The Padé Table and its Relation to Certain Numerical Algorithms

Habilitationsschrift

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1. INTRODUCTION

The theory of Padé approximation has a long history. Its foundation goes back at least to Cauchy, in 1821. About 25 years later, Jacobi discovered Padé approximation and provided a determinantal formulation. In 1881, Frobenius [44] investigated algebraic properties of Padé approximations and came up with the original concept of the Padé table. In addition, he developed identities relating Padé approximants whose numerators and denominators have degrees differing by at most one. These identities immediately lead to recursive algorithms for computing Padé forms which work under suitable assumptions. In 1892, also Padé [97] proposed to arrange Padé approximants in a semi-infinite table, which was later named the *Padé table*. Padé studied the structure of this table, in particular he treated certain abnormal cases. The block structure of the Padé table is one ot the most fundamental theoretical results known in Padé theory.

While Padé approximation is a very interesting topic by itself, it is even more fascinating – and sometimes also very surprising – that there are connections between the Padé table and other areas of (numerical) analysis and (numerical) linear algebra, that at first sight do not seem to be related at all. Among others we would like to mention continued fractions [13, 52, 93, 94], Rutishauser's quotient difference and LR algorithms [106], the Chebyshev algorithm [28], the Euclidean algorithm for finding the greatest common divisor of two polynomials, the partial realization problem [21, 56], Shank's transformation [110] for accelerating the convergence of a sequence, Wynn's epsilon algorithm [122], Bauer's eta algorithm, Aitken's Δ^2 algorithm, and Kronecker's algorithm [86] for the numerator and denominator coefficients of an antidiagonal sequence in the Padé table [5, §3.7], which was discovered by Chebyshev [29] before. We refer to [4, 5, 51] for details and references.

Most of these algorithms are related to the recursive computation of Padé approximants or Padé forms on a certain path of the Padé table. Among those, famous representatives are algorithms following a diagonal or two adjacent diagonals of the Padé table. These algorithms are related to Hankel matrix factorizations, formally orthogonal polynomials, the Lanczos process based on three-term or coupled two-term recurrences, and to general extrapolation methods. Another important class of algorithms is related to following two adjacent rows of the Padé table. Row algorithms have a close connection to Toeplitz matrix factorizations, formally biorthogonal polynomials, and the isometric Arnoldi process; see Bultheel and van Barel [22] for a recent survey on these relations.

In their original form, these algorithms are direct applications of Frobenius identities. However, they all break down if the path they follow in the Padé table hits the interior of a block of the Padé table. People working in Padé theory have been used to dealing with nonnormal Padé tables. In fact, Magnus [93, 94] described the construction of all regular Padé forms on a certain diagonal in 1962, assuming exact arithmetic, and Chebyshev [29] seems to have been partially aware of this construction in 1870. However, general recurrences for nonnormal Padé forms have not been treated in a unified framework for a long time. In 1983, Draux gave various such recurrences in his thesis [35], but his formulations as well as his proofs turn out to be unnecessary long and complicated. Moreover, all his generalizations are valid in exact arithmetic only. For implementation in finite precision arithmetic, it is much more important to deal with "near breakdowns", which means to overcome instabilities due to a division by a small number. Such algorithms have been studied since the early 1980ies. For the most important application, the nonsymmetric Lanczos process [90], Gragg [52] indicated the main idea to circumvent exact breakdowns. In 1982, Taylor [115] worked out the details for near breakdowns in his thesis, which was published in a joint paper by Parlett, Taylor, and Liu [102] in 1985. In 1992, Gutknecht wrote Part I of his "Completed theory of the look-ahead Lanczos process" [60, 63], which later led to a practical implementation by Freund, Gutknecht, and Nachtigal [39]. Also in 1992, Parlett [100] investigated look-ahead Lanczos by interpreting it as a two-sided block Gram-Schmidt process. At about the same time, extensions of fast Hankel and Toeplitz solvers for curing exact and near breakdowns have been proposed by several authors. We give detailed references to the above mentioned methods, their relations to the Padé table, and their generalizations for exact and finite precision arithmetic in the corresponding chapters.

This thesis contains a unified treatment of generalizations of certain classical algorithms of numerical linear algebra and numerical analysis. From this point of view, it is an extension of the survey paper by Gragg [51], where he discusses the block structure of the Padé table and gives interpretations of certain algorithms in numerical analysis in terms of the Padé table. Here, we consider not only the relations, but we give efficient algorithms that overcome the breakdown problems. The development contains from the very beginning the treatment of exact and near breakdowns. In this point it improves Gutknecht's completed theory of the Lanczos process [60, 63], where the near breakdown case is treated separately in the last two sections of [63]. We would like to emphasize, that once one understands the concept, it is fairly easy to find general recurrences in the Padé table. However, it turns out to be extremely tricky to obtain efficient algorithms. Here we give algorithms which reduce to the classical algorithms if no near breakdowns occur, and which have little overhead when we have to "look ahead", which roughly means to replace those steps that cause difficulties by an appropriate compound step. The complexity of all algorithms is analyzed. Since in this field, herds of indices are around and it is sometimes hard to find out what the recurrences really mean, we illustrate everything by pictures. It is one aim of this thesis, in addition to developing efficient algorithms, to make "look ahead" understandable without forcing the reader to get into the details. For most of the material it should be possible to understand what it is about *without* reading the theorems and *without* checking the proofs. Nevertheless, if the reader wants to know the details, he or she will find them here too.

1.1 Summary

The thesis is organized as follows: Chapter 2 contains basic definitions and theoretical properties of Padé forms and Padé approximants. Among other things, we discuss the block structure of the Padé table, one of the most fundamental results in Padé theory. We introduce the notation of regularity of Padé forms in the Padé table and the two-point Padé table, and we generalize this concept to finite precision arithmetic. In particular, we show that an "inexact" Padé table still has some "block structure", although a direct generalization of the block structure theorem does not seem possible. We are not aware of any results in this direction in the literature. This chapter also contains a collection of inversion formulas for Hankel and Toeplitz matrices applicable under various assumptions related to the different kinds of regular Padé forms.

The aim of Chapter 3 is to provide general recurrences to compute Padé forms in a certain region of the Padé table. From this rather technical chapter, the theorems can be skipped on a first reading. Reading the explanations and looking at the pictures should be sufficient to understand the different kinds of recurrences.

Chapter 4 contains recurrences to compute Padé forms on a certain diagonal of the Padé table. The recurrences involve multiplications of a pair of Padé forms with low degree polynomials, so that we call this type of algorithm the "product form". We describe efficient implementations of look-ahead Levinson and Schur type algorithms, which correspond to computing denominators or residuals of Padé forms, respectively. These algorithms can be combined with recursive doubling in order to obtain a look-ahead version of the superfast algorithm [54].

In Chapter 5, we give the connection of Padé forms on a diagonal of the Padé table to formally orthogonal polynomials and we show how the algorithms proposed in Chapter 4 can be extended to provide a complete basis of formally orthogonal polynomials or complete block factorizations of Hankel matrices. For this extension, we introduce *underdetermined Padé forms* and show their relation to polynomials satisfying block orthogonality conditions.

For the Lanczos process discussed in Chapter 6, the product form of the algorithms described so far is not feasible. Hence we give alternative recurrences involving underdetermined Padé forms. Using underdetermined Padé forms to construct general recurrences in the Padé table appears to be new. We show how these recurrences lead to more efficient look-ahead algorithms than the ones from the previous chapter. These recurrences can be applied in such a way that each step of the Lanczos process requires only the minimal number of matrix vector multiplications. From the connection to the Padé table, it is natural how the implementations proposed in [39, 63] can be simplified so that work and storage is reduced. Besides the three-term version of the Lanczos process, we also discuss a coupled two-term version, which is related to Padé forms on two adjacent diagonals of the Padé table. Here we can use our results on the block structure of the inexact Padé table from Chapter 2 to justify that breakdowns on the two adjacent diagonals should not be considered independent, as was done in [40]. Again, the recurrences improve the ones proposed previously in [40, 63].

Chapter 7 contains the product form of algorithms related to Padé forms on two adjacent rows of the Padé table. These turn out to be more complicated than recurrences for diagonals, because they require the more general concept of two-point Padé approximation. We give efficient look-ahead Levinson and Schur algorithms in product form, which can be extended to a superfast look-ahead Toeplitz solver.

The connection of Padé forms on two adjacent rows of the Padé table to formally biorthogonal polynomials is made in Chapter 8. We generalize the concept of underdetermined Padé forms, by introducing *left and right underdetermined Padé forms* to fill gaps between regular Padé forms, and show the connection to Toeplitz matrix factorizations. Finally, we present a new matrix formulation of our look-ahead Levinson and Schur algorithms, which is a generalization of the Bareiss-Delosme-Ipsen formulation [6, 32, 81] of the Schur algorithm.

Chapter 9 gives new alternative row recurrences, which involve left and right underdetermined Padé forms. These alternative recurrences lead to new look-ahead algorithms for constructing the complete block factorization of a Toeplitz matrix, which are cheaper than any other method known today. We also discuss the relation to the look-ahead algorithms proposed by Freund and Zha [43] and Freund [38], and show how computational overhead of look-ahead steps of these methods can be reduced by a factor up to two by exploiting the Padé connection. The second part of this chapter then interprets the Levinson algorithm as an Arnoldi process for isometric operators. This relation was described in a special case by Gragg [53] and can be interpreted as the isometric analogue of the Lanczos process. The new algorithm can be used for computing biorthogonal polynomials with respect to a bilinear form from modified moments. To the best of our knowledge, this is the first algorithm which neither requires the moments explicitly nor assumes that regular formally biorthogonal polynomials exist for every degree n.

Extrapolation algorithms and their relation to Padé approximation are considered in Chapter 10, where extensions for their application to nonnormal Padé tables are developed.

As we mentioned before, row recurrences have a close relation to Toeplitz matrix factorizations. For this particular application, we discuss look-ahead strategies and stability issues in Chapter 11. Here we also describe various options for solving Toeplitz systems from the output obtained from look-ahead Levinson and Schur algorithms. We have written a C package containing all the different versions of our look-ahead Levinson and Schur algorithms combined with several options for computing the solution of the linear system. Numerical examples obtained with this package complete this work.

1.2 Outlook

In this thesis, we consider only Padé approximations of formal power and formal Laurent series, but it seems possible to extend most of the work also to vector and matrix Padé approximations [9, 87, 88, 89]. This then ultimately yields algorithms for block-Toeplitz and block-Hankel matrices [24, 119, 121]. Other possible generalizations are related to more general rational interpolation problems [61, 65]. Moreover, we discuss here only algorithms related to diagonals and rows of the Padé table. From this treatment it is obvious how to obtain algorithms related to others paths in the Padé table, for instance columns or anti-diagonals. Finally, we have not included superfast versions of look-ahead Hankel and Toeplitz solvers although they are obtained immediately from the product forms of our algorithms described in Chapters 4 and 7; see [1, 25, 54, 55, 62, 66, 67].

For our new look-ahead Lanczos process based on coupled two-term recurrences, we do not discuss normalization, further practical aspects of look-ahead strategies, or reorthogonalization techniques [31]. These topics will be the subject of future work.

1.3 General comments

In this thesis we will use the common term "Padé approximant" although "Padé interpolant" or "Padé fraction" would be more appropriate, because the use of Padé approximants throughout this thesis is totally formal. If (p, q) is a Padé form of a formal power series or a formal Laurent series, then we will call p its *numerator* and q its *denominator*. Moreover, we denote any algorithm which computes an inverse LDU decomposition of a Hankel or a Toeplitz matrix or – equivalently – denominators of certain Padé forms a *Levinson-type algorithm*. In contrast, we denote any algorithm which provides an LDU decomposition or – equivalently – residuals and numerators of certain Padé forms a *Schur-type algorithm*.

In our pictures that illustrate the recurrences, squares represent underdetermined Padé forms, circles stand for Padé forms and a line indicates that Padé approximants at its end points are different from each other. In other words, such lines always cross the border of a block in the Padé table.

For the solution of structured linear systems of equations, an alternative to look-ahead algorithms is to exploit the *displacement structure* [83] of the coefficient matrix; see, *e.g.*, Gu [58] and Sayed and Kailath [108]. Here we would like to mention the recent survey paper by Kailath and Sayed [84] for theoretical aspects of this subject and the paper by Gallivan, Thirumalai, Van Dooren, and Vermaut [45] for high performance algorithms for Toeplitz and block Toeplitz matrices. Very recently, transformation techniques became popular. The idea is to transform a matrix whose structure is destroyed by pivoting into another structured matrix, for which pivoting preserves the structure. For instance, Hankel and Toeplitz matrices can be transformed by fast Fourier transformation into Cauchy like matrices; see, *e.g.*, Gohberg, Kailath, and Olshevsky [46] and Heinig [73, 74]. We will not discuss these approaches here, because they do not fit into the framework of this thesis, where we only want to consider algorithms which reduce to the classical ones if no breakdown or stability problems arise. The latter is not true for the algorithms we just mentioned. Moreover, these techniques only work for the solution of linear systems with structured matrices. By far the more important applications are, however, the stable implementation of Lanczos type algorithms and the construction of complete bases of formally orthogonal or biorthogonal polynomials. Here, look-ahead is the only choice.

1.4 Notation

We denote by $\mathbb{Z}$ the set of all integers, by $\mathbb{N}$ the set of all nonnegative integers, and by $\mathbb{N}^+$ the set of all positive integers. Moreover, $\mathbb{C}$ is the set of all complex numbers.

By $\mathcal{L}$ we denote the set of formal Laurent series

$$h(\zeta) = \sum_{k=-\infty}^{\infty} \mu_k \zeta^k, \qquad \mu_k \in \mathbb{C},$$

and by

$$\begin{aligned}
\mathcal{L}_{l:m} &:= \{h \in \mathcal{L}\,;\ \mu_k = 0 \text{ if } k < l \text{ or } k > m\},\\
\mathcal{L}_{l} &:= \mathcal{L}_{l:\infty} = \{h \in \mathcal{L}\,;\ \mu_k = 0 \text{ if } k < l\},\\
\mathcal{L}_{m}^{*} &:= \mathcal{L}_{-\infty:m} = \{h \in \mathcal{L}\,;\ \mu_k = 0 \text{ if } k > m\},\\
\mathcal{L}_{0} &:= \mathcal{L}_{0:\infty} := \text{formal power series in } \zeta,\\
\mathcal{L}_{0}^{*} &:= \mathcal{L}_{-\infty:0} := \text{power series in } \zeta^{-1},\\
\mathcal{P}_{m} &:= \mathcal{L}_{0:m} := \text{polynomials in } \zeta \text{ of degree } m,\\
\mathcal{P} &:= \bigcup \mathcal{P}_m := \text{polynomials in } \zeta,\\
\mathcal{R}_{m,n} &:= \text{rational functions of type } (m,n)
\end{aligned}$$

certain subsets of $\mathcal{L}$.

A rational function r of type (m,n) is a function that can be represented as the quotient of two polynomials, $r = p/q$, where the numerator p has degree at most m, and the denominator q has degree at most n and is not the zero polynomial. When p and q have a common factor, it gets cancelled; hence, r does not depend on this factor.

For $h \in \mathcal{L}_m^*$ or $h \in \mathcal{P}$ we define the *exact degree* ∂h by

$$\partial h := \max\{n \in \mathbb{Z}\,;\ \mu_n \neq 0\}$$

and for $h \in \mathcal{L}_l$ we define the *exact codegree* $\partial^* h$ by

$$\partial^* h := \min\{n \in \mathbb{Z}\,;\ \mu_n \neq 0\}.$$

We write $h(\zeta) = O_+(\zeta^l)$ if $h(\zeta) \in \mathcal{L}_l$ and $h(\zeta) = O_-(\zeta^m)$ if $h(\zeta) \in \mathcal{L}_m^*$.

Moreover, we let

$$\Pi_{l:m} h(\zeta) := \sum_{k=l}^{m} \mu_k \zeta^k$$

be the formal projection of $h \in \mathcal{L}$ into $\mathcal{L}_{l:m}$ and $\Pi_m h(\zeta) := \mu_m$ be its mth coefficient.

When $f \in \mathcal{L}_l$ and $g \in \mathcal{L}_0$ with $g(0) \neq 0$, then the quotient f/g is well defined in $\mathcal{L}_l$, and we write $L_+(f/g)$ for it, as in [19]. Likewise, when $f \in \mathcal{L}_m^*$ and $g \in \mathcal{L}_0^*$ with $g(0) \neq 0$, then $L_-(f/g)$ is well defined in $\mathcal{L}_m^*$. For convenience, we write

$$\begin{aligned} h(0) &= \Pi_0 h(z) \quad \text{if} \quad h(\zeta) = O_+(0), \\ h(\infty) &= \Pi_0 h(z) \quad \text{if} \quad h(\zeta) = O_-(0). \end{aligned}$$

1.5 Acknowledgements

Work on the subject of this thesis started when I was visiting the Swiss Center for Scientific Computing (SCSC), formerly the Interdisciplinary Project Center for Supercomputing (IPS), at ETH Zürich in 1992. During this time, Martin Gutknecht introduced me into the topic and aroused my interest in the relation of the Padé table to several other numerical algorithms. I would like to thank him for his support during the last years, for making several visits to Zürich possible and enjoyable, and for his comments on an earlier version of this thesis.

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2. PADÉ FORMS AND THE PADÉ TABLE

This chapter contains a collection of definitions and properties of Padé forms and Padé approximants of formal power series and Laurent series. The recursive algorithms considered in the following chapters depend strongly on these results.

After some basic definitions and theoretical properties of Padé approximants, we discuss the block structure of the Padé table of a formal Laurent series. The block structure theorem is one of the most fundamental results in Padé theory. Next we give a short overview on options to compute Padé forms. Most of our algorithms are based on certain pairs of Padé forms, which made us add two sections on properties of various types of pairs. While Padé forms can be computed by solving linear systems with Hankel or Toeplitz coefficient matrices, it is also true that there are explicit formulas for the inverses of Hankel or Toeplitz matrices in terms of the coefficients of certain Padé forms. Hence, we present inversion formulas applicable under various assumptions. Up to this point, everything was done for exact arithmetic. However, the aim of this thesis is to develop reliable algorithms for finite precision arithmetic. At the end of this chapter, we generalize some of the results of the previous sections to justify our approaches for designing algorithms for finite precision arithmetic. In particular, we discuss the structure of an "inexact" Padé table. We are not aware of any results in this direction in the literature.

2.1 Basic definitions

The most general definition of a Padé form which will be used in this thesis is a *Laurent Padé form* of a quotient of a formal Laurent series and a formal power series.

Definition 2.1: *Given $g \in \mathcal{L}_0$ with $g(0) \neq 0$, $f \in \mathcal{L}_{-N}$ ($N = \infty$ is allowed when $g \equiv -1$), $m \in \mathbb{Z}$, $m \geq -N$, and $n \in \mathbb{N}$, any nonzero pair $(p, q) \in \mathcal{L}_{-N:m} \times (\mathcal{P}_n \setminus \{0\})$ satisfying*

$$g(\zeta)p(\zeta) + f(\zeta)q(\zeta) = O_+(\zeta^{m+n+1}) \tag{2.1}$$

is an (m, n) **Padé form (PF)** *of (f, g). The* **residual** *of (p, q) is the formal power series $e \in \mathcal{L}_0$ defined by*

$$g(\zeta)p(\zeta) + f(\zeta)q(\zeta) = \zeta^{m+n+1}e(\zeta). \tag{2.2}$$

If N is finite, then the rational function

$$r(\zeta) = \frac{p(\zeta)}{q(\zeta)}$$

is called the (m,n) **Padé approximant** *of (f,g). When $N = \infty$ and $g \equiv -1$, then the formal Laurent series*

$$L_+ r(\zeta) = f(\zeta) - L_+ \left(\frac{f(\zeta)q(\zeta) - p(\zeta)}{q(\zeta)} \right) \tag{2.3}$$

is called the (m,n) **Padé approximant** *of $f \in \mathcal{L}$.*

There are some special cases of this definition, which ought to be mentioned explicitly:

- $f \in \mathcal{L}_0$, $g \equiv -1$: $(p,q) \in \mathcal{P}_m \times \mathcal{P}_n$ satisfying (2.1) is an (m,n) Padé form of a formal power series f. This is probably the best known type of Padé form, where p and q are both polynomials.
- $f, g \in \mathcal{L}_0$, $f(0) \neq 0$ or $g(0) \neq 0$: $(p,q) \in \mathcal{P}_m \times \mathcal{P}_n$ satisfying (2.1) is an (m,n) Padé form of (f,g). This case is a generalization of the previous one, but now we are no longer approximating a single formal power series but a quotient of two formal power series; see Lemma 2.1 below.
- If N is a finite number we can multiply f and p by ζ^N, which results in a polynomial $\zeta^N p \in \mathcal{P}_{m+N}$ and a formal power series $\zeta^N f \in \mathcal{L}_0$. Hence we are back in the previous case. However, we allow $N = \infty$, in which case this interpretation is no longer possible. Here, the quotient p/q (as a Laurent series in ζ) is not defined, which made the careful definition (2.3) of a Padé approximant necessary.
- $f \in \mathcal{L}_{-N}$, $g \equiv -1$: $(p,q) \in \mathcal{L}_{-N:m} \times (\mathcal{P}_n \setminus \{0\})$ satisfying (2.1) is an (m,n) (Laurent) Padé form of the formal Laurent series f.

There is a close relation between Padé forms of a formal Laurent series and those of a quotient of a Laurent series and a power series:

Lemma 2.1: *$(p,q) \in \mathcal{L}_{-N:m} \times (\mathcal{P}_n \setminus \{0\})$ is an (m,n) Padé form of $(f,g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ with $g(0) \neq 0$ if and only if (p,q) is an (m,n) Padé form of h, where $h \equiv -f/g \in \mathcal{L}_{-N}$ if $g(0) \neq 0$*

Proof. The statement follows by dividing (2.1) by $-g$, because $g(0) \neq 0$ by assumption. □

Due to this Lemma, we will show most of our statements for Padé forms of a formal Laurent series $h \in \mathcal{L}_{-N}$ or a formal power series $h \in \mathcal{L}_0$ only. The definition than simplifies in the following way: any nonzero pair $(p,q) \in \mathcal{L}_{-N:m} \times \mathcal{P}_n$ satisfying

$$h(\zeta)q(\zeta) - p(\zeta) = O_+(\zeta^{m+n+1}) \tag{2.4}$$

is an (m,n) Padé form of

$$h(\zeta) = \sum_{k=-N}^{\infty} \mu_k \zeta^k \tag{2.5}$$

with complex coefficients $\mu_k \in \mathbb{C}$.

It is easy to see that Padé forms exists for any (m,n). In fact, (2.4) summarizes n linear conditions for the polynomial q, namely, the vanishing of the coefficients of $\zeta^{m+1}, \zeta^{m+2}, \cdots, \zeta^{m+n}$ in the formal Laurent series $hq - p$, because one can set $p = \Pi_{-N:m}(hq)$. Since these conditions are homogeneous and since q contains $n+1$ parameters (of which one is redundant), there are always nontrivial solutions $(p,q) \neq (0,0)$ of (2.4). For Padé forms of a formal power series, the existence was shown by Frobenius [44] already in 1881; see [51, Theorem 3.1].

Clearly, Padé forms are never unique; but nevertheless Padé approximants are:

Lemma 2.2: *Given $h \in \mathcal{L}_{-N}$, $N \in \mathbb{N}$, $m \in \mathbb{Z}$, and $n \in \mathbb{N}$, there always exist (m,n) Padé forms of h, and, after the cancellation of common factors, they all yield the same rational function p/q, which is the (m,n) Padé approximant of h.*

Proof. We have already seen that Padé forms always exist. To show uniqueness of p/q, assume that both (p,q) and $(\tilde{p},\tilde{q})$ are (m,n) Padé forms. Then,

$$\begin{aligned} \tilde{q}(\zeta)[h(\zeta)q(\zeta) - p(\zeta)] &= O_+(\zeta^{m+n+1}), \\ q(\zeta)[h(\zeta)\tilde{q}(\zeta) - \tilde{p}(\zeta)] &= O_+(\zeta^{m+n+1}), \end{aligned}$$

and by subtraction we get $q(\zeta)\tilde{p}(\zeta) - \tilde{q}(\zeta)p(\zeta) = O_+(\zeta^{m+n+1})$. Since $q\tilde{p} - \tilde{q}p \in \mathcal{L}^*_{m+n}$, it must be identical to zero; hence, $q\tilde{p} = \tilde{q}p$. □

An immediate consequence of the proof is that

$$h(\zeta) - L_+ r(\zeta) = O_+(\zeta^{m+n+1-\sigma}), \tag{2.6}$$

where $\sigma = \partial^* q$ is the multiplicity of a zero of q at $\zeta = 0$. Since $r(\zeta) = p(\zeta)/q(\zeta) = \tilde{p}(\zeta)/\tilde{q}(\zeta)$, we also have

$$h(\zeta)\tilde{q}(\zeta) - \tilde{p}(\zeta) = O_+(\zeta^{m+n+1-\sigma}). \tag{2.7}$$

The set of solutions of (2.4) clearly forms a linear space. A generalization of [51, Theorem 3.2], which can be found in [62, Theorem 2.1] or [19, Chapter 11], characterizes this set:

Theorem 2.3: *Given $h \in \mathcal{L}_{-N}$, $m \in \mathbb{Z}$ and $n \in \mathbb{N}$, the general solution $(p,q) \in \mathcal{L}_{-N:m} \times (\mathcal{P}_n \backslash \{0\})$ of (2.4) is*

$$(p(z), q(z)) = (z^\sigma \tilde{p}(z)\, w(z), z^\sigma \tilde{q}(z)\, w(z)), \tag{2.8}$$

where $\tilde{p} \in \mathcal{L}_{-N:m}$ and $\tilde{q} \in \mathcal{P}_n$ with $\tilde{q}(0) = 1$ are uniquely determined and relatively prime (except that $\tilde{p}$ can be the zero polynomial, in which case $\tilde{q}(z) :\equiv 1$);

$$\sigma := \sigma_{m,n} := \max\{0, m+n+1 - \partial^*(h\tilde{q} - \tilde{p})\} \tag{2.9}$$

is a fixed integer satisfying

$$0 \le \sigma \le \delta := \delta_{m,n} := \min\{m - \partial\tilde{p}, n - \partial\tilde{q}\}, \tag{2.10}$$

and $w \in \mathcal{P}_{\delta-\sigma}$ *is arbitrary. The Padé approximant* $r = p/q = \tilde{p}/\tilde{q}$ *is uniquely determined.*

Proof. The proof presented here is similar to [59].

By Lemma 2.2, every solution of (2.4) yields the same fraction p/q, which we may write as $\tilde{p}/\tilde{q}$ with relatively prime $\tilde{p}$ and $\tilde{q}$. Therefore, every such solution can be written in the form (2.8), where $0 \le \sigma \le \delta \equiv \delta_{m,n}$ and $w \in \mathcal{P}_{\delta-\sigma}$. If $\sigma_{m,n}$ defined by (2.9) is positive, $(\tilde{p}, \tilde{q})$ is not a solution of (2.4) (*i.e.*, it is not an (m,n) Padé form), but $(\zeta^{\sigma_{m,n}}\tilde{p}, \zeta^{\sigma_{m,n}}\tilde{q})$ is one, and actually one where the order is exactly $m+n+1$:

$$h(\zeta)\zeta^{\sigma_{m,n}}\tilde{q}(\zeta) - \zeta^{\sigma_{m,n}}\tilde{p}(\zeta) \equiv O_+(\zeta^{m+n+1}) \quad \text{if } \sigma_{m,n} > 0. \tag{2.11}$$

Any other (m,n) Padé form must also contain the common factor $\zeta^{\sigma_{m,n}}$ in order to fulfill (2.4). Hence, we may assume that, in (2.8), $\sigma = \sigma_{m,n}$, since any additional common factor ζ can be incorporated into w.

It remains to verify that, conversely, an arbitrary $w \in \mathcal{P}_{\delta-\sigma}$ in (2.8) yields a solution of (2.4). Clearly, the restriction to degree at most $\delta - \sigma$ is chosen such that $(p,q) \in \mathcal{L}_{-N:m} \times \mathcal{P}_n$. But this is the only restriction that has to be fulfilled. If $\sigma > 0$, then multiplication of (2.11) by any such polynomial w yields (2.4). If $\sigma = 0$, the pair $(\tilde{p}, \tilde{q})$ is itself a Padé form satisfying (2.4), and multiplication by w can only increase the order $O_+(\zeta^{m+n+1})$. □

Definition 2.2: *The nonnegative integer* σ *defined in* (2.9) *is the* **deficiency index** *of* r. *If* $\sigma > 0$, *we call* r **deficient**. *The nonnegative integer* δ *defined in* (2.10) *is called the* **defect** *of* $(\tilde{p}, \tilde{q})$ *in* $\mathcal{R}_{m,n}$.

Theorem 2.4: *A rational function* $r = p/q$ *with* $(p,q) \in \mathcal{L}_{-N:m} \times \mathcal{P}_n$ *with defect* δ *is the* (m,n) *Padé approximant of* $h \in \mathcal{L}_{-N}$ *if and only if*

$$h(\zeta) - L_+ r(\zeta) = O_+(\zeta^{m+n-\delta+1}). \tag{2.12}$$

Proof. First, assume that r is the (m,n) Padé approximant of h, and let again $\tilde{p}/\tilde{q}$ be a reduced representation of r. By definition of σ, (2.7) holds, which implies (2.6) and (2.12), since $\sigma \le \delta$.

Conversely, assume that (2.12) holds for $r = \tilde{p}/\tilde{q}$. Consider any (m,n) PF (p,q), and conclude as in the proof of Lemma 2.2 that $\tilde{q}(\zeta)p(\zeta) - \tilde{p}(\zeta)q(\zeta) = O_+(\zeta^{m+n+1-\delta})$, and, hence, $p/q = \tilde{p}/\tilde{q}$.

This proof also applies in the case $r = 0$, where $\delta = n$. □

While for diagonal recurrences in the Padé table we will see that standard Padé forms are sufficient to construct recursive algorithms, this is no longer true if we want to follow rows or columns in the Padé table. This application requires the more general concept of two-point Padé forms. We will use the definition from [62] of a quadruple of formal Laurent series $(f^-, g^-; f^+, g^+)$ given by

$$f^-(\zeta) =: \sum_{k=1}^{\infty} \phi_k^- \zeta^{-k}, \qquad f^+(\zeta) =: \sum_{k=0}^{\infty} \phi_k^+ \zeta^{k}, \tag{2.13}$$

$$g^-(\zeta) =: \sum_{k=0}^{\infty} \gamma_k^- \zeta^{-k}, \qquad g^+(\zeta) =: \sum_{k=0}^{\infty} \gamma_k^+ \zeta^{k}. \tag{2.14}$$

We assume that these formal Laurent series fulfill at least one of the following four pairs of conditions

$$\phi_1^- \neq 0 \quad \text{and} \quad \gamma_0^+ \neq 0, \tag{2.15}$$

$$\gamma_0^- \neq 0 \quad \text{and} \quad \gamma_0^+ \neq 0, \tag{2.16}$$

$$\phi_1^- \neq 0 \quad \text{and} \quad \phi_0^+ \neq 0, \tag{2.17}$$

$$\gamma_0^- \neq 0 \quad \text{and} \quad \phi_0^+ \neq 0. \tag{2.18}$$

Equivalently, the conditions can be expressed in the short form

$$(\phi_1^- \neq 0 \text{ or } \gamma_0^- \neq 0) \text{ and } (\phi_0^+ \neq 0 \text{ or } \gamma_0^+ \neq 0). \tag{2.19}$$

The following definition is equivalent to that of McCabe and Murphy, Draux [35], and Cooper, Magnus and McCabe [30]. Other definitions are due to Sidi [111], Bultheel [19], Thron, and Magnus; see [62] for details and references.

Definition 2.3: *Given a pair $[l;k]$ of integers satisfying $|l| < k$ or $|l| = k > 0$, a pair $(u,v) \in \mathcal{P}_{k-1} \times \mathcal{P}_k$ is an $[l;k]$* **two-point Padé form** *of $(f^-, g^-; f^+, g^+)$ if*

$$\begin{aligned} g^-(\zeta)u(\zeta) + f^-(\zeta)v(\zeta) &= O_-(\zeta^{l-1}) \in \mathcal{L}_{l-1}^*, \\ g^+(\zeta)u(\zeta) + f^+(\zeta)v(\zeta) &= O_+(\zeta^{k+l}) \in \mathcal{L}_{k+l}. \end{aligned} \tag{2.20}$$

The rational function $u(\zeta)/v(\zeta)$ is said to be the $[l;k]$ **two-point Padé approximant** *of $(f^-, g^-; f^+, g^+)$. The* **residual** *of (u,v) consists of two series $(e^-; e^+) \in \mathcal{L}_0^* \times \mathcal{L}_0$ defined by*

$$\begin{aligned} g^-(\zeta)u(\zeta) + f^-(\zeta)v(\zeta) &= \zeta^{l-1}e^-(\zeta), \\ g^+(\zeta)u(\zeta) + f^+(\zeta)v(\zeta) &= \zeta^{k+l}e^+(\zeta). \end{aligned} \tag{2.21}$$

A standard two-point Padé problem is a special case of this definition, where $g^- \equiv g^+ \equiv -1$. For this case, Sidi [111] proved existence of two-point Padé forms and uniqueness of two-point Padé approximants. Moreover, Bultheel [19, Theorem 11.1] gives a theorem analogous to Theorem 2.3 for two-point Padé forms.

2.2 The Padé table

Given a formal Laurent series h, which may result from a quotient f/g according to Lemma 2.1, we have already seen that unique Padé approximants exist for every index pair $(m,n) \in \mathbb{Z}\times\mathbb{N}$. These Padé approximants can be listed in a table, the famous Padé table introduced by Padé [97], in which we let the m-axis point to the bottom and the n-axis point to the right.

One of the most important properties of the Padé table is its block structure: equal (nonzero) Padé approximants occur in square blocks in the Padé table. Special situations arise only if h is itself rational or if some Padé approximants are identical to the zero function. For formal power series, the following block structure theorem can be found in [51, Theorem 3.2]. Its generalization for formal Laurent series is given in [19, Theorem 11.3]. Due to Lemma 2.1, it is sufficient to state it for Laurent series and not for the more general Definition 2.1.

Theorem 2.5: *Let $h(\zeta) := \sum_{k=-N}^{\infty} \mu_k \zeta^k$, $N \in \mathbb{Z}$, with $\mu_{-N} \neq 0$, and let $m \in \mathbb{Z}$ and $n \in \mathbb{N}$. Then the (m,n) Padé approximant of h is zero for $m < -N$. For $m \geq -N$ no (m,n) Padé approximant is identically zero.*

For any Padé approximant $r \neq 0$ of h, let $r = \tilde{p}/\tilde{q}$ be a reduced representation and thus $(\partial\tilde{p}, \partial\tilde{q})$ be the exact type of r. Moreover, let

$$k \equiv \partial^*(h - L_+ r) = \partial^*(h\tilde{q} - \tilde{p}) \quad (\leq \infty) \tag{2.22}$$

be the order of interpolation of this Padé approximant and set

$$\Lambda \equiv k - \partial\tilde{p} - \partial\tilde{q}. \tag{2.23}$$

Then r is the (m,n) Padé approximant of h in the whole square

$$\partial\tilde{p} \leq m < \partial\tilde{p} + \Lambda, \quad \partial\tilde{q} \leq n < \partial\tilde{q} + \Lambda, \tag{2.24}$$

but nowhere else.

The case $\Lambda = \infty$ occurs if and only if h is rational and $r = h$.

Proof. The pair $(0, \zeta^n)$ is an (m,n) Padé form of h if and only if $h = O_+(\zeta^{m+1})$. Hence, the zero function is the (m,n) Padé approximant whenever $m + 1 \leq -N$ but nowhere else.

From now on assume that $r = \tilde{p}/\tilde{q} \neq 0$. The index pairs (m,n) in the square (2.24) satisfy $m + n \leq \partial\tilde{p} + \partial\tilde{q} + \delta + \Lambda - 1$ since $\partial\tilde{p} + \delta = m$ or $\partial\tilde{q} + \delta = n$ by definition of δ. Hence, by (2.22) and (2.23), condition (2.12) is seen to hold:

$$\partial^*(h - L_+ r) = k = \Lambda + \partial\tilde{p} + \partial\tilde{q} \geq m + n + 1 - \delta.$$

This proves that r is the (m,n) Padé approximant in this square. Conversely, beyond the square, $m + n \geq \partial\tilde{p} + \partial\tilde{q} + \delta + \Lambda$, which yields

$$\partial^*(h - L_+ r) = k = \Lambda + \partial\tilde{p} + \partial\tilde{q} \leq m + n - \delta.$$

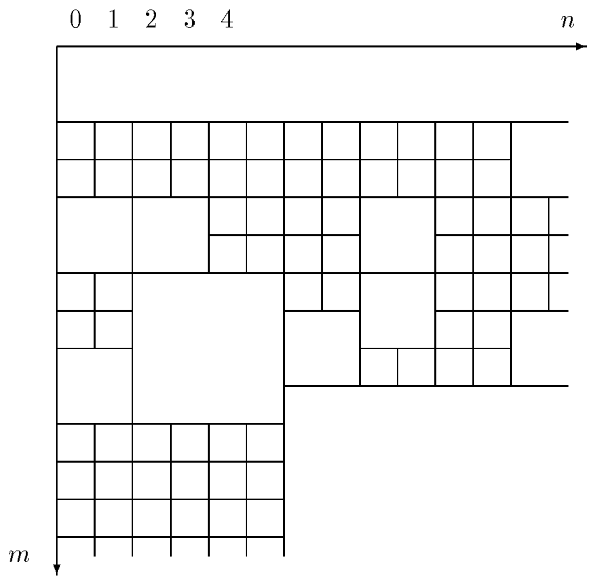


Figure 2.1: Block structure of a Padé table containing a zero block on top, an infinite block in its lower right corner, and square blocks of various dimensions.

Thus, according to Theorem 2.4, r cannot be a Padé approximant there. Finally, $\Lambda = \infty$ implies $k = \infty$, and this clearly means that $r = h$. □

The different situations mentioned in the previous theorem, a zero block, an infinite block, and square blocks, which may arise in a Padé table are illustrated in Figure 2.1.

In [61] the more general case of multipoint Padé approximation is discussed. This treatment shows that for the special case of two-point Padé approximation singular blocks in the two-point Padé table are still square. The case that the data satisfies (2.16) allows an elegant treatment: dividing (2.20) by g^- and g^+, respectively, yields a standard two-point Padé problem for which the block structure was established in [30]. Earlier results are due to Draux [35], but his definition of two-point Padé forms is not as general as the one used here and the proofs are fairly complicated.

2.3 Computation of Padé forms

Mainly to introduce the notation, and to keep this work self contained, we briefly recall how to compute Padé forms and two-point Padé forms. This also shows the close relation to the solution of Hankel and Toeplitz systems of equations.

To compute an (m,n) Padé form of $(f,g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ one may want to rewrite the problem of approximating a quotient of a formal Laurent series and a formal power series according to Lemma 2.1. Then one first has to compute from the first N coefficients of f and g the first N coefficients of $h \equiv -f/g$, *e.g.*, by fast Fourier transformation [76]. Assume that $h \in \mathcal{L}_{-N}$ is given by (2.5) and

$$p(\zeta) = \sum_{k=-N}^{m} \pi_{m-k}\zeta^k, \qquad q(\zeta) = \sum_{k=0}^{n} \rho_k \zeta^k, \tag{2.25}$$

then (2.4) is equivalent to solving the linear system

$$n\left\{\underbrace{\begin{bmatrix} \mu_{m+1} & \mu_m & \cdots & \mu_{m-n+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{m+n} & \mu_{m+n-1} & \cdots & \mu_m \end{bmatrix}}_{n+1}\right. \begin{bmatrix} \rho_0 \\ \rho_1 \\ \vdots \\ \rho_n \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix} \tag{2.26}$$

and setting

$$p = \Pi_{-N:m}(hq). \tag{2.27}$$

The residual with coefficients denoted by

$$e(\zeta) = \sum_{k=0}^{\infty} \varepsilon_{n+k} z^k \tag{2.28}$$

is obtained from the formal projection

$$e = \zeta^{-(m+n+1)}\Pi_{m+n+1:\infty}(hq). \tag{2.29}$$

If the Padé form satisfies $\rho_0 = q(0) \neq 0$, then one can use this coefficient for normalization. Moving the first column of the matrix in (2.26) to the right-hand side one ends up with the well-known Yule-Walker equation

$$\mathbf{T}_{m,n} \begin{bmatrix} \rho_1 \\ \vdots \\ \rho_n \end{bmatrix} = -\rho_0 \begin{bmatrix} \mu_{m+1} \\ \vdots \\ \mu_{m+n} \end{bmatrix}, \tag{2.30}$$

where

$$\mathbf{T}_{m,n} := \begin{bmatrix} \mu_m & \cdots & \mu_{m-n+1} \\ \vdots & \ddots & \vdots \\ \mu_{m+n-1} & \cdots & \mu_m \end{bmatrix} \in \mathbb{C}^{n,n}$$

is an $n \times n$ Toeplitz matrix.

Alternatively, one can solve the linear system which results directly from comparing coefficients in (2.1) [51, Theorem 4.1]. For the special case that f and g are formal power series with coefficients

$$f(\zeta) = \sum_{k=0}^{\infty} \phi_k \zeta^k \quad \text{and} \quad g(\zeta) = \sum_{k=0}^{\infty} \gamma_k \zeta^k$$

with $\gamma_0 \neq 0$ or $\phi_0 \neq 0$, we obtain

$$
m+n+1\left\{\left[\underbrace{\begin{array}{cccc} \gamma_0 & & & \\ \gamma_1 & \gamma_0 & & \\ \vdots & \vdots & \ddots & \\ \gamma_m & \gamma_{m-1} & \cdots & \gamma_0 \\ \vdots & \vdots & & \vdots \\ \gamma_{m+n} & \gamma_{m+n-1} & \cdots & \gamma_n \end{array}}_{m+1}\middle|\underbrace{\begin{array}{cccc} \phi_0 & & & \\ \phi_1 & \phi_0 & & \\ \vdots & \vdots & \ddots & \\ \phi_n & \phi_{n-1} & \cdots & \phi_0 \\ \vdots & \vdots & & \vdots \\ \phi_{m+n} & \phi_{m+n-1} & \cdots & \phi_m \end{array}}_{n+1}\right]\right. \begin{bmatrix} \pi_0 \\ \vdots \\ \pi_m \\ \hline \rho_0 \\ \vdots \\ \rho_n \end{bmatrix} = 0. \tag{2.31}
$$

The two approaches are clearly equivalent by Lemma 2.1. The coefficient matrix of the linear system (2.31) is called a *Sylvester matrix* [25].

Another equivalent problem is obtained by putting the coefficients ρ_j in (2.30) in reverse order:

$$
\mathbf{H}_{m,n} \begin{bmatrix} \rho_n \\ \vdots \\ \rho_1 \end{bmatrix} = -\rho_0 \begin{bmatrix} \mu_{m+1} \\ \vdots \\ \mu_{m+n} \end{bmatrix}, \tag{2.32}
$$

where

$$
\mathbf{H}_{m,n} := \begin{bmatrix} \mu_{m-n+1} & \cdots & \mu_m \\ \vdots & \ddots & \vdots \\ \mu_m & \cdots & \mu_{m+n-1} \end{bmatrix} \in \mathbb{C}^{n,n}
$$

is an $n \times n$ Hankel matrix.

The solution of Hankel systems of equations is closely related to computing diagonal entries of the Padé table of the symbol h of the Hankel matrix and also to computing formally orthogonal polynomials; see Chapters 4 and 5. In this application, h is a formal power series which corresponds to the case $N = 0$ in the equations above.

For the solution of Toeplitz systems of equations we need recurrences for adjacent rows of the Padé table, as will be discussed in Chapter 7. Some of the recurrences we propose make use of two-point Padé forms. Denominators of Padé forms in adjacent rows of the Padé table can be interpreted as formally biorthogonal polynomials with respect to a certain bilinear form. This will be the topic of Chapter 8.

To compute two-point Padé forms, things get a little bit more complicated. If we assume that (u, v) is an $[l; k]$ two-point Padé form of the quadruple (f^-, g^-, f^+, g^+) defined in (2.13), (2.14) and write

$$
u(\zeta) = \sum_{j=0}^{k-1} \alpha_j \zeta^j, \quad v(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j, \tag{2.33}
$$

then the conditions (2.20) are equivalent to

$$\left[\begin{array}{ccc|ccc}
\gamma^-_{-l} & \cdots & \gamma^-_{k-l-1} & \phi^-_{-l} & \cdots & \phi^-_{k-l} \\
\ddots & & \vdots & \ddots & & \vdots \\
 & \gamma^-_0 & \gamma^-_1 & & \phi^-_1 & \phi^-_2 \\
 & & \gamma^-_0 & & & \phi^-_1 \\
\hline
\gamma^+_0 & & & \phi^+_0 & & \\
\gamma^+_1 & \gamma^+_0 & & \phi^+_1 & \phi^+_0 & \\
\vdots & & \ddots & \vdots & & \ddots \\
\gamma^+_{k+l-1} & \cdots & \gamma^+_l & \phi^+_{k+l-1} & \cdots & \phi^+_{l-1}
\end{array}\right]
\left[\begin{array}{c}
\alpha_0 \\ \vdots \\ \alpha_{k-1} \\ \hline \beta_0 \\ \vdots \\ \beta_k
\end{array}\right] = \mathbf{0}; \tag{2.34}$$

see also (3.20) in [62]. The coefficient matrix is a $2k \times (2k+1)$ *mosaic Toeplitz matrix* [72].

2.4 Regularity of Padé forms

For the construction of recursive algorithms following a certain path in the Padé table, we will not use arbitrary Padé forms but only certain pairs, whose numerator and denominator degree differ by at most one and which are located in different blocks of the Padé table. We will actually use four different kinds of pairs of Padé forms defined as follows:

Definition 2.4: *Let (p,q) be an (m,n) Padé form of $(f,g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ with $g(0) \neq 0$, and let $r = p/q$ be the (m,n) Padé approximant of (f,g), $(p^\uparrow, q^\uparrow)$ be an $(m-1,n)$ Padé form of (f,g) and $r^\uparrow = p^\uparrow/q^\uparrow$ be the $(m-1,n)$ Padé approximant. Moreover, let $r^\nwarrow$ and $r^\leftarrow$ be the $(m-1,n-1)$ and the $(m,n-1)$ Padé approximant of (f,g), respectively. Then we call the index pair (m,n) and the Padé form*

(i) (p,q) **row regular** *iff $r \neq r^\leftarrow$;*
(ii) (p,q) **column regular** *iff $r \neq r^\uparrow$;*
(iii) (p,q) **regular** (*diagonally regular*) *iff $r \neq r^\nwarrow$;*
(iv) $(p^\uparrow, q^\uparrow)$ **anti-diagonally regular** *iff $r^\uparrow \neq r^\leftarrow$.*

In order to make the notation more illustrative, we use arrows to indicate the location of neighboring Padé forms with respect to a regular (m,n) Padé form (p,q) of (f,g), as we did in the above definition. Hence, we denote by $(p^\nwarrow, q^\nwarrow)$ the $(m-1,n-1)$ Padé form, by $(p^\uparrow, q^\uparrow)$ the $(m-1,n)$ Padé form, and by $(p^\leftarrow, q^\leftarrow)$ the $(m,n-1)$ Padé forms. The corresponding residuals are denoted in the same way. The following picture shows the location of these Padé forms and illustrates the notation.

$$\boxed{\begin{array}{lcc}
m-1 & q^\nwarrow & q^\uparrow \\
m & q^\leftarrow & q \\
 & & \\
 & n-1 & n
\end{array}} \tag{2.35}$$

All the algorithms discussed here will be based on some kind of "regular" pairs. For instance, if we want to proceed along a diagonal in the Padé table, then using regular pairs is the most natural choice. To follow a single row, one should base the construction on row-regular pairs, and so on.

Recall from the Block Structure Theorem 2.5 and Theorem 2.3, that Padé forms that are uniquely determined up to scaling are those lying along the border of a block. From (2.8) we know that if (p, q) is a such a Padé form, then it satisfies $q(0) \neq 0$ if and only if it lies in the first row or column of its block or, equivalently, if it is regular. Consequently, for a fixed $\rho_0 \neq 0$, the Yule-Walker equation (2.30) has a unique solution if and only if (p, q) is regular, and $\mathbf{T}_{m,n}$ is nonsingular if and only if (m, n) is a regular index.

For later use, we next give some further equivalent definitions of the different kinds of regularity of Padé forms. Some of the results can be found in [51, Theorem 5.4] and [62]. We have chosen to include the proofs to emphasize their simplicity.

Lemma 2.6: *Let (p, q) be an (m, n) Padé form, and $(p^{\leftarrow}, q^{\leftarrow})$ be an $(m, n-1)$ Padé form of $(f, g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ with $g(0) \neq 0$. Then, the following statements are equivalent when $n > 0$:*

(i) *(p, q) is row-regular, i.e., $pq^{\leftarrow} - p^{\leftarrow}q \neq 0 \ \in \mathcal{L}^*_{m+n}$;*
(ii) *the Toeplitz matrices $\mathbf{T}_{m,n}$ and $\mathbf{T}_{m+1,n}$ are nonsingular;*
(iii) *the Yule-Walker equation (2.30) with $\rho_0 = 1$ has a unique solution which satisfies $\partial q = n$;*
(iv) *$e^{\leftarrow}(0) \neq 0$ and $q(0) \neq 0$;*
(v) *$pq^{\leftarrow} - p^{\leftarrow}q = \Delta^{\leftarrow}\zeta^{m+n} \neq 0$, $\Delta^{\leftarrow} \in \mathbb{C}$;*
(vi) *$\partial p^{\leftarrow} = m$ and $\partial q = n$.*

Proof. (i)⇔(ii)⇔(iii) follows from the Block Structure Theorem 2.5, as we have explained above. Here we have exploited that the lower neighbor of a row-regular Padé form must be a regular Padé form, and that if $\partial q < n$, then the (m, n) Padé form (p, q) is also an $(m, n-1)$ Padé form and thus cannot be row-regular.

