal{E}(f,f) + \frac{2\tilde{\beta}(s)R^2}{1-2\tilde{\beta}(s)\varepsilon(R)}\mu(\phi|f|)^2 \\ &\le r\mathcal{E}(f,f) + \frac{2\tilde{\beta}(s)R^2}{1-2\tilde{\beta}(s)\varepsilon(R)}\mu(\phi|f|)^2.\end{aligned}$$

Therefore, (3.1) holds for

$$\beta(r) = \inf\left\{\frac{2\tilde{\beta}(s)R^2}{1-2\tilde{\beta}(s)\varepsilon(R)} : (s,R) \in A_r\right\} < \infty, \quad r > r_0.$$

Hence it remains to prove $\varepsilon(R) \to 0$ as $R \to \infty$. Since B is compact, for any $\varepsilon > 0$ there exist $f_1, \dots, f_m \in B$ such that $\cup_{i=1}^m B(f_i, \varepsilon) \supset B$. Then for any $g \in B$, there exists $1 \le i \le m$ such that $g \in B(f_i, \varepsilon)$. In particular, there exists a constant $C > 0$ such that $\mu(g^2) \le C$ for all $g \in B$. Thus,

$$\begin{aligned}\mu(g^2 1_{\{|g|>\phi R\}}) - 2\varepsilon^2 &\le 2\mu(f_i^2 1_{\{|g|>\phi R\}}) \\ &\le 2\mu(f_i^2 1_{\{\phi\le R^{-1/2}\}}) + 2\mu(f_i^2 1_{\{|g|>R^{1/2}\}}) \\ &\le 2\mu(f_i^2 1_{\{\phi\le R^{-1/2}\}}) + 2M\mu(|g| > R^{1/2}) + 2\mu(f_i^2 1_{\{f_i^2>M\}}) \\ &\le 2\mu(f_i^2 1_{\{\phi\le R^{-1/2}\}}) + 2\mu(f_i^2 1_{\{f_i^2>M\}}) + \frac{2MC}{R}.\end{aligned}$$

This implies that

$$\varepsilon(R) \le 2\sum_{i=1}^m \left\{\mu(f_i^2 1_{\{\phi\le R^{-1/2}\}}) + 2\mu(f_i^2 1_{\{f_i^2>M\}})\right\} + \frac{2MC}{R} + 2\varepsilon^2.$$

Therefore,

$$\lim_{R\to\infty}\varepsilon(R) \le 2\varepsilon^2 + 2\sum_{i=1}^m \mu(f_i^2 1_{\{f_i^2>M\}}).$$

By the dominated convergence theorem, letting first $M \to \infty$, then $\varepsilon \to 0$, we complete the proof. □

According to Theorem 2.2, to prove that (3.1) implies $\sigma_{\rm ess}(-L) \subset [r_0^{-1}, \infty)$, we need to verify that $P_t B_\phi$ is relatively compact for some $t > 0$. To this end, we assume that P_t has a density $p_t(x,y)$ with respect to μ. The following theorem is due to [25] and [17].

Theorem 3.2. *Assume that for some $t > 0$ the operator P_t has a density $p_t(x, y)$ with respect to μ, i.e.,*

$$P_t f = \int_E p_t(\cdot, y) f(y) \mu(\mathrm{d}y)$$

holds in $L^2(\mu)$. Then for any positive $\phi \in L^2(\mu)$ and $\beta\colon (r_0, \infty) \to (0, \infty)$, (3.1) implies $\sigma_{\mathrm{ess}}(-L) \subset [r_0^{-1}, \infty)$.

Proof. By Theorem 2.2, it suffices to show that $P_t B_\phi$ is relatively compact, i.e., for any sequence $\{f_n\} \subset B_\phi$, the sequence $\{P_t f_n\}$ has a convergent subsequence. Since $|f_n| \le \phi$, the sequence $\{\frac{f_n}{\phi}\}$ is bounded in $L^\infty(\mu)$ and hence, is weak*-relatively compact. Let $g \in L^\infty(\mu)$ and $\{f_{n_k}\}$ be a subsequence of $\{f_n\}$ such that $f_{n_k} \to g$ in $L^\infty(\mu)$ in the weak*-topology, i.e.,

$$\lim_{k\to\infty} \mu(h(f_{n_k}\phi^{-1} - g)) = 0, \quad h \in L^1(\mu).$$

Since for μ-a.e. x,

$$P_t\phi(x) = \int_E p_t(x, y)\phi(y)\mu(\mathrm{d}y) < \infty,$$

we have $p_t(x, \cdot)\phi \in L^1(\mu)$ and hence,

$$\begin{aligned} &\lim_{k\to\infty} |P_t f_{n_k}(x) - P_t(g\phi)(x)| \\ &= \lim_{k\to\infty} \big|\mu\big((f_{n_k} - g)\phi^{-1} \cdot \{p_t(x, \cdot)\phi\}\big)\big| = 0, \quad \mu\text{- a.e.} \end{aligned}$$

Moreover, since $|f_{n_k}| \le \phi$,

$$|P_t f_{n_k}| + |P_t(gh)| \le (1 + \|g\|_\infty) P_t\phi \in L^2(\mu).$$

By the dominated convergence theorem $\|P_t f_{n_k} - P_t(g\phi)\|_2 \to 0$ as $k \to \infty$. □

Remark 3.3. The assumption on the existence of density in Theorem 3.2 can be replaced by the existence of asymptotic density: *a linear operator is said to have asymptotic density w.r.t. μ if there exists a sequence of linear operators $\{P_n\}$ having densities w.r.t. μ such that $\|P_n - P\|_2 \to 0$ as $n \to \infty$.* A fact is that *any compact operator has asymptotic density.* See §3.1.3 in [31] for details.

Due to this remark, we have the following consequences.

Corollary 3.4. *Assume that P_t has asymptotic density for some $t > 0$. Then the following are equivalent:*

(1) *There exist $\phi > 0$ in $L^2(\mu)$ and some $\beta\colon (r_0, \infty) \to (0, \infty)$ such that (3.1) holds.*

(2) *For any $\phi > 0$ in $L^2(\mu)$, there exists $\beta\colon (r_0, \infty) \to (0, \infty)$ such that (3.1) holds.*

(3) $\sigma_{\mathrm{ess}}(-L) \subset [r_0^{-1}, \infty)$.