Multiplying (2.2) (for (p, q) and $(p^{\leftarrow}, q^{\leftarrow})$) by $q^{\leftarrow}$ and q, respectively, and subtracting yields

$$\underbrace{pq^{\leftarrow}}_{\mathcal{L}^*_{m+n-1}} - \underbrace{p^{\leftarrow}q}_{\mathcal{L}^*_{m+n}} = \zeta^{m+n}(\underbrace{\zeta e q^{\leftarrow}}_{\mathcal{L}_1} - \underbrace{e^{\leftarrow}q}_{\mathcal{L}_0})\underbrace{g^{-1}}_{\mathcal{L}_0} \in \mathcal{L}_{m+n}.$$

Here, the left-hand side is in $\mathcal{L}^*_{m+n}$ and the right-hand side is in $\mathcal{L}_{m+n}$, which means that both sides are scalar multiples of ζ^{m+n}. Comparing coefficients yields

$$p^{\leftarrow}(\infty)\rho_n = e^{\leftarrow}(0)\rho_0/g(0),$$

which proves the remaining equivalences. □

Lemma 2.7: *Let (p, q) be an (m, n) Padé form, and $(p^{\uparrow}, q^{\uparrow})$ be an $(m-1, n)$ Padé form of $(f, g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ with $g(0) \neq 0$. Then, the following statements are equivalent when $n > 0$:*

(i) *(p,q) is column-regular, i.e., $pq^{\uparrow} - p^{\uparrow}q \neq 0 \in \mathcal{L}^*_{m+n}$;*
(ii) *the Toeplitz matrices $\mathbf{T}_{m,n}$ and $\mathbf{T}_{m,n+1}$ are nonsingular;*
(iii) *the Yule-Walker equation (2.30) with $\rho_0 = 1$ has a unique solution and the corresponding numerator polynomial $p = \Pi_{0:m}(hq)$ satisfies $\partial p = m$.*
(iv) *$e^{\uparrow}(0) \neq 0$ and $q(0) \neq 0$;*
(v) *$pq^{\uparrow} - p^{\uparrow}q = \Delta^{\uparrow}\zeta^{m+n} \neq 0$, $\Delta^{\uparrow} \in \mathbb{C}$;*
(vi) *$\partial p = m$ and $\partial q^{\uparrow} = n$.*

Proof. (i)⇔(ii)⇔(iii) follows from the Block Structure Theorem 2.5, the remaining equivalences from

$$\underbrace{pq^{\uparrow}}_{\mathcal{L}^*_{m+n}} - \underbrace{p^{\uparrow}q}_{\mathcal{L}^*_{m+n-1}} = \zeta^{m+n}(\underbrace{\zeta e q^{\uparrow}}_{\mathcal{L}_1} - \underbrace{e^{\uparrow}q}_{\mathcal{L}_0})\underbrace{g^{-1}}_{\mathcal{L}_0} \in \mathcal{L}_{m+n}.$$

□

Lemma 2.8: *Let (p,q) be an (m,n) Padé form, and $(p^{\nwarrow}, q^{\nwarrow})$ be an $(m-1,n-1)$ Padé form of $(f,g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ with $g(0) \neq 0$. Then, the following statements are equivalent when $n > 0$:*
(i) *(p,q) is regular, i.e., $pq^{\nwarrow} - p^{\nwarrow}q \neq 0 \in \mathcal{L}^*_{m+n-1}$;*
(ii) *the Toeplitz matrix $\mathbf{T}_{m,n}$ is nonsingular;*
(iii) *the Yule-Walker equation (2.30) with $\rho_0 = 1$ has a unique solution.*
(iv) *$e^{\nwarrow}(0) \neq 0$ and $q(0) \neq 0$;*
(v) *$pq^{\nwarrow} - p^{\nwarrow}q = \Delta^{\nwarrow}\zeta^{m+n-1} \neq 0$, $\Delta^{\nwarrow} \in \mathbb{C}$.*
Moreover, if (p,q) is regular, then
(vi) *$(\partial p = m$ and $\partial q^{\nwarrow} = n-1)$ or $(\partial q = n$ and $\partial p^{\nwarrow} = m-1)$. But, in general, the converse is not true.*

Proof. (i)⇔(ii)⇔(iii) follows from the Block Structure Theorem 2.5, the remaining equivalences from

$$\underbrace{pq^{\nwarrow}}_{\mathcal{L}^*_{m+n-1}} - \underbrace{p^{\nwarrow}q}_{\mathcal{L}^*_{m+n-1}} = \zeta^{m+n-1}(\underbrace{\zeta^2 e q^{\nwarrow}}_{\mathcal{L}_2} - \underbrace{e^{\nwarrow}q}_{\mathcal{L}_0})\underbrace{g^{-1}}_{\mathcal{L}_0} \in \mathcal{L}_{m+n-1}. \tag{2.36}$$

□

Lemma 2.9: *Let $(p^{\uparrow}, q^{\uparrow})$ be an $(m-1,n)$ Padé form, and $(p^{\leftarrow}, q^{\leftarrow})$ be an $(m,n-1)$ Padé form of $(f,g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ with $g(0) \neq 0$. Then, the following statements are equivalent when $n > 0$:*
(i) *$(p^{\uparrow}, q^{\uparrow})$ is anti-diagonally regular, i.e., $p^{\uparrow}q^{\leftarrow} - p^{\leftarrow}q^{\uparrow} \neq 0 \in \mathcal{L}^*_{m+n}$;*
(ii) *the Toeplitz matrix $\mathbf{T}_{m,n}$ is nonsingular;*
(iii) *the Yule-Walker equation*

$$\mathbf{T}_{m,n}\begin{bmatrix} \rho_0^{\uparrow} \\ \vdots \\ \rho_{n-1}^{\uparrow} \end{bmatrix} = -\rho_n^{\uparrow}\begin{bmatrix} \mu_{m-n} \\ \vdots \\ \mu_{m-1} \end{bmatrix}, \tag{2.37}$$

with $\rho_n^{\uparrow} = 1$ has a unique solution.

(iv) $\partial p^{\leftarrow} = m$ *and* $\partial q^{\uparrow} = n$;
(v) $p^{\uparrow} q^{\leftarrow} - p^{\leftarrow} q^{\uparrow} = \Delta^{\nearrow} \zeta^{m+n} \neq 0$, $\Delta^{\nearrow} \in \mathbb{C}$;

Moreover, if $(p^{\uparrow}, q^{\uparrow})$ *is anti-diagonally regular, then*

(vi) $(e^{\uparrow}(0) \neq 0$ *and* $q^{\leftarrow}(0) \neq 0)$ *or* $(e^{\leftarrow}(0) \neq 0$ *and* $q^{\uparrow}(0) \neq 0)$. *But, in general, the converse is not true.*

Proof. (i)$\Leftrightarrow$(ii)$\Leftrightarrow$(iii) follows from the Block Structure Theorem 2.5, the remaining equivalences from

$$\underbrace{p^{\uparrow} q^{\leftarrow}}_{\mathcal{L}^*_{m+n-2}} - \underbrace{p^{\leftarrow} q^{\uparrow}}_{\mathcal{L}^*_{m+n}} = \zeta^{m+n} (\underbrace{e^{\uparrow} q^{\leftarrow}}_{\mathcal{L}_0} - \underbrace{e^{\leftarrow} q^{\uparrow}}_{\mathcal{L}_0}) \underbrace{g^{-1}}_{\mathcal{L}_0} \in \mathcal{L}_{m+n}. \tag{2.38}$$

□

An immediate consequence of Lemmas 2.8 and 2.9 is

Corollary 2.10: *Let* (p, q) *be an* (m, n) *Padé form of* $(f, g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ *with* $g(0) \neq 0$, *and* $(p^{\uparrow}, q^{\uparrow})$ *be an* $(m-1, n)$ *Padé form of* (f, g). *Then* (p, q) *is regular if and only if* $(p^{\uparrow}, q^{\uparrow})$ *is anti-diagonally regular.*

The short proofs of the above Lemmas also show the following identities written in the notation (2.25) and the analogous one for $q^{\uparrow}$, $q^{\leftarrow}$, and $q^{\nwarrow}$:

Corollary 2.11: *Let* (p, q), $(p^{\leftarrow}, q^{\leftarrow})$, $(p^{\nwarrow}, q^{\nwarrow})$, $(p^{\uparrow}, q^{\uparrow})$ *be Padé forms illustrated in* (2.35) *of* $h = -f/g \in \mathcal{L}_{-N}$, *where* $f \in \mathcal{L}_{-N}$, $g \in \mathcal{L}_0$, *and* $g(0) \neq 0$. *Then the following identities are valid:*

(i) $-\pi_0^{\leftarrow} \rho_n = e^{\leftarrow}(0) \rho_0$;
(ii) $\pi_0 \rho_n^{\uparrow} = e^{\uparrow}(0) \rho_0$;
(iii) $\pi_0 \rho_{n-1}^{\nwarrow} - \pi_0^{\nwarrow} \rho_n = e^{\nwarrow}(0) \rho_0$;
(iv) $\pi_0^{\leftarrow} \rho_n^{\uparrow} = e^{\uparrow}(0) \rho_0^{\leftarrow} - e^{\leftarrow}(0) \rho_0^{\uparrow}$;

Now assume that (m, n) is a regular index, *i.e.*, that the Toeplitz matrix $\mathbf{T}_{m,n}$ is nonsingular. Then the coefficients of q and $q^{\uparrow}$ are determined by the Yule-Walker equations (2.30) and (2.37) and the coefficients of $q^{\leftarrow}$ and $q^{\nwarrow}$ are solutions of

$$\mathbf{T}_{m,n} \begin{bmatrix} \rho_0^{\leftarrow} \\ \vdots \\ \rho_{n-1}^{\leftarrow} \end{bmatrix} = \pi_0^{\leftarrow} \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \qquad \mathbf{T}_{m,n} \begin{bmatrix} \rho_0^{\nwarrow} \\ \vdots \\ \rho_{n-1}^{\nwarrow} \end{bmatrix} = e^{\nwarrow}(0) \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}. \tag{2.39}$$

This can be seen by extending (2.26) (where n is replaced by $n-1$) by one more equation such that the coefficient matrix remains Toeplitz. If we write this equation on top of the first one in (2.26), then this matrix becomes $\mathbf{T}_{m,n}$, and the right-hand side is equal to $\Pi_m(hq^{\leftarrow})\mathbf{e}_0 = \pi_0^{\leftarrow}\mathbf{e}_0$ by (2.27). If we write it after the last one and replace additionally m by $m-1$, the coefficient matrix is again $\mathbf{T}_{m,n}$ and the right-hand side becomes $\Pi_{m+n-1}(hq^{\nwarrow})\mathbf{e}_{n-1} = e^{\nwarrow}(0)\mathbf{e}_{n-1}$ by (2.29).

These equations are also called *fundamental equations* by Heinig and Rost [75] and their solutions are called *generators* in the context of displacement structure [84]. Since (m,n) is a regular index, we clearly have

$$\rho_0 \neq 0, \quad \rho_n^{\uparrow} \neq 0, \quad \pi_0^{\leftarrow} \neq 0, \quad e^{\nwarrow}(0) \neq 0.$$

We can therefore use the freedom we have in scaling Padé forms by setting these quantities to one and assume in the following the normalizations

$$\rho_0 = 1, \quad \rho_n^{\uparrow} = 1, \quad \pi_0^{\leftarrow} = 1, \quad e^{\nwarrow}(0) = 1. \tag{2.40}$$

2.5 Regularity of two-point Padé forms

Definition 2.4 can be generalized in an obvious fashion to two-point Padé forms:

Definition 2.5: *Let (u,v) be an $[m;n]$ two-point Padé form of $(f^-,g^-;f^+,g^+) \in \mathcal{L}_{-1}^* \times \mathcal{L}_0^* \times \mathcal{L}_0 \times \mathcal{L}_0$ satisfying* (2.19) *and let $r = u/v$ be the $[m;n]$ two-point Padé approximant of $(f^-,g^-;f^+,g^+)$, $(u^{\uparrow},v^{\uparrow})$ be an $[m-1;n]$ two-point Padé form of $(f^-,g^-;f^+,g^+)$, and $r^{\uparrow} = u^{\uparrow}/v^{\uparrow}$ be the $[m-1;,n]$ two-point Padé approximant. Moreover, let $r^{\nwarrow}$ and $r^{\leftarrow}$ be the $[m-1;n-1]$ and the $[m;n-1]$ two-point Padé approximant of $(f^-,g^-;f^+,g^+)$, respectively. Then we call the index pair $[m;n]$ and the two-point Padé form*

(i) (u,v) **row regular** *iff $r \neq r^{\leftarrow}$;*
(ii) (u,v) **column regular** *iff $r \neq r^{\uparrow}$;*
(iii) (u,v) **regular** (*diagonally regular*) *iff $r \neq r^{\nwarrow}$;*
(iv) $(u^{\uparrow},v^{\uparrow})$ **anti-diagonally regular** *iff $r^{\uparrow} \neq r^{\leftarrow}$.*

We next give the generalizations of Lemmas 2.6–2.9 to two-point Padé forms. Parts of the first three Lemmas presented in this section have been proved in a different way in [62, Lemma 3.4–3.6] and [66, Lemma 4.2]. The proofs given here are simpler and give additional information.

Lemma 2.12: *Let (u,v) be an $[m;n]$ two-point Padé form, and $(u^{\leftarrow},v^{\leftarrow})$ be an $[m;n-1]$ two-point Padé form of $(f^-,g^-;f^+,g^+) \in \mathcal{L}_{-1}^* \times \mathcal{L}_0^* \times \mathcal{L}_0 \times \mathcal{L}_0$ satisfying* (2.19). *Then, the following statements are equivalent when $n > 0$ and $|m| \leq n-1$:*

(i) *(u,v) is row-regular;*
(ii) *$uv^{\leftarrow} - vu^{\leftarrow} = \Delta^{\leftarrow}\zeta^{m+n-1} \neq 0$, $\Delta^{\leftarrow} \in \mathbb{C}$;*
(iii) *$e^{\leftarrow +}(0) \neq 0$ and $e^{\leftarrow -}(\infty) \neq 0$;*
(iv) *$e^{\leftarrow +}(0) \neq 0$ and ($v(0) \neq 0$ if $\gamma_0^+ \neq 0$ and $u(0) \neq 0$ if $\phi_0^+ \neq 0$);*
(v) *$e^{\leftarrow -}(\infty) \neq 0$ and ($\partial u = n-1$ if $\phi_1^- \neq 0$ and $\partial v = n$ if $\gamma_0^- \neq 0$).*

Proof. The proof is done analogously to the proof of the corresponding statement for row-regular one-point Padé forms in Lemma 2.6. We multiply (2.21) (for (u,v) and for $(u^{\leftarrow},v^{\leftarrow})$) by $u^{\leftarrow}$ and u, respectively, and subtract the two equations for the approximation in zero and the two equations containing the approximation in infinity from each other. This results in

$$uv^{\leftarrow} - vu^{\leftarrow} = \begin{cases} \zeta^{m-1}(\underbrace{e^{-}v^{\leftarrow}}_{\mathcal{L}^*_{n-1}} - \underbrace{e^{\leftarrow -}v}_{\mathcal{L}^*_{n}})\underbrace{(g^{-})^{-1}}_{\mathcal{L}^*_0} \in \mathcal{L}^*_{m+n-1}, & \text{if } \gamma_0^- \neq 0 \\ \zeta^{m-1}(\underbrace{e^{\leftarrow -}u}_{\mathcal{L}^*_{n}} - \underbrace{e^{-}u^{\leftarrow}}_{\mathcal{L}^*_{n-1}})\underbrace{(f^{-})^{-1}}_{\mathcal{L}^*_1} \in \mathcal{L}^*_{m+n-1}, & \text{if } \phi_1^- \neq 0 \\ \zeta^{m+n-1}(\underbrace{\zeta e^{+}v^{\leftarrow}}_{\mathcal{L}_1} - \underbrace{e^{\leftarrow +}v}_{\mathcal{L}_0})\underbrace{(g^{+})^{-1}}_{\mathcal{L}_0} \in \mathcal{L}_{m+n-1}, & \text{if } \gamma_0^+ \neq 0 \\ \zeta^{m+n-1}(\underbrace{e^{\leftarrow +}u}_{\mathcal{L}_0} - \underbrace{\zeta e^{+}u^{\leftarrow}}_{\mathcal{L}_1})\underbrace{(f^{+})^{-1}}_{\mathcal{L}_0} \in \mathcal{L}_{m+n-1}, & \text{if } \phi_0^+ \neq 0. \end{cases}$$

The left-hand side is a polynomial of degree $2(n-1)$, the right-hand side is seen to be a scalar multiple of ζ^{m+n-1}, because it lies in $\mathcal{L}_{m+n-1} \cap \mathcal{L}^*_{m+n-1}$. Comparing coefficients for ζ^{m+n-1} proves the equivalences. □

Lemma 2.13: *Let (u, v) be an $[m; n]$ two-point Padé form, and $(u^{\uparrow}, v^{\uparrow})$ be an $[m-1; n]$ two-point Padé form of $(f^-, g^-; f^+, g^+) \in \mathcal{L}^*_{-1} \times \mathcal{L}^*_0 \times \mathcal{L}_0 \times \mathcal{L}_0$ satisfying* (2.19)*. Then, the following statements are equivalent when $n > 0$ and $-n+1 \leq m \leq n$:*

(i) *(u, v) is column-regular;*
(ii) *$uv^{\uparrow} - vu^{\uparrow} = \Delta^{\uparrow}\zeta^{m+n-1} \neq 0$, $\Delta^{\uparrow} \in \mathbb{C}$;*
(iii) *$e^{\uparrow +}(0) \neq 0$ and $e^{-}(\infty) \neq 0$;*
(iv) *$e^{\uparrow +}(0) \neq 0$ and ($v^{\uparrow}(0) \neq 0$ if $\gamma_0^+ \neq 0$ and $u^{\uparrow}(0) \neq 0$ if $\phi_0^+ \neq 0$);*
(v) *$e^{-}(\infty) \neq 0$ and ($\partial u^{\uparrow} = n-1$ if $\phi_1^- \neq 0$ and $\partial v^{\uparrow} = n$ if $\gamma_0^- \neq 0$).*

Proof.

$$uv^{\uparrow} - vu^{\uparrow} = \begin{cases} \zeta^{m}(\underbrace{\zeta e^{-}v^{\uparrow}}_{\mathcal{L}^*_{n+1}} - \underbrace{e^{\uparrow -}v}_{\mathcal{L}^*_{n}})\underbrace{(g^{-})^{-1}}_{\mathcal{L}^*_0} \in \mathcal{L}^*_{m+n-1}, & \text{if } \gamma_0^- \neq 0 \\ \zeta^{m}(\underbrace{e^{\uparrow -}u}_{\mathcal{L}^*_{n-1}} - \underbrace{\zeta e^{-}u^{\uparrow}}_{\mathcal{L}^*_{n}})\underbrace{(f^{-})^{-1}}_{\mathcal{L}^*_1} \in \mathcal{L}^*_{m+n-1}, & \text{if } \phi_1^- \neq 0 \\ \zeta^{m+n-1}(\underbrace{\zeta e^{+}v^{\uparrow}}_{\mathcal{L}_1} - \underbrace{e^{\uparrow +}v}_{\mathcal{L}_0})\underbrace{(g^{+})^{-1}}_{\mathcal{L}_0} \in \mathcal{L}_{m+n-1}, & \text{if } \gamma_0^+ \neq 0 \\ \zeta^{m+n-1}(\underbrace{e^{\uparrow +}u}_{\mathcal{L}_0} - \underbrace{\zeta e^{+}u^{\uparrow}}_{\mathcal{L}_1})\underbrace{(f^{+})^{-1}}_{\mathcal{L}_0} \in \mathcal{L}_{m+n-1}, & \text{if } \phi_0^+ \neq 0 \end{cases}$$

□

Lemma 2.14: *Let (u, v) be an $[m; n]$ two-point Padé form, and $(u^{\nwarrow}, v^{\nwarrow})$ be an $[m-1; n-1]$ two-point Padé form of $(f^-, g^-; f^+, g^+) \in \mathcal{L}^*_{-1} \times \mathcal{L}^*_0 \times \mathcal{L}_0 \times \mathcal{L}_0$ satisfying* (2.19)*. Then, the following statements are equivalent when $n \geq 2$ and $-n+2 \leq m \leq n-1$:*

(i) *(u, v) is regular;*
(ii) *$uv^{\nwarrow} - vu^{\nwarrow} = \Delta^{\nwarrow}\zeta^{m+n-2} \neq 0$, $\Delta^{\nwarrow} \in \mathbb{C}$;*

(iii) $e^{\nwarrow +}(0) \neq 0$ *and* $(e^{-}(\infty) \neq 0$ *or* $e^{\nwarrow -}(\infty) \neq 0)$*;*
(iv) $e^{\nwarrow +}(0) \neq 0$ *and* $v(0) \neq 0$.

Moreover, if (u, v) *is regular, then*

(v) $(e^{-}(\infty) \neq 0$ *and* $\partial v^{\nwarrow} = n-1)$ *or* $(e^{\nwarrow -}(\infty) \neq 0$ *and* $\partial v = n)$ *if* $\gamma_0^- \neq 0$, *and* $(e^{-}(\infty) \neq 0$ *and* $\partial u^{\nwarrow} = n-2)$ *or* $(e^{\nwarrow -}(\infty) \neq 0$ *and* $\partial u = n-1)$ *if* $\phi_1^- \neq 0$.
In both cases $e^{\nwarrow -}(\infty) \neq 0$ *or* $e^{-}(\infty) \neq 0$.

Proof.

$$uv^{\nwarrow} - vu^{\nwarrow} = \begin{cases} \zeta^{m-2}(\underbrace{\zeta e^{-} v^{\nwarrow}}_{\mathcal{L}_n^*} - \underbrace{e^{\nwarrow -} v}_{\mathcal{L}_n^*}) \underbrace{(g^{-})^{-1}}_{\mathcal{L}_0^*} \in \mathcal{L}_{m+n-2}^*, & \text{if } \gamma_0^- \neq 0 \\ \zeta^{m-2}(\underbrace{e^{\nwarrow -} u}_{\mathcal{L}_{n-1}^*} - \underbrace{\zeta e^{-} u^{\nwarrow}}_{\mathcal{L}_{n-1}^*}) \underbrace{(f^{-})^{-1}}_{\mathcal{L}_1^*} \in \mathcal{L}_{m+n-2}^*, & \text{if } \phi_1^- \neq 0 \\ \zeta^{m+n-2}(\underbrace{\zeta^2 e^{+} v^{\nwarrow}}_{\mathcal{L}_2} - \underbrace{e^{\nwarrow +} v}_{\mathcal{L}_0}) \underbrace{(g^{+})^{-1}}_{\mathcal{L}_0} \in \mathcal{L}_{m+n-2}, & \text{if } \gamma_0^+ \neq 0 \\ \zeta^{m+n-2}(\underbrace{e^{\nwarrow +} u}_{\mathcal{L}_0} - \underbrace{\zeta^2 e^{+} u^{\nwarrow}}_{\mathcal{L}_2}) \underbrace{(f^{+})^{-1}}_{\mathcal{L}_0} \in \mathcal{L}_{m+n-2}, & \text{if } \phi_0^+ \neq 0 \end{cases}$$

□

Lemma 2.15: *Let* $(u^{\uparrow}, v^{\uparrow})$ *be an* $[m-1; n]$ *two-point Padé form, and* $(u^{\leftarrow}, v^{\leftarrow})$ *be an* $[m; n-1]$ *two-point Padé form of* $(f^-, g^-; f^+, g^+) \in \mathcal{L}_{-1}^* \times \mathcal{L}_0^* \times \mathcal{L}_0 \times \mathcal{L}_0$ *satisfying* (2.19). *Then, the following statements are equivalent when* $n \geq 1$ *and* $-m+1 \leq n \leq m-1$*:*

(i) $(u^{\uparrow}, v^{\uparrow})$ *is anti-diagonally regular;*
(ii) $u^{\leftarrow} v^{\uparrow} - v^{\leftarrow} u^{\uparrow} = \Delta^{\nearrow} \zeta^{m+n-1} \neq 0$, $\Delta^{\nearrow} \in \mathbb{C}$*;*
(iii) $e^{\leftarrow -}(\infty) \neq 0$ *and* $(e^{\leftarrow +}(0) \neq 0$ *or* $e^{\uparrow +}(0) \neq 0)$*;*
(iv) $e^{\leftarrow -}(\infty) \neq 0$ *and* $(\partial v^{\uparrow} = n$ *if* $\gamma_0^- \neq 0$ *and* $\partial u^{\uparrow} = n-1$ *if* $\phi_1^- \neq 0)$.

Moreover, if $(u^{\uparrow}, v^{\uparrow})$ *is anti-diagonally regular, then*

(v) $e^{\leftarrow +}(0) \neq 0$ *or* $e^{\uparrow +}(0) \neq 0$.

Proof.

$$u^{\leftarrow} v^{\uparrow} - v^{\leftarrow} u^{\uparrow} = \begin{cases} \zeta^{m-2}(\underbrace{\zeta e^{\leftarrow -} v^{\uparrow}}_{\mathcal{L}_{n+1}^*} - \underbrace{e^{\uparrow -} v^{\leftarrow}}_{\mathcal{L}_{n-1}^*}) \underbrace{(g^{-})^{-1}}_{\mathcal{L}_0^*} \in \mathcal{L}_{m+n-1}^*, & \text{if } \gamma_0^- \neq 0 \\ \zeta^{m-2}(\underbrace{e^{\uparrow -} u^{\leftarrow}}_{\mathcal{L}_{n-1}^*} - \underbrace{\zeta e^{\leftarrow -} u^{\uparrow}}_{\mathcal{L}_n^*}) \underbrace{(f^{-})^{-1}}_{\mathcal{L}_1^*} \in \mathcal{L}_{m+n-1}^*, & \text{if } \phi_1^- \neq 0 \\ \zeta^{m+n-1}(\underbrace{e^{\leftarrow +} v^{\uparrow}}_{\mathcal{L}_0} - \underbrace{e^{\uparrow +} v^{\leftarrow}}_{\mathcal{L}_0}) \underbrace{(g^{+})^{-1}}_{\mathcal{L}_0} \in \mathcal{L}_{m+n-1}, & \text{if } \gamma_0^+ \neq 0 \\ \zeta^{m+n-1}(\underbrace{e^{\uparrow +} u^{\leftarrow}}_{\mathcal{L}_0} - \underbrace{e^{\leftarrow +} u^{\uparrow}}_{\mathcal{L}_0}) \underbrace{(f^{+})^{-1}}_{\mathcal{L}_0} \in \mathcal{L}_{m+n-1}, & \text{if } \phi_0^+ \neq 0 \end{cases}$$

□

2.6 Inversion formulas

In Section 2.3 we have seen that Padé forms can be computed by solving linear systems with Toeplitz or Hankel matrices. It is also well known that the inverses of Toeplitz and Hankel matrices are given explicitly in terms of the coefficients of the denominators of certain Padé forms; see *e.g.*, [75]. Moreover, there is a close connection between certain inversion formulas and the Christoffel-Darboux formula. We refer to [22, 52, 85] for details.

The first inversion formula gives the inverse of a Hankel matrix, the remaining ones consider Toeplitz matrices under various assumptions. These assumptions correspond to the different types of regularity we discussed in the previous two sections.

Theorem 2.16: [75, Theorem 1.1'] *Let (p, q) be a regular (m, n) Padé form of $h \in \mathcal{L}$, $(p^{\nwarrow}, q^{\nwarrow})$ be an $(m-1, n-1)$ Padé form of h, normalized by* (2.40). *Then $\mathbf{H}_{m,n}$ is nonsingular, and*

$$
\begin{aligned}
\mathbf{H}_{m,n}^{-1} = {} & \begin{bmatrix} \rho^{\nwarrow}_{n-1} & & & \mathbf{0} \\ \rho^{\nwarrow}_{n-2} & \rho^{\nwarrow}_{n-1} & & \\ \vdots & \ddots & \ddots & \\ \rho^{\nwarrow}_{0} & \cdots & \rho^{\nwarrow}_{n-2} & \rho^{\nwarrow}_{n-1} \end{bmatrix} \begin{bmatrix} \rho_{n-1} & \cdots & \rho_1 & \rho_0 \\ \vdots & ⋰ & ⋰ & \\ \rho_1 & \rho_0 & & \\ \rho_0 & & & \mathbf{0} \end{bmatrix} \\
& - \begin{bmatrix} \rho_n & & & \mathbf{0} \\ \rho_{n-1} & \rho_n & & \\ \vdots & \ddots & \ddots & \\ \rho_1 & \cdots & \rho_{n-1} & \rho_n \end{bmatrix} \begin{bmatrix} \rho^{\nwarrow}_{n-2} & \cdots & \rho^{\nwarrow}_{0} & 0 \\ \vdots & ⋰ & ⋰ & \\ \rho^{\nwarrow}_{0} & 0 & & \\ 0 & & & \mathbf{0} \end{bmatrix}.
\end{aligned}
\tag{2.41}
$$

There is also an inversion formula based on anti-diagonally regular pairs [75, Theorem 1.2'], but we do not need it here.

The following theorem gives the inverse of a Toeplitz matrix in terms of the coefficients of a regular or an anti-diagonally regular pair of Padé forms.

Theorem 2.17: [75, Theorem 1.1, Remark 1.1] *Let (p, q) be a regular (m, n) Padé form of $h \in \mathcal{L}$, $(p^{\nwarrow}, q^{\nwarrow})$ be an $(m-1, n-1)$, $(p^{\uparrow}, q^{\uparrow})$ be an $(m-1, n)$, and $(p^{\leftarrow}, q^{\leftarrow})$ be an $(m, n-1)$ Padé form of h, normalized by* (2.40). *Then $\mathbf{T}_{m,n}$ is nonsingular,*

$$
\begin{aligned}
\mathbf{T}_{m,n}^{-1} = {} & \begin{bmatrix} \rho^{\nwarrow}_{n-1} & \rho^{\nwarrow}_{n-2} & \cdots & \rho^{\nwarrow}_{0} \\ & \rho^{\nwarrow}_{n-1} & \ddots & \vdots \\ & & \ddots & \rho^{\nwarrow}_{n-2} \\ \mathbf{0} & & & \rho^{\nwarrow}_{n-1} \end{bmatrix} \begin{bmatrix} \rho_0 & & & \mathbf{0} \\ \rho_1 & \rho_0 & & \\ \vdots & \ddots & \ddots & \\ \rho_{n-1} & \cdots & \rho_1 & \rho_0 \end{bmatrix} \\
& - \begin{bmatrix} \rho_n & \rho_{n-1} & \cdots & \rho_1 \\ & \rho_n & \ddots & \vdots \\ & & \ddots & \rho_{n-1} \\ \mathbf{0} & & & \rho_n \end{bmatrix} \begin{bmatrix} 0 & & & \mathbf{0} \\ \rho^{\nwarrow}_{0} & 0 & & \\ \vdots & \ddots & \ddots & \\ \rho^{\nwarrow}_{n-2} & \cdots & \rho^{\nwarrow}_{0} & 0 \end{bmatrix},
\end{aligned}
$$

and

$$
\begin{aligned}
\mathbf{T}_{m,n}^{-1} = {} & \begin{bmatrix} \rho_0^{\leftarrow} & & & \mathbf{0} \\ \rho_1^{\leftarrow} & \rho_0^{\leftarrow} & & \\ \vdots & \ddots & \ddots & \\ \rho_{n-1}^{\leftarrow} & \cdots & \rho_1^{\leftarrow} & \rho_0^{\leftarrow} \end{bmatrix} \begin{bmatrix} \rho_n^{\uparrow} & \rho_{n-1}^{\uparrow} & \cdots & \rho_1^{\uparrow} \\ & \rho_n^{\uparrow} & \ddots & \vdots \\ & & \ddots & \rho_{n-1}^{\uparrow} \\ \mathbf{0} & & & \rho_n^{\uparrow} \end{bmatrix} \\
& - \begin{bmatrix} \rho_0^{\uparrow} & & & \mathbf{0} \\ \rho_1^{\uparrow} & \rho_0^{\uparrow} & & \\ \vdots & \ddots & \ddots & \\ \rho_{n-1}^{\uparrow} & \cdots & \rho_1^{\uparrow} & \rho_0^{\uparrow} \end{bmatrix} \begin{bmatrix} 0 & \rho_{n-1}^{\leftarrow} & \cdots & \rho_1^{\leftarrow} \\ & 0 & \ddots & \vdots \\ & & \ddots & \rho_{n-1}^{\leftarrow} \\ \mathbf{0} & & & 0 \end{bmatrix}.
\end{aligned} \tag{2.42}
$$

The next inversion formula based on column-regular pairs is due to Gohberg and Semencul [47], where it was derived without the Padé connection.

Theorem 2.18: [75, Theorem 1.2] *Let (p,q) be a column-regular (m,n) Padé form of $h \in \mathcal{L}$, and $(p^{\uparrow}, q^{\uparrow})$ be an $(m-1,n)$ Padé form of h, normalized by* (2.40). *Then $\pi_0 = e^{\uparrow}(0) \neq 0$, $\mathbf{T}_{m,n+1}$ is nonsingular,*

$$
\begin{aligned}
\mathbf{T}_{m,n+1}^{-1} = {} & \frac{1}{\pi_0} \begin{bmatrix} \rho_0 & & & \mathbf{0} \\ \rho_1 & \rho_0 & & \\ \vdots & \ddots & \ddots & \\ \rho_n & \cdots & \rho_1 & \rho_0 \end{bmatrix} \begin{bmatrix} \rho_n^{\uparrow} & \rho_{n-1}^{\uparrow} & \cdots & \rho_0^{\uparrow} \\ & \rho_n^{\uparrow} & \ddots & \vdots \\ & & \ddots & \rho_{n-1}^{\uparrow} \\ \mathbf{0} & & & \rho_n^{\uparrow} \end{bmatrix} \\
& - \frac{1}{\pi_0} \begin{bmatrix} 0 & & & \mathbf{0} \\ \rho_0^{\uparrow} & 0 & & \\ \vdots & \ddots & \ddots & \\ \rho_{n-1}^{\uparrow} & \cdots & \rho_0^{\uparrow} & 0 \end{bmatrix} \begin{bmatrix} 0 & \rho_n & \cdots & \rho_1 \\ & 0 & \ddots & \vdots \\ & & \ddots & \rho_n \\ \mathbf{0} & & & 0 \end{bmatrix},
\end{aligned} \tag{2.43}
$$

and

$$
\begin{aligned}
\mathbf{T}_{m,n}^{-1} = {} & \frac{1}{\pi_0} \begin{bmatrix} \rho_0 & & & \mathbf{0} \\ \rho_1 & \rho_0 & & \\ \vdots & \ddots & \ddots & \\ \rho_{n-1} & \cdots & \rho_1 & \rho_0 \end{bmatrix} \begin{bmatrix} \rho_n^{\uparrow} & \rho_{n-1}^{\uparrow} & \cdots & \rho_1^{\uparrow} \\ & \rho_n^{\uparrow} & \ddots & \vdots \\ & & \ddots & \rho_{n-1}^{\uparrow} \\ \mathbf{0} & & & \rho_n^{\uparrow} \end{bmatrix} \\
& - \frac{1}{\pi_0} \begin{bmatrix} \rho_0^{\uparrow} & & & \mathbf{0} \\ \rho_1^{\uparrow} & \rho_0^{\uparrow} & & \\ \vdots & \ddots & \ddots & \\ \rho_{n-1}^{\uparrow} & \cdots & \rho_1^{\uparrow} & \rho_0^{\uparrow} \end{bmatrix} \begin{bmatrix} \rho_n & \rho_{n-1} & \cdots & \rho_1 \\ & \rho_n & \ddots & \vdots \\ & & \ddots & \rho_{n-1} \\ \mathbf{0} & & & \rho_n \end{bmatrix}.
\end{aligned} \tag{2.44}
$$

Finally, an analogous formula based on row-regular pairs is

Theorem 2.19: [68, Theorem 2.4] *Let (p,q) be a row-regular (m,n) Padé form of $h \in \mathcal{L}$, and $(p^{\leftarrow}, q^{\leftarrow})$ be an $(m, n-1)$ Padé form of h, normalized by* (2.40). *Then $\rho_n =$*

$-e^{\leftarrow}(0) \neq 0$, $\mathbf{T}_{m+1,n}$ *is nonsingular,*

$$\mathbf{T}_{m+1,n}^{-1} = \frac{1}{\rho_n}\begin{bmatrix} \rho_n & \rho_{n-1} & \cdots & \rho_1 \\ & \rho_n & \ddots & \vdots \\ & & \ddots & \rho_{n-1} \\ \mathbf{0} & & & \rho_n \end{bmatrix}\begin{bmatrix} 0 & & & \mathbf{0} \\ \rho_0^{\leftarrow} & 0 & & \\ \vdots & \ddots & \ddots & \\ \rho_{n-2}^{\leftarrow} & \cdots & \rho_0^{\leftarrow} & 0 \end{bmatrix} - \frac{1}{\rho_n}\begin{bmatrix} \rho_{n-1}^{\leftarrow} & \rho_{n-2}^{\leftarrow} & \cdots & \rho_0^{\leftarrow} \\ & \rho_{n-1}^{\leftarrow} & \ddots & \vdots \\ & & \ddots & \rho_{n-2}^{\leftarrow} \\ \mathbf{0} & & & \rho_{n-1}^{\leftarrow} \end{bmatrix}\begin{bmatrix} \rho_0 & & & \mathbf{0} \\ \rho_1 & \rho_0 & & \\ \vdots & \ddots & \ddots & \\ \rho_{n-1} & \cdots & \rho_1 & \rho_0 \end{bmatrix}, \tag{2.45}$$

and

$$\mathbf{T}_{m,n}^{-1} = \frac{1}{\rho_n}\begin{bmatrix} \rho_n & \rho_{n-1} & \cdots & \rho_1 \\ & \rho_n & \ddots & \vdots \\ & & \ddots & \rho_{n-1} \\ \mathbf{0} & & & \rho_n \end{bmatrix}\begin{bmatrix} \rho_0^{\leftarrow} & & & \mathbf{0} \\ \rho_1^{\leftarrow} & 0 & & \\ \vdots & \ddots & \ddots & \\ \rho_{n-1}^{\leftarrow} & \cdots & \rho_1^{\leftarrow} & \rho_0^{\leftarrow} \end{bmatrix} - \frac{1}{\rho_n}\begin{bmatrix} 0 & \rho_{n-1}^{\leftarrow} & \cdots & \rho_1^{\leftarrow} \\ & 0 & \ddots & \vdots \\ & & \ddots & \rho_{n-1}^{\leftarrow} \\ \mathbf{0} & & & 0 \end{bmatrix}\begin{bmatrix} \rho_0 & & & \mathbf{0} \\ \rho_1 & \rho_0 & & \\ \vdots & \ddots & \ddots & \\ \rho_{n-1} & \cdots & \rho_1 & \rho_0 \end{bmatrix}.$$

It was shown in [68] that evaluating these inversion formulas is weakly stable [23] under suitable assumptions. To be more precise, the formulas of Theorem 2.17 are forward stable if $\mathbf{T}_{m,n}$ is well conditioned, those of Theorem 2.18 are forward stable if $\mathbf{T}_{m,n}$ and $\mathbf{T}_{m,n+1}$ are well conditioned, and finally, the formulas of Theorem 2.18 require well-conditioned matrices $\mathbf{T}_{m,n}$ and $\mathbf{T}_{m+1,n}$ to guarantee forward stability.

2.7 Well-conditioned Padé forms

Most of the theorems and properties we have seen so far are based on assumptions like "one Padé approximant is identical to another" or "certain coefficients are different from zero". However, our main interest is in the development of algorithms for recursively computing Padé approximants or Padé forms in certain regions of the Padé table. Clearly, such assumptions and properties are not sufficient if we want to do our computations in finite precision arithmetic. They do help, in some sense, as they tell us what to look for. However, we will show next that a straightforward generalization which replaces the assumption of a certain matrix to be "nonsingular" by "well conditioned" and some quantities to be different from "zero" by "not too small" is sufficient to make all our algorithms work also in finite precision arithmetic. The definition is motivated by the characterization of the four types of regularity in Lemmas 2.6–2.9 (ii).

Definition 2.6: *Let (p, q) be an (m, n) Padé form of $(f, g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ with $g(0) \neq 0$, and $(p^\uparrow, q^\uparrow)$ be an $(m-1, n)$ Padé form of (f, g). Then we call the index pair (m, n) and the Padé form*

(i) (p, q) **row well-conditioned** *iff $\mathbf{T}_{m,n}$ and $\mathbf{T}_{m+1,n}$ are well conditioned;*
(ii) (p, q) **column well-conditioned** *iff $\mathbf{T}_{m,n}$ and $\mathbf{T}_{m,n+1}$ are well conditioned;*
(iii) (p, q) **well conditioned** *iff $\mathbf{T}_{m,n}$ is well conditioned;*
(iv) $(p^\uparrow, q^\uparrow)$ **anti-diagonally well-conditioned** *iff $\mathbf{T}_{m,n}$ is well conditioned.*

However, for simplification we will use "regular" instead of "well conditioned" most of the time and hope that this will not result in any confusion. "Regular" should be interpreted as "well conditioned", whenever the computations are done in finite precision arithmetic.

Although one probably cannot expect to prove an immediate generalization of the Block Structure Theorem 2.5, we can show that something similar is still true. None of our algorithms will use Padé forms in the interior of a block of the Padé table, so we do not bother with those. However, we are interested in well-conditioned or anti-diagonally well-conditioned pairs and we will show that such pairs cannot occur isolated. In exact arithmetic, this follows for regular or anti-diagonally regular pairs from Jacobi's identity [51, Theorem 5.1]

$$\det \mathbf{T}_{m-1,n} \det \mathbf{T}_{m+1,n} + \det \mathbf{T}_{m,n-1} \det \mathbf{T}_{m,n+1} = (\det \mathbf{T}_{m,n})^2,$$

which follows from Sylvester's determinant identity [51, Theorem 2.6]. Here is an illustration of what this identity tells us: if the entry of the Padé table represented by the filled circle is nonsingular, then one can conclude that at least one of the entries represented by crosses is nonsingular, too.

$$\boxed{\begin{array}{cccc} \begin{array}{cc} \bullet & \times \\ \times & \end{array} & \begin{array}{cc} \times & \bullet \\ & \times \end{array} & \begin{array}{cc} \times & \\ \bullet & \times \end{array} & \begin{array}{cc} & \times \\ \times & \bullet \end{array} \\ \\ \text{Theorem 2.20} & \text{Theorem 2.21} & \text{Theorem 2.22} & \text{Theorem 2.23} \end{array}} \tag{2.46}$$

The theorems indicated in the picture give a generalization of Jacobi's identity, where "nonsingular" is replaced by "well conditioned".

Theorem 2.20: *Let $\mathbf{T}_{m,n}$ be well conditioned and assume that $\|\mathbf{T}_{m,n+1}\| \leq \Lambda$. Then*

$$\|\mathbf{T}_{m,n+1}^{-1}\| \leq 4n \|\mathbf{T}_{m,n}^{-1}\| \sqrt{1 + \Lambda^2 \|\mathbf{T}_{m,n}^{-1}\|^2}$$

or

$$\|\mathbf{T}_{m+1,n}^{-1}\| \leq 4n(\Lambda + 1) \|\mathbf{T}_{m,n}^{-1}\|^2,$$

i.e., $\mathbf{T}_{m,n+1}$ is well conditioned or $\mathbf{T}_{m+1,n}$ is well conditioned. (If one of the matrices is singular, then we set the norm of its inverse to infinity.)

Proof. By the Block Structure Theorem 2.5, $\mathbf{T}_{m+1,n}$ or $\mathbf{T}_{m,n+1}$ is nonsingular. Let us first assume that both are nonsingular.

From the Yule-Walker equations (2.30) and (2.37) we obtain

$$\|\mathbf{q}\|^2 = 1 + \|[\ \rho_1 \ \ \cdots \ \ \rho_n \ ]^T\|^2 \leq 1 + \Lambda^2 \|\mathbf{T}_{m,n}^{-1}\|^2$$

and

$$\|\mathbf{q}^{\uparrow}\|^2 = 1 + \|[\ \rho_0^{\uparrow} \ \ \cdots \ \ \rho_{n-1}^{\uparrow} \ ]^T\|^2 \leq 1 + \Lambda^2 \|\mathbf{T}_{m,n}^{-1}\|^2, \tag{2.47}$$

where

$$\mathbf{q} = [\ \rho_0 \ \ \cdots \ \ \rho_n \ ]^T \quad \text{and} \quad \mathbf{q}^{\uparrow} = [\ \rho_0^{\uparrow} \ \ \cdots \ \ \rho_n^{\uparrow} \ ]^T$$

with $\rho_0 = \rho_n^{\uparrow} = 1$ by (2.40). Moreover by the normalization (2.40) and from (2.39) we have

$$\|\mathbf{q}^{\leftarrow}\| \leq \|\mathbf{T}_{m,n}^{-1}\| \quad \text{and} \quad \|\mathbf{q}^{\nwarrow}\| \leq \|\mathbf{T}_{m,n}^{-1}\|, \tag{2.48}$$

where

$$\mathbf{q}^{\leftarrow} = [\ \rho_0^{\leftarrow} \ \ \cdots \ \ \rho_{n-1}^{\leftarrow} \ ]^T \quad \text{and} \quad \mathbf{q}^{\nwarrow} = [\ \rho_0^{\nwarrow} \ \ \cdots \ \ \rho_{n-1}^{\nwarrow} \ ]^T.$$

Therefore, the assumption that $\mathbf{T}_{m,n}$ is well conditioned guarantees that the norms of the fundamental solutions cannot be large.

Next we have from the inversion formulas (2.43) and (2.45) the upper bounds

$$\|\mathbf{T}_{m,n+1}^{-1}\| \leq \|\mathbf{T}_{m,n+1}^{-1}\|_F \leq \frac{2n}{|\pi_0|} \|\mathbf{q}\| \, \|\mathbf{q}^{\uparrow}\| \tag{2.49}$$

and

$$\|\mathbf{T}_{m+1,n}^{-1}\| \leq \|\mathbf{T}_{m+1,n}^{-1}\|_F \leq \frac{2n}{|\rho_n|} \|\mathbf{q}\| \, \|\mathbf{q}^{\leftarrow}\|.$$

It is therefore sufficient to show that $|\rho_n|$ and $|\pi_0|$ are not both small.

If we add another row to (2.30) and move the right-hand side to the left, then $\mathbf{q}$ satisfies

$$\mathbf{T}_{m,n+1}\mathbf{q} = \left[\begin{array}{ccc|c} & & & \mu_{m-n} \\ & \mathbf{T}_{m,n} & & \vdots \\ & & & \mu_{m-1} \\ \hline \mu_{m+n} & \cdots & \mu_{m+1} & \mu_m \end{array}\right] \mathbf{q} = \pi_0 \mathbf{e}_0. \tag{2.50}$$

This implies

$$\begin{bmatrix} \rho_0 \\ \vdots \\ \rho_{n-1} \end{bmatrix} = \mathbf{T}_{m,n}^{-1} \left(-\rho_n \begin{bmatrix} \mu_{m-n} \\ \vdots \\ \mu_{m-1} \end{bmatrix} + \pi_0 \mathbf{e}_0 \right)$$

and thus

$$\|\mathbf{q}\|^2 \leq \|\mathbf{T}_{m,n}^{-1}\|^2 \left(|\rho_n| \, \Lambda + |\pi_0|\right)^2 + |\rho_n|^2 \leq \|\mathbf{T}_{m,n}^{-1}\|^2 \left(|\rho_n| \, (\Lambda + 1) + |\pi_0|\right)^2.$$

The last inequality shows that

$$\max\{\, |\rho_n|\,(\Lambda+1), |\pi_0|\,\} \geq \frac{\|\mathbf{q}\|}{2\|\mathbf{T}_{m,n}^{-1}\|} \tag{2.51}$$

and therefore one of the following upper bounds is valid:

$$\|\mathbf{T}_{m,n+1}^{-1}\| \leq 4n\|\mathbf{T}_{m,n}^{-1}\|\,\|\mathbf{q}^{\uparrow}\| \tag{2.52}$$

or

$$\|\mathbf{T}_{m+1,n}^{-1}\| \leq 4n(\Lambda+1)\|\mathbf{T}_{m,n}^{-1}\|\,\|\mathbf{q}^{\leftarrow}\|, \tag{2.53}$$

which are even sharper than those stated in the theorem according to (2.47) and (2.48).

The second case, that either $\mathbf{T}_{m+1,n}$ or $\mathbf{T}_{m,n+1}$ is exactly singular is equivalent to either ρ_n or π_0 being exactly zero by Lemmas 2.6 and 2.7, respectively. The statement then follows again from (2.51). □

The upper bound (2.49) was used by Ammar and Gragg [1] in their numerical experiments on superfast Toeplitz solvers for the positive definite case.

The bad news from this theorem is that in terms of the condition numbers of the matrix $\mathbf{T}_{m,n}$ and its "neighbors" $\mathbf{T}_{m+1,n}$, $\mathbf{T}_{m,n+1}$, the bounds involve the square of the condition number of $\mathbf{T}_{m,n}$. Hence, this result is not strong enough to guarantee a certain structure for large blocks in an "inexact" Padé table. However, it seems to be useful for algorithms working with well-conditioned pairs of one of the types defined in Definition 2.6. The previous theorem means that a well-conditioned pair must be column well-conditioned or row well-conditioned (or both). Since we can show the analogous theorems for the other neighbors of a well-conditioned Padé form in Picture (2.46), this implies, for example, that well-conditioned pairs on two adjacent diagonals cannot occur independently, as was shown in [63] for the exact Padé table. The next three theorems contain the remaining cases.

Theorem 2.21: *Let $\mathbf{T}_{m,n}$ be well conditioned and assume that $\|\mathbf{T}_{m,n+1}\| \leq \Lambda$. Then*

$$\|\mathbf{T}_{m+1,n}^{-1}\| \leq 4n\|\mathbf{T}_{m,n}^{-1}\|\sqrt{1+\Lambda^2\|\mathbf{T}_{m,n}^{-1}\|^2}$$

or

$$\|\mathbf{T}_{m,n-1}^{-1}\| \leq 4n(\Lambda+1)\|\mathbf{T}_{m,n}^{-1}\|^2,$$

i.e., $\mathbf{T}_{m+1,n}$ is well conditioned or $\mathbf{T}_{m,n-1}$ is well conditioned.

Proof. The proof is similar to the proof of Theorem 2.20. The block structure theorem tells us that at least one of the matrices $\mathbf{T}_{m+1,n}$ or $\mathbf{T}_{m,n-1}$ is nonsingular. We again first assume that both matrices are nonsingular.

Applying the inversion formula (2.44) with n replaced by $n-1$ and taking the different normalization into account yields

$$\|\mathbf{T}_{m,n-1}^{-1}\| \leq \frac{2n}{|\rho_0^{\leftarrow}|}\|\mathbf{q}^{\leftarrow}\|\,\|\mathbf{q}^{\nwarrow}\|.$$

Next we have from (2.39)

$$\mathbf{T}_{m,n+1}\begin{bmatrix}\mathbf{q}^{\leftarrow}\\ 0\end{bmatrix}=\left[\begin{array}{c|ccc}\mu_m & \mu_{m-1} & \cdots & \mu_{m-n}\\ \hline \mu_{m+1} & & & \\ \vdots & & \mathbf{T}_{m,n} & \\ \mu_{m+n} & & & \end{array}\right]\begin{bmatrix}\mathbf{q}^{\leftarrow}\\ 0\end{bmatrix}=\mathbf{e}_0+e^{\leftarrow}(0)\mathbf{e}_n,$$

and hence

$$\|\mathbf{q}^{\leftarrow}\|\leq\|\mathbf{T}_{m,n}^{-1}\|\left(|\rho_0^{\leftarrow}|(\Lambda+1)+|e^{\leftarrow}(0)|\right).$$

This yields the lower bound

$$\max\{\,|\rho_0^{\leftarrow}|\,(\Lambda+1),|e^{\leftarrow}(0)|\,\}\geq\frac{\|\mathbf{q}^{\leftarrow}\|}{2\|\mathbf{T}_{m,n}^{-1}\|}. \tag{2.54}$$

Here, $e^{\leftarrow}(0)=-\rho_n$ by Theorem 2.19 or Corollary 2.11.

The remaining part of the proof is done similarly to the previous theorem:

$$\|\mathbf{T}_{m,n-1}^{-1}\|\leq 4n(\Lambda+1)\|\mathbf{T}_{m,n}^{-1}\|\,\|\mathbf{q}^{\nwarrow}\|$$

or

$$\|\mathbf{T}_{m+1,n}^{-1}\|\leq 4n\|\mathbf{T}_{m,n}^{-1}\|\,\|\mathbf{q}\|.$$

□

Analogously to Theorem 2.20 there also holds

Theorem 2.22: *Let $\mathbf{T}_{m,n}$ be well conditioned and assume that $\|\mathbf{T}_{m,n+1}\|\leq\Lambda$. Then*

$$\|\mathbf{T}_{m,n+1}^{-1}\|\leq 4n\|\mathbf{T}_{m,n}^{-1}\|\sqrt{1+\Lambda^2\|\mathbf{T}_{m,n}^{-1}\|^2}$$

or

$$\|\mathbf{T}_{m-1,n}^{-1}\|\leq 4n(\Lambda+1)\|\mathbf{T}_{m,n}^{-1}\|^2,$$

i.e., $\mathbf{T}_{m,n+1}$ is well conditioned or $\mathbf{T}_{m-1,n}$ is well conditioned.

Theorem 2.23: *Let $\mathbf{T}_{m,n}$ be well conditioned and assume that $\|\mathbf{T}_{m,n+1}\|\leq\Lambda$. Then*

$$\|\mathbf{T}_{m-1,n}^{-1}\|\leq 4n\|\mathbf{T}_{m,n}^{-1}\|\sqrt{1+\Lambda^2\|\mathbf{T}_{m,n}^{-1}\|^2}$$

or

$$\|\mathbf{T}_{m,n-1}^{-1}\|\leq 4n(\Lambda+1)\|\mathbf{T}_{m,n}^{-1}\|^2,$$

i.e., $\mathbf{T}_{m,n-1}$ is well conditioned or $\mathbf{T}_{m-1,n}$ is well conditioned.

In a very vague formulation, we can now prove a block structure theorem for the "inexact" Padé table. To make it readable, we leave it in this very imprecise form. Precise results can be taken from the proof. The previous theorems gave bounds for the condition number of direct neighbors of well-conditioned Padé forms. These bounds already involved the square of the condition number of the well-conditioned Padé form. We will see that the bounds of Padé forms which are j rows or columns away from a well-conditioned Padé form can grow like the $(j+1)$st power of this condition number. However, it seems to be worth mentioning, that a block structure can be established under suitable assumptions.

Theorem 2.24: *The "inexact" Padé table consists of square blocks, where the entries on the left and upper border of a block are "well conditioned" and the other entries correspond to "ill-conditioned" Toeplitz matrices.*

Proof. From Theorems 2.20–2.23, we conclude that all blocks must be convex, hence rectangular. This is best seen from the Picture (2.46). It remains to show that the rectangles are squares. Assume that $(m+j,n)$ and $(m,n+k)$ are well-conditioned indices for $j=0,\dots,J-1$ and $k=0,\dots,K-1$, *i.e.*, that the block is of size $J\times K$ and let $\|\mathbf{T}_{m+J,n+K}\|\leq\Lambda$. Denote as usual by (p_n,q_n) the regular (m,n) Padé form of h, which is located in the upper left corner of the block.

We start with the case $K>J>1$ and assume $j+1\leq K-1$. From (2.50) we conclude that

$$\mathbf{T}_{m+j+1,n+1}\mathbf{q}_n=\sum_{l=0}^{j}\varepsilon_{n+l,n}\mathbf{e}_{n-j+l}.$$

Moreover, we have

$$\mathbf{T}_{m,n+j+1}\begin{bmatrix}\mathbf{q}_n\\ \mathbf{0}_j\end{bmatrix}=\pi_{0,n}\mathbf{e}_0+\sum_{l=0}^{j-1}\varepsilon_{n+l,n}\mathbf{e}_{n+l+1},$$

where the residual e_n of (p_n,q_n) is denoted by

$$e_n(\zeta)=\sum_{l=0}^{\infty}\varepsilon_{n+l,n}\zeta^l.$$

We next show that the norm of the vector

$$\begin{bmatrix}\varepsilon_{n,n} & \cdots & \varepsilon_{n+j-1,n}\end{bmatrix}^T$$

is small. From the fundamental equations (2.39) and the normalization (2.40) we obtain

$$\mathbf{d}_{n+j}:=\mathbf{q}_{n+j}-\pi_{0,n+j}\begin{bmatrix}\mathbf{q}^{\leftarrow}_{n+j}\\ 0\end{bmatrix}=\pi_{0,n+j}e^{\leftarrow}_{n+j}(0)\mathbf{T}^{-1}_{m,n+j+1}\mathbf{e}_{n+j}$$

and thus

$$\|\mathbf{d}_{n+j}\| \le \delta_{n+j} := |\pi_{0,n+j} e^{\leftarrow}_{n+j}(0)| \cdot \|\mathbf{T}^{-1}_{m,n+j+1}\|.$$

Recall that by assumption, $\mathbf{T}_{m,n+j+1}$ is well conditioned but $\mathbf{T}_{m+1,n+j+1}$ is ill conditioned. The latter implies that $|e^{\leftarrow}_{n+j}(0)|$ is small (otherwise inversion formula (2.45) would show that $\mathbf{T}_{m+1,n+j+1}$ is well conditioned), which makes δ_{n+j} small. Moreover, the maximum in (2.51) is attained for $\pi_{0,n+j}$, which shows that

$$|\pi_{0,n+j}| \ge \frac{\|\mathbf{q}_{n+j}\|}{2\Lambda \|\mathbf{T}^{-1}_{m,n+j}\|}.$$

By induction we conclude

$$\|\mathbf{q}_{n+j} - \nu_{n+j} \begin{bmatrix} \mathbf{q}_n \\ \mathbf{0}_j \end{bmatrix}\| \le \sum_{l=1}^{j} \delta_{n+l}, \quad \nu_{n+j} := \pi_{0,n+1} \cdots \pi_{0,n+j} \cdot \rho^{\leftarrow}_{0,n+1} \cdots \rho^{\leftarrow}_{0,n+j},$$

which gives in view of (2.50)

$$\begin{aligned} \mathbf{T}_{m,n+j+1}\mathbf{q}_{n+j} &= \pi_{0,n+j}\mathbf{e}_0 \\ &= \mathbf{T}_{m,n+j+1}\left(\nu_{n+j}\begin{bmatrix} \mathbf{q}_n \\ \mathbf{0}_j \end{bmatrix} + \sum_{l=1}^{j}\begin{bmatrix} \mathbf{d}_{n+l} \\ \mathbf{0}_{j-l} \end{bmatrix}\right) \\ &= \nu_{n+j}\left(\pi_{0,n}\mathbf{e}_0 + \sum_{l=0}^{j-1} \varepsilon_{n+l,n}\mathbf{e}_{n+l+1}\right) + \mathbf{T}_{m,n+j+1}\sum_{l=1}^{j}\begin{bmatrix} \mathbf{d}_{n+l} \\ \mathbf{0}_{j-l} \end{bmatrix}. \end{aligned}$$

For $\rho^{\leftarrow}_{0,n+j}$, we have the upper bound (2.54):

$$|\rho^{\leftarrow}_{0,n+j}| \ge \frac{\|\mathbf{q}^{\leftarrow}\|}{2(\Lambda+1)\|\mathbf{T}^{-1}_{m,n+j}\|}$$

This finally yields

$$\|[\ \varepsilon_{n,n} \ \ \cdots \ \ \varepsilon_{n+j-1,n}\ ]^T\| \le \frac{\Lambda}{\nu_{n+j}} \sum_{l=1}^{j} \delta_{n+l},$$

where $|\nu_{n+j}|$ cannot be small due to the upper bounds on $\rho^{\leftarrow}_{n+j}$ and $\pi_{0,n+j}$. However, we also have

$$\|\mathbf{T}^{-1}_{m+j+1,n+1}\| \ge \|\mathbf{q}_n\| \frac{1}{\|[\ \varepsilon_{n,n} \ \ \cdots \ \ \varepsilon_{n+j-1,n}\ ]^T\|}.$$

Therefore, $\mathbf{T}_{m+j+1,n+1}$ is ill conditioned, which shows that $K = J$.

The case $J > K > 1$ is done analogously. □

Note that we did not characterize the condition of Padé forms in the interior of a block quantitatively, because, as we mentioned before, we are not interested in Padé forms in the interior of a block for the purpose of this thesis.

We would like to stress that none of our algorithms will make use of the fact that blocks in the Padé table are square. However, for some of the algorithms, we will exploit the statements of Theorems 2.20–2.23.

Probably, one could show similar results for two-point Padé forms, but we do not pursue this further.

3. GENERAL RECURRENCES

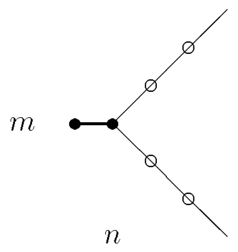
The aim of this chapter is to provide general recurrences to compute Padé forms in a certain region of the Padé table. All the recurrences presented here start from one of the four types of regular pairs and yield a Padé form located in a sector with opening angle of 90 degree to the right of the pair we started.

This chapter is rather technical. On a first reading, the theorems can be omitted. Reading the explanations and looking at the pictures should be sufficient to understand the different kinds of recurrences and to see which Padé forms can be computed with these results and which Padé forms are required to perform this computation.

Most of the recurrences given in this section have been proved in [62], [66], and [69]. While these papers mainly contain recurrences which compute a fixed type of regular pairs, *e.g.*, they compute a column-regular pair from another column-regular pair, here we include also so-called "mixed" recurrences, *i.e.*, recurrences which start from a (row-/column-/anti-diagonally) regular pair and yield a (row-/column-/anti-diagonally) regular pair with all its possible combinations. We have shown in [69] how to take advantage of these mixed recurrences in order to develop algorithms which are optimal in the sense that none of the other recurrences require less computational work. To the best of our knowledge, the recurrences for two-point Padé forms based on anti-diagonally regular pairs are new. For Padé forms recurrences based on anti-diagonally regular pairs have been established independently in [120]. We use these recurrences to develop yet another variant of algorithm which is similar to the one we presented in [69] in Chapters 7–9. Since the proofs of the different types of recurrences are similar and those of row regular, column regular, and regular pairs have been proved elsewhere [62, 66], we only prove the statements for anti-diagonally regular pairs.

3.1 Recurrences based on row-regular pairs

The following theorem gives recurrences based on row-regular pairs for the one-point Padé table. The picture shows the region in the Padé table for which the assumptions of the theorem are fulfilled. The filled circles represent an (m,n) Padé form and its left neighbor, an $(m,n-1)$ Padé form. The thick line connecting these two Padé forms indicates that the corresponding Padé approximants belong to different blocks of the Padé table, *i.e.*, that the (m,n) Padé form is row-regular.



Theorem 3.1: *Assume $N \in \mathbb{Z}$ and $(l,k),(m,n) \in \mathbb{Z} \times \mathbb{N}^+$ such that $m > -N$, $|l| < k$ or $|l| = k > 0$. Let (p_n, q_n) be a row-regular (m,n) Padé form of $(f,g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ with $g(0) \neq 0$ (or $f \in \mathcal{L}$ and $g \equiv -1$) with residual e_n, and let $(p_n^{\leftarrow}, q_n^{\leftarrow})$ and $e_n^{\leftarrow}$ be an $(m, n-1)$ Padé form and its residual.*

If $(u_k^{(n)}, v_k^{(n)})$ is an $[l;k]$ two-point Padé form with residual (e_k^-, e_k^+) of

$$(f^-, g^-; f^+, g^+) := (\zeta^{-m-1} p_n, \zeta^{-m} p_n^{\leftarrow}; e_n, e_n^{\leftarrow}), \tag{3.1}$$

then

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ \zeta^{k+l} e_{n+k} \end{bmatrix} := \begin{bmatrix} \zeta p_n^{\leftarrow} & p_n \\ \zeta q_n^{\leftarrow} & q_n \\ e_n^{\leftarrow} & e_n \end{bmatrix} \begin{bmatrix} u_k^{(n)} \\ v_k^{(n)} \end{bmatrix}$$

yields an $(m+l, n+k)$ Padé form (p_{n+k}, q_{n+k}) of (f,g) and its residual e_{n+k}, which is equal to e_k^+, while e_k^- is equal to $\zeta^{-m-l} p_{n+k}$.

For the special case that $l = 0$ and that we compute *all* row-regular Padé forms of the mth row of the Padé table, a recurrence relation between the denominators of three consecutive Padé forms on one row has been given by Draux [35, Proprieté 4.17]. To be more precise, assume that $n-j$,n, and $n+k$ are three consecutive row-regular indices. Then Draux's result exploits the fact that, up to scaling, $q_n^{\leftarrow} = \zeta^{\sigma} q_{n-j}$ by Theorem 2.3, which is clearly applicable in exact arithmetic only. The above theorem is much more general, in particular, it can be used for algorithms implemented in finite precision arithmetic also. Moreover, we would like to mention that although Draux treats two-point Padé forms in his thesis [35], he did not seem to be aware of the fact that his recursions are related to certain two-point Padé forms.

The analogous result for two-point Padé forms gives

Theorem 3.2: *Assume (k,l), $(m,n) \in \mathbb{Z} \times \mathbb{N}^+$ such that $|l| < k$ or $|l| = k > 0$, and $|m| < n$ or $|m| = n > 0$. Let $(u_n, v_n) = (u_{m;n}, v_{m;n})$ be a row-regular $[m;n]$ two-point Padé form of a quadruple $(f^-, g^-; f^+, g^+)$ satisfying (2.16) and $(u_n^{\leftarrow}, v_n^{\leftarrow}) = (u_{m;n-1}, v_{m;n-1})$ be an $[m;n-1]$ two-point Padé form. Finally, let (e_n^-, e_n^+) and $(e_n^{\leftarrow -}, e_n^{\leftarrow +})$ be the residuals of (u_n, v_n) and $(u_n^{\leftarrow}, v_n^{\leftarrow})$, respectively.*

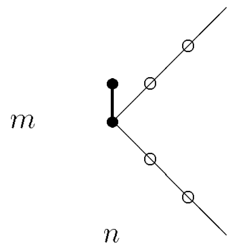
If $(u_k^{(n)}, v_k^{(n)}) = (u_{l;k}, v_{l;k})$ *is an* $[l;k]$ *two-point Padé form of* $(\zeta^{-1}e_n^-, e_n^{\leftarrow -}; e_n^+, e_n^{\leftarrow +})$ *with residual* $(e_k^{(n)-}, e_k^{(n)+})$, *then*

$$\begin{bmatrix} u_{n+k} \\ v_{n+k} \\ \zeta^{l-1}e_{n+k}^- \\ \zeta^{k+l}e_{n+k}^+ \end{bmatrix} := \begin{bmatrix} \zeta u_n^{\leftarrow} & u_n \\ \zeta v_n^{\leftarrow} & v_n \\ e_n^{\leftarrow -} & \zeta^{-1}e_n^- \\ e_n^{\leftarrow +} & e_n^+ \end{bmatrix} \begin{bmatrix} u_k^{(n)} \\ v_k^{(n)} \end{bmatrix}$$

yields an $[m+l; n+k]$ *two-point Padé form* $(u_{n+k}, v_{n+k}) := (u_{m+l;n+k}, v_{m+l;n+k})$ *of* $(f^-, g^-; f^+, g^+)$ *and its residual* (e_{n+k}^-, e_{n+k}^+), *which is equal to* $(e_k^{(n)-}, e_k^{(n)+})$.

3.2 Recurrences based on column-regular pairs

Next, we consider the corresponding recurrences based on column-regular pairs. We again start with the one-point Padé table.



Theorem 3.3: *Assume* $N \in \mathbb{Z}$ *and* $(l,k), (m,n) \in \mathbb{Z} \times \mathbb{N}^+$ *such that* $|l| < k$ *or* $|l| = k > 0$. *Let* (p_n, q_n) *be a column-regular* (m,n) *Padé form of* $(f,g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ *with* $g(0) \neq 0$ *(or* $f \in \mathcal{L}$ *and* $g \equiv -1$*) with residual* e_n, *and let* $(p_n^{\uparrow}, q_n^{\uparrow})$ *and* $e_n^{\uparrow}$ *be an* $(m-1, n)$ *Padé form and its residual.*

If $|l| < k$ *or* $|l| = k > 0$, *and if* $(u_k^{(n)}, v_k^{(n)})$ *is an* $[l;k]$ *two-point Padé form with residual* (e_k^-, e_k^+) *of*

$$(f^-, g^-; f^+, g^+) := (\zeta^{-m-1}p_n, \zeta^{-m}p_n^{\uparrow}; e_n, e_n^{\uparrow}),$$

then $\partial v_k \leq k-1$ *holds, and the recurrence formula*

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ \zeta^{k+l}e_{n+k} \end{bmatrix} := \begin{bmatrix} \zeta p_n^{\uparrow} & p_n \\ \zeta q_n^{\uparrow} & q_n \\ e_n^{\uparrow} & e_n \end{bmatrix} \begin{bmatrix} u_k^{(n)} \\ v_k^{(n)} \end{bmatrix}$$

yields an $(m+l, n+k)$ *Padé form* (p_{n+k}, q_{n+k}) *of* (f,g) *and its residual* e_{n+k}, *which is equal to* e_k^+, *while* e_k^- *is equal to* $\zeta^{-m-l}p_{n+k}$.

Recursions for two-point Padé forms based on column-regular pairs of two-point Padé forms are given in the following

Theorem 3.4: *Assume (k,l), $(m,n) \in \mathbb{Z} \times \mathbb{N}^+$ such that $|l| < k$ or $|l| = k > 0$, and $-n+1 \leq m \leq n$. Let $(u_n, v_n) = (u_{m;n}, v_{m;n})$ be a column-regular $[m;n]$ two-point Padé form of a quadruple $(f^-, g^-; f^+, g^+)$ satisfying (2.16) and $(u_n^{\uparrow}, v_n^{\uparrow}) = (u_{m-1;n}, v_{m-1;n})$ be an $[m-1;n]$ two-point Padé form. Finally, let (e_n^-, e_n^+) and $(e_n^{\uparrow -}, e_n^{\uparrow +})$ be the residuals of (u_n, v_n) and $(u_n^{\uparrow}, v_n^{\uparrow})$, respectively.*

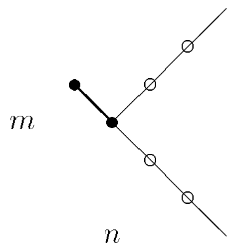
If $(u_k^{(n)}, v_k^{(n)}) = (u_{l;k}, v_{l;k})$ is an $[l;k]$ two-point Padé form of $(\zeta^{-1} e_n^-, \zeta^{-1} e_n^{\uparrow -}; e_n^+, e_n^{\uparrow +})$ with residual $(e_k^{(n)-}, e_k^{(n)+})$, then $\partial v_k^{(n)} \leq k-1$ holds and the recurrence formula

$$\begin{bmatrix} u_{n+k} \\ v_{n+k} \\ \zeta^l e_{n+k}^- \\ \zeta^{k+l} e_{n+k}^+ \end{bmatrix} := \begin{bmatrix} \zeta u_n^{\uparrow} & u_n \\ \zeta v_n^{\uparrow} & v_n \\ e_n^{\uparrow -} & e_n^- \\ e_n^{\uparrow +} & e_n^+ \end{bmatrix} \begin{bmatrix} u_k^{(n)} \\ v_k^{(n)} \end{bmatrix}$$

yields an $[m+l; n+k]$ two-point Padé form $(u_{n+k}, v_{n+k}) := (u_{m+l;n+k}, v_{m+l;n+k})$ of $(f^-, g^-; f^+, g^+)$ and its residual (e_{n+k}^-, e_{n+k}^+), which is equal to $(e_k^{(n)-}, e_k^{(n)+})$.

3.3 Recurrences based on regular pairs

Recall that, for a regular pair, the second member of this pair is row regular or column regular. Hence, there exist more regular pairs than row-regular or column-regular pairs in the Padé table, which turns out to be favorable for some applications.



Theorem 3.5: *Assume $N \in \mathbb{Z}$ and $(l,k), (m,n) \in \mathbb{Z} \times \mathbb{N}^+$ such that $m > -N+1, |l| \leq k$. Let (p_n, q_n) be a regular (m,n) Padé form of $(f,g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ with $g(0) \neq 0$ (or $f \in \mathcal{L}$ and $g \equiv -1$) with residual e_n, and let $(p_n^{\nwarrow}, q_n^{\nwarrow})$ and $e_n^{\nwarrow}$ be an $(m-1, n-1)$ Padé form and its residual.*

If $(u_k^{(n)}, v_k^{(n)})$ is an $[l;k]$ two-point Padé form with residual (e_k^-, e_k^+) of

$$(f^-, g^-; f^+, g^+) := (\zeta^{-m-1} p_n, \zeta^{-m+1} p_n^{\nwarrow}; e_n, e_n^{\nwarrow}), \tag{3.2}$$

then

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ \zeta^{k+l} e_{n+k} \end{bmatrix} := \begin{bmatrix} \zeta^2 p_n^{\nwarrow} & p_n \\ \zeta^2 q_n^{\nwarrow} & q_n \\ e_n^{\nwarrow} & e_n \end{bmatrix} \begin{bmatrix} u_k^{(n)} \\ v_k^{(n)} \end{bmatrix} \tag{3.3}$$

yields an $(m+l, n+k)$ *Padé form* (p_{n+k}, q_{n+k}) *of* (f, g) *and its residual* e_{n+k}, *which is equal to* e_k^+, *while* e_k^- *is equal to* $\zeta^{-m-l} p_{n+k}$.

For two-point Padé forms we have

Theorem 3.6: *Assume* (k, l), $(m, n) \in \mathbb{Z} \times \mathbb{N}^+$ *such that* $|l| < k$ *or* $|l| = k > 0$, *and* $-n+1 \le m \le n$. *Let* $(u_n, v_n) = (u_{m;n}, v_{m;n})$ *be a regular* $[m; n]$ *two-point Padé form of a quadruple* $(f^-, g^-; f^+, g^+)$ *satisfying* (2.15) *or* (2.16) *and* $(u_n^{\nwarrow}, v_n^{\nwarrow}) = (u_{m-1;n-1}, v_{m-1;n-1})$ *be an* $[m-1; n-1]$ *two-point Padé form. Finally, let* (e_n^-, e_n^+) *and* $(e_n^{\nwarrow -}, e_n^{\nwarrow +})$ *be the residuals of* (u_n, v_n) *and* $(u_n^{\nwarrow}, v_n^{\nwarrow})$, *respectively.*

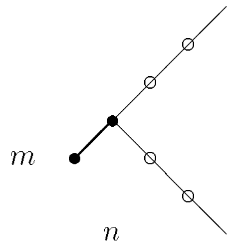
If $(u_k^{(n)}, v_k^{(n)}) = (u_{l;k}, v_{l;k})$ *is an* $[l; k]$ *two-point Padé form of* $(\zeta^{-1} e_n^-; e_n^{\nwarrow -}; e_n^+, e_n^{\nwarrow +})$ *with residual* $(e_k^{(n)-}, e_k^{(n)+})$, *then the recurrence formula*

$$\begin{bmatrix} u_{n+k} \\ v_{n+k} \\ \zeta^{l-1} e_{n+k}^- \\ \zeta^{k+l} e_{n+k}^+ \end{bmatrix} := \begin{bmatrix} \zeta^2 u_n^{\nwarrow} & u_n \\ \zeta^2 v_n^{\nwarrow} & v_n \\ e_n^{\nwarrow -} & \zeta^{-1} e_n^- \\ e_n^{\nwarrow +} & e_n^+ \end{bmatrix} \begin{bmatrix} u_k^{(n)} \\ v_k^{(n)} \end{bmatrix} \tag{3.4}$$

yields an $[m+l; n+k]$ *two-point Padé form* $(u_{n+k}, v_{n+k}) := (u_{m+l;n+k}, v_{m+l;n+k})$ *of* $(f^-, g^-; f^+, g^+)$ *and its residual* (e_{n+k}^-, e_{n+k}^+), *which is equal to* $(e_k^{(n)-}, e_k^{(n)+})$.

3.4 Recurrences based on anti-diagonally regular pairs

The last type of pairs we want to consider are anti-diagonally regular pairs. Since, by Corollary 2.10, $(p_n^{\uparrow}, q_n^{\uparrow})$ and $(p_n^{\leftarrow}, q_n^{\leftarrow})$ are an anti-diagonally regular pair if and only if (p_n, q_n) and $(p_n^{\nwarrow}, q_n^{\nwarrow})$ are a regular pair, anti-diagonally regular pairs are suited equally well as regular pairs. Since the Padé forms of such a pair match the Laurent series up to the same O_+ order, the recurrences even look a little nicer for anti-diagonally regular pairs than for regular pairs.



Theorem 3.7: *Assume* $N \in \mathbb{Z}$ *and* $(l, k), (m, n) \in \mathbb{Z} \times \mathbb{N}^+$ *such that* $m > -N+1$, $|l+1| < k$ *or* $|l+1| = k > 0$. *Let* $(p_n^{\uparrow}, q_n^{\uparrow})$ *be an anti-diagonally regular* $(m-1, n)$ *Padé form of* $(f, g) \in \mathcal{L}_{-N} \times \mathcal{L}_0$ *with* $g(0) \neq 0$ *(or* $f \in \mathcal{L}$ *and* $g \equiv -1$*) with residual* $e_n^{\uparrow}$, *and let* $(p_n^{\leftarrow}, q_n^{\leftarrow})$ *and* $e_n^{\leftarrow}$ *be an* $(m, n-1)$ *Padé form and its residual.*

If $(u_k^{(n)}, v_k^{(n)})$ *is an* $[l+1;k]$ *two-point Padé form with residual* (e_k^-, e_k^+) *of*

$$(f^-, g^-; f^+, g^+) := (\zeta^{-m} p_n^{\uparrow}, \zeta^{-m} p_n^{\leftarrow}; e_n^{\uparrow}, e_n^{\leftarrow}), \tag{3.5}$$

then

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ \zeta^{k+l+1} e_{n+k} \end{bmatrix} := \begin{bmatrix} p_n^{\leftarrow} & p_n^{\uparrow} \\ q_n^{\leftarrow} & q_n^{\uparrow} \\ e_n^{\leftarrow} & e_n^{\uparrow} \end{bmatrix} \begin{bmatrix} u_k^{(n)} \\ v_k^{(n)} \end{bmatrix} \tag{3.6}$$

yields an $(m+l, n+k)$ *Padé form* (p_{n+k}, q_{n+k}) *of* (f,g) *and its residual* e_{n+k}*, which is equal to* e_k^+*, while* e_k^- *is equal to* $\zeta^{-m-l} p_{n+k}$*.*

Proof. For simplicity we delete the upper index $^{(n)}$ in the proof.

The data (3.5) satisfy (2.17) or (2.18) since, by Lemma 2.9, we have $\partial p_n^{\leftarrow} = m$ and $e_n^{\uparrow}(0) \neq 0$ or $e_n^{\leftarrow}(0) \neq 0$.

It is obvious that $q_{n+k} \in \mathcal{P}_{n+k}$. Then it remains to prove the following statements:

$$\partial p_{n+k} \leq m+l, \tag{3.7}$$

$$f q_{n+k} + g p_{n+k} = \zeta^{m+l+n+k+1} e_{n+k} \tag{3.8}$$

$$e_{n+k} \in \mathcal{L}_0, \tag{3.9}$$

Since (u_k, v_k) as an $[l+1;k]$ two-point Padé form we have

$$g^- u_k + f^- v_k = \zeta^{-m}(p_n^{\leftarrow} u_k + p_n^{\uparrow} v_k) = \zeta^l e_k^- = O_-(\zeta^l).$$

Therefore,

$$p_{n+k} = p_n^{\leftarrow} u_k + p_n^{\uparrow} v_k = \zeta^{m+l} e_k^- = O_-(\zeta^{m+l}),$$

i.e., (3.7), and $e_k^- = \zeta^{-m-l} p_{n+k}$. From

$$g^+ u_k + f^+ v_k = e_n^{\leftarrow} u_k + e_n^{\uparrow} v_k = \zeta^{k+l+1} e_k^+ = O_+(\zeta^{k+l+1})$$

it follows that

$$e_{n+k} = \zeta^{-k-l-1}(e_n^{\leftarrow} u_k + e_n^{\uparrow} v_k) = e_k^+ = O_+(1).$$

This proves (3.9). (3.8) follows from

$$f q_{n+k} + g p_{n+k} = \zeta^{m+n}(e_n^{\leftarrow} u_k + e_n^{\uparrow} v_k) = \zeta^{m+n+k+l+1} e_k^+,$$

which completes the proof. □

Theorem 3.8: *Assume* $(k,l), (m,n) \in \mathbb{Z} \times \mathbb{N}^+$ *such that* $|l+1| < k$ *or* $|l+1| = k > 0$*, and* $-n+1 \leq m \leq n-1$*. Let* $(u_n^{\uparrow}, v_n^{\uparrow}) = (u_{m-1;n}, v_{m-1;n})$ *be an anti-diagonally regular* $[m-1;n]$ *two-point Padé form of a quadruple* $(f^-, g^-; f^+, g^+)$ *satisfying* (2.17) *or* (2.18) *and* $(u_n^{\leftarrow}, v_n^{\leftarrow}) = (u_{m;n-1}, v_{m;n-1})$ *be an* $[m; n-1]$ *two-point Padé form. Finally, let* $(e_n^{\uparrow -}, e_n^{\uparrow +})$ *and* $(e_n^{\leftarrow -}, e_n^{\leftarrow +})$ *be the residuals of* (u_n, v_n) *and* $(u_n^{\leftarrow}, v_n^{\leftarrow})$*, respectively.*

If $(u_k^{(n)}, v_k^{(n)}) = (u_{l;k}, v_{l;k})$ *is an* $[l;k]$ *two-point Padé form of* $(\zeta^{-1}e_n^{\uparrow -}; e_n^{\leftarrow -}; e_n^{+}, e_n^{\leftarrow +})$ *with residual* $(e_k^{(n)-}, e_k^{(n)+})$*, then the recurrence formula*

$$\begin{bmatrix} u_{n+k} \\ v_{n+k} \\ \zeta^l e_{n+k}^- \\ \zeta^{k+l} e_{n+k}^+ \end{bmatrix} := \begin{bmatrix} u_n^{\leftarrow} & u_n^{\uparrow} \\ v_n^{\leftarrow} & v_n^{\uparrow} \\ e_n^{\leftarrow -} & \zeta^{-1} e_n^{\uparrow -} \\ e_n^{\leftarrow +} & e_n^{\uparrow +} \end{bmatrix} \begin{bmatrix} u_k^{(n)} \\ v_k^{(n)} \end{bmatrix}$$

yields an $[m+l; n+k]$ *two-point Padé form* $(u_{n+k}, v_{n+k}) := (u_{m+l;n+k}, v_{m+l;n+k})$ *of* $(f^-, g^-; f^+, g^+)$ *and its residual* (e_{n+k}^-, e_{n+k}^+)*, which is equal to* $(e_k^{(n)-}, e_k^{(n)+})$*.*

Proof. The data satisfy (2.17) or (2.18) since, by Lemma 2.15, $e_n^{\leftarrow -}(\infty) \neq 0$ and $e_n^{\leftarrow +}(0) \neq 0$ or $e_n^{\uparrow +}(0) \neq 0$.

To prove the theorem, the following properties must be verified:

$$(u_{n+k}, v_{n+k}) \in (\mathcal{P}_{n+k-1}, \mathcal{P}_{n+k}), \tag{3.10}$$
$$g^- u_{n+k} + f^- v_{n+k} = \zeta^{m+l-1} e_{n+k}^-, \tag{3.11}$$
$$g^+ u_{n+k} + f^+ v_{n+k} = \zeta^{n+k+m+l-1} e_{n+k}^+, \tag{3.12}$$
$$(e_{n+k}^-, e_{n+k}^+) \in (\mathcal{L}_0^*, \mathcal{L}_0). \tag{3.13}$$

From $(u_n^{\leftarrow}, v_n^{\leftarrow}) \in \mathcal{P}_{n-2} \times \mathcal{P}_{n-1}$ and $(u_n^{\uparrow}, v_n^{\uparrow}) \in \mathcal{P}_{n-1} \times \mathcal{P}_n$ we obtain (3.10). By assumption, $(u_k^{(n)}, v_k^{(n)})$ is an $[l;k]$ two-point Padé form. Hence

$$\begin{aligned} g^- u_{n+k} + f^- v_{n+k} &= (g^- u_n^{\leftarrow} + f^- v_n^{\leftarrow}) u_k^{(n)} + (g^- u_n^{\uparrow} + f^- v_n^{\uparrow}) v_k^{(n)} \\ &= \zeta^{m-1}(e_n^{\leftarrow -} u_k^{(n)} + \zeta^{-1} e_n^{\uparrow -} v_k^{(n)}) \\ &= \zeta^{m+l-1} e_k^{(n)-} = O_-(\zeta^{m+l-1}) \end{aligned}$$

and

$$\begin{aligned} g^+ u_{n+k} + f^+ v_{n+k} &= (g^+ u_n^{\leftarrow} + f^+ v_n^{\leftarrow}) u_k^{(n)} + (g^+ u_n^{\uparrow} + f^+ v_n^{\uparrow}) v_k^{(n)} \\ &= \zeta^{m+n-1}(e_n^{\leftarrow +} u_k^{(n)} + e_n^{\uparrow +} v_k^{(n)}) \\ &= \zeta^{m+n+k+l} e_k^{(n)+} = O_+(\zeta^{m+n+k+l}). \end{aligned}$$

This proves (3.11) and (3.12). Moreover, it follows that $(e_{n+k}^-; e_{n+k}^+) = (e_k^{(n)-}; e_k^{(n)+})$, hence (3.13). □

3.5 *Preserving regularity*

The previous sections have shown that one can compute all Padé forms in a sector with angle of 90 degree from a (row-/column-/anti-diagonally) regular pair of Padé forms. For the efficiency of recursive algorithms it is important to decide whether a new Padé form is regular of a certain type *before* one actually computes it. The reason is that computing the Padé forms is usually the dominant part of the computation, so the length k of a step in the algorithm should be determined before the step is completed. The next theorem provides a simple way to make this decision, based upon the two-point Padé form used in the recursion. Usually k is small, mostly $k=1$, so that the criterion is very efficient.

Theorem 3.9: *Let the assumptions of one of the previous Theorems* 3.1, 3.3, 3.5, *or* 3.7 *be valid. Then the following conclusions hold:*

(i) $(u_k^{(n)}, v_k^{(n)})$ *is row regular iff* (p_{n+k}, q_{n+k}) *is row regular.*
(ii) $(u_k^{(n)}, v_k^{(n)})$ *is column regular iff* (p_{n+k}, q_{n+k}) *is column regular.*
(iii) $(u_k^{(n)}, v_k^{(n)})$ *is regular iff* (p_{n+k}, q_{n+k}) *is regular.*
(iv) $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)})$ *is anti-diagonally regular iff* $(p_{n+k}^{\uparrow}, q_{n+k}^{\uparrow})$ *is anti-diagonally regular.*

Proof. We prove the theorem only for the one-point Padé table and for the recurrences based on anti-diagonally regular pairs, *i.e.*, for the assumptions of Theorem 3.7. All the other cases can be handled completely analogously.

(i) We start by applying Theorem 3.7 with k replaced by $k-1$. This yields additionally for an $[l+1;k-1]$ two-point Padé form $(u_k^{\leftarrow(n)}, v_k^{\leftarrow(n)})$ of (3.5) an $(m+l, n+k-1)$ Padé form $(p_{n+k}^{\leftarrow}, q_{n+k}^{\leftarrow})$ of (f,g). Putting both recurrences together gives

$$\begin{bmatrix} p_{n+k}^{\leftarrow} & p_{n+k} \\ q_{n+k}^{\leftarrow} & q_{n+k} \end{bmatrix} = \begin{bmatrix} p_n^{\leftarrow} & p_n^{\uparrow} \\ q_n^{\leftarrow} & q_n^{\uparrow} \end{bmatrix} \begin{bmatrix} u_k^{\leftarrow(n)} & u_k^{(n)} \\ v_k^{\leftarrow(n)} & v_k^{(n)} \end{bmatrix}.$$

Taking determinants proves the statement.

(ii) Similarly we now apply Theorem 3.7 with l replaced by $l-1$. This yields for an $[l;k]$ two-point Padé form $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)})$ of (3.5) an $(m+l-1, n+k)$ Padé form $(p_{n+k}^{\uparrow}, q_{n+k}^{\uparrow})$ of (f,g):

$$\begin{bmatrix} p_{n+k}^{\uparrow} & p_{n+k} \\ q_{n+k}^{\uparrow} & q_{n+k} \end{bmatrix} = \begin{bmatrix} p_n^{\leftarrow} & p_n^{\uparrow} \\ q_n^{\leftarrow} & q_n^{\uparrow} \end{bmatrix} \begin{bmatrix} u_k^{\uparrow(n)} & u_k^{(n)} \\ v_k^{\uparrow(n)} & v_k^{(n)} \end{bmatrix}.$$

Taking determinants proves the statement.

(iii) Here we replace l by $l-1$ and k by $k-1$ in Theorem 3.7. This yields for an $[l;k-1]$ two-point Padé form$(u_k^{\nwarrow(n)}, v_k^{\nwarrow(n)})$ of (3.5) an $(m+l-1, n+k-1)$ Padé form $(p_{n+k}^{\nwarrow}, q_{n+k}^{\nwarrow})$ of (f,g):

$$\begin{bmatrix} p_{n+k}^{\nwarrow} & p_{n+k} \\ q_{n+k}^{\nwarrow} & q_{n+k} \end{bmatrix} = \begin{bmatrix} p_n^{\leftarrow} & p_n^{\uparrow} \\ q_n^{\leftarrow} & q_n^{\uparrow} \end{bmatrix} \begin{bmatrix} u_k^{\nwarrow(n)} & u_k^{(n)} \\ v_k^{\nwarrow(n)} & v_k^{(n)} \end{bmatrix}.$$

Again, taking determinants proves the statement.

(iv) We combine the arguments in (i) and (ii):

$$\begin{bmatrix} p_{n+k}^{\leftarrow} & p_{n+k}^{\uparrow} \\ q_{n+k}^{\leftarrow} & q_{n+k}^{\uparrow} \end{bmatrix} = \begin{bmatrix} p_n^{\leftarrow} & p_n^{\uparrow} \\ q_n^{\leftarrow} & q_n^{\uparrow} \end{bmatrix} \begin{bmatrix} u_k^{\leftarrow(n)} & u_k^{\uparrow(n)} \\ v_k^{\leftarrow(n)} & v_k^{\uparrow(n)} \end{bmatrix}.$$

Taking determinants finishes the proof. □

The analogous statement for two-point Padé forms is:

Theorem 3.10: *Let the assumptions of one of the previous Theorems* 3.2, 3.4, 3.6, *or* 3.8 *be valid. Then the following conclusions hold:*

(i) $(u_k^{(n)}, v_k^{(n)})$ *is row regular iff* (u_{n+k}, v_{n+k}) *is row regular.*

(ii) $(u_k^{(n)}, v_k^{(n)})$ *is column regular iff* (u_{n+k}, v_{n+k}) *is column regular.*

(iii) $(u_k^{(n)}, v_k^{(n)})$ *is regular iff* (u_{n+k}, v_{n+k}) *is regular.*

(iv) $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)})$ *is anti-diagonally regular iff* $(u_{n+k}^{\uparrow}, v_{n+k}^{\uparrow})$ *is anti-diagonally regular.*

4. RECURRENCES FOR DIAGONALS IN THE PADÉ TABLE

In this chapter we want to derive efficient recurrences to compute the elements of a certain diagonal of the Padé table. A classical algorithm, which can be applied if all Padé forms on the considered diagonal are regular, was probably first discovered by Chebyshev [28] in 1859. The required recurrences also fall in the class discussed by Frobenius [44] in 1881. A generalization of the Chebyshev algorithm which avoids exact breakdowns was proposed by Golub and Gutknecht [48], continued fractions which relate to distinct entries on a diagonal of the Padé table were introduced by Magnus [93, 94]. The same continued fractions were already used by Chebyshev [29]. Related work for curing exact breakdowns in algorithms connected to Padé forms on a diagonal of the Padé table is due to Struble [112], Rissanen [105], Gragg [52], Nuttall and Singh [96], Bultheel [18], Draux [35], Gragg and Lindquist [56], Heinig [71], Heinig and Rost [75], Pal and Kailath [99], and many others. In contrast to these papers, which only deal with exactly singular blocks in the Padé table, here we treat the more general case of near breakdowns.

As we mentioned in Chapter 2, Padé forms located on a certain diagonal of the Padé table are closely related to the solution of Hankel systems of equations. If the Hankel system we want to solve is positive definite applying the classical algorithm of Trench [117], which consists of the famous three-term recurrences for formally orthogonal polynomials, is "safe", although it should be mentioned that in general, such matrices are ill conditioned. However, for indefinite systems, singular blocks in the Padé table can arise and then one has to generalize these recurrences. One option for generalizations is to *look-ahead*, which roughly means to jump over these singular blocks. This was done in a lot of papers recently, *e.g.*, Brent, Gustavson, and Yun [10], Cabay and Meleshko [25], Freund and Zha [43], Gragg and Gutknecht [55], and Van Barel and Bultheel [119], to mention only a few.

The diagonal recurrences described in this chapter are identical to those described by Cabay and Meleshko [25] and by Gragg and Gutknecht [55], except for a different normalization in [25] and that both papers do not consider recurrences for two-point Padé forms. Cabay and Meleshko prove weak stability of their algorithm. Their proof is applicable to our situation also. While the algorithm [25] was proposed for computing Padé approximants, *i.e.*, numerators and denominators of Padé forms, we will present *Levinson-* and *Schur-type* versions of this algorithm and show how they can be implemented with very little overhead. Note that we call an algorithm a Levinson-type algorithm, if the computed quantities belong to an inverse LDU decomposition of a Hankel matrix or, equivalently, if it provides denominators of Padé forms. We call it a Schur-type algorithm, if it yields at least parts of the LDU decomposition, which means that it computes residuals of Padé forms. From a computational point of view, the main difference is that a Levinson-type algorithm requires inner products but a Schur-type algorithm does not. For the Levinson-type algorithms we present here and in the following chapters, we show that they require the same number of inner inner products as the classical Levinson-type algorithm. This answers an open question posed in [55].

There are also close connections to formally orthogonal polynomials and to the Lanczos process. These will be discussed in Chapters 5 and 6.

4.1 Fast algorithms

We start by collecting the relevant recurrences from Chapter 3 since they simplify in our particular situation. Clearly, for computing Padé forms along a diagonal of the Padé table, we will use recurrences based on regular pairs.

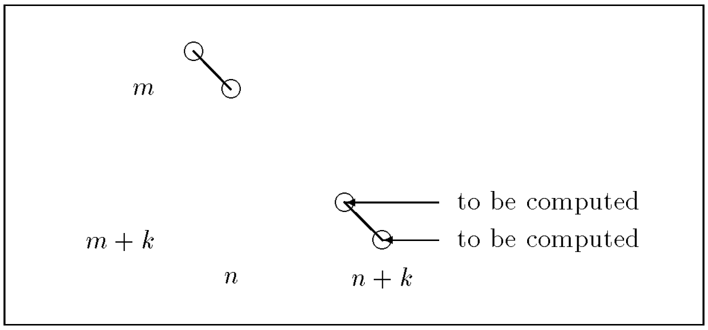
Corollary 4.1: *Let the assumptions of Theorem* 3.5 *be valid. If* $(u_k^{(n)}, v_k^{(n)})$ *is a* $(k-1,k)$ *Padé form of* $(e_n, e_n^{\nwarrow})$, *then* (3.3) *yields an* $(m+k, n+k)$ *Padé form of* (f,g) *with residual* $e_{n+k} = e_k^{(n)}$.

Proof. The statement follows immediately from Theorem 3.5 by using the fact that a $[k;k]$ two-point Padé form of (3.2) is a $(k-1,k)$ Padé form of $(e_n, e_n^{\nwarrow})$. □

If we want to advance on a diagonal of the two-point Padé table, we can use

Corollary 4.2: *Let the assumptions of Theorem* 3.6 *be valid. If* $(u_k^{(n)}, v_k^{(n)})$ *is a* $(k-1,k)$ *Padé form of* $(e_n^+, e_n^{\nwarrow +})$, *then* (3.4) *yields an* $[m+k; n+k]$ *two-point Padé form of* $(f^-, g^-; f^+, g^+)$ *with residual* $e_{n+k}^+ = e_k^{(n)+}$.

These corollaries show that we do not need two-point Padé forms in algorithms following diagonals of the Padé table. This simplifies matters considerably. An illustration of the recurrences based on regular pairs gives



Here, and in following, circles represent Padé forms in the Padé table at the indicated positions. We print lines between Padé forms when their corresponding Padé approximants are different from each other. So this picture shows that one can proceed from one regular pair to another. The decision whether the new $(m+k, n+k)$ Padé form is regular or not can be made upon checking if the small $(k-1, k)$ Padé form $(u_k^{(n)}, v_k^{(n)})$ is regular by Theorem 3.9.