Corollary 3.5. *The following are equivalent:*

(1) P_t *is compact for some/any* $t > 0$.

(2) P_t *has asymptotic density for some* $t > 0$ *and there exist* $\phi > 0$ *in* $L^2(\mu)$ *and some* $\beta\colon (0,\infty) \to (0,\infty)$ *such that* (3.1) *holds for* $r_0 = 0$.

(3) P_t *has asymptotic density for any* $t > 0$, *and for any* $\phi > 0$ *in* $L^2(\mu)$ *there exists* $\beta\colon (0,\infty) \to (0,\infty)$ *such that* (3.1) *holds for* $r_0 = 0$.

(4) $\sigma_{\text{ess}}(-L) = \emptyset$.

As a conclusion of this section, we present the following result on (3.1) which can be easily verified by splitting arguments.

Proposition 3.6. *If* (3.1) *holds for some positive* $\phi \in L^2(\mu)$ *and some* $\beta\colon (r_0,\infty) \to (0,\infty)$, *then for any* $\tilde{\phi} > 0$ *such that* $\tilde{\phi} \in L^2(\mu)$ *there exists* $\tilde{\beta}\colon (r_0,\infty) \to (0,\infty)$ *such that*

$$\mu(f^2) \le r\mathcal{E}(f,f) + \tilde{\beta}(r)\mu(\tilde{\phi}|f|)^2, \quad f \in \mathcal{D}(\mathcal{E}),\ r > r_0.$$

4 Exponential decay of the semigroup in the tail norm

Let P be a bounded linear operator on $L^2(\mu)$. For any $\phi, \psi > 0$ with $\phi, \psi \in L^2(\mu)$ we have

$$\lim_{R\to\infty} \sup_{\|f\|_2\le 1} \|(Pf)1_{\{|Pf|>R\psi\}}\|_2 = \lim_{R\to\infty} \sup_{\|f\|_2\le 1} \mu\big((|Pf| - R\phi)^+{}^2\big)^{1/2}.$$

So, the above limits are independent of the choices of ϕ and ψ. We call the limit *tail norm* of P, and denote it by $\|P\|_T$.

Theorem 4.1. *Let* $r_0 \ge 0$ *be fixed. Then*

(1) (3.1) *implies* $\|P_t\|_T \le \mathrm{e}^{-t/r_0}$ *for all* $t \ge 0$;

(2) *if* $\|P_t\|_T \le \mathrm{e}^{-t/r_0}$ *holds for some* $t > 0$, *then for any strictly positive* $\phi \in L^2(\mu)$ *there exists* $\beta\colon (r_0,\infty) \to (0,\infty)$ *such that* (3.1) *holds.*

Proof. (1) For $\in L^2(\mu)$ with $\|f\|_2 \le 1$, let $h(t) = \mu((P_t f)^2)$, $t \ge 0$. Then (3.1) implies

$$\begin{aligned} h'(t) &= -2\mathcal{E}(P_t f, P_t f) \\ &\le -\frac{2}{r}h(t) + \frac{2\beta(r)}{r}\mu(\phi|P_t f|)^2 \\ &\le -\frac{2}{r}h(t) + \frac{2\beta(r)}{r}\mu(|f|P_t\phi)^2, \quad r > r_0. \end{aligned}$$

By Gronwall's lemma

$$\mu((P_t f)^2) \le \mathrm{e}^{-2t/r} + \frac{2\beta(r)}{r}\mathrm{e}^{-2t/r}\int_0^t \mathrm{e}^{2s/r}\mu(|f|P_s\phi)^2\mathrm{d}s$$

for $r > r_0$. Since due to Jensen's inequality $(P_t f)^+ \le P_t f^+$, for any $R > 0$ we have

$$\begin{aligned}\mu\big((|P_t f| - RP_t\phi)^{+2}\big) &\le \mu\big((P_t(|f| - R\phi)^+)^2\big)\\ &\le \mathrm{e}^{-2t/r} + \frac{2\beta(r)}{r}\int_0^t \mu\big((|f| - R\phi)^+ P_s\phi\big)^2\mathrm{d}s\\ &\le \mathrm{e}^{-2t/r} + \frac{2\beta(r)}{r}\int_0^t \mu\big(1_{\{|f|>R\phi\}}(P_s\phi)^2\big)\mathrm{d}s, \quad r > r_0.\end{aligned}$$

In the last step we have used the fact that

$$\begin{aligned}\mu\big((|f| - R\phi)^+ P_s\phi\big)^2 &\le \mu\big(1_{\{|f|>R\phi\}}(P_s\phi)^2\big)\mu\big((|f| - R\phi)^{+2}\big)\\ &\le \mu\big(1_{\{|f|>R\phi\}}(P_s\phi)^2\big).\end{aligned}$$

Moreover,

$$\begin{aligned}&\mu((P_s\phi)^2 1_{\{|f|>R\phi\}})\\ &\quad\le \mu((P_s\phi)^2 1_{\{\phi<R^{-1/2}\}}) + \mu((P_s\phi)^2 1_{\{|f|>R^{1/2}\}})\\ &\quad\le \mu((P_s\phi)^2 1_{\{\phi<R^{-1/2}\}}) + \mu((P_s\phi)^2 1_{\{P_s\phi>R^{1/4}\}}) + R^{1/2}\mu(|f| > R^{1/2})\\ &\quad\le \mu((P_s\phi)^2 1_{\{\phi<R^{-1/2}\}}) + \mu((P_s\phi)^2 1_{\{P_s\phi>R^{1/4}\}}) + R^{-1/2} =: \varepsilon_R(s) \to 0\end{aligned}$$

as $R \to \infty$. So, by the dominated convergence theorem,

$$\begin{aligned}\|P_t\|_T^2 - \mathrm{e}^{-2t/r} &\le \lim_{R\to\infty}\sup_{|f|_2\le 1}\mu\big((|P_t f| - RP_t\phi)^{+2}\big)\\ &\le \frac{2\beta(r)}{r}\lim_{R\to\infty}\int_0^t \varepsilon_R(s)\mathrm{d}s = 0, \quad r > r_0.\end{aligned}$$

This implies $\|P_t\|_T \le \mathrm{e}^{-t/r_0}$ by letting $r \downarrow r_0$.