A sketch of a look-ahead algorithm for computing regular pairs of Padé forms located on a diagonal of the Padé table is

Algorithm 4.1: Look-ahead algorithm for diagonals in the Padé table.
INPUT: $h \in \mathcal{L}$, m, N;
OUTPUT: *regular* $(m+L, L)$ *Padé form* (p_L, q_L) *of* h *for largest possible* $L \le N$;
Set $n = 0$, $q_0 = 1$, $p_0 = \Pi_{-\infty:m} h$, $e_0 = \Pi_{m+1:\infty} h$, $q_0^{\nwarrow} = 0$, $p_0^{\nwarrow} = 1$, $e_0^{\nwarrow} = -1$;
while $n < N$
  determine the smallest $k > 1$ *such that* $n + k$ *is a regular index;*
  if $n + k < N$
    if $k = 1$
      set $(p_{n+1}^{\nwarrow}, q_{n+1}^{\nwarrow}, e_{n+1}^{\nwarrow}) = (p_n, q_n, e_n)$;
    else
      (*apply Corollary* 4.1)
      compute a $(k-1, k)$ *Padé form* $(u_k^{(n)}, v_k^{(n)})$ *of* $(e_n, e_n^{\nwarrow})$ *and then* (p_{n+k}, q_{n+k});
      compute a $(k-2, k-1)$ *Padé form* $(u_k^{\nwarrow(n)}, v_k^{\nwarrow(n)})$ *of* $(e_n, e_n^{\nwarrow})$ *and then* $(p_{n+k}^{\nwarrow}, q_{n+k}^{\nwarrow})$;
  else
    set $L = n$;
  set $n = n + k$;

Recall that the Padé forms are normalized according to (2.40).

4.2 Computation of recurrence coefficients

To apply Corollary 4.1 we have to compute a $(k-1, k)$ Padé form of $(e_n, e_n^{\nwarrow})$, where $e_n^{\nwarrow}(0) \ne 0$ since (p_n, q_n) is a regular Padé form of $h = f/g$. Therefore, we have to solve (2.31) (where we have to set $m = k-1$, $n = k$, replace π_j by $\alpha_j^{(n)}$, ρ_j by $\beta_j^{(n)}$, with $\alpha_j^{(n)}$, $\beta_j^{(n)}$ defined in (2.33), and set $\gamma_j = \varepsilon_{n+j,n}^{\nwarrow}$, and $\phi_j = \varepsilon_{n+j,n}$). From the normalization (2.40) and the first equation in (2.31) we obtain

$$\beta_0^{(n)} = 1 \qquad \text{and} \qquad \alpha_0^{(n)} = -\frac{\varepsilon_{n,n}}{\varepsilon_{n,n}^{\nwarrow}}. \tag{4.1}$$

Recall that $\varepsilon_{n,n} = e_n(0)$ and $\varepsilon_{n,n}^{\nwarrow} = e_n^{\nwarrow}(0)$, according to the notation introduced in (2.28). Moving the respective columns for $\alpha_0^{(n)}$ and $\beta_0^{(n)}$ to the right-hand side we end up with the linear system

$$\mathbf{S}_{k,n}\begin{bmatrix}\alpha_1^{(n)}\\ \vdots\\ \alpha_{k-1}^{(n)}\\ \hline \beta_1^{(n)}\\ \vdots\\ \beta_k^{(n)}\end{bmatrix} = -\begin{bmatrix}\varepsilon^{\nwarrow}_{n+1,n}\\ \vdots\\ \varepsilon^{\nwarrow}_{n+2k-1,n}\end{bmatrix}\alpha_0^{(n)} - \begin{bmatrix}\varepsilon_{n+1,n}\\ \vdots\\ \varepsilon_{n+2k-1,n}\end{bmatrix}\beta_0^{(n)}, \tag{4.2}$$

with the Sylvester matrix

$$\mathbf{S}_{k,n} := \left[\begin{array}{ccc|cccc} \varepsilon^{\nwarrow}_{n,n} & & & \varepsilon_{n,n} & & & \\ \vdots & \ddots & & \vdots & \ddots & & \\ \varepsilon^{\nwarrow}_{n+k-2,n} & \cdots & \varepsilon^{\nwarrow}_{n,n} & \varepsilon_{n+k-2,n} & \cdots & \varepsilon_{n,n} & 0\\ \varepsilon^{\nwarrow}_{n+k-1,n} & \cdots & \varepsilon^{\nwarrow}_{n+1,n} & \varepsilon_{n+k-1,n} & \cdots & \varepsilon_{n+1,n} & \varepsilon_{n,n}\\ \vdots & & \vdots & \vdots & & \vdots & \vdots\\ \varepsilon^{\nwarrow}_{n+2k-2,n} & \cdots & \varepsilon^{\nwarrow}_{n+k,n} & \varepsilon_{n+2k-2,n} & \cdots & \varepsilon_{n+k-2,n} & \varepsilon_{n+k-1,n} \end{array}\right] \in \mathbb{C}^{2k-1,2k-1}.$$

To compute the upper left neighbor, we have to solve the linear system (2.31) for $m = k-2$ and $n = k-1$. In this case, we add a row to bring the normalization (2.40) for $e^{\nwarrow}_{n+k}$ into play:

$$\left[\begin{array}{ccc|ccc}\varepsilon^{\nwarrow}_{n+2k-2,n} & \cdots & \varepsilon^{\nwarrow}_{n+k,n} & \varepsilon_{n+2k-2,n} & \cdots & \varepsilon_{n+k-1,n}\end{array}\right]\begin{bmatrix}\mathbf{a}^{\nwarrow}_k\\ \mathbf{b}^{\nwarrow}_k\end{bmatrix} = \varepsilon^{\nwarrow}_{n+k,n+k},$$

where

$$\mathbf{a}^{\nwarrow}_k := [\,\alpha_0^{\nwarrow(n)} \ \cdots \ \alpha_{k-2}^{\nwarrow(n)}\,]^T, \qquad \mathbf{b}^{\nwarrow}_k := [\,\beta_0^{\nwarrow(n)} \ \cdots \ \beta_{k-1}^{\nwarrow(n)}\,]^T.$$

Then we have to solve

$$\mathbf{S}_{k,n}\begin{bmatrix}\mathbf{a}^{\nwarrow}_k\\ \mathbf{b}^{\nwarrow}_k\end{bmatrix} = \mathbf{e}_{2k-2}\varepsilon^{\nwarrow}_{n+k,n+k} \tag{4.3}$$

with the same coefficient matrix as in (4.2).

We next show that the matrix $\mathbf{S}_{k,n}$ can be used to determine the size k of a look-ahead step in Algorithm 4.1.

Lemma 4.3: *The $(k-1,k)$ Padé form $(u_k^{(n)}, v_k^{(n)})$ of $(e_n, e^{\nwarrow}_n)$ is regular if and only if the matrix $\mathbf{S}_{k,n}$ is nonsingular.*

Proof. (i) If $\mathbf{S}_{k,n}$ is singular, then a nontrivial solution of (4.3) with $e^{\nwarrow}_{n+k,n+k} = 0$ exists. This then yields a $(k-2,k-1)$ Padé form $(u_k^{\nwarrow(n)}, v_k^{\nwarrow(n)})$ of $(e_n, e^{\nwarrow}_n)$ with residual $e_k^{\nwarrow(n)}$ with $e_k^{\nwarrow(n)}(0) = 0$. Thus, by Lemma 2.8, the corresponding $(k-1,k)$ Padé form cannot be regular.

(ii) Now let $\mathbf{S}_{k,n}$ be nonsingular. Then we obtain from (4.2) and (4.3) a $(k-1,k)$ Padé form $(u_k^{(n)}, v_k^{(n)})$ with $v_k^{(n)}(0) \neq 0$ and its upper neighbor which satisfies $e_k^{\nwarrow(n)}(0) \neq 0$. By Lemma 2.8, $(u_k^{(n)}, v_k^{(n)})$ is regular. □

Recall that, by Theorem 3.9, the $(m+k, n+k)$ Padé form (p_{n+k}, q_{n+k}) is regular if and only if the $(k-1,k)$ Padé form $(u_k^{(n)}, v_k^{(n)})$ is regular. Therefore, Lemma 4.3 provides an efficient criterion to determine the step length k. In practice, one will keep the smallest singular value of $\mathbf{S}_{k,n}$ above some prescribed tolerance or the condition number of $\mathbf{S}_{k,n}$ bounded to determine the end of a look-ahead step. Various look-ahead strategies are discussed in Chapter 11.

4.3 Implementation details

In the classical algorithm, where no look-ahead is performed, the recurrence coefficients are fully determined by (4.1) and the solution of (4.2) for $k = 1$:

$$\beta_1^{(n)} = -\left(\varepsilon_{n+1,n}^{\nwarrow}\alpha_0^{(n)} + \varepsilon_{n+1,n}\beta_0^{(n)}\right)/\varepsilon_{n,n}. \tag{4.4}$$

Here, and in the more general case of look-ahead steps, the coefficients $\varepsilon_{n+k,n}^{\nwarrow}$ and $\varepsilon_{n+k,n}$ of $e_n^{\nwarrow}$ and e_n can be computed according to the definitions of $e_n^{\nwarrow}$ and e_n if $q_n^{\nwarrow}$ and q_n are available. If g is a constant, this requires one inner product for each new coefficient and two otherwise. We call the resulting algorithm for computing diagonal Padé forms a *Levinson-type algorithm.*

Another option is to directly compute the residuals $e_n^{\nwarrow}$ and e_n. Then the recurrence coefficients that appear in (4.1) and (4.2) are available without knowledge of $q_n^{\nwarrow}$ and q_n. This variant is called a *Schur-type algorithm.* It does not require any inner products.

Next we want to show that our look-ahead extension of the classical Levinson-type algorithm can be implemented with the same number of inner products as the latter. There we have $e_n^{\nwarrow} = e_{n-1}$, and thus it is sufficient to compute $\varepsilon_{n,n}$ and $\varepsilon_{n+1,n}$ by inner products. However, in a look-ahead step, we further need $\varepsilon_{n+2,n}, \ldots, \varepsilon_{n+2k-1,n}$ and $\varepsilon_{n+2,n}^{\nwarrow}, \ldots, \varepsilon_{n+2k-1,n}^{\nwarrow}$. Since we always start a look-ahead step with a regular pair, which satisfies $\rho_{0,n}\varepsilon_{n,n}^{\nwarrow} \neq 0$ by Lemma 2.8(iv), we compute $\varepsilon_{n+j,n}$, $j = 1, \ldots, 2k-1$ by inner products and $\varepsilon_{n+j,n}^{\nwarrow}$, $j = 1, \ldots, 2k-1$ recursively from the equalities in Lemma 2.8(v) and (2.36):

$$e_n^{\nwarrow}q_n = \zeta^2 e_n q_n^{\nwarrow} + \Delta_n^{\nwarrow} = \zeta^2 e_n q_n^{\nwarrow} + \varepsilon_{n,n}^{\nwarrow}, \tag{4.5}$$

which is equivalent to

$$\begin{bmatrix} \rho_{2,n} & \rho_{1,n} & \rho_{0,n} & & \\ \vdots & & & \ddots & \\ \rho_{2k,n} & \cdots & \cdots & \cdots & \rho_{0,n} \end{bmatrix} \begin{bmatrix} e_{n,n}^{\nwarrow} \\ \vdots \\ e_{n+2k,n}^{\nwarrow} \end{bmatrix} = \begin{bmatrix} \rho_{0,n}^{\nwarrow} & & \\ \vdots & \ddots & \\ \rho_{2k-2,n}^{\nwarrow} & \cdots & \rho_{0,n}^{\nwarrow} \end{bmatrix} \begin{bmatrix} \varepsilon_{n,n} \\ \vdots \\ \varepsilon_{n+2k,n} \end{bmatrix}.$$

Recall that $\varepsilon^{\nwarrow}_{n,n}$ and $\varepsilon^{\nwarrow}_{n+1,n}$ are known from the previous step if this was a regular step. If it was a look-ahead step, then due to the normalization (2.40) we have $\varepsilon^{\nwarrow}_{n,n} = 1$. Moreover, $\varepsilon^{\nwarrow}_{n+1,n}$ can be computed recursively from quantities available from the previous step via the recurrence for $e^{\nwarrow}_n$ alluded to Corollary 4.1. Since $\rho_{0,n} = 1$, we can then compute $\varepsilon^{\nwarrow}_{n+j,n}$, $j = 2, \ldots, 2k-1$ recursively from (4.5). This means that to proceed k columns in the Padé table, we need exactly $2k$ inner products, no matter whether we perform only regular or also look-ahead steps. If we make only regular steps, then we have to compute $\varepsilon_{n+j,n+j}$ and $\varepsilon_{n+j+1,n+j}$, $j = 0, \ldots, k-1$. In a look-ahead step of size k we have to compute $\varepsilon_{n+j,n}$, $j = 0, \ldots, 2k-1$.

After these efficiency considerations, we are now ready to give a more detailed sketch of two versions of Algorithm 4.1. The first is a Levinson-type algorithm, which computes the denominators of the Padé forms and the coefficients of the residuals, which are required for the recurrence coefficients.

Algorithm 4.2: Look-ahead Levinson-type algorithm for diagonals in the Padé table.
INPUT: $h \in \mathcal{L}$, m, N;
OUTPUT: *denominator* q_N *of regular* $(m+L, L)$ *Padé form of* h *for largest possible* $L \leq N$;
Set $n = 0$, $q_0 = 1$, $q^{\nwarrow}_0 = 0$, $\varepsilon^{\nwarrow}_{0,0} = -1$, $\varepsilon^{\nwarrow}_{1,0} = 0$;
while $n < N$
  set $k = 1$; *compute* $\varepsilon_{n,n} = \Pi_{m+2n+1}(hq_n)$, $\varepsilon_{n+1,n} = \Pi_{m+2n+2}(hq_n)$;
  while $\sigma_{\min}(\mathbf{S}_{k,n}) < tol$ *and* $n + k < N$
    set $k = k + 1$;
    set $\varepsilon_{n+2k-2,n} = \Pi_{m+2n+2k-1}(hq_n)$, $\varepsilon_{n+2k-1,n} = \Pi_{m+2n+2k}(hq_n)$;
    compute $\varepsilon^{\nwarrow}_{n+2k-2,n}$, $\varepsilon^{\nwarrow}_{n+2k-1}$ *from* (4.5);
  solve (4.2) *for the coefficients of* $u_k \in \mathcal{P}_{k-1}$ *and* $v_k \in \mathcal{P}_k$;
  compute $q_{n+k} = \zeta^2 q^{\nwarrow}_n u_k + q_n v_k$ (*Corollary* 4.1);
  if $n + k < N$
    if $k = 1$
      set $q^{\nwarrow}_{n+1} = q_n$, $\varepsilon^{\nwarrow}_{n+1,n+1} = \varepsilon_{n,n}$, $\varepsilon^{\nwarrow}_{n+2,n+1} = \varepsilon_{n+1,n}$;
    else
      solve (4.3) *for the coefficients of* $u^{\nwarrow}_k \in \mathcal{P}_{k-2}$ *and* $v^{\nwarrow}_k \in \mathcal{P}_{k-1}$;
      compute $q^{\nwarrow}_{n+k} = \zeta^2 q^{\nwarrow}_n u^{\nwarrow}_k + q_n v^{\nwarrow}_k$ (*Corollary* 4.1);
      set $\varepsilon^{\nwarrow}_{n+k,n+k} = 1$ *and compute* $\varepsilon^{\nwarrow}_{n+k+1,n+k} = \Pi_{2k-1}(e^{\nwarrow}_n u^{\nwarrow}_k + e_n v^{\nwarrow}_k)$,
      where $e^{\nwarrow}_n = \sum_{j=0}^{2k-1} \varepsilon^{\nwarrow}_{n+j,n} \zeta^j$ *and* $e_n = \sum_{j=0}^{2k-1} \varepsilon_{n+j,n} \zeta^j$;
  else
    set $L = n$;
  set $n = n + k$;

Next we discuss an analogue algorithm of Schur type. It computes only the residuals of Padé forms. This algorithm does not require any inner products; all coefficients are computed recursively.

Algorithm 4.3: Look-ahead Schur-type algorithm for diagonals in the Padé table.
INPUT: $h \in \mathcal{L}$, m, N;
OUTPUT: *residual* e_N *of regular* $(m+L, L)$ *Padé form of* h *for largest possible* $L \leq N$;
Set $n = 0$, $e_0 = \Pi_{m+1:\infty} h$, $e_0^{\nwarrow} = -1$;
while $n < N$
  set $k = 1$;
  while $\sigma_{\min}(\mathbf{S}_{k,n}) < tol$ *and* $n + k < N$
    set $k = k + 1$;
  solve (4.2) *for the coefficients of* $u_k \in \mathcal{P}_{k-1}$ *and* $v_k \in \mathcal{P}_k$;
  compute $e_{n+k} = \zeta^{-2k}(e_n^{\nwarrow} u_k + e_n v_k)$ (*Corollary* 4.1);
  if $n + k < N$
    if $k = 1$
      set $e_{n+1}^{\nwarrow} = e_n$;
    else
      solve (4.3) *for the coefficients of* $u_k^{\nwarrow} \in \mathcal{P}_{k-2}$ *and* $v_k^{\nwarrow} \in \mathcal{P}_{k-1}$;
      compute $e_{n+k}^{\nwarrow} = \zeta^{-2k+2}(e_n^{\nwarrow} u_k^{\nwarrow} + e_n v_k^{\nwarrow})$;
  else
    set $L = n$;
  set $n = n + k$;

In practice one will apply the above algorithm only for Laurent series with finitely many nonzero coefficients. Then the number of relevant nonzero elements of the residuals computed in this algorithm decreases from step to step. For example, if this algorithm is used to compute the LDU decomposition of an $N \times N$ Hankel matrix, then h is a formal power series. For a regular index n, $2(N-n)+1$ elements of e_n and $2(N-n)+3$ of $e_n^{\nwarrow}$ have to be computed; see Section 5.3 below. Table 4.1 summarizes the operations for the two algorithms. At first sight, the Schur-type algorithm looks less expensive, but as we have just explained, the SAXPYs are in average twice as long as for the Levinson-type algorithm, so that this levels out the arithmetic operations for the inner products.

The two algorithms we just described compute only the minimal information which is required to proceed along a diagonal of the Padé table. Of course one always has the option to compute additionally numerators and/or residuals in the Levinson-type algorithm and numerators and/or denominators in the Schur-type algorithm according to the recurrences referred to in Corollary 4.1.

Operations in a block of size $k \geq 1$	Levinson-type	Schur-type
inner products	$2k$	–
SAXPYs	$4k-2$	$4k-2$

Table 4.1: Operation counts for Algorithms 4.2 and 4.3

5. FORMALLY ORTHOGONAL POLYNOMIALS

As we mentioned before, there is a close relation of Padé forms located on a diagonal of the Padé table and formally orthogonal polynomials (FOPs) [12, 22, 55, 60, 119]. In the previous chapter we have established algorithms which proceed from one regular pair to another (not necessarily the next one). If not all Padé forms on the considered diagonal are regular, then this produces gaps between two regular pairs. We will therefore define *underdetermined* Padé forms to fill the gaps in between. These can be used to compute block factorizations of Hankel matrices or complete polynomial bases with weakened orthogonality properties.

In the context of formally orthogonal polynomials, this has been done before by different authors, which call these polynomials *quasi orthogonal* [8, 35] or *inner* [39, 43, 56, 60]. In contrast to these authors, we will introduce this concept solely from the Padé point of view, as it was sketched in [52] for exact arithmetic. This approach is advantageous because numerators, residuals, and denominators of Padé forms satisfy the same recurrence relations, so that one statement and one proof serve for different applications, *e.g.*, for Levinson and Schur type algorithms. We will exploit this further in the next chapter, where this uniform treatment will lead to different recurrences.

We restrict ourselves to Padé forms of a formal power series in this and the following chapter.

5.1 *Formally orthogonal polynomials and Padé approximation*

Given $h \in \mathcal{L}_0$ with coefficients (2.5), or equivalently, the semi-infinite sequence $\{\mu_k\}_{k=0}^{\infty}$ of moments, we define a sequence of linear functionals $\{\Phi_m\}_{m\geq 0}$ on $\mathcal{P}$ by its values

$$\Phi_m(\zeta^j) := \mu_{j+m}, \quad j \in \mathbb{N}. \tag{5.1}$$

For arbitrary polynomials s and t of degree less than n represented by

$$s(\zeta) =: \sum_{j=0}^{n} \sigma_j \zeta^j, \quad t(\zeta) =: \sum_{j=0}^{n} \tau_j \zeta^j,$$

we set $\sigma_j = \tau_j = 0$ for $j > n$ and introduce the infinite coefficient vectors

$$\mathbf{s} := [\ \sigma_0 \ \cdots \ \sigma_n \ 0 \ \cdots\ ]^T, \quad \mathbf{t} := [\ \tau_0 \ \cdots \ \tau_n \ 0 \ \cdots\ ]^T.$$

Then, the value of the linear functional of the product st is

$$\Phi_m(st) = \sum_{i,j=0}^{\infty} \sigma_i \mu_{i+j+m} \tau_j = \mathbf{s}^T \mathbf{H}\, \mathbf{t}, \tag{5.2}$$

where $\mathbf{H} := [\mu_{i+j+m}]_{i,j=0}^{\infty}$ is the Hankel operator with symbol $\sum_{k=0}^{\infty} \mu_{k+m} \zeta^k$.

Definition 5.1: *The polynomial $s \in \mathcal{P}_n \backslash \mathcal{P}_{n-1}$ is called an nth* **formally orthogonal polynomial** (**FOP**) *with respect to Φ_m if*

$$\Phi_m(\zeta^j s) = 0, \quad j = 0, \ldots, n-1. \tag{5.3}$$

An nth FOP is said to be **regular** *if it is uniquely determined up to scaling; otherwise, it is* **singular**.

Using (5.2) with $t(\zeta) = \zeta^j$, (5.3) reads

$$\sum_{i=0}^{n} \sigma_i \mu_{i+j+m} = 0, \qquad j = 0, \ldots, n-1.$$

If we further define the reflected polynomial s^* of a polynomial $s \in \mathcal{P}_n$ by

$$s^*(\zeta) := \zeta^n s(\zeta^{-1}) = \sum_{i=0}^{n} \sigma_{n-i} \zeta^i, \tag{5.4}$$

then, in view of

$$(hs^*)(\zeta) = \sum_{j=0}^{\infty} \sum_{i=0}^{n} \sigma_{n-i} \mu_{j-i} \zeta^j = \sum_{j=0}^{\infty} \sum_{k=0}^{n} \sigma_k \mu_{j+k-n} \zeta^j,$$

(where $\mu_j = \sigma_j = 0$ for $j < 0$), (5.3) can be written as

$$\Pi_{m+n:m+2n-1}(hs^*) = 0. \tag{5.5}$$

Thus, we have the following

Lemma 5.1: *The reflected polynomial s^* of an nth FOP s with respect to Φ_m is equal to the denominator q_n of an $(m+n-1, n)$ Padé form (p_n, q_n) of $h \in \mathcal{L}_0$. It is regular if and only if the $(m+n-1, n)$ Padé form is regular.*

Proof. The first part is proved by (5.5). For the second statement, note that FOPs need to have exact degree n, and hence can be normalized to be monic. Then the condition (5.3), when expressed in terms of the polynomial coefficients, becomes exactly the Yule-Walker equation (2.32) with $\rho_0 = 1$ and where m is replaced by $m+n-1$. The required uniqueness of a regular normalized FOP is thus seen to be equivalent to the nonsingularity of $\mathbf{T}_{m+n-1,n}$ or $\mathbf{H}_n := \mathbf{H}_{m+n-1,n}$. By Lemma 2.8, this is equivalent to the regularity of the $(m+n-1, n)$ Padé form of h. □

In the following we will keep the index m of the linear functional Φ_m fixed and therefore use only one index for Padé forms and FOPs indicating the degree of the denominator of the Padé form or the degree of the FOP, respectively, whenever this can be done without causing confusion.

Not every $(m+n-1, n)$ Padé form of h is necessarily regular and for those n, for which it is not regular, no regular FOP of degree n exists. If one still wants to compute a complete basis of $\mathcal{P}_N$, then one has to weaken the orthogonality condition (5.3) and compute denominators of so called *underdetermined* Padé forms. We next define underdetermined Padé forms and show how they can be computed efficiently. Again, the study of FOPs, with respect to different Φ_m, is made more transparent because of the, more general, Padé table, and the block structure theorem or its generalization presented in Section 2.7.

5.2 Inner FOPs and underdetermined Padé forms

In the following we denote by $\{n_j\}_{j\geq 0}$ a monotone increasing sequence of indices for which regular $(m+n-1, n)$ Padé forms exist. It is crucial that this sequence is not requested to contain *all* regular $(m+n-1, n)$ Padé forms; in practice, we want to exclude nearly singular ones and include only well-conditioned Padé forms introduced in Definition 2.6.

Definition 5.2: *For $n_l = n < n+k < n_{l+1}$, an $(n+k)$th* **inner FOP** *with respect to Φ_m is any polynomial $s \in \mathcal{P}_{n+k} \setminus \mathcal{P}_{n+k-1}$ satisfying*

$$\Phi_m(s\zeta^i) = 0, \qquad i = 0\ldots, n-1. \tag{5.6}$$

Next we give equivalent conditions for characterizing inner polynomials.

Lemma 5.2: *Let $h \in \mathcal{L}_0$ and the associated linear functional $\Phi_m(\cdot)$ specified by (5.1) be given, and let $k, n \geq 0$. For $q_{n+k} \in \mathcal{P}_{n+k}$ the following statements are equivalent:*

(i) $\Phi_m(q^*_{n+k}\zeta^i) = 0$ *for* $i = 0, \ldots, n-1$*;*

(ii) $\Pi_{m+n+k:m+2n+k-1}(hq_{n+k}) = 0$*;*

(iii) *there exists $p_{n+k} \in \mathcal{P}_{m+n+k-1}$ such that*

$$hq_{n+k} - p_{n+k} = \zeta^{m+2n+k}e_{n+k} = O_+(\zeta^{m+2n+k}). \tag{5.7}$$

Proof. Let $\mu_j = \rho_{j,n+k} = 0$ for $j < 0$. Then in view of

$$(hq_{n+k})(\zeta) = \sum_{i=0}^{\infty}\sum_{\ell=0}^{n+k} \mu_\ell \rho_{i-\ell,n+k}\zeta^i = \sum_{i=0}^{\infty}\sum_{\ell=0}^{n+k} \mu_{i-\ell}\rho_{\ell,n+k}\zeta^i \tag{5.8}$$

and

$$\Phi_m(q^*_{n+k}\zeta^i) = \mathbf{e}_i^T \mathbf{H}_{n+k+1} \begin{bmatrix} \rho_{n+k,n+k} \\ \vdots \\ \rho_{0,n+k} \end{bmatrix} = \sum_{\ell=0}^{n+k} \mu_{i+n+k-\ell+m}\rho_{\ell,n+k} \tag{5.9}$$

the first two statements are equivalent. The third statement is equivalent to the second since we can define $p_{n+k} = \Pi_{0:m+n+k-1}(hq_{n+k})$ and $e_{n+k} = \zeta^{-(m+2n+k)}\Pi_{m+2n+k:\infty}(hq_{n+k})$. $\square$

If n is a regular index, then the special case of $k = 0$ in Lemma 5.2 shows that

$$\Phi_m(\zeta^i q_n^*) = 0 \qquad \text{for} \quad i = 0, \ldots, n-1 \tag{5.10}$$
$$\Phi_m(\zeta^i q_n^{\nwarrow *}) = 0 \qquad \text{for} \quad i = 0, \ldots, n-2, \tag{5.11}$$

i.e., $q_n^* \in \mathcal{P}_n$ is a regular nth FOP with respect to Φ_m and $q_n^{\nwarrow *} \in \mathcal{P}_{n-1}$ is orthogonal to all polynomials of degree at most $n-2$ with respect to Φ_m. It is important to understand that $q_n^{\nwarrow *}$ is in general not an FOP of degree $n-1$, because it is not guaranteed that it has exact degree $n-1$. To be more precise, if $n-1$ is not a regular index, then $q_n^{\nwarrow *}$ is not a scalar multiple of the inner FOP q_{n-1}^*.

Definition 5.3: *For $n_l = n < n+k < n_{l+1}$ and $h \in \mathcal{L}_0$, any pair $(p_{n+k}, q_{n+k}) \in \mathcal{P}_{m+n+k-1} \times \mathcal{P}_{n+k}$ with $q_{n+k}(0) \neq 0$ satisfying (5.7) is called an $(m+n+k-1, n+k)$* **underdetermined Padé form** *and e_{n+k} is called its residual.*

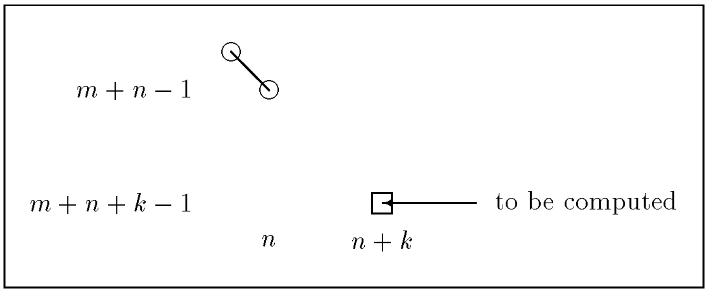
Next we relate modified moments of the linear functional Φ_m to coefficients of the residuals of (possibly underdetermined) Padé forms.

Lemma 5.3: *Let n be a regular index or $k = 0$. If (p_{n+k}, q_{n+k}) is an $(m+n+k-1, n+k)$ underdetermined Padé form of $h \in \mathcal{L}_0$ with residual e_{n+k}, or an $(m+n-1, n)$ Padé form of h if $k = 0$, then*

$$e_{n+k}(\zeta) = \sum_{j=0}^{\infty} \Phi_m(q_{n+k}^* \zeta^{n+j})\zeta^j. \tag{5.12}$$

Proof. The equality (5.12) follows immediately from (5.8) and (5.9). $\square$

The following picture and theorem show how to construct inner FOPs from a regular pair.



(5.13)

In this and all the forthcoming pictures squares represent underdetermined Padé forms. As before, circles stand for Padé forms and a line indicates that Padé approximants at its end points are different from each other. In other words, such lines always cross the border of a block in the Padé table.

Theorem 5.4: *Let (p_n, q_n) be a regular $(m+n-1, n)$ Padé form of $h \in \mathcal{L}_0$, and let $(p_n^{\nwarrow}, q_n^{\nwarrow})$ be its upper left neighbor, i.e., an $(m+n-2, n-1)$ Padé form of h. Moreover, let e_n and $e_n^{\nwarrow}$ be the residuals these Padé forms, $k \geq 1$, and*

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ \zeta^k e_{n+k} \end{bmatrix} := \begin{bmatrix} \zeta^2 p_n^{\nwarrow} & p_n \\ \zeta^2 q_n^{\nwarrow} & q_n \\ e_n^{\nwarrow} & e_n \end{bmatrix} \begin{bmatrix} u_k^{(n)} \\ v_k^{(n)} \end{bmatrix},$$

where $(u_k^{(n)}, v_k^{(n)}) \in \mathcal{P}_{k-1} \times \mathcal{P}_k$ is a solution of

$$e_n^{\nwarrow} u_k^{(n)} + e_n v_k^{(n)} = O_+(\zeta^k) \tag{5.14}$$

with $v_k(0) \neq 0$.

Then, q_{n+k}^* is an inner FOP with respect to Φ_m, i.e., it is orthogonal to every polynomial of degree less than n, and p_{n+k}, q_{n+k}, and e_{n+k} satisfy (5.7).

Proof. Obviously, $q_{n+k} \in \mathcal{P}_{n+k}$, $p_{n+k} \in \mathcal{P}_{m+n+k-1}$, and $q_{n+k}(0) \neq 0$. It remains to verify Condition (iii) in Lemma 5.2: if $u_k^{(n)}$, $v_k^{(n)}$ are chosen according to (5.14), then we have

$$hq_{n+k} - p_{n+k} = \zeta^{m+2n}(e_n^{\nwarrow} u_k^{(n)} + e_n v_k^{(n)}) = O_+(\zeta^{m+2n+k}),$$

and e_{n+k} satisfies (5.7). □

For our purposes it is sufficient to compute one particularly simple solution:

Corollary 5.5: *Let the assumptions of Theorem 5.4 be valid. Then there exists a unique solution of (5.14) if we set $v_k^{(n)} \equiv 1$.*

Proof. By Lemma 2.8, $e_n^{\nwarrow}(0) \neq 0$. Then

$$u_k^{(n)} = -\Pi_{0:k-1} L_+(e_n / e_n^{\nwarrow}), \tag{5.15}$$

is the unique solution of (5.14) for $v_k^{(n)} \equiv 1$. □

Let

$$u_k^{(n)}(\zeta) = \sum_{j=0}^{k-1} \gamma_j^{(n)} \zeta^j,$$

then the coefficients $\gamma_j^{(n)}$ of the solution (5.15) are determined by the following lower triangular Toeplitz system

$$\begin{bmatrix} \varepsilon_{n,n}^{\nwarrow} & & \\ \vdots & \ddots & \\ \varepsilon_{n+k-1,n}^{\nwarrow} & \cdots & \varepsilon_{n,n}^{\nwarrow} \end{bmatrix} \begin{bmatrix} \gamma_0^{(n)} \\ \vdots \\ \gamma_{k-1}^{(n)} \end{bmatrix} = - \begin{bmatrix} \varepsilon_{n,n} \\ \vdots \\ \varepsilon_{n+k-1,n} \end{bmatrix}.$$

Due to the structure of this linear system we have by induction

$$\varepsilon_{n,n}^{\nwarrow} \gamma_k^{(n)} = -\varepsilon_{n,n+k}, \qquad k = 1, 2, \ldots \tag{5.16}$$

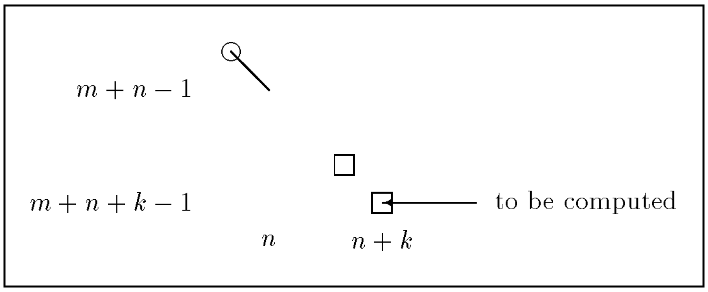
Moreover, $u_k^{(n)}$ is obtained from the recurrence

$$u_1^{(n)} = \gamma_0^{(n)}, \qquad u_k^{(n)} = u_{k-1}^{(n)} + \gamma_{k-1}^{(n)}\zeta^{k-1}, \qquad k = 1, 2, \ldots,$$

and hence

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ \zeta^k e_{n+k} \end{bmatrix} = \begin{bmatrix} p_{n+k-1} \\ q_{n+k-1} \\ \zeta^{k-1} e_{n+k-1} \end{bmatrix} + \begin{bmatrix} \zeta^2 p_n^{\nwarrow} \\ \zeta^2 q_n^{\nwarrow} \\ e_n^{\nwarrow} \end{bmatrix} \gamma_{k-1}^{(n)} \zeta^{k-1}, \qquad k = 1, 2, \ldots. \tag{5.17}$$

Here is a picture of this update formula. The reader should compare it to (5.13) to visualize the difference.



(5.18)

5.3 *Hankel matrix factorizations*

Assume for a moment that regular FOPs q_n^* with respect to the linear functional $\Phi_m(\cdot)$ defined in (5.1) exist for every $n \leq N$. Then, from (5.3) we have for the FOPs of degree j and k, respectively:

$$\Phi_m(q_j^* q_k^*) = 0 \quad j \neq k. \tag{5.19}$$

If we define the upper triangular matrix $\mathbf{R} := \mathbf{R}_N \in \mathbb{C}^{N,N}$, where

$$\mathbf{R}_N := \begin{bmatrix} \rho_{0,0} & \rho_{1,1} & \cdots & \rho_{N-1,N-1} \\ & \rho_{0,1} & \cdots & \rho_{N-2,N-1} \\ & & \ddots & \vdots \\ & & & \rho_{0,N-1} \end{bmatrix}, \tag{5.20}$$

then we obtain from (5.2) and (5.19)

$$\mathbf{R}^T \mathbf{H}_N \mathbf{R} = \mathbf{D}_N, \tag{5.21}$$

with a diagonal matrix $\mathbf{D} := \mathbf{D}_N = \operatorname{diag}(\delta_{0,0}, \ldots, \delta_{N-1,N-1})$, where

$$\delta_{n,k} := \Phi_m(q_n^* q_k^*).$$

We have normalized regular Padé forms by $q_n(0) = 1$, so that the corresponding FOPs are monic. Therefore, we have by (5.12),

$$\delta_{n,n} = \Phi_m(q_n^* q_n^*) = \Phi_m(\zeta^n q_n^*) = \Pi_{m+2n}(hq_n) = \varepsilon_{n,n}, \quad n = 0, \ldots, N-1. \tag{5.22}$$

However, if regular FOPs do not exist for every degree $n < N$, then a factorization (5.21) no longer exists with a diagonal matrix $\mathbf{D}$. In this case we can complete the sequence of regular FOPs by inner FOPs such that the full set of polynomials q_n^* leads to a block LDU decomposition of $\mathbf{H}_N^{-1}$ with a well-conditioned block diagonal matrix $\mathbf{D} = (\delta_{jk})$, *i.e.*, we obtain an "inverse" block factorization of the Hankel matrix $\mathbf{H}_N$ ($N = \infty$ is allowed). In many situations it is desirable to compute this factorization and not only the last pair of polynomials $q_N^{\nwarrow}$ and q_N that allows us to represent $\mathbf{H}_N^{-1}$ by an inversion formula, *e.g.*, the one of Theorem 2.16.

Clearly, the matrix $\mathbf{D}$ in (5.21) is still (complex) symmetric. Moreover, due to our special choice of inner polynomials, we can even show that it is a block diagonal matrix whose blocks inherit the Hankel structure of $\mathbf{H}_N$:

Theorem 5.6: *If the upper triangular matrix* $\mathbf{R}$ *defined in* (5.20) *contains in its* $(n+1)$*st column* $(0 \leq n < N)$ *the coefficients of an nth regular or inner FOP, where the latter is constructed according to Corollary* 5.5, *then the matrix* $\mathbf{D}$ *in* (5.21) *is block diagonal. The blocks of* $\mathbf{D}$ *always start with a regular index and each block is a Hankel matrix. Moreover, the* $n \times n$ *principal submatrix* $\mathbf{D}_n$ *of* $\mathbf{D}$ *is nonsingular if and only if* $\mathbf{H}_n$ *is nonsingular.*

Proof. The weakened orthogonality conditions (5.6) imply that the matrix $\mathbf{D}$ in (5.21) is block diagonal. Clearly, every block of $\mathbf{D}$ starts with a regular index. Recall that n is a regular index if and only if $\mathbf{H}_n$ is nonsingular.

Let $n = n_l$ be a regular index, and let $n < n+j < n_{l+1}$, $n \leq n+k < n_{l+1}-1$. From (5.17) we obtain the following recurrence for the reflected polynomials:

$$q_{n+j}^* = \zeta^{n+j} q_{n+j}(\zeta^{-1}) = \zeta q_{n+j-1}^* + \gamma_{j-1}^{(n)} q_n^{\nwarrow *}. \tag{5.23}$$

From the definition of inner polynomials and in view of $q_n^{\nwarrow *} \in \mathcal{P}_{n-1}$ we have

$$\begin{aligned} \Phi_m(q_{n+j}^* q_{n+k}^*) &= \Phi_m((\zeta q_{n+j-1}^* + \gamma_{j-1}^{(n)} q_n^{\nwarrow *}) q_{n+k}^*) \\ &= \Phi_m(\zeta q_{n+j-1}^* q_{n+k}^*) \\ &= \Phi_m(q_{n+j-1}^* (q_{n+k+1}^* - \gamma_k^{(n)} q_n^{\nwarrow *})) \\ &= \Phi_m(q_{n+j-1}^* q_{n+k+1}^*). \end{aligned}$$

Hence, the blocks of $\mathbf{D}$ are Hankel matrices.

The last statement of the theorem follows from (5.21) because $\mathbf{R}$ is unit upper triangular and thus nonsingular. Hence, $\mathbf{H}_n$ and the $n \times n$ submatrix of $\mathbf{D}$ are of same rank. □

If we consider exact breakdowns only, then the diagonal blocks of $\mathbf{D}$ are not only Hankel but right lower triangular [52, 56, 60]. However, if we allow building blocks in the case of near breakdowns, then the left upper triangles of the diagonal blocks of $\mathbf{D}$ are no longer zero but they still inherit the Hankel structure.

Let us now take a closer look at the structure of the upper triangular matrix $\mathbf{R}$. Assume that regular FOPs of degree n_l and n_{l+1} ($l \geq 1$) exist, and define $\mathbf{r}_l \in \mathbb{C}^{h_l}$ and $\mathbf{R}^{(l)} \in \mathbb{C}^{h_l,h_l}$ by the following $(h_l+1) \times (h_l+1)$ submatrix of $\mathbf{R}$, where $h_l := n_{l+1} - n_l$

$$\begin{bmatrix} 1 & \mathbf{r}_l^T \\ 0 & \mathbf{R}^{(l)} \end{bmatrix} := \left[\begin{array}{c|ccc} \rho_{0,n_l-1} & \rho_{1,n_l} & \cdots & \rho_{h_l,n_{l+1}-1} \\ \hline & \rho_{0,n_l} & \cdots & \rho_{h_l-1,n_{l+1}-1} \\ & & \ddots & \vdots \\ & & & \rho_{0,n_{l+1}-1} \end{array}\right]. \tag{5.24}$$

The matrix $\mathbf{R}^{(l)}$ corresponds to the lth block of the inverse factorization (5.21).

Lemma 5.7: *For $l = 1, 2, \ldots$, the submatrix defined in* (5.24) *is a unit upper triangular Toeplitz matrix. For $l = 0$, we have $\mathbf{R}_0 = \mathbf{I}_{h_0}$.*

Proof. The statement for $l = 0$ is obvious from the recursion (5.17), because there we have $q_0^{\nwarrow} = 0$ and $q_0 = 1$.

For $l \geq 1$, we let $1 \leq m \leq k \leq h_l$. Rewriting (5.17) in terms of the coefficients of ζ^m yields

$$\rho_{m,n_l+k} = \rho_{m,n_l+k-1},$$

since the second term in (5.17) is $O_+(\zeta^{k+1})$. This establishes the Toeplitz structure of the submatrix (5.24). □

So far, we have shown that the coefficients of the denominators of diagonal (underdetermined) Padé forms lead to an inverse LDU decomposition of the Hankel matrix $\mathbf{H}_N$. We next want to show, that the LDU decomposition itself can also be computed by means of Padé forms, without inverting the upper triangular matrix $\mathbf{R}$.

Theorem 5.8: *Let the assumptions of Theorem* 5.6 *be valid. Then*

$$\mathbf{L} := \mathbf{L}_N := \mathbf{H}_N \mathbf{R}_N \tag{5.25}$$

is a block lower triangular matrix which contains in its $(n+1)$st column $(0 \leq n < N)$ the coefficients of the residual e_n of the (possibly underdetermined) $(m+n-1, n)$ Padé form of h. Moreover,

$$\mathbf{H}_N = \mathbf{L}\mathbf{D}^{-1}\mathbf{L}^T \tag{5.26}$$

is a block LDU decomposition of $\mathbf{H}_N$.

Proof. To simplify the notation, let $n = n_l + k < n_{l+1}$ be an index in the lth block of the LDU decomposition and (p_n, q_n) be the $(m+n-1, n)$ Padé form of h if $k = 0$, or the particular underdetermined Padé form of Corollary 5.5 if $k > 0$. Then we have by Definition 5.3

$$hq_n - p_n = \zeta^{m+2n_l+k} e_n.$$

Moreover from Lemma 5.2 and (5.12) we obtain

$$\Phi_m(q_n^* \zeta^i) = \mathbf{e}_i^T \mathbf{H}_N \mathbf{R} \mathbf{e}_n = \mathbf{e}_i^T \mathbf{L} \mathbf{e}_n = 0, \qquad i = 0, \ldots, n_l - 1$$

and $\mathbf{e}_i^T \mathbf{H}_N \mathbf{R} \mathbf{e}_n = \varepsilon_{i,n}$ for $i \geq n_l$. This shows that $\mathbf{L} := \mathbf{H}_N \mathbf{R} = (\varepsilon_{i,j})_{i,j=0}^{N-1}$ is block lower triangular.

Finally, the LDU decomposition (5.26) follows from (5.21) and (5.25). □

In view of (5.21) and (5.25), we can compute the block diagonal matrix $\mathbf{D}$ via

$$\mathbf{D} = \mathbf{R}^T \mathbf{L}. \tag{5.27}$$

In Levinson-type algorithms we only compute the matrix $\mathbf{R}$ and just a few entries of $\mathbf{L}$, while in Schur-type algorithms, we do not have any entries of $\mathbf{R}$ available, except that we know that $\mathbf{R}$ has unit diagonal. This is sufficient for the diagonal entries of $\mathbf{D}$, as was shown in (5.22), but it is not obvious how to determine a complete diagonal block of $\mathbf{D}$ in a look-ahead step. Next we show, how one can obtain the matrix $\mathbf{D}$ with negligible computational work even in a look-ahead step. We start with the Levinson-type algorithm, where $\mathbf{R}$ is known. Note that due to the Hankel structure of the blocks of

$$\mathbf{D} = \operatorname{diag}(\mathbf{D}^{(0)}, \ldots, \mathbf{D}^{(J)})$$

it is sufficient to compute the first and the last column of each block. Since $\mathbf{R}$ is unit upper triangular, the elements of the first column of $\mathbf{D}^{(l)}$ are the coefficients $\varepsilon_{n_l,n_l}, \ldots, \varepsilon_{n_{l+1}-1,n_l}$ of the (n_l)th residual e_{n_l}. These have been computed explicitly by inner products in Algorithm 4.2. Since we even have $\varepsilon_{n_l,n_l}, \ldots, \varepsilon_{n_l+2h_l-1,n_l}$ and $\varepsilon^{\nwarrow}_{n_l,n_l}, \ldots, \varepsilon^{\nwarrow}_{n_l+2h_l-1,n_l}$ available, we can use the third line of the recurrence (5.17) to compute the first h_l coefficients of $e_{n_{l+1}-1}$. These are exactly those entries of $\mathbf{L}$ that are required to compute the last column of $\mathbf{D}^{(l)}$ via (5.27).

For the Schur-type algorithm, things get a little trickier in case of a look-ahead step. The key point is the Toeplitz structure of the submatrix (5.24) of $\mathbf{R}$. Lemma 5.7 states that it is sufficient to compute the first $h_l - 1$ components of the vector $\mathbf{r}_l$ in order to know the complete submatrix $\mathbf{R}^{(l)}$. The procedure described below was previously described by Freund [38, Lemma 3.4] for his look-ahead Bareiss algorithm for Toeplitz matrices. For completeness, we also present the proof here.

Lemma 5.9: *For $l \geq 1$, the elements $\rho_{1,n_l+1}, \ldots, \rho_{h_l-1,n_l+h_l-1}$ of the matrix $\mathbf{R}^{(l)} \in \mathbb{C}^{h_l,h_l}$ satisfy the recurrence*

$$\rho_{j+1,n_l+j+1} = -[\ \rho_{j,n_l+j} \ \ \cdots \ \ \rho_{1,n_l+1} \ \ 1 \ \ \mathbf{0}^T_{N-n_l-j-1}\ ]\mathbf{c}_{l-1}, \quad j = 0, 1, \ldots, h_l - 2, \tag{5.28}$$

where

$$\mathbf{c}_{l-1} = \tilde{\mathbf{L}}^{(l-1)}(\mathbf{L}^{(l-1)})^{-1}\mathbf{e}_{h_l-1}.$$

Here, $\mathbf{L}^{(l-1)} = \mathbf{L}_{n_{l-1}:n_l-1,n_{l-1}:n_l-1}$ *denotes the* $(l-1)$*st diagonal block of* $\mathbf{L}$ *and* $\tilde{\mathbf{L}}^{(l-1)} = \mathbf{L}_{n_{l-1}:N-1,n_{l-1}:n_l-1}$ *denotes the part of the* $(l-1)$*st block column of* $\mathbf{L}$ *below the diagonal block.*

Proof. We consider the lth block row and the $(l-1)$st block column of (5.27). Since this is not a diagonal block, we have

$$\mathbf{0} = [\ \star \quad \mathbf{r}_l\ ]\mathbf{L}^{(l-1)} + [\ (\mathbf{R}^{(l)})^T \quad \mathbf{0}\ ]\tilde{\mathbf{L}}^{(l-1)}.$$

Multiplying from the right by $(\mathbf{L}^{(l-1)})^{-1}$ and taking the (h_l-1)st column yields

$$\mathbf{r}_l = -[\ (\mathbf{R}^{(l)})^T \quad \mathbf{0}\ ]\tilde{\mathbf{L}}^{(l-1)}(\mathbf{L}^{(l-1)})^{-1}\mathbf{e}_{h_l-1} = -[\ (\mathbf{R}^{(l)})^T \quad \mathbf{0}\ ]\mathbf{c}_{l-1}.$$

Note that the vector $\mathbf{r}_l$ contains the desired coefficients ρ_{j,n_l+j}, $j = 1,\ldots,h_l-1$ so that the recurrence (5.28) follows. □

With this lemma, we can finally compute $\mathbf{R}^{(l)}$ in a Schur-type algorithm which then yields $\mathbf{D}^{(l)} = (\mathbf{R}^{(l)})^T\mathbf{L}^{(l)}$.

If we extend Algorithms 4.2 and 4.3 such that they compute the complete block factorizations of $\mathbf{H}_N$, then the operation count is additional $k-1$ SAXPYs for the inner FOPs or its residuals. The operation count is summarized in Table 5.1. Compared to the classical algorithm, the overhead is now $3(k-1)$ SAXPYs in a block of size k.

We will develop a variant with less overhead in the next chapter.