(2) On the other hand, suppose that $\|P_t\|_T \le \mathrm{e}^{-t/r_0}$ holds for some $t > 0$. For any strictly positive $\phi \in L^2(\mu)$ we intend to construct $\beta\colon (r_0,\infty) \to (0,\infty)$ such that (3.1) holds. For any $r > r_0$, let $r_1 = \frac{1}{2}(r + r_0) \in (r_0, r)$. So, there exists $R_r > 0$ such that

$$\sup_{\|f\|_2\le 1}\mu\big((P_t f)^2 1_{\{|P_t f|>\phi R_r\}}\big) \le \mathrm{e}^{-2t/r_1}.$$

This implies

$$\mu((P_t f)^2) \le \mathrm{e}^{-2t/r_1} + R_r\mu(\phi|P_t f|), \quad \mu(f^2) = 1.$$

Let $\{E_\lambda\}_{\lambda\geq 0}$ be the spectral family of $-L$. Then $\lambda \mapsto E_\lambda(f,f)$ is a probability distribution function on $[0,\infty)$. By the Jensen inequality,

$$\begin{aligned}\mu((P_s f)^2) &= \int_0^\infty \mathrm{e}^{-\lambda s}\mathrm{d}E_\lambda(f,f)\\ &\leq \left(\int_0^\infty \mathrm{e}^{-\lambda t}\mathrm{d}E_\lambda(f,f)\right)^{s/t} = \mu((P_t f)^2)^{s/t}, \quad s\in(0,t).\end{aligned}$$

Therefore,

$$\mu((P_s f)^2) \leq \left\{\mathrm{e}^{-2t/r_1} + R_r\mu(\phi|P_t f|)\right\}^{s/t}, \quad s\in(0,t).$$

Since equality holds at $s=0$, we are able to take derivatives for both sides to derive

$$\begin{aligned}-2\mathscr{E}(f,f) &\leq \frac{1}{t}\log\left\{\mathrm{e}^{-2t/r_1} + R_r\mu(\phi|P_t f|)\right\} \leq -\frac{1}{t}\cdot\frac{2t}{r_1} + \frac{1}{t}R_r\mathrm{e}^{2t/r_1}\mu(\phi|P_t f|)\\ &\leq -\frac{2}{r_1} + \frac{1}{t}R_r\mathrm{e}^{2t/r_1}\mu((P_t\phi)|f|) \leq -\frac{2}{r} + C(t,r)\mu((P_t\phi)|f|)^2,\end{aligned}$$

where $C(t,r) = \frac{1}{4}(\frac{2}{r_1}-\frac{2}{r})^{-1}\frac{R_r^2}{t^2}\mathrm{e}^{4t/r_1}$.

$$\mu(f^2) \leq r\mathscr{E}(f,f) + \frac{1}{2}C(t,r)\mu((P_t\phi)|f|)^2, \quad r > r_0.$$

Since $P_t\phi \in L^2(\mu)$, this implies that for any $\phi > 0$ with $\phi \in L^2(\mu)$ there exists $\beta\colon (r_0,\infty)\to(0,\infty)$ such that (3.1) holds. □

Corollary 4.2. *The following statements are equivalent to each other:*

(1) (3.1) *holds for* $r_0 = 0$, *some positive* $\phi \in L^2(\mu)$ *and some* $\beta\colon (0,\infty)\to(0,\infty)$.

(2) $\|P_t\|_T = 0$ *for all* $t > 0$.

(3) $\|P_t\|_T = 0$ *for some* $t > 0$.

5 Links to transportation-cost inequalities

Let (E,ρ) be a Polish space and μ a probability measure on E. For $p\geq 1$ we define the L^p-Wasserstein distance (or the L^p-transportation cost) by

$$W_p^\rho(\mu_1,\mu_2) := \left\{\inf_{\pi\in\mathscr{C}(\mu_1,\mu_2)}\int_{E\times E}\rho(x,y)^p\pi(\mathrm{d}x,\mathrm{d}y)\right\}^{1/p}$$

for probability measures μ_1, μ_2 on E, where $\mathscr{C}(\mu_1,\mu_2)$ is the class of probability measures on $E\times E$ with marginal distributions μ_1 and μ_2.

According to [9], Corollary 4,

$$W_p^\rho(f\mu,\mu)^{2p} \leq C\mu(f\log f), \quad f\geq 0,\ \mu(f)=1,$$

holds for some $C > 0$ provided $\mu(\mathrm{e}^{\lambda\rho(o,\cdot)^{2p}}) < \infty$ for some $\lambda > 0$, where $o \in E$ is a fixed point. See also [15] for $p = 1$. Furthermore, applying Theorem 1.15 in [18] with $c(x, y) = \rho(x, y)^q$ and $\alpha(r) = r^{2p}$, we conclude that for any $q \in [1, 2p)$,

$$W_q^\rho(f\mu, \mu)^{2p} \le C\mu(f \log f), \quad f \ge 0,\ \mu(f) = 1, \tag{5.1}$$

holds for some $C > 0$ if and only if $\mu(\mathrm{e}^{\lambda\rho(o,\cdot)^{2p}}) < \infty$ for some $\lambda > 0$.

In general, however, this concentration of μ does not imply (5.1) for $q = 2p$. For instance, due to [5], there exist plentiful examples with $\mu(\mathrm{e}^{\lambda\rho(o,\cdot)^2}) < \infty$ for some $\lambda > 0$ but the Poincaré inequality does not hold, which is weaker than the Talagrand inequality (see [20], Section 7, or [4], Section 4.1):

$$W_2^\rho(f\mu, \mu)^2 \le C\mu(f \log f), \quad f \ge 0,\ \mu(f) = 1.$$

Therefore, to derive (5.1) with $q = 2p$, one needs something stronger than the corresponding concentration of μ.