Operations in a block of size $k \geq 1$	Levinson-type	Schur-type
inner products	$2k$	–
SAXPYs	$5k-3$	$5k-3$

Table 5.1: Operation counts for Algorithms 4.2 and 4.3 combined with inner FOPs

6. LANCZOS ALGORITHM

In this chapter we want to interpret the Levinson-type look-ahead algorithm discussed in the previous chapters in terms of the Lanczos process [90]. The connection of the Lanczos process to the Padé table has been discussed by Gragg [52], Gutknecht [60, 63], and by Gragg and Lindquist [56] in the context of the partial realization problem. Extensions of the Lanzcos algorithms which can overcome exact as well as near breakdowns have been proposed by Taylor [115], Parlett, Taylor, and Liu [102], Brezinski, Redivo-Zaglia, and Sadok [14, 15], Nachtigal [95], Parlett [100], Hochbruck [78], Freund, Gutknecht, and Nachtigal [39], Gutknecht [63], and Joubert [82].

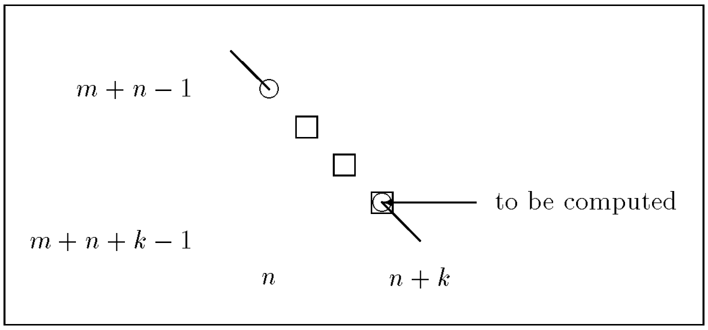
Here, we will not only deal with algorithms for computing Padé forms on a certain diagonal of the Padé table but also consider algorithms for two adjacent diagonals. The most important application of such recurrences is the look-ahead Lanczos method based on coupled two-term recurrences, with the biconjugate gradient method [91] as its famous representative. For exact breakdowns, this has been discussed in detail by Gutknecht [63]. An implementation which works for near breakdowns also is described by Freund and Nachtigal [40]. In contrast to [40] we discuss such coupled recurrences from the Padé point of view and show that this connection can help to make the algorithm of [40] more efficient. The first algorithm for computing Padé forms on a staircase diagonal which can deal with singular blocks in the Padé table is due to Berlekamp and Massey described in [5, Chapter 4, §4]. There is however an important difference to the algorithms we propose: Berlekamp and Massey define underdetermined Padé forms to fill the gaps between two regular pairs in such a way that the Padé forms have the correct O_+ order of their residual, but numerators and denominators are allowed to have higher degree. The latter makes their definition useless for the Lanczos process or for computing a basis of FOPs.

We do not consider implementation issues of the Lanczos process here, in particular, we do not discuss normalization, further practical aspects of look-ahead strategies, or reorthogonalization techniques [31]. These issues will be described elsewhere.

6.1 Alternative recurrences using inner FOPs

So far we computed regular pairs from regular pairs. If inner polynomials were constructed they solely served for completing block LDU decompositions, but they were not incorporated into the computation of the next regular pair. Here, we show how to make use of the computed inner polynomials. This will then illustrate the ultimate connection to the look-ahead Levinson-type Hankel solver proposed by Freund and Zha [43] and the look-ahead Lanczos algorithm by Freund, Gutknecht, and Nachtigal [39, 60, 63].

To visualize the recurrences we present pictures before we state the theorems. The symbols in the pictures have been introduced in Chapter 4 and 5: circles stand for Padé forms, squares represent underdetermined Padé forms, and a line indicates that Padé approximants located at the end points of the line – even if they are not involved in the recurrence – are different from each other. The Padé form indicated by an arrow is the one we want to compute. The remaining (underdetermined) Padé forms displayed in the picture are involved in the recurrence for this Padé form.



We will continue to use the recurrence (5.17) illustrated in (5.18) for inner FOPs and give new recurrences only for computing a new regular pair.

Theorem 6.1: *Let (p_n, q_n) be a regular $(m+n-1, n)$ Padé form of $h \in \mathcal{L}_0$ with residual e_n and let (p_{n+j}, q_{n+j}) be arbitrary $(m+n+j-1, n+j)$ underdetermined Padé forms with residuals e_{n+j}.*

If a nontrivial solution of the linear system

$$\begin{bmatrix} \varepsilon_{n,n} & \cdots & \varepsilon_{n+k-1,n} \\ \vdots & & \vdots \\ \varepsilon_{n+k-1,n} & \cdots & \varepsilon_{n+k-1,n+k-1} \end{bmatrix} \begin{bmatrix} \theta_0^{\nwarrow} \\ \vdots \\ \theta_{k-1}^{\nwarrow} \end{bmatrix} = \mathbf{e}_{k-1} e_{n+k}^{\nwarrow}(0) \tag{6.1}$$

exists, then $(p_{n+k}^{\nwarrow}, q_{n+k}^{\nwarrow})$ with

$$\begin{bmatrix} p_{n+k}^{\nwarrow} \\ q_{n+k}^{\nwarrow} \\ \zeta^{k-1} e_{n+k}^{\nwarrow} \end{bmatrix} = \sum_{j=0}^{k-1} \begin{bmatrix} \zeta^{k-1-j} p_{n+j} \\ \zeta^{k-1-j} q_{n+j} \\ e_{n+j} \end{bmatrix} \theta_j^{\nwarrow} \tag{6.2}$$

is an $(m+n+k-2, n+k-1)$ Padé form of h with residual $e_{n+k}^{\nwarrow}$.

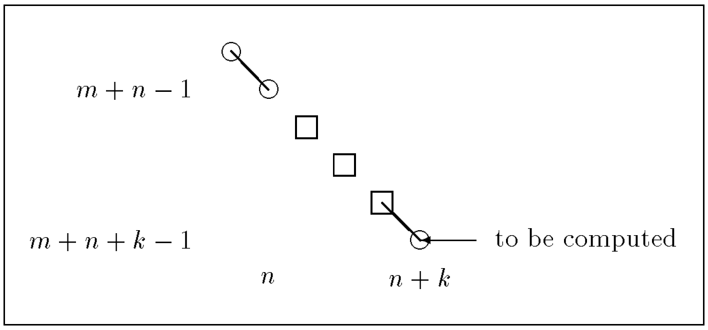
Proof. We use (6.2) as the definition of $p_{n+k}^{\nwarrow}$ and $q_{n+k}^{\nwarrow}$. First of all observe that $p_{n+k}^{\nwarrow} \in \mathcal{P}_{m+n+k-2}$ and $q_{n+k}^{\nwarrow} \in \mathcal{P}_{n+k-1}$. By Definition 5.3, we have

$$h q_{n+k}^{\nwarrow} - p_{n+k}^{\nwarrow} = \zeta^{m+2n+k-1} \sum_{j=0}^{k-1} e_{n+j} \theta_j^{\nwarrow}.$$

This is in $\mathcal{L}_{m+2n+2k-2}$, and thus $(p^{\nwarrow}_{n+k}, q^{\nwarrow}_{n+k})$ is an $(m+n+k-2, n+k-1)$ Padé form of h, if and only if

$$\Pi_{0:k-2}\left(\sum_{j=0}^{k-1} e_{n+j}\theta^{\nwarrow}_j\right) = 0,$$

or, equivalently, if (6.1) holds. □



Theorem 6.2: *Let the assumptions of Theorem* 6.1 *be valid, and let in addition* $(p^{\nwarrow}_n, q^{\nwarrow}_n)$ *be an* $(m+n-2, n-1)$ *Padé form with residual* $e^{\nwarrow}_n$. *Moreover, define*

$$\vartheta_{n+k} = -e_{n+k-1}(0)/e^{\nwarrow}_n(0). \tag{6.3}$$

If a solution of

$$\begin{bmatrix} \varepsilon_{n,n} & \cdots & \varepsilon_{n,n+k-1} \\ \vdots & & \vdots \\ \varepsilon_{n+k-1,n} & \cdots & \varepsilon_{n+k-1,n+k-1} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \vdots \\ \theta_{k-1} \end{bmatrix} = - \begin{bmatrix} \varepsilon_{n+1,n+k-1} \\ \vdots \\ \varepsilon_{n+k,n+k-1} \end{bmatrix} - \begin{bmatrix} \varepsilon^{\nwarrow}_{n+1,n} \\ \vdots \\ \varepsilon^{\nwarrow}_{n+k,n} \end{bmatrix} \vartheta_{n+k} \tag{6.4}$$

exists, then (p_{n+k}, q_{n+k}) *with*

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ \zeta^k e_{n+k} \end{bmatrix} = \begin{bmatrix} p_{n+k-1} \\ q_{n+k-1} \\ \zeta^{-1} e_{n+k-1} \end{bmatrix} + \sum_{j=0}^{k-1} \begin{bmatrix} \zeta^{k-j} p_{n+j} \\ \zeta^{k-j} q_{n+j} \\ e_{n+j} \end{bmatrix} \theta_j + \begin{bmatrix} \zeta^{k+1} p^{\nwarrow}_n \\ \zeta^{k+1} q^{\nwarrow}_n \\ \zeta^{-1} e^{\nwarrow}_n \end{bmatrix} \vartheta_{n+k} \tag{6.5}$$

is an $(m+n+k-1, n+k)$ *Padé form of* h *with* $q_{n+k}(0) \neq 0$ *and residual* e_{n+k}.

Proof. Clearly, $p^{\nwarrow}_{n+k} \in \mathcal{P}_{m+n+k-2}$ and $q^{\nwarrow}_{n+k} \in \mathcal{P}_{n+k-1}$. From Lemma 5.2 we have

$$hq_{n+k} - p_{n+k} = \zeta^{m+2n+k}\left(\zeta^{-1}(e_{n+k-1} + e^{\nwarrow}_n \vartheta_{n+k}) + \sum_{j=0}^{k-1} e_{n+j}\theta_j\right).$$

The condition $hq_{n+k} - p_{n+k} = O_+(\zeta^{m+2n+2k})$ is equivalent to (6.3) and (6.4). Finally $q_{n+k}(0) = q_{n+k-1}(0) \neq 0$ by Definition 5.3 □

We next prove a lemma concerning the length k of a look-ahead step. It is the counterpart of Lemma 4.3 for the new recurrences of the previous two theorems.

Lemma 6.3: *Let $n = n_l$ be a regular index. Then $n+k$ is a regular index if and only if the coefficient matrix $\mathbf{L}^{(l)} = (\varepsilon_{n+i,n+j})_{i,j=0}^{k-1}$ arising in* (6.1) *and* (6.4) *is nonsingular.*

Proof. $\mathbf{H}_{n+k} = \mathbf{H}_{m+n+k-1,n+k}$ is nonsingular if and only if $\mathbf{T}_{m,n+k}$ is nonsingular, which is equivalent to $n+k$ being a regular index by Lemma 2.8. It follows from Theorem 5.8 (where $N = n+k$) that $\mathbf{H}_{n+k}$ and $\mathbf{L}$ are of same rank since $\mathbf{R}$ is unit upper triangular. Since n is a regular index, $\mathbf{H}_n$ is regular and thus all previous diagonal blocks of $\mathbf{L}$ are nonsingular. Hence, $\mathbf{H}_{n+k}$ is nonsingular if and only if $\mathbf{L}^{(l)}$ is. □

The previous two theorems provide an alternative way of implementing look-ahead steps in the Levinson- or Schur-type algorithms of Chapter 4: we no longer have to multiply by polynomials u_k, v_k of degree greater than one, but instead form linear combinations of underdetermined Padé forms. This turns out to require fewer SAXPYs per look-ahead step ($k > 1$) than the version we had before. Compare Tables 4.1 and 6.1.

Here is the complete new version of the Levinson-type Algorithm 4.2, which uses the normalization (2.40) and the same number of inner products as the classical Levinson algorithm.

Algorithm 6.1: Look-ahead Levinson-type algorithm for diagonals in the Padé table using inner FOPs.
INPUT: $h \in \mathcal{L}_0$, m, N;
OUTPUT: *denominator q_N of regular $(m+L, L)$ Padé form of h for largest possible $L \le N$;*
Set $n = 0$, $l = 0$, $q_0 = 1$, $q_0^{\nwarrow} = 0$, $\varepsilon_{0,0}^{\nwarrow} = 1$, $\varepsilon_{1,0}^{\nwarrow} = 0$;
while $n < N$
  Set $k = 1$; *compute* $\varepsilon_{n,n} = \Pi_{m+2n+1}(hq_n)$, $\varepsilon_{n+1,n} = \Pi_{m+2n+2}(hq_n)$; *set* $\mathbf{L}^{(l)} = \varepsilon_{n,n}$;
  while $\sigma_{\min}(\mathbf{L}^{(l)}) < tol$ *and* $n+k \le N$
    compute kth inner FOP of lth block by (5.17) *and* (5.16):

$$q_{n+k} = q_{n+k-1} - \zeta^{k+1} q_n^{\nwarrow} \varepsilon_{n,n+k-1};$$

    set $\varepsilon_{n+2k,n} = \Pi_{m+2n+2k+1}(hq_n)$, $\varepsilon_{n+2k+1,n} = \Pi_{m+2n+2k+2}(hq_n)$;
    compute $\varepsilon_{n+2k,n}^{\nwarrow}$, $\varepsilon_{n+2k+1,n}^{\nwarrow}$ *from* (4.5);
    compute the kth row and column of $\mathbf{L}^{(l)} = (\varepsilon_{n+i,n+j})_{i,j=0}^{k-1}$ *from* (5.17);
    set $k = k+1$;
  solve (6.4) *for the coefficients* θ_j, $j = 0, \dots, k-1$ *and compute from* (6.5)

$$q_{n+k} = q_{n+k-1} + \sum_{j=0}^{k-1} \zeta^{k-j} q_{n+j} \theta_j + \zeta^{k+1} q_n^{\nwarrow} \vartheta_{n+k};$$

  if $n+k < N$
    if $k = 1$
      set $q_{n+1}^{\nwarrow} = q_n$, $\varepsilon_{n+1,n+1}^{\nwarrow} = \varepsilon_{n,n}$, $\varepsilon_{n+2,n+1}^{\nwarrow} = \varepsilon_{n+1,n}$;
    else

solve (6.1) *for the coefficients* $\theta_j^{\nwarrow}$, $j = 0, \ldots, k-1$ *and compute from* (6.2)

$$q_{n+k}^{\nwarrow} = \sum_{j=0}^{k-1} \zeta^{k-1-j} q_{n+j} \theta_j^{\nwarrow};$$

set $\varepsilon_{n+k,n+k}^{\nwarrow} = 1$ *and compute* $\varepsilon_{n+k+1,n+k}^{\nwarrow} = \Pi_k \left(\sum_{j=0}^{k-1} e_{n+j} \theta_j^{\nwarrow} \right)$ *from* (6.2);

else

set $L = n$;

set $n = n + k$, $l = l + 1$;

A new version of the Schur-type Algorithm 4.3, which uses again the normalization (2.40) is

Algorithm 6.2: Look-ahead Schur-type algorithm for diagonals in the Padé table using inner residuals.

INPUT: $h \in \mathcal{L}_0$, m, N;

OUTPUT: *residual* e_N *of regular* $(m+L, L)$ *Padé form of* h *for largest possible* $L \leq N$;

Set $n = 0$, $l = 0$, $e_0 = \Pi_{m+1:\infty} h$, $e_0^{\nwarrow} = 1$;

while $n < N$

Set $k = 1$ *and* $\mathbf{L}^{(l)} = \varepsilon_{n,n}$;

while $\sigma_{\min}(\mathbf{L}^{(l)}) < tol$ *and* $n + k \leq N$

compute kth inner residual of lth block by (5.17) *and* (5.16):

$$e_{n+k} = \zeta^{-1}(e_{n+k-1} - e_n^{\nwarrow} \varepsilon_{n,n+k-1});$$

set $\mathbf{L}^{(l)} = (\varepsilon_{n+i,n+j})_{i,j=0}^{k-1}$ *and* $k = k + 1$;

solve (6.4) *for the coefficients* θ_j, $j = 0, \ldots, k-1$ *and compute from* (6.5)

$$e_{n+k} = \zeta^{-k} \left(\zeta^{-1}(e_{n+k-1} + e_n^{\nwarrow} \vartheta_{n+k}) + \sum_{j=0}^{k-1} e_{n+j} \theta_j \right);$$

if $n + k < N$

if $k = 1$

set $e_{n+1}^{\nwarrow} = e_n$;

else

solve (6.1) *for the coefficients* $\theta_j^{\nwarrow}$, $j = 0, \ldots, k-1$ *and compute from* (6.2)

$$e_{n+k}^{\nwarrow} = \zeta^{-k+1} \left(\sum_{j=0}^{k-1} \zeta^{k-1-j} q_{n+j} \theta_j^{\nwarrow} \right);$$

else

set $L = n$;

set $n = n + k$, $l = l + 1$;

Operations in a block of size k	Levinson-type		Schur-type	
	regular step	inner step	regular step	inner step
inner products/step	2	2	–	–
SAXPYs/step	$2k$	1	$2k$	1
inner products	$2k$		–	
SAXPYs	$3k-1$		$3k-1$	

Table 6.1: Operation counts for Algorithms 6.1 and 6.2.

In Table 6.1 we give the operation counts for Algorithms 6.1 and 6.2. The top part of the table shows the operations per step, the bottom part the total number of operations per block. If $k = 1$, then these two parts coincide, since no inner steps occur. The $2k$ SAXPYs computed in a regular step come from $k+1$ SAXPYs for q_{n+k} or e_{n+k} plus $k-1$ SAXPYs for $q^{\nwarrow}_{n+k}$ or $e^{\nwarrow}_{n+k}$. The SAXPYs for the Levinson-type algorithm are of size less than or equal to $n+k$. For the Schur-type algorithm, they are of size less than or equal to $2(N-n)+1$. If the algorithm performs a step of length $k = 1$, then no inner FOPs arise, and hence the operation count is two inner products for the Levinson-type algorithm plus two SAXPYs for both types. Thus, a look-ahead step of size k produces on overhead of k SAXPYs only. One has to keep in mind that in average, the SAXPYs in a Schur-type algorithm are of twice the length of the inner products and SAXPYs in a Levinson-type algorithm. However, it is in general not correct to claim that the overhead of the Schur-type algorithm is higher, because the overhead depends on the index n where a look-ahead step occurs. For the Levinson-type algorithm, it is cheaper if it occurs for n small, while for the Schur-type algorithm the opposite is true.

Note that the classical three-term recurrences for FOPs require two SAXPYs and two inner products in the Levinson algorithm. Hence the overhead in a block of size k is $k-1$ SAXPYs but no inner products. There is no overhead if $k = 1$. The same is true for the Schur algorithm.

6.2 *Lanczos algorithm and Padé approximation*

As pointed out by Parlett in a private communication at the Householder meeting 1996, one can formulate the Lanczos process in a very general setting. Assume that $A : \mathcal{H} \to \mathcal{H}$ is a linear operator acting on a linear space $\mathcal{H}$ over the field $\mathbb{C}$ and let $\mathcal{H}'$ be the dual space of $\mathcal{H}$ consisting of all linear functionals on $\mathcal{H}$. Then the adjoint A^T of A is defined by

$$(A^T\mathbf{w})(\mathbf{v}) = \mathbf{w}(A\mathbf{v}) \qquad \forall \mathbf{v} \in \mathcal{H},\ \mathbf{w} \in \mathcal{H}'.$$

For $\mathbf{w} \in \mathcal{H}'$ and $\mathbf{v} \in \mathcal{H}$, we will use the notation

$$\mathbf{w}(\mathbf{v}) := \langle \mathbf{w}, \mathbf{v} \rangle.$$

Obviously, $\langle \cdot, \cdot \rangle$ is a bilinear form on $\mathcal{H}' \times \mathcal{H}$. The aim of the Lanczos process is to construct two sequences of elements of $\mathcal{H}'$ and $\mathcal{H}$, called the left and right Lanczos vectors, which form bases of the nth Krylov space with respect to the adjoint operator A^T and the operator A itself, respectively. The bases are characterized by a certain block duality condition, which means that left and right Lanczos vectors are dual to each other if they are located in different blocks. At first sight, this does not seem to be related to Padé approximation, but in fact it is, as was studied in detail in [60]. At least for special situations, this relation was mentioned before by several authors; see the references in [60, 64]. We will soon see how the framework we derived in the previous section can be extended to the Lanczos algorithm.

Let two arbitrary nonzero elements $\mathbf{v} \in \mathcal{H}$ and $\mathbf{w} \in \mathcal{H}'$ be given. Then the nth Lanczos vectors can be written as

$$\mathbf{v}_n = q_n^*(A)\mathbf{v} \qquad \text{and} \qquad \mathbf{w}_n = q_n^*(A^T)\mathbf{w}, \tag{6.6}$$

where q_n^* is a polynomial of exact degree n such that the matrix

$$(\langle \mathbf{w}_j, A^m \mathbf{v}_k \rangle) \tag{6.7}$$

is block diagonal. The cases $m = 0$ and $m = 1$ are the most interesting ones, because they correspond to dual and A-dual vectors $\mathbf{v}_n$ and $\mathbf{w}_n$.

Here we assume the polynomials to be monic, but of course, if $\mathcal{H}$ is a normed linear space and $\mathcal{H}'$ is its normed dual space, it is possible to introduce scaling factors into (6.6). These scaling factors may then be different for left and right Lanczos vectors.

A special case of this general presentation of the Lanczos algorithm is that $\mathcal{H} = \mathbb{C}^N$. The Riesz representation theorem identifies $\mathcal{H}$ with its dual space $\mathcal{H}'$. Then A and its adjoint A^T can be represented by square $N \times N$ matrices, and the elements of $\mathcal{H}$ and $\mathcal{H}'$ by vectors in $\mathbb{C}^N$. Finally, $\langle \mathbf{w}, \mathbf{v} \rangle = \mathbf{w}^T \mathbf{v}$.

If j and k are indices in different blocks, then the block duality (6.6) is equivalent to $\Phi_m(q_j^* q_k^*) = 0$, where $\Phi_m : \mathcal{P} \to \mathbb{C}$ is the linear functional

$$\Phi_m(st) = \langle s(A^T)\mathbf{w}, A^m t(A)\mathbf{v} \rangle = \langle \mathbf{w}, s(A) A^m t(A) \mathbf{v} \rangle.$$

Therefore, q_n^* is an nth FOP (regular or inner) with respect to Φ_m. The moments of this linear form are $\mu_j = \langle \mathbf{w}, A^j \mathbf{v} \rangle$, $j \geq 0$. They define the *generating function*

$$h(\zeta) = \sum_{j=0}^{\infty} \Phi_0(\zeta^j)\zeta^j = \sum_{j=0}^{\infty} \langle \mathbf{w}, (\zeta A)^j \mathbf{v} \rangle = \langle \mathbf{w}, (I - \zeta A)^{-1} \mathbf{v} \rangle.$$

The Lanczos process can be interpreted as an algorithm to compute FOPs. This is closely related to constructing diagonal sequences of Padé forms, as we have discussed in Chapter 5. So, at least in principle, a Levinson type algorithm can be used to compute the Lanczos vectors. Clearly, we have to use a variant which computes also inner FOPs, since a complete basis of FOPs is desired.

Unfortunately, we run into a number of problems if we want to apply Algorithms 4.2 or 6.1 in its present form:

- So far, our recurrences work with the coefficients of the polynomials $q_n^{\nwarrow}$ and q_n. In a Lanczos algorithm, we never compute these polynomials explicitly, but instead we only have the Lanczos vectors (6.6) available.
- For each step we only want to apply the operators A and A^T once, as in the classical Lanczos algorithm. This corresponds to using recurrences where one only multiplies by polynomials of degree at most one. This excludes Algorithm 4.2 but the recurrences of Algorithm 6.1 look fine.
- Computing the moments μ_j of the formal power series h explicitly is a highly unstable and inefficient process. However, without knowledge of the moments, we cannot compute the coefficients of the residuals e_n and $e_n^{\nwarrow}$, which arise in the linear systems (6.1) and (6.4). A remedy is to evaluate instead the modified moments

$$\langle \mathbf{w}_j, A^m \mathbf{v}_k \rangle = \Phi_m(q_j^* q_k^*) = \delta_{j,k},$$

  which are entries of $\mathbf{D} = (\delta_{j,k})$, the block diagonal matrix defined in (5.21). Hence we have to rewrite the linear systems (6.1) and (6.4) such that they contain only entries of $\mathbf{D}$ and possibly further computable modified moments.

6.3 Look-ahead Lanczos process based on three-term recurrences

To address the problems stated at the end of the previous section assume in the following that $n = n_l$ is a regular index, and that $n_{l+1} = n + k$. If q_n and $q_n^{\nwarrow}$ are the denominators of the $(n-1, n)$ and $(n-2, n-1)$ Padé forms of h, then by (5.10) and (5.11) we have:

$$\begin{aligned} \Phi_m(\zeta^i q_n^{\nwarrow *}) &= 0 \qquad \text{for} \quad i = 0, \ldots, n-2, \\ \Phi_m(\zeta^i q_n^*) &= 0 \qquad \text{for} \quad i = 0, \ldots, n-1. \end{aligned}$$

Since we only want to multiply by polynomials of degree at most one, we use the recurrences of Theorems 6.1 and 6.2 and not those of Corollary 4.1. In terms of the reflected polynomials they become

$$\begin{aligned} q_{n+k}^{\nwarrow *} &= \sum_{j=0}^{k-1} q_{n+j}^* \theta_j^{\nwarrow}, \\ q_{n+k}^* &= \zeta q_{n+k-1}^* + \sum_{j=0}^{k-1} q_{n+j}^* \theta_j + \vartheta_{n+k} q_n^{\nwarrow *}. \end{aligned} \tag{6.8}$$

For inner FOPs, we have (5.23) where $\gamma_{j-1}^{(n)}$ is given by (5.16).

We use the same normalization as before, *i.e.*, (2.40). For the reflected polynomials, this means that q_n^* is monic for every $n \geq 0$, and that in view of Lemmas 5.2 and 5.3

$$\Phi_m(\zeta^{n-1} q_n^{\nwarrow *}) = \Phi_m(q_{n-1}^* q_n^{\nwarrow *}) = e_n^{\nwarrow}(0) = 1 \tag{6.9}$$

for regular indices n.

We cannot use the linear systems (6.1) and (6.4) in their present form, since we do not know the coefficients of the residuals. Next we therefore derive equivalent linear systems which contain only quantities which can be computed in a Lanczos process.

Theorem 6.4: *Assume that $n = n_l$ is a regular index. Let q_n^* be an nth regular FOP, $n = n_l$, let $q_n^{\nwarrow *}$ be a polynomial orthogonal to any polynomial of degree less than or equal to $n-2$ satisfying (6.9), and let q_{n+j}^*, $j = 1, \ldots, k-1$, be inner FOPs. Moreover, assume $\mathbf{D}^{(l)} = (\Phi_m(q_{n+i}^* q_{n+j}^*))_{i,j=0}^{k-1}$ to be nonsingular. Then the following statements hold:*

(i) *If*

$$\vartheta_{n+k} = -\Phi_m(q_{n-1}^* \zeta q_{n+k-1}^*) \tag{6.10}$$

and $\mathbf{d}_n = [\ \theta_0 \ \cdots \ \theta_{k-1}\ ]^T$ is the unique solution of

$$\mathbf{D}^{(l)} \mathbf{d}_n = - \begin{bmatrix} \Phi_m(q_n^* \zeta q_{n+k-1}^*) \\ \vdots \\ \Phi_m(q_{n+k-1}^* \zeta q_{n+k-1}^*) \end{bmatrix}, \tag{6.11}$$

then q_{n+k}^* defined in (6.8) is a regular $(n+k)$th FOP with respect to Φ_m.

(ii) *If $\mathbf{d}_n^{\nwarrow} = [\ \theta_0^{\nwarrow} \ \cdots \ \theta_{k-1}^{\nwarrow}\ ]^T$ is the unique solution of*

$$\mathbf{D}^{(l)} \mathbf{d}_n^{\nwarrow} = \mathbf{e}_{k-1}, \tag{6.12}$$

then $q_{n+k}^{\nwarrow *}$ defined in (6.8) is orthogonal to all polynomials of degree at most $n+k-2$ with respect to Φ_m and normalized by (6.9).

(iii) *If, for $j = 1, \ldots, k-1$,*

$$\gamma_{j-1}^{(n)} = -\Phi_m(q_{n-1}^* \zeta q_{n+j-1}^*), \tag{6.13}$$

then q_{n+j}^* defined by (5.23) is an $(n+j)$th inner FOP with respect to Φ_m.

Proof. (i) By our specific normalization inner FOPs are monic and therefore q_{n+k}^* is monic of degree $n+k$. To prove that it is orthogonal to every polynomial of degree less than $n+k$, we multiply the recurrences of (6.8) by q_i^*, $i = 0, \ldots, n+k-1$, and apply the linear form Φ_m. Using (6.10) and (5.10) we obtain

$$\begin{aligned} \Phi_m(q_i^* q_{n+k}^*) &= \Phi_m(q_i^* \zeta q_{n+k-1}^*) + \sum_{j=0}^{k-1} \Phi_m(q_i^* q_{n+j}^*) \theta_j + \Phi_m(q_i^* q_n^{\nwarrow *}) \vartheta_{n+k} \\ &= \begin{cases} 0, & \text{for} \quad i = 0, \ldots, n-2, \\ \Phi_m(q_i^* \zeta q_{n+k-1}^*) + \Phi_m(q_i^* q_n^{\nwarrow *}) \vartheta_{n+k}, & \text{for} \quad i = n-1, \\ \Phi_m(q_i^* \zeta q_{n+k-1}^*) + \sum_{j=0}^{k-1} \Phi_m(q_i^* q_{n+j}^*) \theta_j & \text{for} \quad i = n, \ldots, n+k-1. \end{cases} \end{aligned}$$

The condition (6.9) and the definition of $\mathbf{D}^{(l)}$ lead to (6.10) and (6.11).

(ii) The same technique applied to the first equation in (6.8) yields

$$\Phi_m(q_i^* q_{n+k}^{\nwarrow *}) = \sum_{j=0}^{k-1} \Phi_m(q_i^* q_{n+j}^*)\theta_j^{\nwarrow} = 0, \quad \text{for} \quad i = 0, \ldots, n-1,$$

while $\Phi_m(q_i^* q_{n+k}^{\nwarrow *}) = 0$ for $i = n, \ldots, n+k-2$ and $\Phi_m(q_{n+k-1}^* q_{n+k}^{\nwarrow *}) = 1$ are equivalent to (6.12).

(iii) Clearly, q_{n+j}^* is monic of degree $n+j$. To see that it is orthogonal to every polynomial of degree less than n we multiply (5.23) by q_i^*, $i \le n-1$, apply the linear form Φ_m and observe again (5.11), (5.10), and (6.9). This finally gives (6.13). □

Recall that a desirable feature of look-ahead Levinson-type and look-ahead Lanczos algorithms is to avoid overhead of inner products. We have shown how this can be accomplished for our Levinson-type algorithm in Sections 4.3 and 6.1. Next we show, that it is also possible for an implementation based on the recurrences in the previous theorem.

From Theorem 5.6 it is known that the blocks $\mathbf{D}^{(l)}$ of the block diagonal matrix $\mathbf{D}$ have Hankel structure. Hence it is sufficient to compute the diagonal and the first superdiagonal of $\mathbf{D}^{(l)}$, which costs $2k-1$ inner products. For the right hand side in (6.11), we have shown in the proof of Theorem 5.6, that for $k \ge 2$, *i.e.*, in a look-ahead step,

$$\Phi_m(q_{n+j}^* \zeta q_{n+k-1}^*) = \Phi_m(q_{n+j+1}^* q_{n+k-1}^*), \qquad \text{for} \quad j = 0, \ldots, k-2. \tag{6.14}$$

This means that the first $k-1$ entries are elements from $\mathbf{D}^{(l)}$, and only the last one, $\Phi_m(q_{n+k-1}^* \zeta q_{n+k-1}^*)$, has to be computed explicitly. Since our FOPs are monic, we have

$$\Phi_m(q_{n-1}^* \zeta q_{n+j}^*) = \Phi_m(\zeta^n q_{n+j}^*) = \Phi_m(q_n^* q_{n+j}^*),$$

and thus we obtain from (6.13)

$$\gamma_j^{(n)} = -\Phi_m(q_n^* q_{n+j}^*), \qquad \text{for} \quad j = 0, \ldots, k-1,$$

so that $\gamma_j^{(n)}$ corresponds to an element in the first row of $\mathbf{D}^{(l)}$. This makes a total of $2k$ inner products for a look-ahead step of size k, which is the minimal possible number.

Theorem 6.4 yields yet another variant of Levinson-type algorithm, this time interpreted for FOPs. We present it here to provide the reader with the algorithmic details. As before, we included only the simplest possible look-ahead strategy.

Algorithm 6.3: Look-ahead Levinson-type algorithm for FOPs.
INPUT: *N, linear form* Φ_m*;*
OUTPUT: *FOPs of degree at most* N *with respect to* Φ_m*;*
Set $n = 0$, $l = 0$, $q_0^* = 1$, $q_0^{\nwarrow *} = 0$, $\varepsilon_0^{\nwarrow} = 1$*;*
while $n < N$

Set $k=1$*; compute* $\delta_{n,n}=\Phi_m(q_n^* q_n^*)$ *and set* $\mathbf{D}^{(l)}=\delta_{n,n}$*;*
while $\sigma_{\min}(\mathbf{D}^{(l)}) < tol$ *and* $n+k \leq N$
set $\gamma_{k-1}^{(n)} = -\delta_{n,n+k-1}/\varepsilon_n^{\nwarrow}$ *and compute the* $(n+k)$*th inner FOP*

$$q_{n+k}^* = \zeta q_{n+k-1}^* + \gamma_{k-1}^{(n)} q_n^{\nwarrow *};$$

set $\delta_{n+k-1,n+k}=\Phi_m(q_{n+k-1}^* q_{n+k}^*)$ *and* $\delta_{n+k,n+k}=\Phi_m(q_{n+k}^* q_{n+k}^*)$*;*
extend the Hankel matrix $\mathbf{D}^{(l)}$ *by one row and column;*
set $k=k+1$*;*
compute $\Phi_m(q_{n+k-1}^*\zeta q_{n+k-1}^*)$*, set* $\vartheta_{n+k}=\delta_{n,n+k-1}/\varepsilon_n^{\nwarrow}$*, and exploit* (6.14) *to solve* (6.11) *for* $\mathbf{d}_n$ *to compute the* $(n+k)$*th regular FOP*

$$q_{n+k}^* = \zeta q_{n+k-1}^* + [\; q_n^* \;\; \cdots \;\; q_{n+k-1}^* \;]\mathbf{d}_n + q_n^{\nwarrow *}\vartheta_{n+k};$$

if $n+k<N$
if $k=1$
set $q_{n+1}^{\nwarrow *} = q_n^*$*,* $\varepsilon_{n+1}^{\nwarrow}=\delta_{n,n}$*;*
else
set $\varepsilon_{n+k}^{\nwarrow}=1$*, solve* (6.12) *for* $\mathbf{d}_n^{\nwarrow}$*, and compute*

$$q_{n+k}^{\nwarrow *} = [\; q_n^* \;\; \cdots \;\; q_{n+k-1}^* \;]\mathbf{d}_n^{\nwarrow};$$

set $n=n+k$*,* $l=l+1$*;*

In compact form and after eliminating the auxiliary $\nwarrow$ polynomials, the recurrence relations for regular and inner FOPs can be written as

$$\zeta\,[\; q_0^* \;\; \cdots \;\; q_{n-1}^* \;] = [\; q_0^* \;\; \cdots \;\; q_n^* \;]\mathbf{G}_n, \tag{6.15}$$

where $\mathbf{G}_n$ is an $(n+1)\times n$ unit upper Hessenberg matrix, which is also block tridiagonal. If all the steps are generic, *i.e.*, if every FOP is regular, then $\mathbf{G}_n$ is tridiagonal.

This algorithm is just the look-ahead Lanczos algorithm for FOPs proposed in [43], which was presented previously in [63, §9] and [78]. It was first shown in [43, p. 307], that one can make use of the polynomials $q_n^{\nwarrow *}$. However, the construction is not evident, because the polynomial $q_n^{\nwarrow *}$ is neither related to an orthogonality condition nor to a Padé form. Since we started from the recurrences in the Padé table, it was natural to base the recurrences on regular pairs and not only on FOPs. Another advantage of our approach is that the same derivation yields recurrences for FOPs, residuals and numerators of Padé forms, and hence leads not only to Levinson-type algorithms but also to Schur-type algorithms.

The operation count for Algorithm 6.3 is the same as for Algorithm 6.1. The operation count given in [43, p. 308] turns out to be incorrect, since the SAXPYs to compute $q_n^{\nwarrow *}$ (denoted by z_l in [43]) are not included.

Algorithm 6.3 can now be translated into a look-ahead Lanczos algorithm. For completeness, we also give this form here for the case $m = 0$. We would like to stress that for this type of algorithm, a reliable criterion to determine the length of a look-ahead step is not obtained as easily as for the Levinson-type algorithm. Different strategies for $\mathcal{H} = \mathbb{C}^N$ have been proposed in [39, 102] and should be included in the algorithm below. We will not discuss look-ahead strategies for this particular application further.

Algorithm 6.4: Look-ahead Lanczos algorithm.
INPUT: *linear operator* $A : \mathcal{H} \to \mathcal{H}$ *and its adjoint operator* $A^T : \mathcal{H}' \to \mathcal{H}'$,
$\mathbf{v}_0 \in \mathcal{H}$, $\mathbf{w}_0 \in \mathcal{H}'$;
OUTPUT: *Lanczos basis vectors* $\mathbf{v}_0, \mathbf{v}_1, \ldots \in \mathcal{H}$, $\mathbf{w}_0, \mathbf{w}_1, \ldots \in \mathcal{H}'$.
Set $n = 0$, $l = 0$; $\mathbf{v}_0^{\nwarrow} = \mathbf{0} \in \mathcal{H}$, $\mathbf{w}_0^{\nwarrow} = \mathbf{0} \in \mathcal{H}'$, $\varepsilon_0^{\nwarrow} = 1$;
while $\mathbf{v}_n \neq \mathbf{0}$ *and* $\mathbf{w}_n \neq \mathbf{0}$
  Set $k = 1$; *compute* $\delta_{n,n} = \langle \mathbf{w}_n, \mathbf{v}_n \rangle$ *and set* $\mathbf{D}^{(l)} = \delta_{n,n}$;
  while $\sigma_{\min}(\mathbf{D}^{(l)}) < tol$ *and* $n + k \leq N$
    set $\gamma_{k-1}^{(n)} = -\delta_{n,n+k-1}/\varepsilon_n^{\nwarrow}$ *and compute the* $(n+k)$*th inner vectors*

$$\begin{aligned} \mathbf{v}_{n+k} &= A\mathbf{v}_{n+k-1} + \gamma_{k-1}^{(n)} \mathbf{v}_n^{\nwarrow} \\ \mathbf{w}_{n+k} &= A^T \mathbf{w}_{n+k-1} + \gamma_{k-1}^{(n)} \mathbf{w}_n^{\nwarrow} \end{aligned}$$

    compute $\delta_{n+k-1,n+k} = \langle \mathbf{w}_{n+k-1}, \mathbf{v}_{n+k} \rangle$ *and* $\delta_{n+k,n+k} = \langle \mathbf{w}_{n+k}, \mathbf{v}_{n+k} \rangle$;
    extend the Hankel matrix $\mathbf{D}^{(l)}$ *by one row and column;*
    set $k = k + 1$;
  compute $\langle \mathbf{w}_{n+k-1}, A\mathbf{v}_{n+k-1} \rangle$, *set* $\vartheta_{n+k} = \delta_{n,n+k-1}/\varepsilon_n^{\nwarrow}$, *exploit* (6.14) *to solve* (6.11) *for* $\mathbf{d}_n$ *and compute the* $(n+k)$*th regular FOP*

$$\begin{aligned} \mathbf{v}_{n+k} &= A\mathbf{v}_{n+k-1} + [\ \mathbf{v}_n \ \cdots \ \mathbf{v}_{n+k-1}\ ]\mathbf{d}_n + \vartheta_{n+k} \mathbf{v}_n^{\nwarrow} \\ \mathbf{w}_{n+k} &= A^T \mathbf{w}_{n+k-1} + [\ \mathbf{w}_n \ \cdots \ \mathbf{w}_{n+k-1}\ ]\mathbf{d}_n + \vartheta_{n+k} \mathbf{w}_n^{\nwarrow} \end{aligned}$$

  if $n + k < N$
    if $k = 1$
      set $\mathbf{v}_{n+1}^{\nwarrow} = \mathbf{v}_n$; $\mathbf{w}_{n+1}^{\nwarrow} = \mathbf{w}_n$; $\varepsilon_{n+1}^{\nwarrow} = \delta_{n,n}$
    else
      set $\varepsilon_{n+k}^{\nwarrow} = 1$, *solve* (6.12) *for* $\mathbf{d}_n^{\nwarrow}$, *and set*

$$\begin{aligned} \mathbf{v}_{n+k}^{\nwarrow} &= [\ \mathbf{v}_n \ \cdots \ \mathbf{v}_{n+k-1}\ ]\mathbf{d}_n^{\nwarrow} \\ \mathbf{w}_{n+k}^{\nwarrow} &= [\ \mathbf{w}_n \ \cdots \ \mathbf{w}_{n+k-1}\ ]\mathbf{d}_n^{\nwarrow} \end{aligned}$$

  set $n = n + k$, $l = l + 1$;

The compact version (6.15) of this algorithm yields the well-known relations

$$\begin{aligned} A[\ \mathbf{v}_0 \ \cdots \ \mathbf{v}_{n-1}\ ] &= [\ \mathbf{v}_0 \ \cdots \ \mathbf{v}_n\ ]\mathbf{G}_n, \\ A^T[\ \mathbf{w}_0 \ \cdots \ \mathbf{w}_{n-1}\ ] &= [\ \mathbf{w}_0 \ \cdots \ \mathbf{w}_n\ ]\mathbf{G}_n \end{aligned}$$

Operations in a block of size k	regular step	inner step
inner products/step	2	2
SAXPYs/step	$4k$	2
matrix vector multiplications/step	2	2
inner products	$2k$	
SAXPYs	$6k-2$	
matrix vector multiplications	$2k$	

Table 6.2: Operation counts for Algorithm 6.4

with a unit upper Hessenberg and block tridiagonal matrix $\mathbf{G}_n$. This algorithm is very similar to the look-ahead Lanczos algorithm proposed in [39, 63]. However, the recurrences in [39] did not make use of the auxiliary vectors $\mathbf{v}_n^{\nwarrow}$ and $\mathbf{w}_n^{\nwarrow}$. Instead, the whole previous block was involved in the recurrences for inner as well as for regular vectors. As we mentioned before the possibility of saving these operations was first exploited in [43] and was also used in [119]. Nevertheless, this does not seem to be well-known for the look-ahead Lanczos process, which can be seen from the fact that it is not yet implemented in the highly recommendable software package QMRPACK by Freund and Nachtigal [41] which is available in NETLIB. We would like to emphasize that using the auxiliary vectors $\mathbf{v}_n^{\nwarrow}, \mathbf{w}_n^{\nwarrow}$ does not only reduce the number of arithmetic operations, but also the storage requirements. If we restrict the maximal block size to $k_{\max}$, then we need in the worst case only $2(k_{\max}+1)$ vectors from previous blocks plus storage for two temporary vectors. In contrast, the implementation proposed in [39] requires to allocate memory for $4k_{\max}$ Lanczos vectors plus two temporary vectors.

Table 6.2 gives the operation counts for Algorithm 6.4. Here again, the top part shows the operations per step, so that one can distinguish between regular and inner steps and the bottom part shows the operations for a complete block. Note that the SAXPYs double compared to Algorithm 6.3, since we have to compute two sequences of vectors, which correspond to only one sequence of FOPs. In each step, regular or inner, we need to apply the operators A and its adjoint A^T only once. The overhead in a step of size k is only $2k-2$ SAXPYs but no overhead in terms of inner products or matrix vector multiplications arises. There is no overhead if $k=1$.

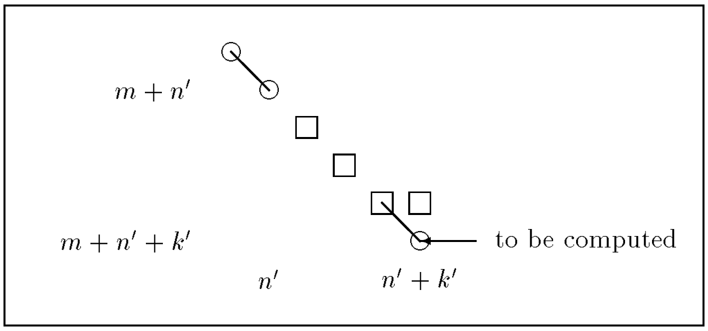
6.4 Recurrences for adjacent diagonals

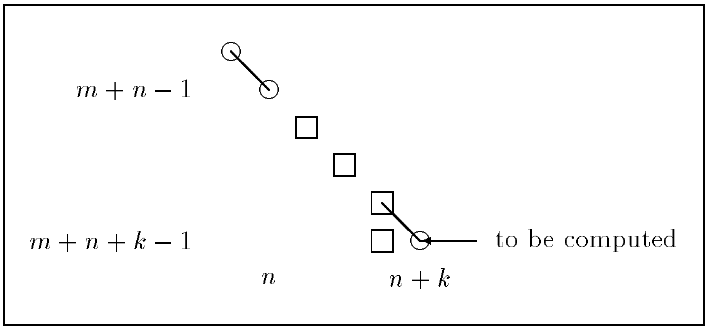
One of the most well-known algorithms for the iterative solution of linear systems $A\mathbf{x} = \mathbf{b}$ is the conjugate gradient method [77]. Basically, it computes two bases of a Krylov space with respect to the Hermitian positive definite coefficient matrix A and the initial residual vector. One basis consists of the residual vectors arising during the iteration, and the second one contains the search directions. The residual vectors are orthogonal to each other, the search directions are A-orthogonal to each other. The fact that A is positive definite ensures that no breakdowns can occur during the course of the computation.

The generalization to non-Hermitian matrices is the biconjugate gradient method [91], which computes two bases of a Krylov space with respect to A and two bases of a Krylov space with respect to A^T. These bases correspond to the Lanczos vectors with respect to the bilinear form (6.7) for $m = 0$ and $m = 1$, respectively. Hence this type of algorithm is related to computing Padé forms on two adjacent diagonals. Here it is possible that breakdowns due to a division by zero or instabilities because of a division of a very small quantity arise.

This important application motivates us to discuss algorithms for staircase diagonals also. We first discuss the general algorithm for the Padé table and give the interpretation for the Lanczos process later in Section 6.5. Another motivation is that there is a widespread belief that coupled two-term recurrences are more stable than three-term recurrences [40]. However, this has only been observed in numerical examples, *e.g.*, in [40], but we are not aware of a proof of this statement. In [101], Parlett discusses this question for the qd algorithm, which is another type of algorithm related to Padé approximation on a staircase diagonal.

The following two pictures illustrate the recurrences of the next theorem.





To avoid a second index for distinguishing Padé forms on the two diagonals we denote Padé forms on the lower diagonal by (u_n, v_n) and their residuals by w_n. The index n

indicates the column in the Padé table or, equivalently, the maximum degree of the denominator v_n. We continue to use the normalization (2.40) for both sequences, *i.e.*, $v_n(0) = 1$ and $w_n^{\nwarrow}(0) = 1$.

Theorem 6.5: *Let (p_n, q_n) be a regular $(m+n-1, n)$ Padé form of $h \in \mathcal{L}_0$ with residual e_n and let $(u_{n'}, v_{n'})$ be a regular $(m+n', n')$ Padé form of h with residual $w_{n'}$. Moreover, assume that $(p_n^{\nwarrow}, q_n^{\nwarrow})$ is an $(m+n-2, n-1)$ Padé form of h with residual $e_n^{\nwarrow}$ and that $(u_{n'}^{\nwarrow}, v_{n'}^{\nwarrow})$ is an $(m+n'-1, n'-1)$ Padé form with residual $w_{n'}^{\nwarrow}$.*

(i) *If $n' \le n$ we let $(p_{n'+k'}, q_{n'+k'})$ be an $(m+n'+k'-1, n'+k')$ underdetermined Padé form (with respect to the regular index n) and $(u_{n'+j}, v_{n'+j})$, $1 \le j \le k'-1$, be $(m+n'+j, n'+j)$ underdetermined Padé forms (with respect to the regular index n') with residuals $e_{n'+k'}$ and $w_{n'+j}$, respectively. Define*

$$\vartheta^{\downarrow}_{n'+k'} = \begin{cases} -e_{n'+k'}(0)/w_{n'}^{\nwarrow}(0) & \textit{for } n' = n, \\ 0 & \textit{for } n' < n. \end{cases} \tag{6.16}$$

If a unique solution of

$$\Pi_{0:k'}\left(\zeta^{n-n'} e_{n'+k'} + w_{n'}^{\nwarrow}\vartheta^{\downarrow}_{n'+k'} + \zeta\sum_{j=0}^{k'-1} w_{n'+j}\theta^{\downarrow}_{n'+j}\right) = 0 \tag{6.17}$$

exists, then $(u_{n'+k'}, v_{n'+k'})$ defined as

$$\begin{bmatrix} u_{n'+k'} \\ v_{n'+k'} \\ \zeta^{k'+1} w_{n'+k'} \end{bmatrix} = \begin{bmatrix} p_{n'+k'} \\ q_{n'+k'} \\ e_{n'+k'} \end{bmatrix} + \sum_{j=0}^{k'-1} \begin{bmatrix} \zeta^{k'-j} u_{n'+j} \\ \zeta^{k'-j} v_{n'+j} \\ w_{n'+j} \end{bmatrix} \theta^{\downarrow}_j + \begin{bmatrix} \zeta^{k'+1} u_{n'}^{\nwarrow} \\ \zeta^{k'+1} v_{n'}^{\nwarrow} \\ w_{n'}^{\nwarrow} \end{bmatrix} \vartheta^{\downarrow}_{n'+k'}, \tag{6.18}$$

is a regular $(m+n'+k', n'+k')$ Padé form of h.