In this section we aim to derive (5.1) with $q = 2p$, i.e.,

$$W_{2p}^\rho(f\mu, \mu)^{2p} \le C\mu(f \log f), \quad f \ge 0,\ \mu(f) = 1, \tag{5.2}$$

on a connected complete Riemannian manifold M for the Riemannian distance ρ, by using the super Poincaré inequalities

$$\mu(f^2) \le r\mu(|\nabla f|^2) + \beta(r)\mu(|f|)^2, \quad r > 0,\ f \in C_b^1(M), \tag{5.3}$$

where $\beta\colon (0, \infty) \to (0, \infty)$ is a decreasing function. The advantage of (5.2) is its tensorization property. More precisely, due to the induction argument in [22], Section 3, if (5.2) holds for pairs (μ_i, ρ_i), $i = 1, \dots, n$, then it also holds for the product measure $\mu_1 \times \cdots \times \mu_n$ and

$$\rho_n(x_1, \dots, x_n; y_1, \dots, y_n) := \Big\{\sum_{i=1}^n \rho_i(x_i, y_i)^{2p}\Big\}^{1/2p}.$$

To derive (5.2) from (5.3), we first prove the weighted log-Sobolev inequality

$$\mu(f^2 \log f^2) \le C\mu(\alpha \circ \rho(o, \cdot)|\nabla f|^2), \quad \mu(f^2) = 1, \tag{5.4}$$

where α is a positive function determined by β in (5.3). By Theorem 1.1 in [29] (see also [20], [4]), (5.4) implies

$$W_2^{\rho_\alpha}(f\mu, \mu)^2 \le C\mu(f \log f), \quad f \ge 0, \mu(f^2) = 1, \tag{5.5}$$

where ρ_α is the Riemannian distance induced by the metric

$$\langle X, Y\rangle' := \frac{1}{\alpha \circ \rho(o, x)}\langle X, Y\rangle, \quad X, Y \in T_x M,\ x \in M.$$

The following result is due to [33].

Theorem 5.1. *Let $\mu(\mathrm{d}x) = \mathrm{e}^{V(x)}\mathrm{d}x$ for some $V \in C(M)$ be a probability measure on M. Assume that (5.3) holds for some positive decreasing $\beta \in C((0,\infty))$ such that*

$$\eta(s) := \big(\log(2s)\big)\big(1 \wedge \beta^{-1}(s/2)\big), \quad s \geq 1$$

is bounded, where $\beta^{-1}(s) := \inf\{t \geq 0 : \ \beta(t) \leq s\}$. Then (5.4) holds for some $C > 0$ and

$$\alpha(s) := \sup\left\{\eta(t) : \ t \geq \frac{1}{\mu(\rho(o,\cdot) \geq s-2)}\right\}, \quad s \geq 0.$$

Consequently, (5.5) holds.

Since $\mu(\rho(o,\cdot) \geq s-2)$ can be estimated by using known concentration of μ induced by the super Poincaré inequality, one may determine the function α in Theorem 5.1 by using β only. But in general the formulation is quite complicated, so we consider below some specific situations as consequences.

Corollary 5.2. *Let $\delta \in (1,2)$.*

(a) *(5.3) with $\beta(r) = \exp[c(1 + r^{-1/\delta})]$ implies (5.4) with*

$$\alpha(s) := (1+s)^{-2(\delta-1)/(2-\delta)}$$

and (5.5) with $\rho_\alpha(x,y)$ replaced by

$$\rho(x,y)(1 + \rho(o,x) \vee \rho(o,y))^{(\delta-1)/(2-\delta)}.$$

Consequently, it implies

$$W_{2/(2-\delta)}^{\rho}(f\mu,\mu)^{2/(2-\delta)} \leq C\mu(f\log f), \quad \mu(f) = 1, \ f \geq 0, \tag{5.6}$$

for some constant $C > 0$.

(b) *If $V \in C^2(M)$ with $\mathrm{Ric} - \mathrm{Hess}_V$ bounded below, then the following are equivalent to each other:*

(1) *(5.3) with $\beta(r) = \exp[c(1 + r^{-1/\delta})]$ for some constant $c > 0$;*

(2) *(5.4) with $\alpha(s) := (1+s)^{-2(\delta-1)/(2-\delta)}$ for some $C > 0$;*

(3) *(5.5) for some $C > 0$ and $\rho_\alpha(x,y)$ replaced by*

$$\rho(x,y)(1 + \rho(o,x) \vee \rho(o,y))^{(\delta-1)/(2-\delta)};$$

(4) *(5.6) for some $C > 0$;*

(5) *$\mu(\exp[\lambda\rho(o,\cdot)^{2/(2-\delta)}]) < \infty$ for some $\lambda > 0$.*

We remark that (5.3) with $\beta(r) = \exp[c(1 + r^{-1/\delta})]$ for some $c > 0$ is equivalent to the following $\log^\delta$-Sobolev inequality (see [24], [25], [17], [31] for more general results on (5.3) and the F-Sobolev inequality)

$$\mu(f^2 \log^\delta(1 + f^2)) \leq C_1\mu(|\nabla f|^2) + C_2, \quad \mu(f^2) = 1.$$

Since due to [25], Corollary 5.3, if (5.3) holds with $\beta(r) = \exp[c(1 + r^{-1/\delta})]$ for some $\delta > 2$ then M has to be compact, as a complement to Corollary 5.2 we consider the critical case $\delta = 2$ in the next corollary.

Corollary 5.3. (5.3) *with* $\beta(r) = \exp[c(1 + r^{-1/2})]$ *for some* $c > 0$ *implies* (5.4) *with* $\alpha(s) := \mathrm{e}^{-c_1 s}$ *for some* $c_1 > 0$ *and* (5.5) *with* $\rho_\alpha(x, y)$ *replaced by*

$$\rho(x, y)\mathrm{e}^{c_2[\rho(o,x)\vee\rho(o,y)]}$$

for some c_2. *If* $\mathrm{Ric} - \mathrm{Hess}_V$ *is bounded below, they are all equivalent to the concentration* $\mu(\exp[\mathrm{e}^{\lambda\rho(o,\cdot)}]) < \infty$ *for some* $\lambda > 0$.

Example 5.4. *Let* Ric *be bounded below. Let* $V \in C(M)$ *be such that* $V + a\rho(o, \cdot)^\sigma$ *is bounded for some* $a > 0$ *and* $\sigma \geq 2$. *By Corollaries* 2.5 *and* 3.3 *in* [24], (5.3) *holds for* $\beta(r) = \exp[c(1 + r^{-\sigma/[2(\sigma-1)}]$. *Then Corollary* 5.2 *implies*

$$W_\sigma^\rho(f\mu, \mu)^\sigma \leq C\mu(f \log f), \quad f \geq 0,\ \mu(f) = 1,$$

for some constant $C > 0$. *In this inequality* σ *cannot not be replaced by any larger number, since* $W_\sigma^\rho \geq W_1^\rho$ *and for any* $p \geq 1$ *the inequality*

$$W_1^\rho(f\mu, \mu)^p \leq C\mu(f \log f), \quad f \geq 0,\ \mu(f) = 1,$$

implies $\mu(\mathrm{e}^{\lambda\rho(o,\cdot)^p}) < \infty$ *for some* $\lambda > 0$, *which fails when* $p > \sigma$ *for* μ *specified above.*

Example 5.5. *In the situation of Example* 5.4 *but let* $V + \exp[c\rho(o, \cdot)]$ *be bounded for some* $c > 0$. *Then by* [24], *Corollaries* 2.5 *and* 3.3, (5.3) *holds with* $\beta(r) = \exp[c'(1 + r^{-1/2})]$ *for some* $c' > 0$. *Hence, by Corollary* 5.3,

$$\inf_{\pi\in\mathcal{C}(\mu,f\mu)} \int_{M\times M} \rho(x, y)^2 \mathrm{e}^{c_1\rho(x,y)}\pi(\mathrm{d}x, \mathrm{d}y) \leq C\mu(f \log f), \quad f \geq 0,\ \mu(f) = 1, \tag{5.7}$$

holds for some $c_1, C > 0$.

On the other hand, it is easy to see that (5.7) *implies* $\mu(\exp[\exp(\lambda\rho(o, \cdot))]) < \infty$ *for any* $\lambda > 0$, *which is the exact concentration property of the given measure* μ.

6 Log-Sobolev inequality with unbounded below curvature

Let M be a d-dimensional complete connected non-compact Riemannian manifold and $V \in C^2(M)$ such that

$$Z := \int_M \mathrm{e}^{V(x)}\mathrm{d}x < \infty, \tag{6.1}$$

where $\mathrm{d}x$ is the volume measure on M. Let $\mu(\mathrm{d}x) = Z^{-1}\mathrm{e}^{V(x)}\mathrm{d}x$. Under (6.1) it is easy to see that $H_0^{2,1}(\mu) = W^{2,1}(\mu)$, where $H_0^{2,1}(\mu)$ is the completion of $C_0^1(M)$ under the Sobolev norm $\|f\|_{2,1} := \mu(f^2 + |\nabla f|^2)^{1/2}$, and $W^{2,1}(\mu)$ is the completion of the class $\{f \in C^1(M) :\ f + |\nabla f| \in L^2(\mu)\}$ under $\|\cdot\|_{2,1}$. Then the L-diffusion process is non-explosive and its semigroup P_t is uniquely determined. Moreover, P_t is symmetric in $L^2(\mu)$ so that μ is P_t-invariant. It is well known by the Bakry–Emery criterion that (see [3])

$$\mathrm{Ric} - \mathrm{Hess}_V \geq K$$

for some constant $K > 0$ implies the Gross log-Sobolev inequality [19]:

$$\mu(f^2 \log f^2) := \int_M f^2 \log f^2 \mathrm{d}\mu \le C\mu(|\nabla f|^2), \quad \mu(f^2) = 1,\ f \in C^1(M), \tag{6.2}$$

for $C = 2/K$. This result was extended by Chen and the author [13] to the situation that $\mathrm{Ric} - \mathrm{Hess}_V$ is uniformly positive outside a compact set. In the case that $\mathrm{Ric} - \mathrm{Hess}_V$ is bounded below, sufficient concentration conditions of μ for (6.2) to hold are presented in [26], [1], [27]. Obviously, for a condition on $\mathrm{Ric} - \mathrm{Hess}_V$ the Ricci curvature and $-\mathrm{Hess}_V$ play the same role.

In this section we aim to study the log-Sobolev inequality with $\mathrm{Ric} - \mathrm{Hess}_V$ unbounded below. We shall search for the weakest possibility of curvature lower bound for the log-Sobolev inequality to hold under the condition

$$-\mathrm{Hess}_V \ge \delta \quad \text{outside a compact set} \tag{6.3}$$

for some constant $\delta > 0$. This condition is reasonable as the log-Sobolev inequality implies $\mu(\mathrm{e}^{\lambda\rho_o^2}) < \infty$ for some $\lambda > 0$.

It turns out that under (6.3) the optimal curvature lower bound condition for (6.2) to hold is of type

$$\inf_M \{\mathrm{Ric} + \sigma^2 \rho_o^2\} > -\infty \tag{6.4}$$

for some constant $\sigma > 0$. The following result is proved in [34].

Theorem 6.1. *Assume that* (6.3) *and* (6.4) *hold for some constants* $c, \delta, \sigma > 0$ *with* $\delta > (1 + \sqrt{2})\sigma\sqrt{d-1}$. *Then* (6.2) *holds for some* $C > 0$.

More precisely, let $\theta_0 > 0$ be the smallest positive constant such that for any connected complete non-compact Riemannian manifold M and $V \in C^2(M)$ such that $Z := \int_M \mathrm{e}^{V(x)}\mathrm{d}x < \infty$, the conditions (6.3) and (6.4) with $\delta > \sigma\theta_0\sqrt{d-1}$ imply (6.2) for some $C > 0$. Due to Theorem 6.1 and Example 6.2 below, we conclude that

$$\theta_0 \in [1, 1 + \sqrt{2}].$$

The exact value of θ_0 however is unknown.