(ii) *If $n' \ge n-1$ we let (u_{n+k-1}, v_{n+k-1}) be an $(m+n+k-1, n+k-1)$ underdetermined Padé form (with respect to the regular index n') and (p_{n+j}, q_{n+j}), $1 \le j \le k-1$, be $(m+n+j-1, n+j)$ underdetermined Padé forms (with respect to the regular index n). Define*

$$\vartheta_{n+k} = \begin{cases} -w_{n+k-1}(0)/e_n^{\nwarrow}(0) & \textit{for } n' = n-1, \\ 0 & \textit{for } n' > n-1. \end{cases} \tag{6.19}$$

If a unique solution of

$$\Pi_{0:k}\left(\zeta^{n'-n+1} w_{n+k-1} + e_n^{\nwarrow}\vartheta_{n+k} + \zeta\sum_{j=0}^{k-1} e_{n+j}\theta_{n+j}\right) = 0 \tag{6.20}$$

exists, then (p_{n+k}, q_{n+k}) defined by

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ \zeta^{k+1} e_{n+k} \end{bmatrix} = \begin{bmatrix} u_{n+k-1} \\ v_{n+k-1} \\ w_{n+k-1} \end{bmatrix} + \sum_{j=0}^{k-1} \begin{bmatrix} \zeta^{k-j} p_{n+j} \\ \zeta^{k-j} q_{n+j} \\ e_{n+j} \end{bmatrix} \theta_j + \begin{bmatrix} \zeta^{k+1} p_n^{\nwarrow} \\ \zeta^{k+1} q_n^{\nwarrow} \\ e_n^{\nwarrow} \end{bmatrix} \vartheta_{n+k}, \tag{6.21}$$

is a regular $(m+n+k-1, n+k)$ Padé form of h with residual e_{n+k}.

Proof. By assumption and by Definition 5.3

$$\begin{aligned} hq_{n+j} - p_{n+j} &= \zeta^{m+2n+j} e_{n+j}, \qquad (p_{n+j}, q_{n+j}) \in \mathcal{P}_{m+n+j-1} \times \mathcal{P}_{n+j}, \\ hv_{n'+j} - u_{n'+j} &= \zeta^{m+2n'+j} w_{n'+j}, \qquad (u_{n'+j}, v_{n'+j}) \in \mathcal{P}_{m+n'+j} \times \mathcal{P}_{n'+j}. \end{aligned}$$

Moreover, since n' and n are regular indices, $e_n^{\nwarrow}(0) \neq 0$ and $w_{n'}^{\nwarrow}(0) \neq 0$, so that $\vartheta^{\downarrow}_{n'+k'}$ and $\vartheta_{n+k'}$ are well defined. Then, $(u_{n'+k'}, v_{n'+k'})$ defined in (6.18) satisfies

$$\begin{aligned} hv_{n'+k'} - u_{n'+k'} &= \zeta^{m+2n+n'-n+k'} e_{n'+k'} + \zeta^{m+2n'+k'+1} \sum_{j=0}^{k'-1} w_{n'+j} \theta_j^{\downarrow} + \zeta^{m+2n'+k'} w_{n'}^{\nwarrow} \vartheta^{\downarrow}_{n'+k'} \\ &= \zeta^{m+2n'+k'} \left(\zeta^{n-n'} e_{n'+k'} + w_{n'}^{\nwarrow} \vartheta^{\downarrow}_{n'+k'} + \zeta \sum_{j=0}^{k'-1} w_{n'+j} \theta_j^{\downarrow} \right). \end{aligned}$$

This shows that a solution of (6.17) yields

$$hv_{n'+k'} - u_{n'+k'} = \zeta^{m+2(n'+k')+1} w_{n'+k'}$$

with $u_{n'+k'} \in \mathcal{P}_{m+n'+k'}$ and $v_{n'+k'} \in \mathcal{P}_{n'+k'}$ which proves (i) by the assumption that the solution is unique.

To prove (ii), we use (6.21) as the definition of its left-hand side and obtain

$$\begin{aligned} hq_{n+k} - p_{n+k} &= \zeta^{m+2n'+n-n'+k} w_{n+k-1} + \zeta^{2n+k} \sum_{j=0}^{k-1} e_{n+j} \theta_j + \zeta^{2n+k-1} e_n^{\nwarrow} \vartheta_{n+k} \\ &= \zeta^{m+2n+k-1} \left(\zeta^{n'-n+1} w_{n+k-1} + e_n^{\nwarrow} \vartheta_{n+k} + \zeta \sum_{j=0}^{k-1} e_{n+j} \theta_j \right). \end{aligned}$$

Clearly, q_{n+k} and p_{n+k} have the correct degree. Hence a solution of (6.20) ensures

$$hq_{n+k} - p_{n+k} = z^{m+2(n+k)} e_{n+k}$$

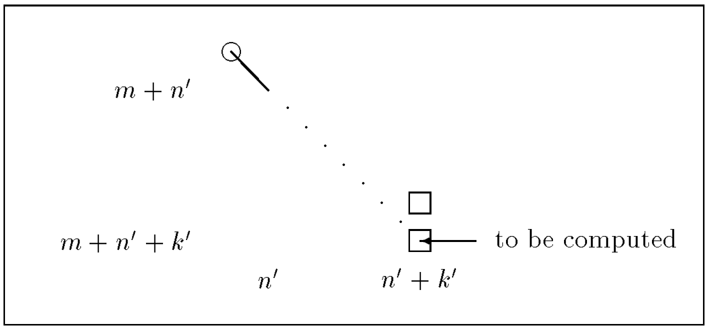
so that (p_{n+k}, q_{n+k}) is an $(m+n+k-1, n+k)$ Padé form. The uniqueness shows that it is regular. □

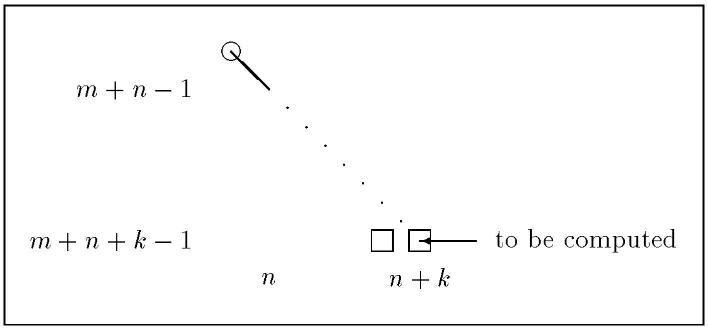
Several remarks are in order.

- In exact arithmetic the block structure of the Padé table ensures that $n' = n$ or $n' = n-1$ in the previous theorem. Then the assumptions in (i) and (ii) are both satisfied. For $n' = n$ the regular Padé form (p_n, q_n) is also row-regular, as was shown in Lemma 2.6 (ii). For $n' = n-1$ the regular Padé form (u_{n-1}, v_{n-1}) is column-regular. See Lemma 2.7 (ii).
- It is clear that the two adjacent diagonals hit a block either at its left border, which yields a row-regular pair or at its upper border, in which case we can work with a column-regular pair. Since all blocks are square a diagonal which enters the block at its left border must leave it at its lower border. One which enters a block at its upper border must leave it at its right border. Therefore, column-regular and row-regular pairs occur alternately.

- In finite precision arithmetic, the theorems proved in Section 2.7 justify the assumption that still $n' = n$ or $n' = n - 1$. However, since Theorem 2.24 is not strong enough to guarantee the existence of well-defined square blocks, the assumption that column well-conditioned and row well-conditioned pairs occur alternately seems no longer justified.
- Since a regular index on one of the diagonals is always related to a column-regular or a row-regular pair, one can always replace one of the recurrences (6.18) or (6.21) by a classical Frobenius identity: from a row-regular pair (p_{n+k}, q_{n+k}), $(u^{\nwarrow}_{n+k}, v^{\nwarrow}_{n+k})$ one can obtain (u_{n+k}, v_{n+k}), and a column-regular pair (u_{n+k}, v_{n+k}), $(p^{\nwarrow}_{n+k}, q^{\nwarrow}_{n+k})$ yields (p_{n+k}, q_{n+k}). So there is only one recurrence which costs more than one SAXPY to compute the next regular Padé forms on both diagonals.
- The theorem can be used even under the more general assumption that regular pairs on adjacent diagonals occur independently from each other. In this situation one has to choose the largest regular indices n and n', respectively, such that the assumptions in (i) and (ii) are satisfied. The reason is that an underdetermined Padé form of index, say j, with respect to a regular index $\tilde{n} > n$ can also be interpreted as an underdetermined Padé form of index j with respect to n. Since then the first $\tilde{n} - n$ coefficients of its residual are equal to zero, the linear system we have to solve decouples. However, the application of classical Frobenius identities is no longer possible if we do not relate the regular pairs on both diagonals. The recurrences are then equivalent to those from [40], but the authors seem to have been unaware of simplifications due to the use of auxiliary Padé forms $(u^{\nwarrow}_{n}, v^{\nwarrow}_{n})$ and $(p^{\nwarrow}_{n}, q^{\nwarrow}_{n})$.
- Recurrences to compute the auxiliary Padé forms $(p^{\nwarrow}_{n+k}, q^{\nwarrow}_{n+k})$ and $(u^{\nwarrow}_{n+k}, v^{\nwarrow}_{n+k})$ have been derived in Theorem 6.1.

Next we consider the computation of underdetermined Padé forms via coupled recurrences. They can be illustrated as follows





Theorem 6.6: *Let the assumptions of Theorem* 6.5 *be valid.*

(i) *If* $n' \leq n$, *then* $(u_{n'+k'}, v_{n'+k'})$ *defined by*

$$\begin{bmatrix} u_{n'+k'} \\ v_{n'+k'} \\ \zeta w_{n'+k'} \end{bmatrix} = \begin{bmatrix} p_{n'+k'} \\ q_{n'+k'} \\ e_{n'+k'} \end{bmatrix} + \begin{bmatrix} \zeta^{k'+1} u_{n'}^{\nwarrow} \\ \zeta^{k'+1} v_{n'}^{\nwarrow} \\ w_{n'}^{\nwarrow} \end{bmatrix} \vartheta_{n'+k'}^{\downarrow},$$

where $\vartheta_{n'+k'}^{\downarrow}$ *is taken from* (6.16) *is an underdetermined* $(m+n'+k', n'+k')$ *Padé form of* h.

(ii) *If* $n' \geq n-1$, *then* (p_{n+k}, q_{n+k}) *defined by*

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ \zeta e_{n+k} \end{bmatrix} = \begin{bmatrix} u_{n+k-1} \\ v_{n+k-1} \\ w_{n+k-1} \end{bmatrix} + \begin{bmatrix} \zeta^{k+1} p_{n}^{\nwarrow} \\ \zeta^{k+1} q_{n}^{\nwarrow} \\ e_{n}^{\nwarrow} \end{bmatrix} \vartheta_{n+k},$$

where ϑ_{n+k} *is taken from* (6.19) *is an underdetermined* $(m+n+k-1, n+k)$ *Padé form of* h *with residual* e_{n+k}.

Proof. The statements follow from the proof of the previous theorem. □

Due to the remarks above we always have $n' = n$ or $n' = n-1$. Therefore, either $\vartheta_{n'+k'}^{\downarrow}$ or ϑ_{n+k} is equal to zero. Hence we get the corresponding underdetermined Padé form for free from its upper or left neighbor, respectively. If $n' = n$, then (p_n, q_n) is a row-regular Padé form, and we have $\vartheta_{n+k} = 0$. In this case, we do not need to compute the upper neighbor $(p_n^{\nwarrow}, q_n^{\nwarrow})$. If $n' = n-1$, then $(u_{n'}, v_{n'})$ is a column-regular Padé form, and then we have $\vartheta_{n'+k'}^{\downarrow} = 0$, so that the computation of $(u_{n'}^{\nwarrow}, v_{n'}^{\nwarrow})$ can be saved. Table 6.3 summarizes the operation count under these assumptions. Note that the classical algorithm requires only 2 SAXPYs per step, so that the overhead is only $\min\{k, k'\}$ SAXPYs. There is again no overhead in terms of inner products, as we will explain in the next section.

Operations in a blocks of size k and k'	regular step	inner step
inner products/step	2	2
SAXPYs/step	$k+k'+1$	1
inner products	$k+k'$	
SAXPYs	$k+k'+\min\{k,k'\}$	

Table 6.3: Operation counts for look-ahead step using coupled two-term recurrences under the assumption that $n'=n$ or $n'=n-1$ and $n'+k'=n+k$ or $n'+k'=n+k-1$ (notation from Theorems 6.5 and 6.6).

6.5 Look-ahead Lanczos process based on coupled two-term recurrences

In order to apply the recurrences from the previous section for computing bases of Krylov spaces, we have to take the problems stated at the end of Section 6.2 into account. We proceed similar to Section 6.3 and write the recurrences in terms of FOPs, *i.e.*, reflected denominators of Padé forms. This yields for regular pairs in the upper diagonal

$$\begin{aligned} q_{n+k}^{\nwarrow *} &= \sum_{j=0}^{k-1} q_{n+j}^{*}\theta_j^{\nwarrow}, \\ q_{n+k}^{*} &= \zeta v_{n+k-1}^{*} + \sum_{j=0}^{k-1} q_{n+j}^{*}\theta_j + q_n^{\nwarrow *}\vartheta_{n+k} \end{aligned} \tag{6.22}$$

and for regular pairs in the lower diagonal

$$\begin{aligned} v_{n'+k}^{\nwarrow *} &= \sum_{j=0}^{k-1} v_{n'+j}^{*}\gamma_j^{\nwarrow}, \\ v_{n'+k}^{*} &= q_{n'+k}^{*} + \sum_{j=0}^{k-1} v_{n'+j}^{*}\theta_j^{\downarrow} + v_{n'}^{\nwarrow *}\vartheta_{n'+k}^{\downarrow}. \end{aligned} \tag{6.23}$$

Inner FOPs in the upper diagonal are given by

$$q_{n+k}^{\nwarrow *} = \zeta v_{n+k-1}^{*} + q_n^{\nwarrow *}\vartheta_{n+k}, \tag{6.24}$$

inner FOPs in the lower diagonal by

$$v_{n'+k}^{\nwarrow *} = q_{n'+k}^{*} + v_{n'}^{\nwarrow *}\vartheta_{n'+k}^{\downarrow}. \tag{6.25}$$

Next we give the recurrence coefficients in terms of modified moments.

Theorem 6.7: *Let q_n^* be an nth regular FOP with respect to Φ_m, let $q_n^{\nwarrow *}$ be a polynomial orthogonal to any polynomial of degree less than or equal to $n-2$ satisfying (6.9), and let q_{n+j}^*, $j=1,\ldots,k-1$, be inner FOPs with respect to Φ_m. Moreover, let $v_{n'}^*$ be an n'th* *regular FOP with respect to* Φ_{m+1}, *let* $v_{n'}^{\nwarrow *}$ *be a polynomial orthogonal to any polynomial of degree less than or equal to* $n'-2$ *satisfying* (6.9), *and let* $v_{n'+j}^*$, $j = 1, \ldots, k'-1$, *be inner FOPs with respect to* Φ_{m+1}.

Then the following statements hold:

(i) *If* $\mathbf{D}^{\downarrow(l')} = (\Phi_{m+1}(v_{n'+i}^* v_{n'+j}^*))_{i,j=0}^{k'-1}$ *is nonsingular and if*

$$\vartheta_{n'+k'}^{\downarrow} = \begin{cases} -\Phi_{m+1}(v_{n'-1}^* q_{n'+k'}^*) & \text{for } n' = n-1, \\ 0 & \text{for } n' > n-1. \end{cases}$$

and $\mathbf{d}_{n'}^{\downarrow} = [\begin{array}{ccc} \theta_0^{\downarrow} & \cdots & \theta_{k'-1}^{\downarrow} \end{array}]^T$ *is the unique solution of*

$$\mathbf{D}^{\downarrow(l')} \mathbf{d}_{n'}^{\downarrow} = - \begin{bmatrix} \Phi_m(v_{n'}^* \zeta q_{n'+k'-1}^*) \\ \vdots \\ \Phi_m(v_{n'+k'-1}^* \zeta q_{n'+k'-1}^*) \end{bmatrix},$$

then $v_{n'+k'}^*$ *defined in* (6.23) *is a regular* $(n'+k')$*th FOP with respect to* Φ_{m+1}.

(ii) *If* $\mathbf{D}^{(l)} = (\Phi_m(q_{n+i}^* q_{n+j}^*))_{i,j=0}^{k-1}$ *is nonsingular and if*

$$\vartheta_{n+k} = \begin{cases} -\Phi_m(q_{n-1}^* \zeta v_{n+k-1}^*) & \text{for } n' = n-1, \\ 0 & \text{for } n' > n-1. \end{cases}$$

and $\mathbf{d}_n = [\begin{array}{ccc} \theta_0 & \cdots & \theta_{k-1} \end{array}]^T$ *is the unique solution of*

$$\mathbf{D}^{(l)} \mathbf{d}_n = - \begin{bmatrix} \Phi_m(q_n^* \zeta v_{n+k-1}^*) \\ \vdots \\ \Phi_m(q_{n+k-1}^* \zeta v_{n+k-1}^*) \end{bmatrix}$$

then q_{n+k}^* *defined in* (6.22) *is a regular* $(n+k)$*th FOP with respect to* Φ_m.

(iii) *If, for* $j = 1, \ldots, k'-1$, $v_{n'+j}^*$ *defined by* (6.25) *is an* $(n'+j)$*th inner FOP with respect to* Φ_{m+1}.

(iv) *If, for* $j = 1, \ldots, k-1$, q_{n+j}^* *defined by* (6.24) *is an* $(n+j)$*th inner FOP with respect to* Φ_m.

Proof. The proof is done similarly to the proof of the three-term recurrences in Theorem 6.4. We therefore omit the details here. □

For the upper neighbors of regular FOPs with respect to Φ_m and Φ_{m+1} we have to solve

$$\mathbf{D}^{(l)} \mathbf{d}^{\nwarrow} = \mathbf{e}_{k-1},$$

where $\mathbf{d}^{\nwarrow} = [\begin{array}{ccc} \theta_0^{\nwarrow} & \cdots & \theta_{k-1}^{\nwarrow} \end{array}]$ and

$$\mathbf{D}_{l'}^{\downarrow} \mathbf{c}^{\nwarrow} = \mathbf{e}_{k'-1},$$

where $\mathbf{c}^{\nwarrow} = [\ \gamma_0^{\nwarrow} \ \cdots \ \gamma_{k'-1}^{\nwarrow}\ ]$. This was shown in Theorem 6.4(ii).

After eliminating the auxiliary $\nwarrow$ vectors, the recurrence relations (6.22)–(6.25) can be written in compact form as

$$\begin{aligned} [\ q_0^* \ \cdots \ q_{n-1}^*\ ] &= [\ v_0^* \ \cdots \ v_{n-1}^*\ ]\mathbf{V}_n, && (6.26)\\ \zeta[\ v_0^* \ \cdots \ v_{n-1}^*\ ] &= [\ q_0^* \ \cdots \ q_n^*\ ]\mathbf{V}_n^{\downarrow}, && (6.27)\end{aligned}$$

where $\mathbf{V}_n = (\nu_{i,j})$ is an $n\times n$ unit upper triangular and $\mathbf{V}_n^{\downarrow} = (\nu_{i,j}^{\downarrow})$ is an $(n+1)\times n$ unit upper Hessenberg matrix. Both matrices are block bidiagonal, with block sizes equal to the maximal length of a look-ahead step. In the generic case, where all steps are regular steps with $k = k' = 1$, both matrices are bidiagonal.

Inserting one of these equations into the other decouples the FOPs with respect to Φ_m and Φ_{m+1} again:

$$\begin{aligned} \zeta[\ q_0^* \ \cdots \ q_{n-1}^*\ ] &= [\ q_0^* \ \cdots \ q_n^*\ ]\mathbf{V}_n^{\downarrow}\mathbf{V}_n,\\ \zeta[\ v_0^* \ \cdots \ v_{n-1}^*\ ] &= [\ v_0^* \ \cdots \ v_n^*\ ]\mathbf{V}_n\mathbf{V}_n^{\downarrow},\end{aligned}$$

Note that the coefficient matrices on the right-hand sides are both banded upper Hessenberg matrices, or, to be more precise, they are block tridiagonal in the general case and tridiagonal in the generic case. Hence, one can interpret the recurrences for adjacent diagonals as building the factors of an LU-factorization of the block tridiagonal matrix in (6.15) instead of the tridiagonal matrix itself. This corresponds to the well-known connection between the the conjugate gradient method and the Lanczos process (based on three-term recurrences); see, *e.g.*, [49, Section 10.2.6]. Clearly, the classical algorithm breaks down not only if a regular FOP does not exist, but in addition, it also stops early if an LU-factorization does not exist. It is therefore surprising that a method which is susceptible to a second kind of breakdown nevertheless is often numerically preferable.

By now it should no longer be surprising that the look-ahead Lanczos algorithm based on coupled two-term recurrences can also be implemented by evaluating the same number of inner products as in the generic situation without look-ahead. This has been studied in detail in [40]. As in [40], we propose to evaluate only $\delta_{n,n} = \Phi_m(q_n^* q_n^*)$ and $\delta_{n,n}^{\downarrow} = \Phi_{m+1}(v_n^* v_n^*)$ explicitly by inner products. Assume that $\mathbf{D}_{0:n-1,0:n-1}$ and $\left(\Phi_m(q_i^*\zeta v_j^*)\right)_{i,j=0,\ldots,n-2}$ is known from previous steps. Then we obtain from (6.27)

$$\begin{aligned} \left(\Phi_m(q_i^*\zeta v_j^*)\right)_{i,j=0,\ldots,n-1} &= \left(\Phi_m(q_i^*[\ q_0^* \ \cdots \ q_{j+1}^*\ ]\mathbf{V}_{0:j+1,j}^{\downarrow})\right)_{i,j=0,\ldots,n-1}\\ &= \mathbf{D}_{0:n-1,0:n}\mathbf{V}_{0:n,0:n-1}^{\downarrow}\\ &= \mathbf{D}_{0:n-1,0:n-1}\mathbf{V}_{0:n-1,0:n-1}^{\downarrow} + \mathbf{D}_{0:n-1,n}\mathbf{e}_n^T,\end{aligned}$$

so that we can compute $\left(\Phi_m(q_{n-1}^*\zeta v_j^*)\right)_{j=0,\ldots,n-2}$ and $\left(\Phi_m(q_i^*\zeta v_{n-1}^*)\right)_{j=0,\ldots,n-1}$ from known quantities. Moreover, the formula yields the $(n+1)$st column of $\mathbf{D}$.

Once we have all the elements of this matrix, we can use (6.26) to compute its transpose

$$\begin{aligned}\Big(\Phi_m(v_i^*\zeta q_j^*)\Big)_{i,j=0,\ldots,n-1} &= \Big(\Phi_{m+1}(v_i^*[\ v_0^* \ \ \cdots \ \ v_j^*\ ]\mathbf{V}_{0:j,j})\Big)_{i,j=0,\ldots,n-1} \\ &= \mathbf{D}^{\downarrow}_{0:n-1,0:n-1}\mathbf{V}_n.\end{aligned}$$

This yields $\mathbf{D}^{\downarrow}_{n-1,0:n-2}$. The last column of $\mathbf{D}^{\downarrow}_{0:n-2,n-1}$ is obtained from symmetry, the diagonal element was computed explicitly.

Clearly, the same arguments can be applied for the look-ahead Levinson-type algorithm to compute (underdetermined) Padé forms on two adjacent diagonals.

Details of an implementation of a new version of a look-ahead Lanczos process based on coupled two-term recurrences exploiting the simplifications developed in this chapter will be presented elsewhere.

7. RECURRENCES FOR ADJACENT ROWS IN THE PADÉ TABLE

We have now spent three chapters on different types of algorithms for computing Padé forms located on a certain diagonal or on two adjacent diagonals of the Padé table. Now we want to switch to recurrences following rows in the Padé table of a formal Laurent series. It is well-known that this problem is related to Gaussian quadrature on the unit circle [53] and to Toeplitz matrix factorizations [19, 51, 62]. For the latter application, numerous papers have appeared that generalize the classical Levinson [37, 92, 116, 124] and Schur algorithm [6, 109]. The work started with algorithms which can overcome exact breakdowns, *e.g.*, by Genin, and Kamp [34], Gover and Barnett [50], Heinig [71], Heinig and Rost [75], Pal and Kailath [98], Pombra, Lev-Ari, and Kailath [103], Sugiyama [113], Tyrtyshnikov [118], and Zarowski [123]. Algorithms which work for near-breakdowns also are described *e.g.*, by Chan and Hansen [26, 27], Sweet [114], Freund [38], Freund and Zha [42], Gu [58], Gutknecht [62], Gutknecht and Hochbruck [66, 67, 69], Hochbruck [79], Sayed and Kailath [108], Van Barel and Bultheel [120, 121].

The algorithms we develop here are based on anti-diagonally regular and column-regular pairs. One could also use regular pairs, as was done in [62, 69], but the recurrences for anti-diagonally regular pairs somehow look nicer because both Padé forms involved match the Laurent series up to the same O_+ order.

Algorithms for adjacent rows are more complicated than algorithms for diagonals. The reason is that in order to compute a Padé form in the $(n+k)$th position of a certain diagonal from a pair of Padé forms in the $(n-1)$st and the nth position of the same diagonal, we only need to compute a small $(k-1, k)$ Padé form. In other words, we can recursively compute Padé forms on a diagonal from other small Padé forms. The key point is that on a diagonal the numerator and the denominator degree grow simultaneously. In contrast, recurrences for Padé forms located on adjacent rows need a different concept, namely two-point Padé forms, because the recurrence coefficients must keep the numerator degree fixed and at the same time increase the denomintor in such a way, that the correct O_+ order is achieved. Another algorithmic difficulty is that a straightforward generalization of the classical Levinson [92] and Schur algorithm [109] is not optimal, because such an algorithm would be based on column-regular pairs [66, 67]. Recall that a Padé form is column-regular if and only if two consecutive principal submatrices of the Toeplitz operator are nonsingular. So the blocks of an algorithm based on column-regular pairs are always larger by at most one than the blocks of an algorithm which uses regular or anti-diagonally regular pairs. However, using only regular pairs is not desirable either, because in a generic step, the recurrences are more expensive than the classical algorithms which are based on column-regular pairs. Such algorithms have been proposed in [62] and have been generalized for solving block Toeplitz systems by Van Barel and Bultheel [121]. Their proof of weak stability of the algorithm for block systems is applicable to our algorithms too.

Since we do not want to waste any arithmetic operations if it is not necessary we here consider only look-ahead variants which reduce to the classical algorithms in the case that no look-ahead steps are performed. This is not the case for the algorithms [62, 121]. We therefore propose mixing the recurrences, *i.e.*, using column-regular pairs whenever possible and anti-diagonally regular pairs otherwise [69].

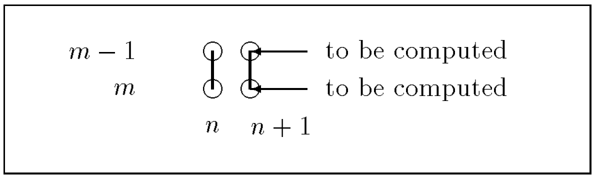
This first chapter on row recurrences contains algorithms to proceed from one anti-diagonally regular pair to another anti-diagonally regular or column-regular pair. From a computational point of view the recurrences of these algorithms consist of polynomial multiplications. We therefore call this type of algorithm the *product form* of a look-ahead row algorithm.

7.1 Fast algorithm

Using the notation introduced in (2.35), recall that an $(m-1, n)$ Padé form $(p_n^{\uparrow}, q_n^{\uparrow})$ is anti-diagonally regular if and only if $p_n^{\leftarrow}/q_n^{\leftarrow} \neq p_n^{\uparrow}/q_n^{\uparrow}$. Equivalently, $(p_n^{\uparrow}, q_n^{\uparrow})$ is anti-diagonally regular if and only if (p_n, q_n) is regular; see Lemmas 2.8 and 2.9. An (m, n) Padé form (p_n, q_n) is column-regular if and only if $p_n/q_n \neq p_n^{\uparrow}/q_n^{\uparrow}$. The coefficients of the (m, n) Padé form (p_n, q_n) and its residual e_n are denoted by (2.25) and (2.28), respectively, as in the previous chapters. Analogous notation is used for those of its neighbors.

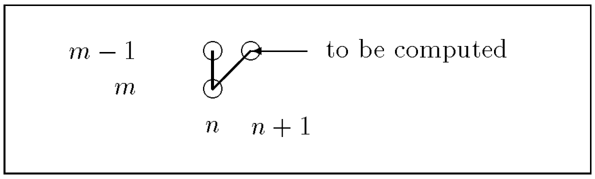
We again illustrate the different types of recurrences by pictures, which can be interpreted in the Padé table as well as in the two-point Padé table. As before, circles represent Padé forms and a line between two Padé forms indicates that these Padé forms belong to different blocks of the Padé table.

(i) Regular step: use a column-regular pair to compute the next column-regular pair. These are the classical recurrences used in the algorithms of Levinson [92] and Schur [109], which are based on Frobenius identities [51]; see Theorems 3.3 and 3.4.



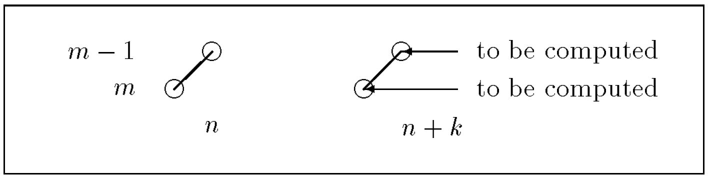
(7.1)

(ii) Switch to the sawtooth algorithm: use a column-regular pair to compute the next anti-diagonally regular pair. This is again done with the classical recurrences of the Levinson or Schur algorithm; see Theorems 3.3 and 3.4.



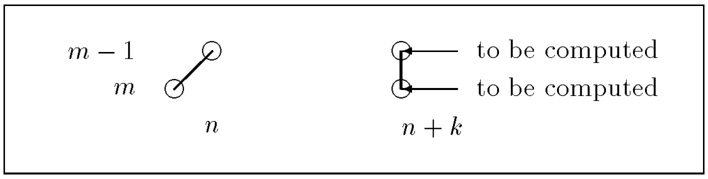
(7.2)

(iii) Look-ahead step: use an anti-diagonally regular pair to compute the next anti-diagonally regular pair (Theorems 3.7 and 3.8). This requires the computation of an anti-diagonally regular $[0;k]$ two-point Padé form and the corresponding $[1;k-1]$ two-point Padé form.



(7.3)

(iv) Switch back to the Levinson or Schur algorithm: use an anti-diagonally regular pair to compute the next column-regular pair (Theorems 3.7 and 3.8). This requires the computation of a column-regular $[1;k]$ two-point Padé form and the corresponding $[0;k]$ two-point Padé form.



(7.4)

We are now in position to present a first version of a fast $(O(N^2))$ algorithm which is "optimal" in the sense that it performs look-ahead steps of minimal size and uses the cheapest possible recurrences. In each step of the algorithm we refer to the pictures above to illustrate what kind of recurrence we actually use.

Algorithm 7.1: Optimized look-ahead algorithm for adjacent rows in the Padé table using anti-diagonally regular pairs of Padé forms
INPUT: $h \in \mathcal{L}$, *m*, *N*;
OUTPUT: *anti-diagonally regular* $(m-1, L)$ *Padé form of* h *for largest possible* $L \leq N$;
Set $n = 0$, $l = 0$, *initialize* (p_0, q_0) *and* $(p_0^{\uparrow}, q_0^{\uparrow})$ *and residuals* $e_0, e_0^{\uparrow}$;
if 0 *is not a column-regular index*
  initialize $(p_0^{\leftarrow}, q_0^{\leftarrow})$ *and residual* $e_0^{\leftarrow}$;
while $n < N$
  if n *is a column-regular index*
    compute $(p_{n+1}^{\uparrow}, q_{n+1}^{\uparrow})$ *(picture* (7.2)*)*;

if $n+1$ *is a column-regular index*
  compute (p_{n+1}, q_{n+1}) *(picture* (7.1)*);*
set $n = n+1$, $l = l+1$*;*
else
  find smallest k *such that* $n+k$ *is an anti-diagonally regular index;*
  if $n+k \le N$
    compute anti-diagonally regular $(p^{\uparrow}_{n+k}, q^{\uparrow}_{n+k})$ *(pictures* (7.3) *or* (7.4)*);*
    if $n+k$ *is a column-regular index*
      compute (p_{n+k}, q_{n+k}) *(picture* (7.4)*);*
    else
      compute $(p^{\leftarrow}_{n+k}, q^{\leftarrow}_{n+k})$ *(picture* (7.3)*);*
  else
    set $L = n$*;*
  set $n = n+k$, $l = l+1$

Algorithm 7.1 can be used in at least three different ways. The first is to compute an $(m-1, N)$ Padé form of h. In this case, numerators and denominators of the anti-diagonally regular pairs in the mth row must be computed, while only a few coefficients of the residuals are required. If Algorithm 7.1 is applied for factoring a Toeplitz matrix or for solving a linear system with Toeplitz coefficient matrix, then we have the option to view it as a look-ahead Levinson-type or as a look-ahead Schur-type algorithm; see [19, 67]. One then usually sets $m = 0$ and $\mu_k = 0$ for $|k| > N$. Levinson-type algorithms compute the denominators of the anti-diagonally regular pairs and a few coefficients of the numerators and residuals; how many depends on the size of the look-ahead step. In contrast, Schur-type algorithms do not require the denominators, but instead work with numerators and residuals only. Details on an efficient implementation of Algorithm 7.1 can be found in Section 7.3 below.

We continue to normalize Padé forms according to (2.40).

7.2 Computation of two-point Padé forms

It has been shown in Section 2.3 that the coefficients of an $[l;k]$-two-point Padé form can be computed by solving the linear system (2.34). For row recurrences in the Padé table, and in particular for the solution of Toeplitz systems of equations, the cases $l = 0$ and $l = -1$ are relevant. Therefore we next want to describe in detail the linear systems that must be solved for determining the coefficients of the two-point Padé forms.

Let us start with the recurrences to compute $(p^{\uparrow}_{n+k}, q^{\uparrow}_{n+k})$ from an anti-diagonally regular pair $(p^{\uparrow}_n, q^{\uparrow}_n)$ and $(p^{\leftarrow}_n, q^{\leftarrow}_n)$. The target Padé form is illustrated as the upper circle in (7.3) or (7.4). From Theorem 3.7 it becomes clear that we have to compute a $[0;k]$ two-point Padé form of the quadruple

$$(f^-, g^-; f^+, g^+) := (p^{\uparrow}_n, p^{\leftarrow}_n; e^{\uparrow}_n, e^{\leftarrow}_n). \tag{7.5}$$

Hence we can use (2.34) for $l = 0$, with $\gamma_j^- = \pi_{j,n}^{\leftarrow}$, $\phi_j^- = \pi_{j-1,n}^{\uparrow}$, $\gamma_j^+ = \varepsilon_{n+j,n}^{\leftarrow}$, and $\phi_j^+ = \varepsilon_{n+j,n}^{\uparrow}$. The normalization of $q_{n+k}^{\uparrow}$ being monic immediately translates into

$$\beta_k^{\uparrow(n)} = 1.$$

Therefore, we can move the last column of the linear system (2.34) to the right-hand side. Moreover, from the kth equation in (2.34), we can eliminate $\alpha_{k-1}^{\uparrow(n)}$:

$$\alpha_{k-1}^{\uparrow(n)} = -\pi_{0,n}^{\uparrow}\beta_k^{\uparrow(n)}/\pi_{0,n}^{\leftarrow}. \tag{7.6}$$

Recall that by Lemma 2.9, $\pi_{0,n}^{\leftarrow} \neq 0$ since n is an anti-diagonally regular index. Then we move the $(k-1)$st column of (2.34) to the right-hand side and drop the kth row. This gives the following linear system:

$$\mathbf{M}_{k,n} \left[\begin{array}{c} \alpha_0^{\uparrow(n)} \\ \vdots \\ \alpha_{k-2}^{\uparrow(n)} \\ \hline \beta_0^{\uparrow(n)} \\ \vdots \\ \beta_{k-1}^{\uparrow(n)} \end{array} \right] = - \left[\begin{array}{c} \pi_{k-1,n}^{\leftarrow} \\ \vdots \\ \pi_{1,n}^{\leftarrow} \\ \hline 0 \\ \vdots \\ 0 \\ \varepsilon_{n,n}^{\leftarrow} \end{array} \right] \alpha_{k-1}^{\uparrow(n)} - \left[\begin{array}{c} \pi_{k-1,n}^{\uparrow} \\ \vdots \\ \pi_{1,n}^{\uparrow} \\ \hline 0 \\ \vdots \\ 0 \\ 0 \end{array} \right] \beta_k^{\uparrow(n)} \tag{7.7}$$

with

$$\mathbf{M}_{k,n} := \left[\begin{array}{ccc|cccc} \pi_{0,n}^{\leftarrow} & \cdots & \pi_{k-2,n}^{\leftarrow} & 0 & \pi_{0,n}^{\uparrow} & \cdots & \pi_{k-2,n}^{\uparrow} \\ & \ddots & \vdots & & & \ddots & \vdots \\ \mathbf{0} & & \pi_{0,n}^{\leftarrow} & \mathbf{0} & & & \pi_{0,n}^{\uparrow} \\ \hline \varepsilon_{n,n}^{\leftarrow} & & \mathbf{0} & \varepsilon_{n,n}^{\uparrow} & & & \mathbf{0} \\ \vdots & \ddots & & \vdots & \ddots & & \\ \vdots & & \varepsilon_{n,n}^{\leftarrow} & \vdots & & \ddots & \\ \varepsilon_{n+k-1,n}^{\leftarrow} & \cdots & \varepsilon_{n+1,n}^{\leftarrow} & \varepsilon_{n+k-1,n}^{\uparrow} & \cdots & \cdots & \varepsilon_{n,n}^{\uparrow} \end{array} \right] \in \mathbb{C}^{2k-1,2k-1}. \tag{7.8}$$

Next we consider the computation of $(p_{n+k}^{\leftarrow}, q_{n+k}^{\leftarrow})$ in (7.3), which is necessary if $n+k$ is not a column-regular index. By Theorem 3.7, we must look for a $[1; k-1]$ two-point Padé form of (7.5), which means that we must set $l = 1$ and replace k by $k-1$ in (2.34). Recall that we want to use the normalization (2.40) and, therefore, we extend the linear system (2.34) by the additional equation

$$\left[\begin{array}{ccc|cccc} \pi_{0,n}^{\leftarrow} & \cdots & \pi_{k-2,n}^{\leftarrow} & 0 & \pi_{0,n}^{\uparrow} & \cdots & \pi_{k-2,n}^{\uparrow} \end{array} \right] \left[\begin{array}{c} \mathbf{a}_k^{\leftarrow} \\ \mathbf{b}_k^{\leftarrow} \end{array} \right] = \pi_{0,n+k}^{\leftarrow},$$

where $\pi^{\leftarrow}_{0,n+k} = 1$ and

$$\mathbf{a}^{\leftarrow}_k := [\ \alpha_0^{\leftarrow(n)} \ \cdots \ \alpha_{k-2}^{\leftarrow(n)}\ ]^T, \qquad \mathbf{b}^{\leftarrow}_k := [\ \beta_0^{\leftarrow(n)} \ \cdots \ \beta_{k-1}^{\leftarrow(n)}\ ]^T.$$

It is easy to see that we end up with the linear system

$$\mathbf{M}_{k,n} \begin{bmatrix} \mathbf{a}^{\leftarrow}_k \\ \mathbf{b}^{\leftarrow}_k \end{bmatrix} = \mathbf{e}_0 \pi^{\leftarrow}_{0,n+k} \tag{7.9}$$

with the same coefficient matrix as in (7.7).

Finally, we consider (7.4), which we want to use if $n+k$ is a column-regular index. Then we need to compute a $[1;k]$ two-point Padé form of (7.5), *i.e.*, solve (2.34) for $l=1$ such that $q_{n+k}(0)=1$. Combining the equation for the constant term of q_{n+k} (see the second row of (3.6)) with the kth equation of (2.34) gives the 2×2 linear system

$$\begin{bmatrix} \rho^{\leftarrow}_{0,n} & \rho^{\uparrow}_{0,n} \\ \varepsilon^{\leftarrow}_{n,n} & \varepsilon^{\uparrow}_{n,n} \end{bmatrix} \begin{bmatrix} \alpha_0^{(n)} \\ \beta_0^{(n)} \end{bmatrix} = \begin{bmatrix} \rho_{0,n+k} \\ 0 \end{bmatrix}. \tag{7.10}$$

The coefficient matrix is nonsingular because its determinant is equal to the coefficient $\Delta^{\nearrow}_n$ in Lemma 2.9 and the anti-diagonally regularity of $(p^{\uparrow}_n, q^{\uparrow}_n)$ ensures that $\Delta^{\nearrow}_n \neq 0$. Recall from Lemma 2.9 and Corollary 2.11 that for an anti-diagonally regular pair $(p^{\uparrow}_n, q^{\uparrow}_n)$, $(p^{\leftarrow}_n, q^{\leftarrow}_n)$ there holds

$$\Delta^{\nearrow}_n = \zeta^{-n}(q^{\leftarrow}_n p^{\uparrow}_n - q^{\uparrow}_n p^{\leftarrow}_n) = -\rho^{\uparrow}_{n,n}\pi^{\leftarrow}_{0,n} = \varepsilon^{\leftarrow}_{n,n}\rho^{\uparrow}_{0,n} - \varepsilon^{\uparrow}_{n,n}\rho^{\leftarrow}_{0,n} = -\pi^{\leftarrow}_{0,n}. \tag{7.11}$$

Thus we can solve (7.10) without knowing $\rho^{\leftarrow}_{0,n}$ and $\rho^{\uparrow}_{0,n}$. Making use of $\rho_{0,n+k}=1$ we obtain

$$\begin{bmatrix} \alpha_0^{(n)} \\ \beta_0^{(n)} \end{bmatrix} = \frac{1}{\pi^{\leftarrow}_{0,n}} \begin{bmatrix} \varepsilon^{\uparrow}_{n,n} \\ -\varepsilon^{\leftarrow}_{n,n} \end{bmatrix}. \tag{7.12}$$

The latter equation can now be used in a Levinson- and in a Schur-type algorithm because all coefficients on the right-hand side are available in both types of algorithms.

After computing the coefficients $\alpha_0^{(n)}$ and $\beta_0^{(n)}$ from (7.10), we can eliminate the corresponding columns and also the kth row in (2.34). Surprisingly, we again end up with a linear system with coefficient matrix $\mathbf{M}_{k,n}$:

$$\mathbf{M}_{k,n} \left[\begin{array}{c} \alpha_1^{(n)} \\ \vdots \\ \alpha_{k-1}^{(n)} \\ \hline \beta_1^{(n)} \\ \vdots \\ \beta_k^{(n)} \end{array}\right] = - \left[\begin{array}{c} 0 \\ \vdots \\ 0 \\ \hline \varepsilon^{\leftarrow}_{n+1,n} \\ \vdots \\ \varepsilon^{\leftarrow}_{n+k,n} \end{array}\right] \alpha_0^{(n)} - \left[\begin{array}{c} 0 \\ \vdots \\ 0 \\ \hline \varepsilon^{\uparrow}_{n+1,n} \\ \vdots \\ \varepsilon^{\uparrow}_{n+k,n} \end{array}\right] \beta_0^{(n)}. \tag{7.13}$$

Hence we have shown that for a look-ahead step of size k it is sufficient to solve linear systems with only one coefficient matrix $\mathbf{M}_{k,n}$ of size $(2k-1)\times(2k-1)$, no matter whether we construct an anti-diagonally regular pair or a column-regular pair.

Lemma 7.1: *The two-point Padé form* $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)})$ *of* $(p_n^{\uparrow}, p_n^{\leftarrow}; e_n^{\uparrow}, e_n^{\leftarrow})$ *is anti-diagonally regular if and only if the matrix* $\mathbf{M}_{k,n}$ *is nonsingular.*

Proof. (i) If $\mathbf{M}_{k,n}$ is singular then a nontrivial solution of (7.7) with $\alpha_{k-1}^{\uparrow(n)} = \beta_k^{\uparrow(n)} = 0$ exists. This yields a $[0;k]$ two-point Padé form $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)})$ with $\partial u_k^{\uparrow(n)} < k-1$ and $\partial v_k^{\uparrow(n)} < k$. By Lemma 2.15, this Padé form cannot be anti-diagonally regular.

(ii) Let $\mathbf{M}_{k,n}$ be nonsingular. Then we obtain from $\beta_k^{\uparrow(n)} = 1$, (7.6), and (7.7) a $[0;k]$ two-point Padé form $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)})$ with $\partial u_k^{\uparrow(n)} = k-1$ and $\partial v_k^{\uparrow(n)} = k$. Moreover, from (7.9) we obtain a $[1;k-1]$ two-point Padé form $(u_k^{\leftarrow(n)}, v_k^{\leftarrow(n)})$ with $e^{\leftarrow -}(\infty) = \pi_{0,n+k}^{\leftarrow} \neq 0$. By Lemma 2.15, $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)})$ is anti-diagonally regular. □

For the efficiency of the algorithm it is important that we first compute the $[0;k]$ two-point Padé form because, once the coefficients of $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)})$ are known, it is possible to check whether $n+k$ is a column-regular index or not, as we have shown in Lemma 3.9. We simply have to check if $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)})$ is column-regular by computing $e_k^{\uparrow +}(0) = e_{n+k}^{\uparrow}(0) = \varepsilon_{n+k,n+k}^{\uparrow}$ from

$$\left[\begin{array}{ccc|ccc} \varepsilon_{n+k,n}^{\leftarrow} & \cdots & \varepsilon_{n+1,n}^{\leftarrow} & \varepsilon_{n+k,n}^{\uparrow} & \cdots & \varepsilon_{n,n}^{\uparrow} \end{array}\right] \left[\begin{array}{c} \mathbf{a}_k^{\uparrow} \\ \mathbf{b}_k^{\uparrow} \end{array}\right] = \varepsilon_{n+k,n+k}^{\uparrow}, \tag{7.14}$$

where

$$\mathbf{a}_k^{\uparrow} := [\ \alpha_0^{\uparrow(n)} \ \cdots \ \alpha_{k-1}^{\uparrow(n)}\ ]^T, \qquad \mathbf{b}_k^{\uparrow} := [\ \beta_0^{\uparrow(n)} \ \cdots \ \beta_k^{\uparrow(n)}\ ]^T.$$

The anti-diagonally regular index $n+k$ is column-regular if and only if $e_{n+k}^{\uparrow}(0) \neq 0$; see Lemma 2.9. This provides an efficient criterion for checking whether to proceed with a column-regular pair (according to (7.4)) or with an anti-diagonally regular pair (according to (7.3)). If we proceed by constructing a column-regular pair, this simply means that we switch back to the classical algorithm. Continuing with an anti-diagonally regular pair is necessary only if two consecutive look-ahead steps occur. If the anti-diagonally regular pair is not column-regular, then it must be row-regular because of the Block Structure Theorem 2.5 or Theorem 2.20 for finite precision arithmetic.

Similar to (7.14) we obtain, for $e_{n+k}^{\leftarrow}(0) = \varepsilon_{n+k,n+k}^{\leftarrow}$,

$$\left[\begin{array}{ccc|ccc} \varepsilon_{n+k,n}^{\leftarrow} & \cdots & \varepsilon_{n+2,n}^{\leftarrow} & \varepsilon_{n+k,n}^{\uparrow} & \cdots & \varepsilon_{n+1,n}^{\uparrow} \end{array}\right] \left[\begin{array}{c} \mathbf{a}_k^{\leftarrow} \\ \mathbf{b}_k^{\leftarrow} \end{array}\right] = \varepsilon_{n+k,n+k}^{\leftarrow} \tag{7.15}$$

which can be computed cheaply.

7.3 Implementation details

The classical Levinson algorithm requires two inner products per step. It computes $\varepsilon_{n,n}$ and $\pi^{\uparrow}_{0,n}$ explicitly by inner products and $\pi_{0,n} = \varepsilon^{\uparrow}_{n,n}$ recursively from known quantities. An efficient implementation of a look-ahead Levinson-type algorithm therefore also evaluates only two inner products per index value. For a look-ahead step, k coefficients of $p^{\leftarrow}_n$ and $p^{\uparrow}_n$ and $k+1$ coefficients of $e^{\leftarrow}_n$ and $e^{\uparrow}_n$ have to be determined; see the linear systems (7.7), (7.9), and (7.13). Recall that $\pi^{\leftarrow}_{0,n} = 1$. In our new algorithm $\varepsilon^{\uparrow}_{n+1,n}, \ldots, \varepsilon^{\uparrow}_{n+k,n}$ and $\pi^{\uparrow}_{0,n}, \ldots, \pi^{\uparrow}_{k-1,n}$ are evaluated by inner products. From these quantities, we can then compute $\varepsilon_{n,n}$ recursively. As we show next, we can compute $\varepsilon^{\leftarrow}_{n,n}, \ldots, \varepsilon^{\leftarrow}_{n+k,n}$ and $\pi^{\leftarrow}_{1,n}, \ldots, \pi^{\leftarrow}_{k-1,n}$ without any (long) inner products, and thus end up with an implementation which requires the same number of inner products as its classical counterpart.

To compute $e^{\leftarrow}_n$, we will use (2.38):

$$e^{\leftarrow}_n q^{\uparrow}_n = e^{\uparrow}_n q^{\leftarrow}_n - \pi^{\leftarrow}_{0,n}. \tag{7.16}$$

Comparing the coefficients of $\zeta^0, \ldots, \zeta^k$ results in the desired coefficients $e^{\leftarrow}_{n,n}, \ldots, e^{\leftarrow}_{n+k,n}$:

$$\begin{bmatrix} \rho^{\uparrow}_{0,n} & & \\ \vdots & \ddots & \\ \rho^{\uparrow}_{k,n} & \cdots & \rho^{\uparrow}_{0,n} \end{bmatrix} \begin{bmatrix} e^{\leftarrow}_{n,n} \\ \vdots \\ e^{\leftarrow}_{n+k,n} \end{bmatrix} = \begin{bmatrix} \rho^{\leftarrow}_{0,n} & & \\ \vdots & \ddots & \\ \rho^{\leftarrow}_{k,n} & \cdots & \rho^{\leftarrow}_{0,n} \end{bmatrix} \begin{bmatrix} e^{\uparrow}_{n,n} \\ \vdots \\ e^{\uparrow}_{n+k,n} \end{bmatrix} - \pi^{\leftarrow}_{0,n}\mathbf{e}_0.$$

Here we have used again that in a look-ahead step starting with index n, this index is a row-regular index. Therefore, we have $\rho^{\uparrow}_{0,n} = q^{\uparrow}_n(0) \neq 0$ so that the above linear system has a unique solution. Moreover, comparing the coefficients of $\zeta^{n-1}, \ldots, \zeta^{n-k+1}$ in

$$p^{\leftarrow}_n q^{\uparrow}_n = p^{\uparrow}_n q^{\leftarrow}_n + \pi^{\leftarrow}_{0,n}\zeta^n, \tag{7.17}$$

which follows again from (2.38), yields a triangular linear system with Toeplitz structure for $\pi^{\leftarrow}_{1,n}, \ldots, \pi^{\leftarrow}_{k-1,n}$ ($\pi^{\leftarrow}_{0,n}$ is known):

$$\begin{bmatrix} 0 & & \\ \rho^{\leftarrow}_{n-1,n} & & \\ \vdots & \ddots & \\ \rho^{\leftarrow}_{n-k+2,n} & \cdots & \rho^{\leftarrow}_{n-1,n} \end{bmatrix} \begin{bmatrix} \pi^{\uparrow}_{0,n} \\ \vdots \\ \pi^{\uparrow}_{k-3,n} \end{bmatrix} = \begin{bmatrix} \rho^{\uparrow}_{n-1,n} & \rho^{\uparrow}_{n,n} & & \\ \vdots & & \ddots & \\ \rho^{\uparrow}_{n-k+1,n} & \cdots & \cdots & \rho^{\uparrow}_{n,n} \end{bmatrix} \begin{bmatrix} \pi^{\leftarrow}_{0,n} \\ \vdots \\ \pi^{\leftarrow}_{k-1,n} \end{bmatrix}.$$

This is all that is needed for a look-ahead Levinson step.

We now give more detailed versions of Algorithm 7.1. The first one is a look-ahead Levinson algorithm. The look-ahead strategy in these algorithms is very simple: we only check the smallest singular value of the coefficient matrix $\mathbf{M}_{k,n}$ arising in the linear systems we have to solve for the recurrence coefficients. We could add other criteria also, but want to present the algorithms in its simplest form here. A more detailed discussion about look-ahead strategies can be found in Section 11.1. Here, we have also included an upper bound $k_{\max}$ on the maximal size of a look-ahead step.

Algorithm 7.2: Look-ahead Levinson-type algorithm for adjacent rows in the Padé table using anti-diagonally regular pairs of LOPs and ROPs.

INPUT: $h \in \mathcal{L}$, m, N, $k_{\max}$;

OUTPUT: *denominator* $q_L^{\uparrow}$ *of an anti-diagonally regular* $(m-1, L)$ *Padé form of* h *for largest possible* $L \leq N$;

Set $n = 0$, $l = 0$, $q_0^{\uparrow} = q_0 = 1$, $\pi_{0,n}^{\uparrow} = \mu_{m-1}$, $\varepsilon_{n,n}^{\uparrow} = \pi_{0,n} = \mu_m$, $\varepsilon_{n,n} = \mu_{m+1}$;

column_regular = $(|\varepsilon_{n,n}^{\uparrow}| > tol)$;

if not column_regular*:*

  set $q_0^{\leftarrow} = 0$, $\pi_{0,n}^{\leftarrow} = 1$, $\varepsilon_{n,n}^{\leftarrow} = -1$, $\sigma_1 = |\varepsilon_{n,n}^{\uparrow}|$;

while $n < N$

  if column_regular

    set $\varepsilon_{n+1,n+1}^{\leftarrow} = \varepsilon_{n,n}$, $\pi_{0,n+1}^{\leftarrow} = \pi_{0,n}$, *and* $q_{n+1}^{\leftarrow} = q_n$;

    compute $\gamma_0^{\uparrow} = -\pi_{0,n}^{\uparrow}/\pi_{0,n}$ *and* $q_{n+1}^{\uparrow} = \zeta q_n^{\uparrow} + q_n\gamma_0^{\uparrow}$;

    set $\varepsilon_{n+1,n+1}^{\uparrow} = \pi_{0,n+1} = \varepsilon_{n,n}(1 - \gamma_0^{\uparrow}/\gamma_0)$ $(= \varepsilon_{n,n}^{\uparrow} + \varepsilon_{n,n}\gamma_0^{\uparrow})$;

    compute $\pi_{0,n+1}^{\uparrow} = \Pi_{m-1}(hq_{n+1}^{\uparrow})$;

    set $n = n+1$, $l = l+1$;

    column_regular = $(|\varepsilon_{n,n}^{\uparrow}| > tol)$, $\sigma_1 = |\varepsilon_{n,n}^{\uparrow}|$;

    if column_regular

      compute $\gamma_0 = -\varepsilon_{n-1,n-1}/\varepsilon_{n-1,n-1}^{\uparrow}$ *and* $q_n = \zeta q_{n-1}^{\uparrow}\gamma_0 + q_{n-1}$;

      compute $\varepsilon_{n,n} = \Pi_{m+n+1}(hq_n)$;

  else

    regular = *false*, $k = 1$,

    compute $\varepsilon_{n+k,n}^{\uparrow} = \Pi_{m+n+k}(hq_n^{\uparrow})$ *and* $\varepsilon_{n+k,n}^{\leftarrow}$ *from* (7.16);

    while ($k < k_{\max}$ *and* $k + n \leq N$ *and not* regular)

      (*construct matrix* $\mathbf{M}_{k,n}$)

      compute $\varepsilon_{n+k+1,n}^{\uparrow} = \Pi_{m+n+k+1}(hq_n^{\uparrow})$ *and* $\pi_{k,n}^{\uparrow} = \Pi_{m-k-1}(hq_n^{\uparrow})$;

      compute $\varepsilon_{n+k+1,n}^{\leftarrow}$ *from* (7.16) *and* $\pi_{k,n}^{\leftarrow}$ *from* (7.17);

      set $k = k+1$; $\sigma_k = \sigma_{\min}(\mathbf{M}_{k,n})$, *where* $\mathbf{M}_{k,n}$ *is defined in* (7.8);

      regular = $(\sigma_k > tol)$;

    if not regular

      (*use optimal* k)*:* $k = \text{argmax}\{\sigma_j,\ 1 \leq j \leq k\}$;

      if $\sigma_k = 0$;

        set $L = n$, *return; matrix is singular;*

      column_regular = $(k = 1)$;

      if column_regular

        compute $\gamma_0 = -\varepsilon_{n-1,n-1}/\varepsilon_{n-1,n-1}^{\uparrow}$ *and* $q_n = \zeta q_{n-1}^{\uparrow}\gamma_0 + q_{n-1}$;

        compute α_0, β_0 *from* (7.12) *and* $\varepsilon_{n,n} = \alpha_0\varepsilon_{n+1,n}^{\leftarrow} + \beta_0\varepsilon_{n+1,n}^{\uparrow}$;

    if ($n + k \leq N$ *and not* column_regular)

      (*compute anti-diagonally regular* $(-1, n+k)$ *Padé form of* h)

      set $\beta_k^{\uparrow} = 1$, *compute* $\alpha_{k-1}^{\uparrow}$ *from* (7.6) *and solve* (7.7) *for* $\alpha_j^{\uparrow}$, $\beta_j^{\uparrow}$;

set $u_k^{\uparrow} = \sum_{j=0}^{k-1} \alpha_j^{\uparrow}\zeta^j$, $v_k^{\uparrow} = \sum_{j=0}^{k} \beta_j^{\uparrow}\zeta^j$ *and compute* $q_{n+k}^{\uparrow} = q_n^{\leftarrow} u_k^{\uparrow} + q_n^{\uparrow} v_k^{\uparrow}$;
compute $\pi_{0,n+k}^{\uparrow} = \Pi_{m-1}(hq_{n+k}^{\uparrow})$ *and* $\varepsilon_{n+k,n+k}^{\uparrow}$ *from* (7.14);
column_regular $= (|\varepsilon_{n+k,n+k}^{\uparrow}| > tol)$;
if column_regular
(*compute column-regular* $(0, n+k)$ *Padé form of* h)
compute α_0, β_0 *from* (7.12) *and solve* (7.13) *for* α_j, β_j;
set $u_k = \sum_{j=0}^{k-1} \alpha_j\zeta^j$, $v_k = \sum_{j=0}^{k} \beta_j\zeta^j$ *and compute* $q_{n+k} = q_n^{\leftarrow} u_k + q_n^{\uparrow} v_k$;
set $\varepsilon_{n+k,n+k} = \Pi_{m+n+k+1}(hq_{n+k})$;
else
set $\pi_{0,n+k}^{\leftarrow} = 1$, *solve* (7.9) *for* $\alpha_j^{\leftarrow}, \beta_j^{\leftarrow}$, *and compute* $\varepsilon_{n+k,n+k}^{\leftarrow}$ *from* (7.15);
set $u_k^{\leftarrow} = \sum_{j=0}^{k-2} \alpha_j^{\leftarrow}\zeta^j$, $v_k^{\leftarrow} = \sum_{j=0}^{k-1} \beta_j^{\leftarrow}\zeta^j$ *and compute* $q_{n+k}^{\leftarrow} = q_n^{\leftarrow} u_k^{\leftarrow} + q_n^{\uparrow} v_k^{\leftarrow}$;
set $n = n+k$, $l = l+1$

The Schur-type algorithm looks a little simpler, since all the quantities for computing the small two-point Padé forms are available and need not be evaluated by inner products or some tricky recursions.

Algorithm 7.3: Optimized look-ahead Schur algorithm for adjacent rows in the Padé table.
INPUT: $h \in \mathcal{L}$, m, N, $k_{\max}$;
OUTPUT: *numerator* $p_L^{\uparrow}$ *and residual* $e_L^{\uparrow}$ *of anti-diagonally regular* $(m-1, L)$ *Padé form of* h *for largest possible* $L \le N$;
Set $n = 0$, $l = 0$, $p_0^{\uparrow} = \Pi_{-\infty:m-1}\, h$, $e_0^{\uparrow} = \Pi_{m:\infty}\, h$; *set* $p_0 = \Pi_{-\infty:m} h$, $e_0 = \Pi_{m+1:\infty}\, h$;
column_regular $= (|\varepsilon_{n,n}^{\uparrow}| > tol)$;
if not column_regular:
set $p_0^{\leftarrow} = 1$, $e_0^{\leftarrow} = -1$, $\sigma_1 = |\varepsilon_{n,n}^{\uparrow}|$;
while $n < N$
if column_regular
set $e_{n+1}^{\leftarrow} = e_n$, $p_{n+1}^{\leftarrow} = p_n$;
compute $\gamma_0^{\uparrow} = -\pi_{0,n}^{\uparrow}/\pi_{0,n}$, $p_{n+1}^{\uparrow} = \zeta p_n^{\uparrow} + p_n\gamma_0^{\uparrow}$ *and* $e_{n+1}^{\uparrow} = e_n^{\uparrow} + e_n\gamma_0^{\uparrow}$;
set $n = n+1$, $l = l+1$;
column_regular $= (|\varepsilon_{n,n}^{\uparrow}| > tol)$, $\sigma_1 = |\varepsilon_{n,n}^{\uparrow}|$;
if column_regular
compute $\gamma_0 = -\varepsilon_{n-1,n-1}/\varepsilon_{n-1,n-1}^{\uparrow}$;
set $p_n = \zeta p_{n-1}^{\uparrow}\gamma_0 + p_{n-1}$ *and* $e_n = \zeta^{-1}(e_{n-1}^{\uparrow}\gamma_0 + e_{n-1})$;
else
regular $=$ *false*, $k = 1$,
compute $\varepsilon_{n+k,n}^{\uparrow} = \Pi_{n+k}(hq_n^{\uparrow})$ *and* $\varepsilon_{n+k,n}^{\leftarrow}$ *from* (7.16);
while ($k < k_{\max}$ *and* $n+k \le N$ *and not* regular)
(*construct matrix* $\mathbf{M}_{k,n}$)
set $k = k+1$;
$\sigma_k = \sigma_{\min}(\mathbf{M}_{k,n})$, *where* $\mathbf{M}_{k,n}$ *is defined in* (7.8);

regular = ($\sigma_k > tol$);
if not regular
  (*use optimal* k): $k = \mathrm{argmax}\{\sigma_j,\ 1 \leq j \leq k\}$;
  if $\sigma_k = 0$;
    set $L = n$, *return; matrix is singular;*
  column_regular = ($k = 1$);
  if column_regular
    compute $\gamma_0 = -\varepsilon_{n-1,n-1}/\varepsilon^{\uparrow}_{n-1,n-1}$;
    $p_n = \zeta p^{\uparrow}_{n-1}\gamma_0 + p_{n-1}$ *and* $e_n = \zeta^{-1}(e^{\uparrow}_{n-1}\gamma_0 + e_{n-1})$;
if ($n + k \leq N$ *and not* column_regular)
  (*compute anti-diagonally regular* $(-1, n+k)$ *Padé form of* h)
  set $\beta^{\uparrow}_k = 1$, *compute* $\alpha^{\uparrow}_{k-1}$ *from* (7.6) *and solve* (7.7) *for* $\alpha^{\uparrow}_j$, $\beta^{\uparrow}_j$;
  set $u^{\uparrow}_k = \sum_{j=0}^{k-1} \alpha^{\uparrow}_j \zeta^j$, $v^{\uparrow}_k = \sum_{j=0}^{k} \beta^{\uparrow}_j \zeta^j$;
  compute $p^{\uparrow}_{n+k} = p^{\leftarrow}_n u^{\uparrow}_k + p^{\uparrow}_n v^{\uparrow}_k$ *and* $e^{\uparrow}_{n+k} = \zeta^{-k}(e^{\leftarrow}_n u^{\uparrow}_k + e^{\uparrow}_n v^{\uparrow}_k)$;
  column_regular = ($|\varepsilon^{\uparrow}_{n+k,n+k}| > tol$);
  if column_regular
    (*compute column-regular* $(0, n+k)$ *Padé form of* h)
    compute α_0, β_0 *from* (7.12) *and solve* (7.13) *for* α_j, β_j;
    set $u_k = \sum_{j=0}^{k-1} \alpha_j \zeta^j$, $v_k = \sum_{j=0}^{k} \beta_j \zeta^j$;
    compute $p_{n+k} = p^{\leftarrow}_n u_k + p^{\uparrow}_n v_k$ *and* $e_{n+k} = \zeta^{-k-1}(e^{\leftarrow}_n u_k + e^{\uparrow}_n v_k)$;
  else
    solve (7.9) *for* $\alpha^{\leftarrow}_j, \beta^{\leftarrow}_j$ *and set* $u^{\leftarrow}_k = \sum_{j=0}^{k-2} \alpha^{\leftarrow}_j \zeta^j$, $v^{\leftarrow}_k = \sum_{j=0}^{k-1} \beta^{\leftarrow}_j \zeta^j$;
    compute $p^{\leftarrow}_{n+k} = p^{\leftarrow}_n u^{\leftarrow}_k + p^{\uparrow}_n v^{\leftarrow}_k$ *and* $e^{\leftarrow}_{n+k} = \zeta^{-k}(e^{\leftarrow}_n u^{\leftarrow}_k + e^{\uparrow}_n v^{\leftarrow}_k)$;
  set $n = n + k$, $l = l + 1$

The operation counts for look-ahead steps in Algorithms 7.2 and 7.3 are listed in Table 7.1. The SAXPYs for the Levinson algorithm result from $2k$ SAXPYs for $q^{\uparrow}_{n+k}$, $2(k-1)$ for $q^{\leftarrow}_{n+k}$, and $2k$ for q_{n+k}. For the Schur algorithm we need $4k$ SAXPYs to compute $p^{\uparrow}_{n+k}$ and $e^{\uparrow}_{n+k}$, $4(k-1)$ to compute $p^{\leftarrow}_{n+k}$ and $e^{\leftarrow}_{n+k}$, and $4k$ for p_{n+k} and e_{n+k}.

Note that the operation counts in Table 7.1 are valid only in a look-ahead step but not in a regular step, since we use recurrences based on column-regular steps whenever possible. If we would base our algorithm on anti-diagonally regular pairs only (as pro-

Operations in a block of size $k > 1$	look-ahead Levinson		look-ahead Schur	
type of step	(7.3)	(7.4)	(7.3)	(7.4)
inner products	$2k$	$2k+1$	–	–
SAXPYs	$2(2k-1)$	$4k$	$4(2k-1)$	$8k$

Table 7.1: Operation counts for Algorithms 7.2 and 7.3

posed in [121]) we would have an overhead of one SAXPY for the Levinson algorithm and two for the Schur algorithm, even in a block of size one. Our optimized algorithm has no overhead in a regular step.

The classical Levinson algorithm requires two SAXPYs and two inner products per step, which makes $2k$ for a block of size k. Thus the overhead is $2(k-1)$ SAXPYs. The classical Schur algorithm requires four SAXPYs per step; hence the overhead is $4(k-1)$ SAXPYs here.

8. FORMALLY BIORTHOGONAL POLYNOMIALS

The previous chapter dealt with computing anti-diagonally regular and column-regular pairs in two adjacent rows of the Padé table of a formal Laurent series. We have seen before that reflected denominators of Padé forms on a certain diagonal of the Padé table of a formal power series are formally orthogonal polynomials with respect to a linear form defined by its moments, which are the coefficients of the power series. For Padé forms on adjacent rows things become a little more complicated. The denominators of Padé forms now correspond to polynomials formally biorthogonal with respect to a bilinear form defined again via moments which are identical to the coefficients of the Laurent series [19, 20, 22, 62]. Therefore, we will generalize the definition of underdetermined Padé forms and define left and right underdetermined Padé forms, which are closely related to left and right inner formally biorthogonal polynomials [42, 62]. We can then show that these formally biorthogonal polynomials define an inverse block LDU decomposition of a Toeplitz matrix and that a block LDU decomposition can be obtained from residuals and numerators. The resulting algorithms therefore generalize the classical Levinson and Schur algorithm in such a way that they use the classical recurrences whenever possible and perform look-ahead steps of minimal length. In [120], Van Barel and Bultheel propose an algorithm to compute right biorthogonal matrix polynomials, which is applicable to block Toeplitz matrices with square blocks. However, their algorithms always use anti-diagonally regular pairs and hence they are more expensive than the classical algorithms even if no look-ahead is necessary. A generalization of our more efficient algorithm to the block case with square blocks is straightforward.

The last section of this chapter contains a generalization of the Bareiss-Delosme-Ipsen matrix formulation [6, 32, 81] of our look-ahead Levinson and Schur algorithms. This generalization will provide an efficient way for solving Toeplitz linear systems with the Schur algorithm as we will see later in Section 11.2. For look-ahead algorithms based on column-regular pairs only, such a matrix formulation was derived in [67]. Here we will extend it further to algorithms which are based on column-regular pairs in generic steps (steps of size one) and on anti-diagonally regular steps otherwise. The derivation is different from the one in [67] which was done solely from a linear algebra point of view.

8.1 Formally biorthogonal polynomials and Padé approximation

Given $h \in \mathcal{L}$, or, equivalently, the doubly infinite sequence $\{\mu_k\}_{k=-\infty}^{\infty}$ of coefficients, we define a bilinear functional $\langle \cdot, \cdot \rangle$ on $\mathcal{P} \times \mathcal{P}$ by its values

$$\langle \zeta^i, \zeta^j \rangle := \mu_{i-j}, \quad (i,j) \in \mathbb{N} \times \mathbb{N}. \tag{8.1}$$

Using the notation introduced in Section 5.1, for $s, t \in \mathcal{P}$ it is well known and easily verified that

$$\langle s, t \rangle = \sum_{i,j=0}^{\infty} \sigma_i \mu_{i-j} \tau_j = \mathbf{s}^T \mathbf{T}\, \mathbf{t}, \tag{8.2}$$

where $\mathbf{T} := [\mu_{i-j}]_{i,j=0}^{\infty}$ is the Toeplitz operator with symbol $h(\zeta) = \sum_{-\infty}^{\infty} \mu_k \zeta^k$.

Definition 8.1: *The polynomial $s \in \mathcal{P}_n \backslash \mathcal{P}_{n-1}$ is called an nth* **left formally biorthogonal polynomial (LOP)***, and the polynomial $t \in \mathcal{P}_n \backslash \mathcal{P}_{n-1}$ is called an nth* **right formally biorthogonal polynomial (ROP)** *if*

$$\langle s, \zeta^j \rangle = 0, \qquad j = 0, \ldots, n-1, \tag{8.3}$$

$$\langle \zeta^i, t \rangle = 0, \qquad i = 0, \ldots, n-1, \tag{8.4}$$

respectively. An nth LOP or ROP is said to be **regular** *if it is uniquely determined up to scaling; otherwise, it is* **singular***.*

In terms of the reflected polynomial $s^\star$ defined in (5.4), the conditions (8.3) and (8.4) can be written as

$$\Pi_{1:n}(hs^\star) = 0 \quad \text{and} \quad \Pi_{0:n-1}(ht) = 0,$$

respectively.

Thus the reflected polynomial $s^\star$ of an nth LOP s is equal to the denominator q_n of a $(0,n)$ Padé form (p_n, q_n) of h, while an nth ROP t is equal to the denominator $q_n^\dagger$ of a $(-1,n)$ Padé form $(p_n^\dagger, q_n^\dagger)$; see also [19, 20]. From now on we therefore denote an nth LOP by $q_n^\star$ and an nth ROP by $q_n^\dagger$. Since both the nth LOP and the nth ROP need to have exact degree n they can be normalized to be monic. This normalization is the same as (2.40) we used before. Then the conditions (8.3) and (8.4), when expressed in terms of the polynomial coefficients, become exactly the Yule-Walker equations (2.30) and (2.37) with $m = 0$ and $\rho_{0,n} = \rho_{n,n}^\dagger = 1$. The required uniqueness of an nth regular normalized LOP is thus seen to be equivalent to the nonsingularity of $\mathbf{T}_n := \mathbf{T}_{0,n}$. The same is true for an nth regular ROP. In particular, it follows that the nth LOP is regular if and only if the nth ROP is and this is equivalent to the $(0,n)$ Padé form being regular (Lemma 2.8) or the $(-1,n)$ Padé form being anti-diagonally regular (Lemma 2.9).

In the generic case, where $q_n^\star$ and $q_n^\dagger$ are regular for every n, these polynomials are called *Szegő polynomials* [7, 85]. When $\mathbf{T}$ is symmetric, $q_n^\star = q_n^\dagger$. When $\mathbf{T}$ is Hermitian, $q_n^\star = \bar{q}_n^\dagger$, where the bar means conjugation of the coefficients. Szegő only considered the special case where $\mathbf{T}$ is additionally positive definite. Then the polynomials are classical polynomials orthogonal on the unit circle.

8.2 Inner biorthogonal polynomials and underdetermined Padé forms

In the following we denote by $\{n_j\}_{j\geq 0}$ a monotone increasing sequence of indices for which anti-diagonally regular $(-1,n)$ Padé forms exist. It is not requested to contain *all* anti-diagonally regular $(-1,n)$ Padé forms; in practice we want to include only well-conditioned ones (Definition 2.6). Our aim is to fill the gaps such that the full sets of polynomials $q_n^\uparrow$ and $q_n^\star$ lead to a block LDU decomposition of $\mathbf{T}^{-1}$ with a well-conditioned block diagonal matrix $\mathbf{D}$. In many situations it is desirable to compute this factorization and not only the last pairs of polynomials q_{N-1} and $q_{N-1}^\uparrow$ or $q_N^\leftarrow$ and $q_N^\uparrow$ that allow us to represent $\mathbf{T}_N^{-1}$ by a suitable inversion formula from Section 2.6.

Definition 8.2: *For $n_l = n < n+k < n_{l+1}$, an $(n+k)$th* **inner LOP** *s_{n+k} and an $(n+k)$th* **inner ROP** *t_{n+k} are any polynomials of exact degree $n+k$ satisfying*

$$\begin{aligned} \langle s_{n+k}, \zeta^i\rangle &= 0, \qquad i = 0\ldots, n-1, && (8.5)\\ \langle \zeta^i, t_{n+k}\rangle &= 0, \qquad i = 0\ldots, n-1, && (8.6)\end{aligned}$$

respectively.

Next we give equivalent conditions for characterizing inner polynomials.

Lemma 8.1: *Let $h \in \mathcal{L}$ and the associated bilinear functional $\langle\cdot,\cdot\rangle$ specified by* (8.1) *be given, and let $k, n \geq 0$. For $q_{n+k} \in \mathcal{P}_{n+k}$ the following statements are equivalent:*

(i) $\langle q_{n+k}^\star, \zeta^i\rangle = 0$ *for* $i = 0,\ldots,n-1$;

(ii) $\Pi_{k+1:n+k}(hq_{n+k}) = 0$;

(iii) *there exists $p_{n+k} \in \mathcal{L}_k^*$ such that*

$$hq_{n+k} - p_{n+k} = \zeta^{n+k+1} e_{n+k} = O_+(\zeta^{n+k+1}). \qquad (8.7)$$

Proof. The statements can be proved by explicitly computing the coefficients of hq_{n+k} and the modified moments of the bilinear form:

$$(hq_{n+k})(\zeta) = \sum_{i=-\infty}^{\infty}\sum_{\ell=0}^{n+k} \mu_{i-l}\rho_{\ell,n+k}\zeta^i \qquad (8.8)$$

and

$$\langle q_{n+k}^*, \zeta^{n+k-i}\rangle = \sum_{\ell=0}^{n+k} \mu_{i-\ell}\rho_{\ell,n+k}, \qquad i \leq n+k. \qquad (8.9)$$

This proves that the first two statements are equivalent. To prove the equivalence to the third statement we define $p_{n+k} = \Pi_{-\infty:k}(hq_{n+k})$ and $e_{n+k} = \zeta^{-n-k-1}\Pi_{n+k+1:\infty}(hq_{n+k})$. □

If n is a regular index, then setting $k=0$ in the previous Lemma shows that

$$\begin{aligned} \langle q_n^*, \zeta^i\rangle &= 0 \qquad \text{for} \quad i = 0,\ldots,n-1,\\ \langle q_n^{\leftarrow *}, \zeta^i\rangle &= 0 \qquad \text{for} \quad i = 0,\ldots,n-2.\end{aligned}$$

Thus, $q_n^* \in \mathcal{P}_n$ is a regular nth LOP if $q_n(0) \neq 0$ and $q_n^{\leftarrow *} \in \mathcal{P}_{n-1}$ is left orthogonal to all polynomials of degree at most $n-2$. The reader should keep in mind that if $n-1$ is not a regular index, then $q_n^{\leftarrow *}$ does not have full degree $n-1$ and thus is not a regular $(n-1)$st LOP. In particular, it is not a multiple of the $(n-1)$st inner LOP q_{n-1}^*.

Lemma 8.2: *Let $h \in \mathcal{L}$ and the associated bilinear functional $\langle \cdot, \cdot \rangle$ specified by* (8.1) *be given, and let $k, n \geq 0$. For $q_{n+k}^{\uparrow} \in \mathcal{P}_{n+k}$ the following statements are equivalent:*

(i) $\langle \zeta^i, q_{n+k}^{\uparrow} \rangle = 0$ *for* $i = 0, \ldots, n-1$;

(ii) $\Pi_{0:n-1}(h q_{n+k}^{\uparrow}) = 0$;

(iii) *there exists* $p_{n+k}^{\uparrow} \in \mathcal{L}_{-1}^*$ *such that*

$$h q_{n+k}^{\uparrow} - p_{n+k}^{\uparrow} = \zeta^n e_{n+k}^{\uparrow} = O_+(\zeta^n). \tag{8.10}$$

Proof. In view of (8.8) and

$$\langle \zeta^i, q_{n+k}^{\uparrow} \rangle = \sum_{\ell=0}^{n+k} \mu_{i-\ell} \rho_{\ell, n+k}^{\uparrow}, \qquad i \geq 0, \tag{8.11}$$

the first two statements are equivalent. The remaining equivalence follows by defining $p_{n+k}^{\uparrow} = \Pi_{-\infty:-1}(h q_{n+k}^{\uparrow})$ and $e_{n+k}^{\uparrow} = \zeta^{-n} \Pi_{n:\infty}(h q_{n+k}^{\uparrow})$. □

Again, if n is a regular index, then setting $k = 0$ in the previous Lemma shows that

$$\langle \zeta^i, q_n^{\uparrow} \rangle = 0 \qquad \text{for} \quad i = 0, \ldots, n-1,$$

which is equivalent to $q_n^{\uparrow} \in \mathcal{P}_n$ being a regular nth ROP if it has full degree n.

Definition 8.3: *For $n_l = n < n+k < n_{l+1}$ and $h \in \mathcal{L}$, any pair $(p_{n+k}, q_{n+k}) \in \mathcal{L}_k^* \times \mathcal{P}_{n+k}$ with $q_{n+k}(0) \neq 0$ satisfying* (8.7) *is called a* $(0, n+k)$ **left underdetermined Padé form** *and e_{n+k} is called its* **residual**.

Any pair $(p_{n+k}^{\uparrow}, q_{n+k}^{\uparrow}) \in \mathcal{L}_{-1}^* \times \mathcal{P}_{n+k}$ with $\partial q_{n+k}^{\uparrow} = n+k$ satisfying (8.10) *is called a* $(-1, n+k)$ **right underdetermined Padé form** *and $e_{n+k}^{\uparrow}$ is called its* **residual**.

The following Lemma shows the relations between the coefficients of underdetermined Padé forms and modified moments of the bilinear form.

Lemma 8.3: *Let n be a regular index or $k = 0$.*

(i) *If (p_{n+k}, q_{n+k}) is a $(0, n+k)$ left underdetermined Padé form with residual e_{n+k}, or a $(0, n)$ Padé form if $k = 0$, then*

$$p_{n+k} = \sum_{i=-\infty}^{k} \langle q_{n+k}^*, \zeta^{n+k-i} \rangle \zeta^i \quad \text{and} \quad e_{n+k} = \sum_{i=0}^{\infty} \langle \zeta^{i+1} q_{n+k}^*, 1 \rangle \zeta^i.$$

(ii) *If $(p_{n+k}^{\uparrow}, q_{n+k}^{\uparrow})$ is a $(-1, n+k)$ right underdetermined Padé form with residual $e_{n+k}^{\uparrow}$, or a $(-1, n)$ Padé form if $k = 0$, then*

$$p_{n+k}^{\uparrow} = \sum_{i=-\infty}^{-1} \langle 1, \zeta^{i+1} q_{n+k}^{\uparrow} \rangle \zeta^i \quad \text{and} \quad e_{n+k}^{\uparrow} = \sum_{i=0}^{\infty} \langle \zeta^{n+i}, q_{n+k}^{\uparrow} \rangle \zeta^i.$$

Proof. The equalities (8.8), (8.9), and (8.11) yield

$$\Pi_i(hq_{n+k}) = \begin{cases} \langle q^*_{n+k}, \zeta^{n+k-i}\rangle, & i \le n+k, \\ \langle \zeta^i, q_{n+k}\rangle, & i \ge 0. \end{cases}$$

From $\mathbf{T}^T = \mathbf{JTJ}$, where $\mathbf{J}$ is the unit antidiagonal matrix, it is easily verified that for arbitrary polynomials $s, t \in \mathcal{P}_n$,

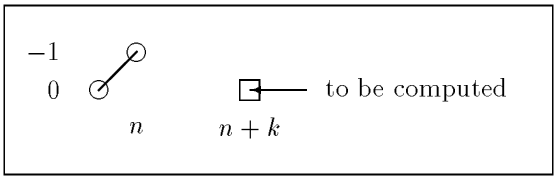
$$\langle s, t\rangle = \langle \zeta^n t(\zeta^{-1}), \zeta^n s(\zeta^{-1})\rangle. \tag{8.12}$$

Hence,

$$\langle \zeta^i, q_{n+k}\rangle = \langle \zeta^{i-n-k} q^*_{n+k}, 1\rangle \qquad \text{for} \quad i \ge n+k.$$

The proof of Part (ii) is done analogously. □

In general, inner LOPs and ROPs are not uniquely determined even if suitably normalized. The following theorem shows how to construct inner LOPs from an anti-diagonally regular pair. In the Padé table, the Padé forms involved in this recurrence are



(8.13)

where the square represents the $(0, n+k)$ left underdetermined Padé form we wish to compute and the two circles show the anti-diagonally regular pair of Padé forms from which it is computed.

Theorem 8.4: *Let $(p_n^{\uparrow}, q_n^{\uparrow})$ be an anti-diagonally regular $(-1, n)$ Padé form, and let $(p_n^{\leftarrow}, q_n^{\leftarrow})$ be its lower left neighbor, i.e., a $(0, n-1)$ Padé form. Moreover, let*

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ \zeta^{k+1} e_{n+k} \end{bmatrix} = \begin{bmatrix} p_n^{\leftarrow} & p_n^{\uparrow} \\ q_n^{\leftarrow} & q_n^{\uparrow} \\ e_n^{\leftarrow} & e_n^{\uparrow} \end{bmatrix} \begin{bmatrix} u_k^{(n)} \\ v_k^{(n)} \end{bmatrix}, \tag{8.14}$$

where $(u_k^{(n)}, v_k^{(n)}) \in \mathcal{P}_k^2$ is a solution of

$$e_n^{\leftarrow} u_k^{(n)} + e_n^{\uparrow} v_k^{(n)} = O_+(\zeta^{k+1}) \tag{8.15}$$

with

$$(q_n^{\leftarrow} u_k^{(n)} + q_n^{\uparrow} v_k^{(n)})(0) \ne 0. \tag{8.16}$$

Then, for $k = 0$, (p_n, q_n) is a regular $(0, n)$ Padé form with residual e_n, and for $k \ge 1$, (p_{n+k}, q_{n+k}) is a left underdetermined $(0, n+k)$ Padé form with residual e_{n+k}.

Proof. We need to show that $p_{n+k} \in \mathcal{L}_k^*$, $q_{n+k} \in \mathcal{P}_{n+k}$, $q_{n+k}(0) \neq 0$, and that (8.7) holds true. From $(u_k^{(n)}, v_k^{(n)}) \in \mathcal{P}_k^2$, $p_n^{\leftarrow} \in \mathcal{L}_0^*$, and $p_n^{\uparrow} \in \mathcal{L}_{-1}^*$, we obtain $p_{n+k} \in \mathcal{L}_k^*$, and similarly, $q_{n+k} \in \mathcal{P}_{n+k}$ since $\partial q_n^{\leftarrow} \leq n-1$ and $\partial q_n^{\uparrow} \leq n$. Moreover, a solution of (8.15) with (8.16) exists, since by Lemma 2.9, $q_n^{\leftarrow}(0) \neq 0$ or $q_n^{\uparrow}(0) \neq 0$.

Next assume that $u_k^{(n)}, v_k^{(n)} \in \mathcal{P}_k$ are chosen according to (8.15). Then we have

$$hq_{n+k} - p_{n+k} = (hq_n^{\leftarrow} - p_n^{\leftarrow})u_k^{(n)} + (hq_n^{\uparrow} - p_n^{\uparrow})v_k^{(n)} = \zeta^n(e_n^{\leftarrow}u_k^{(n)} + e_n^{\uparrow}v_k^{(n)}) = O_+(\zeta^{n+k+1}),$$

and e_{n+k} satisfies (8.7). □

Next we show how one can construct a particularly simple set of inner LOPs.

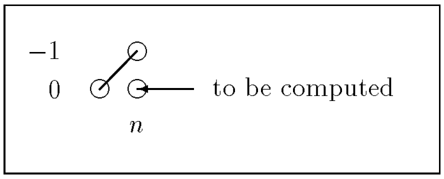
Corollary 8.5: *Let the assumptions of Theorem* 8.4 *be valid and let* $e_n^{\leftarrow}(0) \neq 0$. *Then a unique solution of* (8.15), (8.16) *exists with* $v_k^{(n)} \equiv \beta_0^{(n)} \neq 0$.

Proof. If $e_n^{\leftarrow}(0) \neq 0$, then a solution of (8.15) exists, and hence it is sufficient to show that the solution satisfies $\rho_{0,n+k} = q_{n+k}(0) \neq 0$.

Let $\alpha_0^{(n)} = u_k^{(n)}(0)$, $\varepsilon_{n,n}^{\leftarrow} = e_n^{\leftarrow}(0)$, and $\varepsilon_{n,n}^{\uparrow} = e_n^{\uparrow}(0)$. Comparing the coefficients for ζ^{n+k} in the recursion for q_{n+k} and the constant terms in (8.15) leads to the linear system (7.10). The coefficient matrix is nonsingular by Lemma 2.9. Therefore, if $\rho_{0,n+k}$ vanishes, then it would follow that $\alpha_0^{(n)} = \beta_0^{(n)} = 0$, which contradicts the assumptions in Corollary 8.5. Hence, $\rho_{0,n+k} \neq 0$. □

The assumptions of the previous corollary are satisfied if a $(0, n)$ Padé form (p_n, q_n) is row-regular, *i.e.*, if $(p_n^{\leftarrow}, q_n^{\leftarrow})$ belongs to the last column of a block of the Padé table (Lemma 2.6). This is the only case where we have to compute inner polynomials, because otherwise, since $(p_n^{\uparrow}, q_n^{\uparrow})$ is anti-diagonally regular, (p_n, q_n) is column-regular, which corresponds to the situation illustrated in Picture (7.4). Here, our algorithm switches back to the classical Levinson or Schur algorithm. We clearly do not have to compute inner polynomials then.

Note that if look-ahead steps are necessary, then we always use anti-diagonally regular pairs to proceed. However, pairs of regular formally biorthogonal polynomials of degree n correspond to an anti-diagonally regular $(-1, n)$ Padé form and its lower neighbor. Hence, such a pair of regular biorthogonal polynomials has, with a pair of anti-diagonally regular Padé forms, only the denominator of the upper right Padé form in common. Moreover, it need not correspond to a column-regular pair: the two Padé approximants may lie in the same block of the Padé table. After a look-ahead step, we should first compute the $(0, n)$ Padé form (p_n, q_n) via the recurrences of Theorem 8.4 for $k = 0$. In our algorithm we used the normalization $\rho_{0,n} = q_n(0) = 1$. Then, the recurrence coefficients $(u_0^{(n)}, v_0^{(n)}) = (\alpha_0^{(n)}, \beta_0^{(n)})$ are just the unique solutions of (7.10) given by (7.12). The following picture illustrates this recurrence:



(8.17)

After we have computed (p_n, q_n), we set $\gamma_0^{(n)} = \alpha_0^{(n)}$. Then it is easily seen from (8.15) that the coefficients $\gamma_j^{(n)}$ of

$$u_k^{(n)}(\zeta) = \sum_{j=0}^{k} \gamma_j^{(n)} \zeta^j \tag{8.18}$$

are determined by the following lower triangular Toeplitz system

$$\begin{bmatrix} \varepsilon_{n,n}^{\leftarrow} & & \\ \vdots & \ddots & \\ \varepsilon_{n+k-1,n}^{\leftarrow} & \cdots & \varepsilon_{n,n}^{\leftarrow} \end{bmatrix} \begin{bmatrix} \gamma_1^{(n)} \\ \vdots \\ \gamma_k^{(n)} \end{bmatrix} = - \begin{bmatrix} \varepsilon_{n+1,n}^{\leftarrow} \\ \vdots \\ \varepsilon_{n+k,n}^{\leftarrow} \end{bmatrix} \gamma_0^{(n)} - \begin{bmatrix} \varepsilon_{n+1,n}^{\uparrow} \\ \vdots \\ \varepsilon_{n+k,n}^{\uparrow} \end{bmatrix} \beta_0^{(n)}. \tag{8.19}$$

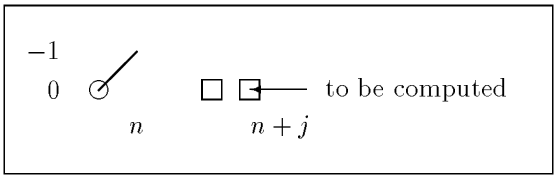
Therefore, $u_k^{(n)}$ is obtained from the recurrence

$$u_0^{(n)} = \gamma_0^{(n)}, \qquad u_j^{(n)} = u_{j-1}^{(n)} + \gamma_j^{(n)} \zeta^j, \qquad j = 1, \ldots, k,$$

and hence

$$\begin{bmatrix} p_{n+j} \\ q_{n+j} \\ \zeta^{j+1} e_{n+j} \end{bmatrix} = \begin{bmatrix} p_{n+j-1} \\ q_{n+j-1} \\ \zeta^j e_{n+j-1} \end{bmatrix} + \begin{bmatrix} p_n^{\leftarrow} \\ q_n^{\leftarrow} \\ e_n^{\leftarrow} \end{bmatrix} \gamma_j^{(n)} \zeta^j, \qquad j = 1, \ldots, k. \tag{8.20}$$

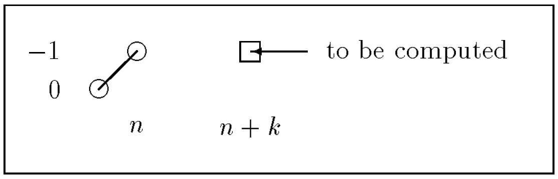
Here is an illustration of this recurrence, which shows that we have eliminated the anti-diagonally regular Padé form of index n and replaced it by the $(0, n+j-1)$st (left underdetermined) Padé form to compute the $(0, n+j)$th left underdetermined Padé form. This reduced the computational cost to only one SAXPY of appropriate length.



A simplification for (8.19) which can be verified directly from (8.20) is

$$\varepsilon_{n,n}^{\leftarrow} \gamma_j^{(n)} = -\varepsilon_{n+j-1,n+j-1}, \qquad j = 1, \ldots, k. \tag{8.21}$$

The next theorem states the analogous result for right underdetermined Padé forms. It is illustrated by



(8.22)

Theorem 8.6: *Let* $(p_n^{\uparrow}, q_n^{\uparrow})$ *be an anti-diagonally regular* $(-1, n)$ *Padé form, and let* $(p_n^{\leftarrow}, q_n^{\leftarrow})$ *be its lower left neighbor, i.e., a* $(0, n-1)$ *Padé form. Moreover, let*

$$\begin{bmatrix} p_{n+k}^{\uparrow} \\ q_{n+k}^{\uparrow} \\ e_{n+k}^{\uparrow} \end{bmatrix} := \begin{bmatrix} p_n^{\leftarrow} & p_n^{\uparrow} \\ q_n^{\leftarrow} & q_n^{\uparrow} \\ e_n^{\leftarrow} & e_n^{\uparrow} \end{bmatrix} \begin{bmatrix} u_k^{\uparrow(n)} \\ v_k^{\uparrow(n)} \end{bmatrix},$$

where $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)}) \in \mathcal{P}_{k-1} \times \mathcal{P}_k$ *is a solution of*

$$p_n^{\leftarrow} u_k^{\uparrow(n)} + p_n^{\uparrow} v_k^{\uparrow(n)} = O_-(\zeta^{-1}) \tag{8.23}$$

with $\partial v_k^{\uparrow(n)} = k$.

Then, $(p_{n+k}^{\uparrow}, q_{n+k}^{\uparrow})$ *is a right underdetermined* $(-1, n+k)$ *Padé form with residual* $e_{n+k}^{\uparrow}$.

Proof. We need to show that $p_{n+k}^{\uparrow} \in \mathcal{L}_{-1}^*$, $q_{n+k}^{\uparrow} \in \mathcal{P}_{n+k}$ is of full degree $n+k$ and that (8.10) is valid. Obviously, we have $q_{n+k}^{\uparrow} \in \mathcal{P}_{n+k}$ and this polynomial is of full degree since, by Lemma 2.9, $\partial q_n^{\uparrow} = n$ and by assumption $\partial v_k^{\uparrow(n)} = k$.

Next assume that $u_k^{\uparrow(n)}$ and $v_k^{\uparrow(n)}$ are chosen as a solution of (8.23). Then we have

$$h q_{n+k}^{\uparrow} - p_{n+k}^{\uparrow} = \zeta^n (e_n^{\leftarrow} u_k^{\uparrow(n)} + e_n^{\uparrow} v_k^{\uparrow(n)}) = O_+(\zeta^n).$$

It remains to show that $p_{n+k}^{\uparrow} \in \mathcal{L}_{-1}^*$. This follows directly from (8.23). □

We now show that a very simple solution exists.

Corollary 8.7: *Let the assumptions of Theorem* 8.4 *be valid. Then a unique solution of* (8.23) *satisfying* (8.16) *exists with* $v_k^{\uparrow(n)} = \zeta^k$.

Proof. By Lemma 2.9, $\partial p_n^{\leftarrow} = 0$. Hence a unique solution of (8.23) exists if one keeps $v_k^{\uparrow(n)}$ fixed. Clearly, $v_k^{\uparrow(n)}$ must have full degree k to ensure that $q_{n+k}^{\uparrow}$ has exact degree $n+k$. Hence, $v_k^{\uparrow(n)} = \zeta^k$ is the simplest possible choice. □

As for left underdetermined Padé forms, we now want to study the recurrences for right underdetermined Padé forms for the particular choice of $v_k^{\uparrow(n)}$ from Corollary 8.7 in more detail. If we define

$$u_k^{\uparrow(n)}(\zeta) = \sum_{j=0}^{k-1} \gamma_{k-j-1}^{\uparrow(n)} \zeta^j, \tag{8.24}$$

then the coefficients $\gamma_j^{\uparrow(n)}$ solve the following upper triangular Toeplitz system

$$\begin{bmatrix} \pi_{0,n}^{\leftarrow} & \cdots & \pi_{k-1,n}^{\leftarrow} \\ & \ddots & \vdots \\ & & \pi_{0,n}^{\leftarrow} \end{bmatrix} \begin{bmatrix} \gamma_{k-1}^{\uparrow(n)} \\ \vdots \\ \gamma_0^{\uparrow(n)} \end{bmatrix} = - \begin{bmatrix} \pi_{k-1,n}^{\uparrow} \\ \vdots \\ \pi_{0,n}^{\uparrow} \end{bmatrix}.$$

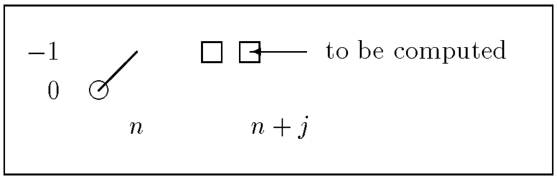
This results again in a simple update formula for $u_k^{\uparrow(n)}$:

$$u_0^{\uparrow(n)} = 0, \qquad u_j^{\uparrow(n)} = \zeta u_{j-1}^{\uparrow(n)} + \gamma_{j-1}^{\uparrow(n)}, \qquad j = 1, \ldots, k-1, \tag{8.25}$$

and hence

$$\begin{bmatrix} p_{n+j}^{\uparrow} \\ q_{n+j}^{\uparrow} \\ e_{n+j}^{\uparrow} \end{bmatrix} = \zeta \begin{bmatrix} p_{n+j-1}^{\uparrow} \\ q_{n+j-1}^{\uparrow} \\ e_{n+j-1}^{\uparrow} \end{bmatrix} + \begin{bmatrix} p_n^{\leftarrow} \\ q_n^{\leftarrow} \\ e_n^{\leftarrow} \end{bmatrix} \gamma_{j-1}^{\uparrow(n)}, \qquad j = 1, \ldots, k-1, \tag{8.26}$$

viz.