Example 6.2. *Let* $M = \mathbb{R}^2$ *be equipped with the rotationally symmetric metric*

$$\mathrm{d}s^2 = \mathrm{d}r^2 + \{r\mathrm{e}^{kr^2}\}^2 \mathrm{d}\theta^2$$

under the polar coordinates $(r, \theta) \in [0, \infty) \times \mathbb{S}^1$ *at* 0, *where* $k > 0$ *is a constant. Then* (*see e.g.* [17])

$$\mathrm{Ric} = -\frac{\frac{\mathrm{d}^2}{\mathrm{d}r^2}(r\mathrm{e}^{kr^2})}{r\mathrm{e}^{kr^2}} = -4k - 4k^2r^2.$$

Thus, (6.4) *holds for* $\sigma = 2k$. *Next, take* $V = -k\rho_o^2 - \lambda(\rho_o^2 + 1)^{1/2}$ *for some* $\lambda > 0$. *By the Hessian comparison theorem and the negativity of the sectional curvature, we obtain* (6.3) *for* $\delta = 2k$. *Since* $d = 2$ *and*

$$\mathrm{e}^{V(x)}\mathrm{d}x = r\mathrm{e}^{-\lambda(1+r^2)^{1/2}}\mathrm{d}r\mathrm{d}\theta, \tag{6.5}$$

one has $Z < \infty$ and $\delta = 2k = \sigma\sqrt{d-1}$. But the log-Sobolev inequality is not valid since by Herbst's inequality it implies $\mu(\mathrm{e}^{r\rho_o^2}) < \infty$ for some $r > 0$, which is however not the case due to (6.5). Since in this example one has $\delta > \sigma\theta\sqrt{d-1}$ for any $\theta < 1$, according to the definition of θ_0 we conclude that $\theta_0 \geq 1$.

7 Functional inequalities on non-convex manifolds

In this part we assume that M is a connected, (non-compact) complete Riemannian manifold with boundary ∂M, and $L = \Delta + \nabla V$ for some V such that $\mu(\mathrm{d}x) = \mathrm{e}^{V(x)}\mathrm{d}x$ is a probability measure on M. We intend to study functional inequalities for the Dirichlet form

$$\mathscr{E}(f,g) = \mu(\langle \nabla f, \nabla g\rangle), \quad f, g \in C_b^1(M).$$

When ∂M is convex, i.e., the second fundamental form $\mathbb{I}$ on ∂M is positive, all known results on functional inequalities proved for manifolds without boundary remain true. In particular, if $\mathrm{Ric} - \mathrm{Hess}_V \geq c$ for some constant $c > 0$ then the log-Sobolev inequality holds:

$$\mu(f^2 \log f^2) \leq \frac{2}{c}\mu(|\nabla f|^2), \quad \mu(f^2) = 1. \tag{7.1}$$

From this one may hope that if $\mathrm{Ric} - \mathrm{Hess}_V \geq c$ for large $c > 0$ and $\mathbb{I} \geq -\varepsilon$ for small $\varepsilon > 0$ there would hold a log-Sobolev inequality.

This is however not true since the second fundamental form and the curvature play different roles in the study of functional inequalities. Indeed, we have the following result due to [35].

Theorem 7.1. *For any $\varepsilon > 0$ and any probability measure μ_0 on $\mathbb{R}^2$ with full support, there exists a smooth connected domain $M \subset \mathbb{R}^2$ with connected ∂M such that $\mathbb{I}_{\partial M} \geq -\varepsilon$, but for any $C > 0$ the Poincaré inequality*

$$\mu_0(f^2 1_M) \leq C\mu_0(1_M|\nabla f|^2), \quad \mu_0(1_M f) = 0$$

does not hold.

So, to study the log-Sobolev inequality on non-convex manifolds, one needs more than lower bounds of the curvature and the second fundamental form.

Theorem 7.2 ([32]). *Let $\mathbb{I} \geq -\sigma$ for some $\sigma > 0$. For any positive function $\varphi \in C^\infty(M)$ such that $N \log\varphi|_{\partial M} \geq \sigma$, the boundary ∂M is convex under the new metric*

$$\langle \cdot, \cdot\rangle_\varphi := \varphi^{-2}\langle \cdot, \cdot\rangle.$$

The above result enables us to derive functional inequalities on non-convex manifolds by using known results established on convex manifolds. For instance, let λ_1 be the first Neumann eigenvalue of Δ on a d-dimensional compact Riemannian manifold M with non-convex boundary ∂M, let μ be the normalized Riemannian volume measure, and let D be the diameter of M.

For any $c \in \mathbb{R}$, $D > 0$ and $d \in \mathbb{N}$, let $\lambda(d, c, D)$ be a universal lower bound estimate for the first Neumann eigenvalue of $L := \Delta + \nabla V$ on a d-dimensional connected compact convex Riemannian manifold with $\mathrm{Ric} - \mathrm{Hess}_V \geq -c$ and diameter $\leq D$.

Let Δ' and ∇' be the Laplacian and gradient of the induced by $\langle \cdot, \cdot \rangle_\varphi$. Let

$$L' := \Delta' + (d-2)\varphi \nabla' \varphi.$$

Then L' is symmetric w.r.t.

$$\mu_\varphi := \varphi^{-2}\mu / \mu(\varphi^{-2}).$$

Moreover,

$$\mu_\varphi(\langle \nabla' f, \nabla' f \rangle') = \frac{\mu(|\nabla f|^2)}{\mu(\varphi^{-2})}.$$

So, letting λ_1' be the first Neumann eigenvalue of L', we have

$$\begin{aligned}(\inf \varphi^{-2})\mathrm{Var}_\mu(f) &\leq \mu(\varphi^{-2})\mathrm{Var}_{\mu_\varphi}(f) \\ &\leq \frac{\mu(\varphi^{-2})}{\lambda_1'}\mu_\varphi(\langle \nabla' f, \nabla' f \rangle') \\ &= \frac{1}{\lambda_1'}\mu(|\nabla f|^2).\end{aligned}$$

Therefore,

$$\lambda_1 \geq \frac{\lambda_1'}{\sup \varphi^2}.$$

To estimate λ_1', we note that

$$\mathrm{Ric}' - (d-2)\mathrm{Hess}'_{\log \varphi} \geq -\varphi^2 K - d|\nabla \varphi|^2 + \frac{1}{2}\Delta \varphi^2,$$

where Ric' and Hess' are the Ricci curvature and the Hess tensor induced by $\langle \cdot, \cdot \rangle_\varphi$ respectively. When $\varphi \geq 1$ one has $D' \leq D$. Therefore:

Theorem 7.3 ([32]). *Let* $\mathrm{Ric} \geq -K, \mathbb{I} \geq -\sigma$. *For any smooth* $\varphi \geq 1$ *such that* $N \log \varphi|_{\partial M} \geq \sigma$, *let*

$$K_\varphi := \sup\left\{\varphi^2 K + d|\nabla \varphi|^2 - \tfrac{1}{2}\Delta \varphi^2\right\}.$$

Then

$$\lambda_1 \geq \frac{\lambda(d, K_\varphi, D)}{\sup \varphi^2}.$$

Taking $\varphi = h \circ \rho_\partial$ for smooth $h \geq 1$ with $h'(0) \geq \sigma h(0)$, and using second variational formula for ρ_∂ in order to estimate K_φ, we obtain explicit lower bounds for λ_1. To make $h \circ \rho_\partial$ smooth, one has to take h to be constant on $[r_0, \infty)$, where r_0 is

the injectivity radius of ∂M. For such a choice of h, one obtains explicit lower bound for λ_1.

In general, we can easily apply the argument to entropy inequalities. Let Φ be a C^2 convex function.

$$\mathrm{Ent}_\mu^\Phi(f) := \mu(\Phi(f)) - \Phi(\mu(f)) \geq 0$$

is called the Φ-entropy w.r.t. μ. Consider the largest constant $\alpha_\Phi \geq 0$ such that

$$\mathrm{Ent}_\mu^\Phi(f) \leq \frac{1}{\alpha_\Phi}\mu(\Phi''(f)|\nabla f|^2).$$

When $\Phi(s) = s\log s$, it reduces to the log-Sobolev inequality.

Let $\alpha_\Phi(d, K, D)$ be a universal lower bound of α_Φ for $\Delta + \nabla V$ on convex connected manifold M of dimensional d, diameter $\leq D$ and $\mathrm{Ric} - \mathrm{Hess}_V \geq -K$. In the same spirit of Theorem 7.3, there holds

$$\alpha_\Phi \geq \frac{\alpha_\Phi(d, K, D)}{\sup\varphi^2}.$$

If ∂M is convex outside a compact set, we only have to make a local change of metric so that the ∂M is convex under the new metric. Since under a local change of metric functional inequalities can be kept up to a constant, some known result on log-Sobolev inequality proved for convex case can be reproved for locally non-convex case. For instance, we have the following result using concentration of μ (see [35]).

Theorem 7.4. *Let $\rho_o = \rho(o, \cdot)$ for a fixed point $o \in M$. Assume that for some compact set $M_0 \subset M$ one has $\mathbb{I}_{\partial M} \geq 0$ on $(\partial M) \setminus M_0$ and $\mathrm{Ric} - \mathrm{Hess}_V \geq -K$ on $M \setminus M_0$ for some $K \in \mathbb{R}$.*

(1) If $\mu(\mathrm{e}^{\lambda\rho_o^2}) < \infty$ holds for some $\lambda > \frac{K}{2}$ then the log-Sobolev inequality (7.1) holds for some $c > 0$.

(2) If $\beta(\lambda) := \mu(\mathrm{e}^{\lambda\rho_o^2}) < \infty$ for any $\lambda > 0$, then the super log-Sobolev inequality

$$\mu(f^2\log f^2) \leq r\mu(|\nabla f|^2) + c(r\wedge 1)^{-d/2}\beta(c/(r\wedge 1)), \quad \mu(f^2) = 1,\ r > 0$$

holds for some constant $c > 0$. Consequently, the Neumann semigroup P_t generated by $L = \Delta + \nabla V$ is supercontractive, i.e., $\|P_t\|_{L^2(\mu)\to L^4(\mu)} < \infty$ for all $t > 0$.

By using a perturbation argument, the log-Sobolev inequality is also established in [35] for a class of globally non-convex manifolds specified in the following result.

Theorem 7.5. *Assume that $\mathbb{I}_{\partial M}$ is bounded, $\mathrm{Ric} \geq -K$ for some $K \geq 0$, the sectional curvature of M is bounded above, and the injectivity radius of ∂M is positive. If $\langle N, \nabla V\rangle$ is bounded below and there exist $\varepsilon, \varepsilon' > 0$ and $\sigma \in (0, 3/4)$ such that $\varepsilon > \varepsilon'\sqrt{(n-1)K}$ and the function*

$$-\sigma|\nabla V|^2 - \Delta V - \varepsilon' V + \varepsilon\rho_o$$

is bounded above on M, then (7.1) holds for some $C > 0$. If furthermore for some $\sigma \in (0, 3/4)$,

$$-r\sigma|\nabla V|^2 - r\Delta V - V + \rho_o \le \phi(r), \quad r > 0,$$

holds for some positive function ϕ on $(0, \infty)$, then the super log-Sobolev inequality

$$\mu(f^2 \log f^2) \le r\mu(|\nabla f|^2) + c + \phi(r) + \frac{d}{2}\log(c(r^{-1}+1)), \quad r > 0,\ \mu(f^2) = 1$$

holds.

To illustrate Theorems 7.4 and 7.5, we present below two examples.

Example 7.6. *Let M be a smooth connected unbounded domain in a Cartan–Hadamard manifold with* Ric $\ge -K_0$ *for some constant $K_0 \ge 0$. Let ∂M be convex outside a compact set and $|V + \lambda\rho_o^p|$ is bounded for some $\lambda, p > 0$ and $o \in M$. If $p = 2$ and $\lambda > K_0/4$ then (7.1) holds for some $C > 0$. If $p > 2$ then the super log-Sobolev inequality holds so that P_t is supercontractive.*

Proof. Since the log-Sobolev inequality is stable under bounded perturbations of V, we may simply assume that $V = -\lambda\rho_o^p$. By the Hessian comparison theorem (recall that the sectional inequalities are non-positive for Cartan–Hadamard manifolds),

$$\text{Ric} - \text{Hess}_V \ge -K_0 + \lambda p(p-2)\rho_o^{p-2}.$$

So, if $p = 2$ then $\text{Ric} - \text{Hess}_V \ge -K$ holds for $K = K_0 - 2\lambda$. Since the Ricci curvature is bounded below, the volume of geodesic balls grows at most exponentially fast in radius. So if $\lambda > K_0/4$ then $\lambda > K/2$ so that for any $\lambda' \in (K/2, \lambda)$ we have

$$\int_M \mathrm{e}^{\lambda'\rho_o^2}\mathrm{d}\mu \le c_2 \int_0^\infty \mathrm{e}^{-(\lambda-\lambda')s^2 + c_1 s}\mathrm{d}s < \infty$$

for some $c_1, c_2 > 0$. Therefore, (7.1) follows by Theorem 7.4. Next, if $p > 2$ then $\mu(\mathrm{e}^{r\rho_o^2}) < \infty$ for all $r > 0$ so that P_t is super contractive due to the same theorem. □

Example 7.7. *Let M satisfy the assumption of Theorem 7.5. Let $h \in C_0^\infty([0, r_0))$ for $r_0 > 0$ smaller than the injectivity radius of ∂M such that $h(0) = 0$ and $h'(0) = 1$. Then $\phi := h \circ \rho_\partial \in C^\infty(M)$ by taking $\phi = 0$ for $\rho_\partial \ge r_0$. If $|V + \lambda(\rho_o^2 - 2\rho_o\phi)|$ is bounded for some $\lambda > 0$ and $o \in \partial M$, then (7.1) holds for some $C > 0$. If moreover $\langle N, \nabla\rho_o^2\rangle$ is bounded above, then (7.1) holds for V such that $|V + \lambda\rho_o^2|$ is bounded for some $\lambda > 0$.*

Proof. Since the log-Sobolev inequality is stable under bounded perturbations of V, for the first case we may assume that $V = -\lambda(\rho_o^2 - 2\rho_o\phi)$. In this case

$$\langle \nabla V, N\rangle = 2\lambda\rho_o(1 - \langle N, \nabla\rho_o\rangle) \ge 0.$$

Since $|\nabla\rho_o| = 1$, $\Delta\rho_o^2 \le C(1+\rho_o)$ for some $C > 0$ and $\Delta\rho_\partial$ is bounded on $\{\rho_\partial \le r_0\}$ by the Laplacian comparison theorems for ρ_o and ρ_∂, there exists a constant $C_1 > 0$ such that

$$-\sigma|\nabla V|^2 - \Delta V - \varepsilon' V + \varepsilon\rho_0 \le (\varepsilon'\lambda - 4\sigma\lambda^2)\rho_o^2 + C_1(1+\rho_o),$$

which is bounded above for $\varepsilon' \in (0, 4\sigma\lambda)$ and $\varepsilon > \varepsilon'\sqrt{(n-1)K}$. Then, by Theorem 7.5, (7.1) holds for some $C > 0$. The proof for the second case is similar. □

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List of Contributors

Jochen Blath, Technische Universität Berlin, Fakultät II, Institut für Mathematik, MA 7-3, Strasse des 17. Juni 136, 10623 Berlin, Germany
blath@math.TU-Berlin.de

Saïd Hamadène, LMM, Université du Maine, Avenue Olivier Messiaen, 72085 Le Mans cedex 9, France
hamadene@univ-lemans.fr

Claudia Klüppelberg, Centre for Mathematical Sciences and Institute for Advanced Study, Technische Universität München, 85748 Garching, Germany
cklu@ma.tum.de

Peter Imkeller, Humboldt-Universität zu Berlin, Institut für Mathematik, Bereich Stochastik, Unter den Linden 6, 10099 Berlin, Germany
imkeller@mathematik.hu-berlin.de

Ross Maller, Centre for Financial Mathematics and School of Finance & Applied Statistics, Australian National University, Canberra, ACT 0200 Australia
Ross.Maller@anu.edu.au

Servet Martínez, Departamento Ingeniería Matemática and Centro Modelamiento Matemático, Universidad de Chile UMI 2807 CNRS, Casilla 170-3 Correo 3, Santiago, Chile
smartine@dim.uchile.cl

Peter Mörters, Department of Mathematical Sciences, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom
maspm@bath.ac.uk

Étienne Pardoux, Laboratoire d'Analyse, Topologie, Probabilités (LATP/UMR 6632), Université de Provence, 39, rue F. Joliot-Curie, 13453 Marseille cedex 13, France
pardoux@cmi.univ-mrs.fr

Gesine Reinert, Department of Statistics, University of Oxford, 1 South Parks Road, Oxford OX1 3TG, United Kingdom
reinert@stats.ox.ac.uk

Sylvie Rœlly, Institut für Mathematik, Universität Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany
roelly@math.uni-potsdam.de

Laurent Saloff-Coste, Department of Mathematics, Cornell University, Malott Hall, Ithaca, NY 14853, U.S.A.
lsc@math.cornell.edu

Jaime San Martín, Departamento Ingeniería Matemática and Centro Modelamiento Matemático, Universidad de Chile UMI 2807 CNRS, Casilla 170-3 Correo 3, Santiago, Chile
jsanmart@dim.uchile.cl

Alexander Schied, Department of Mathematics, Universität Mannheim, A5, 6, 68131 Mannheim, Germany
schied@uni-mannheim.de

Gordon Slade, Department of Mathematics, University of British Columbia, Vancouver, BC, Canada V6T 1Z2
slade@math.ubc.ca

Alla Slynko, Business Campus München, Parkring 11, 85748 Garching-Hochbrück, Germany
alla.a.slynko@gmail.com

Alexander Szimayer, Department of Business Administration III, Universität Bonn, Adenauerallee 24–42, 53113 Bonn, Germany
szimayer@uni-bonn.de

Masayoshi Takeda, Mathematical Institute, Tohoku University, Aoba, Sendai, 980-8578, Japan
takeda@math.tohoku.ac.jp

Anton Wakolbinger, Institut für Mathematik, FB 12, Goethe-Universität, 60054 Frankfurt, Germany
wakolbinger@math.uni-frankfurt.de

Feng-Yu Wang, School of Mathematical Sciences, Beijing Normal University, Beijing 100875, China; and Department of Mathematics, Swansea University, Singleton Park, SA2 8PP, Swansea, United Kingdom
F.-Y.Wang@swansea.ac.uk;wangfy@bnu.edu.cn

Jessica Zúñiga, Department of Mathematics, Building 380, Stanford University, CA 94305, U.S.A.
jzuniga@math.stanford.edu