(8.27)

A simple formula for $\gamma_j^{\uparrow(n)}$ is

$$\pi_{0,n}^{\leftarrow} \gamma_j^{\uparrow(n)} = -\pi_{0,n+j}^{\uparrow}, \qquad j = 0, \ldots, k-1. \tag{8.28}$$

8.3 Toeplitz matrix factorizations

In Section 8.2, we have shown how to compute left and right underdetermined Padé forms, which correspond to inner biorthogonal polynomials and the corresponding numerators and residuals. Let us now consider the inverse block LDU factorization of the Toeplitz matrix $\mathbf{T} = \mathbf{T}_N$ ($N = \infty$ is allowed). If we define $\mathbf{R} = \mathbf{R}_N$ and $\mathbf{R}^\uparrow = \mathbf{R}_N^\uparrow$, where

$$\mathbf{R}_N^\uparrow := \begin{bmatrix} \rho_{0,0}^\uparrow & \rho_{0,1}^\uparrow & \cdots & \rho_{0,N-1}^\uparrow \\ & \rho_{1,1}^\uparrow & \cdots & \rho_{1,N-1}^\uparrow \\ & & \ddots & \vdots \\ & & & \rho_{N-1,N-1}^\uparrow \end{bmatrix}, \qquad \mathbf{R}_N := \begin{bmatrix} \rho_{0,0} & \rho_{1,1} & \cdots & \rho_{N-1,N-1} \\ & \rho_{0,1} & \cdots & \rho_{N-2,N-1} \\ & & \ddots & \vdots \\ & & & \rho_{0,N-1} \end{bmatrix}, \tag{8.29}$$

and $\mathbf{D} = \mathbf{D}_N$ via

$$\mathbf{D} := \mathbf{R}^T \mathbf{T} \mathbf{R}^\uparrow, \tag{8.30}$$

then we can show

Theorem 8.8: *If the upper triangular matrices* $\mathbf{R}$ *and* $\mathbf{R}^\uparrow$ *defined in* (8.29) *contain in their* $(n+1)$*st column* $(0 \le n < N)$ *the coefficients of an nth regular or inner LOP and ROP, respectively, where the latter are constructed according to Corollaries* 8.5 *and* 8.7, *then the matrix* $\mathbf{D}$ *in* (8.30) *is block diagonal. The blocks of* $\mathbf{D}$ *always start with a regular index and each block is a Toeplitz matrix. Moreover, the* $n \times n$ *principal submatrix* $\mathbf{D}_n$ *of* $\mathbf{D}$ *is nonsingular if and only if* $\mathbf{T}_n$ *is nonsingular.*

Proof. The block diagonal structure of $\mathbf{D}$ follows from the weakened biorthogonality conditions (8.5) and (8.6), which also show that the blocks of $\mathbf{D}$ start with regular indices.

From the definition of the bilinear form $\langle \cdot, \cdot \rangle$ defined in (8.1), we have for $\mathbf{D} = (\delta_{j,k})$

$$\delta_{j,k} = \langle q_j^\star, q_k^\uparrow \rangle.$$

Let $n = n_l$ be a regular index and $n = n_l < n+j, n+k < n_{l+1}$. From (8.20), we obtain the following recurrence for the reflected polynomials:

$$q_{n+j}^\star = \zeta^{n+j} q_{n+j}(\zeta^{-1}) = \zeta q_{n+j-1}^\star + \zeta \gamma_j^{(n)} q_n^{\leftarrow *}. \tag{8.31}$$

Moreover, from the definition of the bilinear form (8.1), it is readily seen that for any polynomials s, t

$$\langle s, t \rangle = \langle \zeta s, \zeta t \rangle. \tag{8.32}$$

Finally, the biorthogonality conditions (8.5)–(8.6) ensure that

$$\langle q_{n+j}^\star, t \rangle = 0 = \langle t, q_{n+j}^\uparrow \rangle \ \text{ for all } \ t \in \mathcal{P}_{n-1}. \tag{8.33}$$

Exploiting (8.31)–(8.33) and (8.26), we obtain

$$\begin{aligned}
\langle q^\star_{n+j}, q^\uparrow_{n+k}\rangle &= \langle q^\star_{n+j}, \zeta q^\uparrow_{n+k-1} + \gamma_k^{\uparrow(n)} q_n^\leftarrow\rangle \\
&= \langle q^\star_{n+j}, \zeta q^\uparrow_{n+k-1}\rangle \\
&= \langle \zeta q^\star_{n+j-1} + \zeta \gamma_j^{(n)} q_n^{\leftarrow *}, \zeta q^\uparrow_{n+k-1}\rangle \\
&= \langle q^\star_{n+j-1} + \gamma_j^{(n)}, q^\uparrow_{n+k-1}\rangle \\
&= \langle q^\star_{n+j-1}, q^\uparrow_{n+k-1}\rangle,
\end{aligned}$$

which shows that the blocks of $\mathbf{D}$ have Toeplitz structure.

The last statement follows from (8.30) since $\mathbf{R}$ and $\mathbf{R}^\uparrow$ are unit upper triangular, so that $\mathbf{D}$ and $\mathbf{T}$ have the same rank. Clearly, the same is valid for the principal submatrices. □

Note, that (8.30) is equivalent to

$$\mathbf{T}^{-1} = \mathbf{R}^\uparrow \mathbf{D}^{-1} \mathbf{R}^T,$$

and therefore, the upper triangular matrices $\mathbf{R}$ and $\mathbf{R}^\uparrow$ define an inverse LDU decomposition of $\mathbf{T}$.

In a look-ahead Schur-type algorithm, the coefficients of $p_n^\uparrow, p_n^\leftarrow, e_n^\uparrow, e_n^\leftarrow$ are available, but not the coefficients of the polynomials $q_n^\uparrow$ and $q_n^\leftarrow$. We will show next that these define the LDU decomposition of $\mathbf{T}$; see also [62].

Theorem 8.9: *Let the assumptions of Theorem* 8.8 *be valid and define*

$$\mathbf{L} = \mathbf{T}^T \mathbf{R} \quad \textit{and} \quad \mathbf{L}^\uparrow = \mathbf{T}\mathbf{R}^\uparrow. \tag{8.34}$$

Then, $\mathbf{L}$ *and* $\mathbf{L}^\uparrow$ *are block lower triangular matrices where* $\mathbf{L}$ *contains in its* $(n+1)$*st column the coefficients of* p_n *and* $\mathbf{L}^\uparrow$ *contains in its* $(n+1)$*st column the coefficients of* $e_n^\uparrow$ $(0 \le n < N)$. *Moreover,*

$$\mathbf{T} = \mathbf{L}^\uparrow \mathbf{D}^{-1} \mathbf{L}^T$$

is a block LDU decomposition of $\mathbf{T}$.

Proof. We assume that $n = n_l \le n+k < n_{l+1}$ where n_l and n_{l+1} are regular indices. Let $\mathbf{L} = (\ell_{i,j})$. Then we have from (8.2), Lemma 8.1 and Lemma 8.3(i)

$$\ell_{n+k-i,n+k} = \mathbf{e}_{n+k}^T \mathbf{R}^T \mathbf{T} \mathbf{e}_{n+k-i} = \langle q_{n+k}^{\uparrow *}, \zeta^{n+k-i}\rangle = \begin{cases} 0, & i > k, \\ \pi_{i,n+k}, & i \le k. \end{cases}$$

Similarly, for $\mathbf{L}^\uparrow = (\ell_{i,j}^\uparrow)$, we obtain from Lemma 8.2 and Lemma 8.3(ii)

$$\ell_{i,n+k}^\uparrow = \mathbf{e}_i^T \mathbf{T} \mathbf{R}^\uparrow \mathbf{e}_{n+k} = \langle \zeta^i, q_{n+k}^\uparrow\rangle = \begin{cases} 0, & i \le n-1, \\ \varepsilon_{n+i,n+k}^\uparrow, & i \ge n. \end{cases}$$

Operations in a block of size $k > 1$	look-ahead Levinson		look-ahead Schur	
type of step	(7.3)	(7.4)	(7.3)	(7.4)
inner products	$2k$	$2k+1$	–	–
SAXPYs	$3(2k-1)$	$6k-1$	$5(2k-1)$	$10k-3$

Table 8.1: Operation counts for Algorithms 7.2 and 7.3 combined with underdetermined Padé forms

Therefore, $\mathbf{L}^{\uparrow}$ and $\mathbf{L}$ are block lower triangular. □

To obtain a complete factorization, it remains to show how to determine the matrix $\mathbf{D}$ in both types of algorithms. By (8.34) we can rewrite (8.30) as

$$\mathbf{D} = \mathbf{R}^T \mathbf{L}^{\uparrow} = \mathbf{L}^T \mathbf{R}^{\uparrow}. \tag{8.35}$$

Due to the Toeplitz structure of the blocks in $\mathbf{D}$, the latter matrix is completely determined by the first row and the first column of each block. However, $\mathbf{R}$ and $\mathbf{R}^{\uparrow}$ are unit upper triangular matrices and, therefore, this computation is trivial if we know the coefficients of the corresponding rows of $\mathbf{L}$ and of $\mathbf{L}^{\uparrow}$. Assume that $n = n_l$ and $n + k = n_{l+1}$ are regular indices. Then the $(n+1)$st row of $\mathbf{L}^{\uparrow}$ contains the leading coefficients of $e_n^{\uparrow}, \ldots, e_{n+k-1}^{\uparrow}$, which are available from (8.26). The $(n+1)$st row of $\mathbf{L}$ contains the leading coefficients of $p_n, \ldots, p_{n+k-1}$. The numerator of the regular $(0, n)$ Padé form can be computed via

$$p_n = p_n^{\leftarrow} \alpha_0^{(n)} + p_n^{\uparrow} \beta_0^{(n)}$$

because of Theorem 8.4 for $k = 0$ and (7.10). The numerators $p_{n+1}, \ldots, p_{n+k-1}$ of the underdetermined Padé forms are obtained from (8.20). Since the first coefficients of $p_n^{\leftarrow}$ can be taken from (7.17) and the first coefficients of $p_n^{\uparrow}$ are known from inner products, the block LDU decomposition can be computed without any additional long inner products in the Levinson-type algorithm. For the Schur-type algorithm, there is nothing to compute, because the coefficients of $\mathbf{L}$ and $\mathbf{L}^{\uparrow}$ are determined directly in the algorithm.

In Table 8.1, we list the operation counts for Algorithms 7.2 and 7.3 extended such that they compute the complete block factorization of $\mathbf{T}$. Again we consider all computations which require at most $O(k^3)$ operations as negligible. Starting from Table 7.1, the additional SAXPYs for the Levinson algorithm come from one SAXPY for each of the $k-1$ inner ROPs, one for the regular LOP, and one for each of the $k-1$ inner LOPs. The block LDU decomposition of $\mathbf{T}$ contains only the coefficients of p_n and $e_n^{\uparrow}$. Hence in the Schur type algorithm, we do not have to compute $p_n^{\uparrow}$ and e_n if n is not a regular index. This makes in total again $2k-1$ SAXPYs for the underdetermined Padé forms.

The overhead for these algorithms is $4k-3$ SAXPYs for the Levinson version and $6k-5$ SAXPYs for the Schur algorithm, if $k>1$. There is no overhead for generic steps where $k=1$.

8.4 Matrix formulation of look-ahead algorithms

Bareiss [6] rediscovered the Schur algorithm [109], but presented it in a different form. Starting from two copies of the Toeplitz matrix $\mathbf{T}$ he applied a series of two-dimensional transformations which bring one copy of the matrix into upper triangular form and the other into lower triangular form. Delosme and Ipsen [33, 81] analyzed the Bareiss algorithm further and generalized it to arbitrary matrices with the property that all their contiguous principal submatrices are nonsingular. They showed in particular that the resulting triangular matrices are the second factors in the LU and the UL decomposition of $\mathbf{T}$, and that the first factors can be retrieved from the mentioned two-dimensional transformations. Here, we extend this result to the look-ahead case. In contrast to [6, 33, 81] we work with columns instead of rows. In fact, in its original form, the Bareiss algorithm for $\mathbf{T}$ is the same as the Schur algorithm for $\mathbf{T}^T$. We discuss here the Bareiss-Delosme-Ipsen formulation of the Schur algorithm and its look-ahead extension for Algorithm 7.3 extended by computing underdetermined Padé forms also. This generalizes the formulation in [67, Section 9], where this extension was discussed for look-ahead algorithms based on column-regular pairs only. Using only column-regular pairs made things a little easier, because the algorithms work with quantities which are all contained in the factors of the LDU factorizations of $\mathbf{T}$ and $\mathbf{T}^{-1}$. For the algorithms we proposed in this thesis, this is no longer true: in a look-ahead step, they make use of anti-diagonally regular pairs from which coefficients of the lower left neighbor do in general not appear in the LDU decompositions. The only situation where they are also contained as a column of $\mathbf{R}$ or $\mathbf{L}$ is when we switched from a column-regular step to a look-ahead step; see Picture (7.2). The derivation in [67] was done solely from a linear algebra point of view. Here, we want to present a different derivation, which appears to be simpler because it is based on products of Padé forms, as we will see soon.

The algorithms we want to describe consist of classical steps (column steps), illustrated in (7.1), and look-ahead steps (7.2), whenever necessary. We also describe and solve the problems of switching from classical steps to look-ahead steps (7.2) and vice versa (8.17). We could also use (7.4) for a switch, but prefer to use (8.17) here, since it fits into the framework of both version of look-ahead algorithms: the product form of Section 7.3 based on anti-diagonally pairs only and those of Section 9.1 below, where anti-diagonally regular pairs are computed from underdetermined Padé forms and the last anti-diagonally regular pair.

The key point is to write the recurrences in terms of a sequence of products of 2×2 matrices consisting of numerators and denominators of Padé forms. Details on how to determine the coefficients can be found in this and the previous chapter.

(8a) Classical step (7.1), where n and $n+1$ are column-regular indices

$$\begin{bmatrix} p_{n+1} & p_{n+1}^{\uparrow} \\ q_{n+1} & q_{n+1}^{\uparrow} \end{bmatrix} = \begin{bmatrix} p_n & p_n^{\uparrow} \\ q_n & q_n^{\uparrow} \end{bmatrix} \begin{bmatrix} 1 & \gamma_0^{\uparrow(n)} \\ \zeta\gamma_0^{(n)} & \zeta \end{bmatrix}. \tag{8.36}$$

(8b) Switch from a classical step to a look-ahead step (7.2), where $n-1$ is a column-regular index and thus n is a regular index:

$$\begin{bmatrix} p_n^{\leftarrow} & p_n^{\uparrow} \\ q_n^{\leftarrow} & q_n^{\uparrow} \end{bmatrix} = \begin{bmatrix} p_{n-1} & p_{n-1}^{\uparrow} \\ q_{n-1} & q_{n-1}^{\uparrow} \end{bmatrix} \begin{bmatrix} 1 & \gamma_0^{\uparrow(n-1)} \\ 0 & \zeta \end{bmatrix}. \tag{8.37}$$

(8c) Look-ahead step (7.3), where n and $n+k$ are regular indices

$$\begin{bmatrix} p_{n+k}^{\leftarrow} & p_{n+k}^{\uparrow} \\ q_{n+k}^{\leftarrow} & q_{n+k}^{\uparrow} \end{bmatrix} = \begin{bmatrix} p_n^{\leftarrow} & p_n^{\uparrow} \\ q_n^{\leftarrow} & q_n^{\uparrow} \end{bmatrix} \begin{bmatrix} u_k^{\leftarrow(n)} & u_k^{\uparrow(n)} \\ v_k^{\leftarrow(n)} & v_k^{\uparrow(n)} \end{bmatrix}. \tag{8.38}$$

Here $(u_k^{\leftarrow(n)}, v_k^{\leftarrow(n)}) \in \mathcal{P}_{k-2} \times \mathcal{P}_{k-1}$ and $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)}) \in \mathcal{P}_{k-1} \times \mathcal{P}_k$, with monic $v_k^{\uparrow(n)}$.

(8d) Compute left underdetermined Padé forms (8.13) and right underdetermined Padé forms (8.22), where n and $n+k$ are regular indices

$$\begin{bmatrix} p_{n+j} & p_{n+j}^{\uparrow} \\ q_{n+j} & q_{n+j}^{\uparrow} \end{bmatrix} = \begin{bmatrix} p_n^{\leftarrow} & p_n^{\uparrow} \\ q_n^{\leftarrow} & q_n^{\uparrow} \end{bmatrix} \begin{bmatrix} u_j^{(n)} & u_j^{\uparrow(n)} \\ \beta_0^{(n)} & \zeta^j \end{bmatrix}, \qquad j = 0, \ldots, k-1. \tag{8.39}$$

As in (8.25), we set $u_0^{\uparrow(n)} \equiv 0$. Then this formula is valid also for $j=0$, where it specifies a switch from a look-ahead step to a classical step; see Picture (8.17). Recall that $u_j^{(n)} \in \mathcal{P}_j$ and $u_j^{\uparrow(n)} \in \mathcal{P}_{j-1}$; see Corollaries 8.5 and 8.7.

The idea is now to rewrite these products of Padé forms in terms of matrices. Let $\mathbf{L}_{n;e}^{\uparrow}$, $\mathbf{L}_{n;e}^{\uparrow}$, $\mathbf{R}_{n;e}^{\uparrow}$ and $\mathbf{R}_{n;e}$ be the $N \times n$ matrices consisting of the first n columns of the respective $N \times N$ matrices $\mathbf{L}^{\uparrow}$, $\mathbf{L}$, $\mathbf{R}^{\uparrow}$ and $\mathbf{R}$ defined in (8.29) and (8.34). The additional index e is used to indicate that the matrices are extended versions of the factors of the (inverse) LDU decomposition of the $n \times n$ submatrix $\mathbf{T}_n$ and to distinguish them from the latter. Clearly, for these submatrices there holds also:

$$\mathbf{T}\mathbf{R}_{n;e}^{\uparrow} = \mathbf{L}_{n;e}^{\uparrow} \quad \text{and} \quad \mathbf{R}_{n;e}^{T}\mathbf{T} = \mathbf{L}_{n;e}^{T}. \tag{8.40}$$

Additionally, we introduce the notation

$$\mathbf{L}_{n;e}^{\uparrow(\mathrm{J})} := \mathbf{J}_N \mathbf{L}_{n;e}^{\uparrow} \mathbf{J}_{n;e}, \qquad \text{and} \quad \mathbf{R}_{n;e}^{\uparrow(\mathrm{J})} := \mathbf{J}_N \mathbf{R}_{n;e}^{\uparrow} \mathbf{J}_{n;e},$$

where $\mathbf{J}_n$ denotes the antidiagonal unit matrix or reflection matrix of order n. One obtains $\mathbf{L}_{n;e}^{\uparrow(\mathrm{J})}$ by rotating $\mathbf{L}_n^{\uparrow}$ by 180°. Hence, $\mathbf{L}_{n;e}^{\uparrow(\mathrm{J})}$ is upper triangular and $\mathbf{R}_{n;e}^{\uparrow(\mathrm{J})}$ is lower triangular. The shift matrix (of adaptable size) is denoted by

$$\mathcal{S} := \begin{bmatrix} 0 & & & & \\ 1 & 0 & & & \\ & 1 & 0 & & \\ & & \ddots & \ddots & \\ & & & 1 & 0 \end{bmatrix}$$

and extended versions of $\mathbf{q}_n^{\uparrow}$ and $\mathbf{q}_n$ are given by

$$\mathbf{q}_{n;e}^{\uparrow} := [\rho_{0,n}^{\uparrow} \, \cdots \, \rho_{n,n}^{\uparrow} \, 0 \, \cdots \, 0]^T, \quad \mathbf{q}_{n;e} := [\rho_{0,n} \, \cdots \, \rho_{n,n} \, 0 \, \cdots \, 0]^T \in \mathbb{C}^N.$$

We start with (8.36) and consider the Padé conditions (2.4) (for $m = 0$ and $m = -1$) for a column-regular pair (p_n, q_n), $(p_n^{\uparrow}, q_n^{\uparrow})$. Multiplying (2.4) by ζ^j, $j = 0, \ldots, k-1$, where $k = N - n - 1$ yields in matrix formalism

$$\mathbf{T} \left[\; \mathbf{q}_{n;e} \;\; \cdots \;\; \mathcal{S}^{k-1}\mathbf{q}_{n;e} \;\middle|\; \mathcal{S}\mathbf{q}_{n;e}^{\uparrow} \;\; \cdots \;\; \mathcal{S}^{k}\mathbf{q}_{n;e}^{\uparrow} \; \right] = \mathbf{S}_n^{\circ},$$

where $\mathbf{S}_n^{\circ}$ contains the shifted versions of numerators and residuals of the column-regular pair:

$$\mathbf{S}_n^{\circ} := \mathbf{S}_{N-n-1,n}^{\circ} := \left[\begin{array}{ccc|ccc} \pi_{0,n} & \cdots & \pi_{N-n-2,n} & \pi_{0,n}^{\uparrow} & \cdots & \pi_{N-n-2,n}^{\uparrow} \\ & \ddots & \vdots & & \ddots & \vdots \\ \mathbf{0}_n & & \pi_{0,n} & \mathbf{0}_n & & \pi_{0,n}^{\uparrow} \\ & \ddots & & & \ddots & \\ \varepsilon_{n,n} & & \mathbf{0}_n & \varepsilon_{n,n}^{\uparrow} & & \mathbf{0}_n \\ \vdots & \ddots & & \vdots & \ddots & \\ \varepsilon_{N-2,n} & \cdots & \varepsilon_{n,n} & \varepsilon_{N-2,n}^{\uparrow} & \cdots & \varepsilon_{n,n}^{\uparrow} \end{array} \right].$$

This can be combined with (8.40):

$$\begin{aligned} \mathbf{T} \, [\; \mathbf{R}_{n+1;e} \;\big|\; \mathbf{q}_{n;e} \;\; \cdots \;\; \mathcal{S}^{k-1}\mathbf{q}_{n;e} \;\big|\; \mathcal{S}\mathbf{q}_{n;e}^{\uparrow} \;\; \cdots \;\; \mathcal{S}^{k}\mathbf{q}_{n;e}^{\uparrow} \;\big|\; \mathbf{R}_{n+1;e}^{\uparrow(\mathrm{J})} \;] \\ = [\; \mathbf{L}_{n+1;e} \;\big|\; \mathbf{S}_n^{\circ} \;\big|\; \mathbf{L}_{n+1;e}^{\uparrow(\mathrm{J})} \;]. \end{aligned} \tag{8.41}$$

Note that on the left-hand side $\mathbf{T}$ is multiplied by a matrix whose left half is a square upper triangular block and whose right half is a square lower triangular block. On the right-hand side, the left half of the matrix is a square block with n zero codiagonals above its main diagonal, while the right half is a square block with n zero codiagonals below its main diagonal. If $\mathbf{I} = \mathbf{I}_N$ denotes the unit matrix of order N, then for $n = 0$ this equation reduces to

$$\mathbf{T} \, [\; \mathbf{I} \;\big|\; \mathbf{I} \;] = [\; \mathbf{T} \;\big|\; \mathbf{T} \;], \tag{8.42}$$

while for $n = N-1$ and $\mathbf{J} := \mathbf{J}_N$ we get again

$$\mathbf{T}\,[\ \mathbf{R} \mid \mathbf{R}^{\uparrow(\mathrm{J})}\ ] = [\ \mathbf{L} \mid \mathbf{L}^{\uparrow(\mathrm{J})}\ ]. \tag{8.43}$$

By applying two-dimensional transformations (from the right) the Schur algorithm transforms the right-hand side of (8.42) into the one of (8.43). In contrast, the Levinson algorithm applies the same transformations to the matrices on the left-hand side. If n is a classical step, *i.e.*, if n is a column-regular index, the two-dimensional transformations that are applied at the nth step may be bundled in the $2N \times 2N$ matrix

$$\mathbf{C}_n := \left[\begin{array}{c|c|c|c} \mathbf{I}_{n+1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{N-n-1} & \gamma_0^{\uparrow(n)}\mathbf{I}_{N-n-1} & \mathbf{0} \\ \hline \mathbf{0} & \gamma_0^{(n)}\mathbf{I}_{N-n-1} & \mathbf{I}_{N-n-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I}_{n+1} \end{array}\right], \tag{8.44}$$

with the Schur parameters $\gamma_0^{(n)}$ and $\gamma_0^{\uparrow(n)}$ defined in the algorithms in Section 7.3. Multiplying (8.41) from the right by $\mathbf{C}_n$ yields again (8.41) but with n replaced by $n+1$. This is the matrix formulation of (8.36). If zero is a column-regular index, this statement is also correct for $n = 0$.

If $n-1$ but not n is a column-regular index and if we set $\gamma_0^{(n-1)} = 0$, then (8.44) (for n replaced by $n-1$) yields the transformation for (8.37), but the outcome is now

$$\begin{aligned} \mathbf{T}\,[\ \mathbf{R}_{n;e} \mid \mathbf{q}^{\leftarrow}_{n;e}\ \cdots\ \mathcal{S}^k\mathbf{q}^{\leftarrow}_{n;e} \mid \mathcal{S}\mathbf{q}^{\uparrow}_{n;e}\ \cdots\ \mathcal{S}^k\mathbf{q}^{\uparrow}_{n;e} \mid \mathbf{R}^{\uparrow(\mathrm{J})}_{n+1;e}\ ] \\ = [\ \mathbf{L}_{n;e} \mid \mathbf{M}^{\circ}_n \mid \mathbf{L}^{\uparrow(\mathrm{J})}_{n+1;e}\ ], \end{aligned} \tag{8.45}$$

where $k = N-n-1$ and $\mathbf{M}^{\circ}_n := \mathbf{M}^{\circ}_{k,n}$ is just the matrix $\mathbf{M}_{k,n}$ defined in (7.8) filled with $(n-1)$ zero diagonals in the middle:

$$\mathbf{M}^{\circ}_n := \mathbf{M}^{\circ}_{N-n-1,n} := \left[\begin{array}{ccc|cccc} \pi^{\leftarrow}_{0,n} & \cdots & \pi^{\leftarrow}_{N-n-2,n} & 0 & \pi^{\uparrow}_{0,n} & \cdots & \pi^{\uparrow}_{N-n-2,n} \\ & \ddots & \vdots & & & \ddots & \vdots \\ \mathbf{0}_{n-1} & & \pi^{\leftarrow}_{0,n} & \mathbf{0}_{n-1} & & & \pi^{\uparrow}_{0,n} \\ \varepsilon^{\leftarrow}_{n,n} & \ddots & & \varepsilon^{\uparrow}_{n,n} & \ddots & & \\ \vdots & \ddots & \mathbf{0}_{n-1} & & & \ddots & \\ \vdots & & \varepsilon^{\leftarrow}_{n,n} & \vdots & & \ddots & \mathbf{0}_{n-1} \\ \varepsilon^{\leftarrow}_{N-2,n} & \cdots & \varepsilon^{\leftarrow}_{n+1,n} & \varepsilon^{\uparrow}_{N-2,n} & \cdots & \cdots & \varepsilon^{\uparrow}_{n,n} \end{array}\right].$$

Since in a look-ahead step, the recurrences involve multiplications with two-point Padé forms, *i.e.*, with polynomials of small degree, the matrix $\mathbf{C}_n$ now becomes more complicated than in (8.44). However, it can be easily understood as the matrix formulation of (8.38) and (8.39). Assume that $n = n_l$ is a regular index and that $k = n_{l+1} - n_l$ is the length of the look-ahead step starting with n. Then we have

$$
\mathbf{C}_n^{(L)} := \left[\begin{array}{c|cccccccc|cccccccc|c}
\mathbf{I}_n & \multicolumn{8}{c|}{\mathbf{O}} & \multicolumn{8}{c|}{\mathbf{O}} & \mathbf{O} \\ \hline
 & \gamma_0^{(n)} & \cdots & \gamma_{k-1}^{(n)} & 0 & & & & & 0 & & & & & & & & \\
 & & \ddots & \vdots & \alpha_{k-1}^{\leftarrow(n)} & \ddots & & & & \alpha_{k-1}^{\uparrow(n)} & \ddots & & & & & & & \\
 & & & \gamma_0^{(n)} & \vdots & \ddots & \ddots & & & \vdots & & \ddots & & & & & & \\
\mathbf{O} & & & & \alpha_0^{\leftarrow(n)} & & \ddots & \ddots & & \alpha_0^{\uparrow(n)} & \ddots & & \ddots & & & & & \mathbf{O} \\
 & & & & & \ddots & & \ddots & 0 & & \ddots & \ddots & & 0 & & & & \\
 & & & & & & \ddots & & \alpha_{k-1}^{\leftarrow(n)} & & & \ddots & \ddots & \alpha_{k-1}^{\uparrow(n)} & \gamma_{-1}^{\uparrow(n)} & & & \\
 & & & & & & & \ddots & \vdots & & & & \ddots & \vdots & \vdots & \ddots & & \\
 & & & & & & & & \alpha_0^{\leftarrow(n)} & & & & & \alpha_0^{\uparrow(n)} & \gamma_{k-2}^{\uparrow(n)} & \cdots & \gamma_{-1}^{\uparrow(n)} & \\ \hline
 & \beta_0^{(n)} & & & 0 & & & & & 1 & & & & & & & & \\
 & & \ddots & & \beta_{k-1}^{\leftarrow(n)} & \ddots & & & & \beta_{k-1}^{\uparrow(n)} & \ddots & & & & & & & \\
 & & & \beta_0^{(n)} & \vdots & \ddots & \ddots & & & \vdots & \ddots & \ddots & & & & & & \\
 & & & & \beta_0^{\leftarrow(n)} & & \ddots & \ddots & & \beta_0^{\uparrow(n)} & & \ddots & \ddots & & & & & \\
\mathbf{O} & & & & & \ddots & & \ddots & 0 & & \ddots & & \ddots & 1 & & & & \mathbf{O} \\
 & & & & & & \ddots & & \beta_{k-1}^{\leftarrow(n)} & & & \ddots & & \beta_{k-1}^{\uparrow(n)} & 1 & & & \\
 & & & & & & & \ddots & \vdots & & & & \ddots & \vdots & & \ddots & & \\
 & & & & & & & & \beta_0^{\leftarrow(n)} & & & & & \beta_0^{\uparrow(n)} & & & 1 & \\ \hline
\mathbf{O} & \multicolumn{8}{c|}{\mathbf{O}} & \multicolumn{8}{c|}{\mathbf{O}} & \mathbf{I}_n
\end{array}\right],
$$

where $\alpha_{k-1}^{\leftarrow(n)} = \gamma_{-1}^{\uparrow(n)} = 0$.

After multiplying (8.45) from the right by $\mathbf{C}_n^{(L)}$, we obtain again (8.45) but with n replaced by $n+k$. Note that the last column of $\mathbf{R}_{n+1;e}^{\uparrow}$, which corresponds to the first column of $\mathbf{R}_{n+1;e}^{\uparrow(\mathrm{J})}$, is unchanged after this multiplication, because $\gamma_{-1}^{\uparrow(n)} = 0$ ensures that the $(2N-n)$th column of $\mathbf{C}_n^{(L)}$ is the $(2N-n)$th unit vector.

Similarly, a switch from a look-ahead to a classical step at a column-regular index n can be interpreted from (8.39) as a multiplication with

$$
\mathbf{C}_n^{(S)} := \left[\begin{array}{c|c|c|c}
\mathbf{I}_n & \mathbf{0} & \mathbf{0} & \mathbf{0} \\
\mathbf{0} & \alpha_0^{(n)}\mathbf{I}_{N-n} & \mathbf{0} & \mathbf{0} \\ \hline
\mathbf{0} & \beta_0^{(n)}\mathbf{I}_{N-n} & \mathbf{I}_{N-n} & \mathbf{0} \\
\mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{I}_n
\end{array}\right].
$$

Multiplying (8.45) by $\mathbf{C}_n^{(S)}$ yields (8.41).

The transformation matrix performing a look-ahead step starting at index n and a switch back to classical recurrences at index $n_{l+1} = n+k$ is

$$
\mathbf{C}_n = \mathbf{C}_n^{(L)} \mathbf{C}_{n+k}^{(S)}
$$

while we have

$$\mathbf{C}_n = \mathbf{C}_n^{(L)}$$

if the next step is again a look-ahead step, *i.e.*, if $n_{l+1} > n + k + 1$.

Recall that $n = 0$ is always a regular index. Hence, the matrix $\mathbf{C}_n$ is also correct for $n = n_0 = 0$, if we define $\mathbf{R}_{0;e}$ to be an empty matrix, and as in all our algorithms before, $\pi_0^{\leftarrow} \equiv 1$ and $e_0^{\leftarrow} \equiv -1$. With this notation the transformations implemented in the look-ahead Schur algorithm can be summarized in matrix form as

$$[\ \mathbf{L} \mid \mathbf{L}^{\uparrow(J)}\ ] = \begin{cases} [\ \mathbf{T} \mid \mathbf{T}\ ] \prod_{j=0}^{J-1} \mathbf{C}_{n_j}, & \text{if } n_1 = 1 \\ [\ \mathbf{0} \mid \mathbf{T}\ ] \prod_{j=0}^{J-1} \mathbf{C}_{n_j}, & \text{if } n_1 > 1 \end{cases} \tag{8.46}$$

where J is the number of the last block, *i.e.*, $n_J = N$. Likewise, the look-ahead Levinson algorithm becomes

$$[\ \mathbf{R} \mid \mathbf{R}^{\uparrow(J)}\ ] = \begin{cases} [\ \mathbf{I} \mid \mathbf{I}\ ] \prod_{j=0}^{J-1} \mathbf{C}_{n_j}, & \text{if } n_1 = 1 \\ [\ \mathbf{0} \mid \mathbf{I}\ ] \prod_{j=0}^{J-1} \mathbf{C}_{n_j}, & \text{if } n_1 > 1. \end{cases} \tag{8.47}$$

At the intermediate stages we have either (8.41) or (8.45), depending on whether we are in a generic step (using a column-regular pair) or in a look-ahead step (using an anti-diagonally regular pair).

9. ISOMETRIC ARNOLDI ALGORITHM

By now we have studied in detail how anti-diagonally regular and column-regular pairs can be used to proceed along adjacent rows of the Padé table and to compute LDU or inverse LDU decompositions of a Toeplitz matrix. For the latter, we have introduced left and right underdetermined Padé forms. However, we have used those underdetermined Padé forms only to fill gaps between anti-diagonally regular Padé forms. Next we present alternative recurrences which make use of underdetermined Padé forms, so this chapter can be seen as the counterpart of Chapter 6, where we did the same for diagonal recurrences. For adjacent rows, such recurrences to compute Padé forms have recently been proposed by the author [79], where it was shown that the resulting new variants of the look-ahead Levinson- and Schur algorithm have less overhead than any other available algorithm for computing the complete LDU or inverse LDU decomposition. In contrast to this chapter, regular pairs instead of anti-diagonally regular pairs have been used in [79]. By rewriting the alternative recurrences in product form again, we can also give the matrix formulation of these new algorithms.

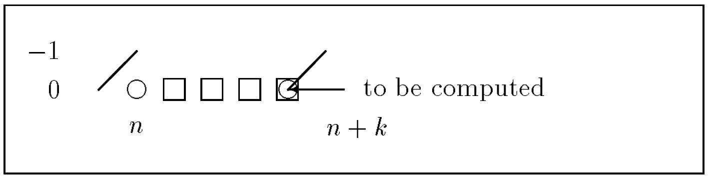
Similar algorithms developed without using the Padé connection have been proposed by Freund and Zha [42] and Freund [38]. We rederive these algorithms in terms of Padé approximation to show how the computational overhead of look-ahead steps of these methods can be reduced by a factor up to two by exploiting the Padé connection.

The second part of this chapter then interprets the Levinson algorithm as an Arnoldi process for isometric operators. This relation was described in a special case by Gragg [53], see also the survey by Watins [107]. The isometric Arnoldi process can be interpreted as the isometric analogue of the Lanczos method. The new algorithm can be used for computing biorthogonal polynomials with respect to a bilinear form from modified moments. To the best of our knowledge, this is the first algorithm which neither requires the moments explicitly nor assumes that regular formally biorthogonal polynomials exist for every degree n.

9.1 Alternative recurrences using inner LOPs and ROPs

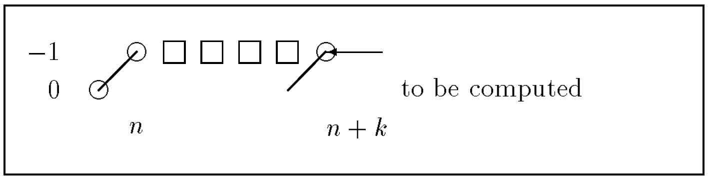
In the following, we assume the normalization (2.40) to be valid for regular as well as for underdetermined Padé forms.

Before stating the theorems we want to illustrate them. We first give two pictures that show which (underdetermined) Padé forms are involved in the recurrences to compute the next anti-diagonally regular pair from the previous anti-diagonally regular pair and subsequent underdetermined Padé forms. Here we assume n and $n+k$ to be regular indices. Picture 9.1 and Theorem 9.1 below show how to compute $(p^{\leftarrow}_{n+k}, q^{\leftarrow}_{n+k})$ from the regular $(0,n)$ Padé form (p_n, q_n) and the left underdetermined $(0,n+1),\ldots,(0,n+k-1)$ Padé forms. The circle inside the right most square represents the Padé form we are looking for.



(9.1)

Picture 9.2 and Theorem 9.2 contain the recurrences to compute the anti-diagonally regular $(-1,n+k)$ Padé form $(p^{\uparrow}_{n+k}, q^{\uparrow}_{n+k})$ from the anti-diagonally regular pair of index n and the $(-1,n+1),\ldots,(-1,n+k-1)$ right underdetermined Padé forms



(9.2)

Theorem 9.1: *Let (p_n, q_n) be a regular $(0,n)$ Padé form of $h \in \mathcal{L}$ (i.e., $(p^{\uparrow}_n, q^{\uparrow}_n)$ be an anti-diagonally regular $(-1,n)$ Padé form) with residual e_n and let (p_{n+j}, q_{n+j}) be $(0,n+j)$ left underdetermined Padé forms with residuals e_{n+j}, $j = 1,\ldots,k-1$.*

If a nontrivial solution of the linear system

$$\begin{bmatrix} \pi_{0,n} & \cdots & \pi_{-k+1,n+k-1} \\ \vdots & & \vdots \\ \pi_{k-1,n} & \cdots & \pi_{0,n+k-1} \end{bmatrix} \begin{bmatrix} \theta^{\leftarrow}_0 \\ \vdots \\ \theta^{\leftarrow}_{k-1} \end{bmatrix} = \mathbf{e}_{k-1} p^{\leftarrow}_{n+k}(\infty) \tag{9.3}$$

exists, then $(p^{\leftarrow}_{n+k}, q^{\leftarrow}_{n+k})$ with

$$\begin{bmatrix} p^{\leftarrow}_{n+k} \\ q^{\leftarrow}_{n+k} \\ e^{\leftarrow}_{n+k} \end{bmatrix} = \sum_{j=0}^{k-1} \begin{bmatrix} \zeta^{k-1-j} p_{n+j} \\ \zeta^{k-1-j} q_{n+j} \\ e_{n+j} \end{bmatrix} \theta^{\leftarrow}_j \tag{9.4}$$

is a $(0,n+k-1)$ Padé form of h with residual $e^{\leftarrow}_{n+k}$.

Proof. We use (9.4) as the definition of $p^{\leftarrow}_{n+k}$ and $q^{\leftarrow}_{n+k}$. Then we have by Lemma 8.1

$$hq^{\leftarrow}_{n+k} - p^{\leftarrow}_{n+k} = \zeta^{n+k} \sum_{j=0}^{k-1} e_{n+j} \theta^{\leftarrow}_j = O_+(\zeta^{n+k}).$$

Moreover, $p^{\leftarrow}_{n+k} \in \mathcal{L}^*_0$ if and only if

$$\Pi_{1:k-1}\left(\sum_{j=1}^{k-1} \zeta^{k-j-1} p_{n+j}\theta^{\leftarrow}_j\right) = 0,$$

or, equivalently, if (9.3) is true. □

Theorem 9.2: *Let $(p^{\uparrow}_n, q^{\uparrow}_n)$ be an anti-diagonally regular $(-1, n)$ Padé form of $h \in \mathcal{L}$ with residual $e^{\uparrow}_n$ and let $(p^{\uparrow}_{n+j}, q^{\uparrow}_{n+j})$ be $(-1, n+j)$ right underdetermined Padé forms with residuals $e^{\uparrow}_{n+j}$, $j = 1, \ldots, k-1$. In addition let $(p^{\leftarrow}_n, q^{\leftarrow}_n)$ be a $(0, n-1)$ Padé form with residual $e^{\leftarrow}_n$ and define*

$$\vartheta^{\uparrow}_{n+k} = -\pi^{\uparrow}_{0,n+k-1}/\pi^{\leftarrow}_{0,n}. \tag{9.5}$$

If a solution of

$$\begin{bmatrix} \varepsilon^{\uparrow}_{n,n} & \cdots & \varepsilon^{\uparrow}_{n,n+k-1} \\ \vdots & & \vdots \\ \varepsilon^{\uparrow}_{n+k-1,n} & \cdots & \varepsilon^{\uparrow}_{n+k-1,n+k-1} \end{bmatrix} \begin{bmatrix} \theta^{\uparrow}_0 \\ \vdots \\ \theta^{\uparrow}_{k-1} \end{bmatrix} = -\begin{bmatrix} 0 \\ \varepsilon^{\uparrow}_{n,n+k-1} \\ \vdots \\ \varepsilon^{\uparrow}_{n+k-2,n+k-1} \end{bmatrix} - \begin{bmatrix} \varepsilon^{\leftarrow}_{n,n} \\ \varepsilon^{\leftarrow}_{n+1,n} \\ \vdots \\ \varepsilon^{\leftarrow}_{n+k-1,n} \end{bmatrix} \vartheta^{\uparrow}_{n+k} \tag{9.6}$$

exists, then $(p^{\uparrow}_{n+k}, q^{\uparrow}_{n+k})$ with

$$\begin{bmatrix} p^{\uparrow}_{n+k} \\ q^{\uparrow}_{n+k} \\ \zeta^k e^{\uparrow}_{n+k} \end{bmatrix} = \zeta \begin{bmatrix} p^{\uparrow}_{n+k-1} \\ q^{\uparrow}_{n+k-1} \\ e^{\uparrow}_{n+k-1} \end{bmatrix} + \sum_{j=0}^{k-1} \begin{bmatrix} p^{\uparrow}_{n+j} \\ q^{\uparrow}_{n+j} \\ e^{\uparrow}_{n+j} \end{bmatrix} \theta^{\uparrow}_j + \begin{bmatrix} p^{\leftarrow}_n \\ q^{\leftarrow}_n \\ e^{\leftarrow}_n \end{bmatrix} \vartheta^{\uparrow}_{n+k} \tag{9.7}$$

is a $(-1, n+k)$ Padé form of h with monic $q^{\uparrow}_{n+k}$ and residual $e^{\uparrow}_{n+k}$.

Proof. Again we interpret (9.7) as the definition of its left-hand side. Since by assumption $p^{\uparrow}_{n+k-1} \in \mathcal{L}^*_{-1}$ and $p^{\leftarrow}_n \in \mathcal{L}^*_0$, (9.5) ensures $p^{\uparrow}_{n+k} \in \mathcal{L}^*_{-1}$. Moreover, by Definition 8.3 of right underdetermined Padé forms and by the normalization (2.40), we have $q^{\uparrow}_{n+k} \in \mathcal{P}_{n+k}$ and $q^{\uparrow}_{n+k}$ monic.

From Lemma 8.2 we obtain

$$hq^{\uparrow}_{n+k} - p^{\uparrow}_{n+k} = \zeta^n\left(\zeta e^{\uparrow}_{n+k-1} + e^{\leftarrow}_n \vartheta^{\uparrow}_{n+k} + \sum_{j=0}^{k-1} e^{\uparrow}_{n+j}\theta^{\uparrow}_j\right).$$

The condition $hq^{\uparrow}_{n+k} - p^{\uparrow}_{n+k} = O_+(\zeta^{n+k})$ is equivalent to (9.6). □

We next prove a lemma concerning the length k of a look-ahead step. It is the counterpart of Lemma 7.1 for the new recurrences given in the previous two theorems.

Lemma 9.3: *Let $n = n_l$ be an anti-diagonally regular index. Then the following two statements are equivalent:*

(i) *the index $n+k$ is a regular index,*
(ii) *the coefficient matrices* $\mathbf{L}^{(l)} = (\pi_{i-j,n+j})_{i,j=0}^{k-1}$ *and* $\mathbf{L}^{\uparrow(l)} = (\varepsilon^{\uparrow}_{n+i,n+j})_{i,j=0}^{k-1}$ *in* (9.3) *and* (9.6) *are nonsingular.*

Proof. Assume that $n+k$ is an anti-diagonally regular index. By Lemma 2.9, this is equivalent to $\mathbf{T}_{n+k} = \mathbf{T}_{0,n+k}$ being nonsingular. By Theorem 8.9, the matrices $\mathbf{L}^{(l)}$ and $\mathbf{L}^{\uparrow(l)}$ are the diagonal blocks of $\mathbf{L}$ and $\mathbf{L}^{\uparrow}$ defined in (8.34). Since $\mathbf{R}$ and $\mathbf{R}^{\uparrow}$ are unit upper triangular, $\mathbf{L}$, $\mathbf{L}^{\uparrow}$, and $\mathbf{T}_N$ are of same rank and the same is true for the principal submatrices of these matrices. Hence, $\mathbf{T}_{n+k}$ is nonsingular if and only if $\mathbf{L}^{(l)}$ and $\mathbf{L}^{\uparrow(l)}$ are nonsingular. □

The previous two theorems provide an alternative way of implementing the Levinson- or Schur-type algorithms of Chapter 7: We no longer have to multiply by polynomials of degree greater than one (the litte two-point Padé forms from Section 7.3) but instead form linear combinations of (underdetermined) Padé forms. As for the Lanczos process, this turns out to be cheaper than the version we had before; see Tables 7.1 and 9.1.

Since the actual computation of the required coefficients of residuals and denominators of the computed formally biorthogonal polynomials turns out to be a little tricky, we now give a detailed complete variant of the Levinson-type Algorithm 7.2. It uses the normalizations (2.40) and requires the same number of inner products as its classical counterpart. In a classical step, inner products are required for computing $\pi^{\uparrow}_{0,n}$ and $\varepsilon_{n,n}$. If we start a look-ahead step, then we can obtain $\varepsilon_{n,n}$ recursively from (8.14). In a look-ahead step, $\varepsilon^{\uparrow}_{n,n}, \ldots, \varepsilon^{\uparrow}_{n+k,n}$ and $\pi^{\uparrow}_{0,n}, \ldots, \pi^{\uparrow}_{k-1,n}$ are computed explicitly by inner products, but all the other coefficients can be updated recursively.

Details of the look-ahead strategy are postponed to Section 11.1. We present here only the simplest possible version, which can deal with look-ahead steps of length at most $k_{\max}$.

Algorithm 9.1: Look-ahead Levinson-type algorithm for adjacent rows in the Padé table using inner LOPs and ROPs.
INPUT: $h \in \mathcal{L}$, N, $k_{\max}$;
OUTPUT: *denominator* $q^{\uparrow}_L$ *of anti-diagonally regular* $(-1, L)$ *Padé form of* h *for largest possible* $L \le N$;
Set $n = 0$, $l = 0$, $q^{\uparrow}_0 = q_0 = 1$, $\pi^{\uparrow}_{0,n} = \mu_{-1}$, $\varepsilon^{\uparrow}_{n,n} = \pi_{0,n} = \mu_0$, $\varepsilon_{n,n} = \mu_1$;
column_regular = $(|\varepsilon^{\uparrow}_{n,n}| > tol)$;
if not column_regular*:*
  set $q^{\leftarrow}_0 = 0$, $\pi^{\leftarrow}_{0,n} = 1$, $\varepsilon^{\leftarrow}_{n,n} = -1$, $\sigma_1 = |\varepsilon^{\uparrow}_{n,n}|$;
while $n < N$
  if column_regular
    set $\varepsilon^{\leftarrow}_{n+1,n+1} = \varepsilon_{n,n}$, $\pi^{\leftarrow}_{0,n+1} = \pi_{0,n}$, *and* $q^{\leftarrow}_{n+1} = q_n$;
    compute $\gamma^{\uparrow}_0 = -\pi^{\uparrow}_{0,n}/\pi_{0,n}$ *and* $\gamma_0 = -\varepsilon_{n,n}/\varepsilon^{\uparrow}_{n,n}$;
    compute $q^{\uparrow}_{n+1} = \zeta q^{\uparrow}_n + q_n\gamma^{\uparrow}_0$ *and* $q_{n+1} = \zeta q^{\uparrow}_n\gamma_0 + q_n$;
    set $\varepsilon^{\uparrow}_{n+1,n+1} = \pi_{0,n+1} = \varepsilon_{n,n}(1 - \gamma^{\uparrow}_0/\gamma_0)$ $(= \varepsilon^{\uparrow}_{n,n} + \varepsilon_{n,n}\gamma^{\uparrow}_0)$;

compute $\pi^{\uparrow}_{0,n+1} = \Pi_{-1}(hq^{\uparrow}_{n+1})$;
set $n = n+1$, $l = l+1$;
column_regular $= (|\varepsilon^{\uparrow}_{n,n}| > tol)$, $\sigma_1 = |\varepsilon^{\uparrow}_{n,n}|$;
if column_regular
compute $\varepsilon_{n,n} = \Pi_{n+1}(hq_n)$;
else
regular = *false*, $k = 1$,
compute $\varepsilon^{\uparrow}_{n+k,n} = \Pi_{n+k}(hq^{\uparrow}_n)$, $\varepsilon^{\leftarrow}_{n+k,n}$ *from* (7.16), *and* $\varepsilon_{n,n}$ *from* (8.14);
while ($k < k_{\max}$ *and* $n+k \le N$ *and not* regular)
(*compute inner LOPs and ROPs and required coefficients*)
compute $\gamma_k^{(n)}$ *from* (8.21), $\gamma_{k-1}^{\uparrow(n)}$ *from* (8.28);
compute q_{n+k} *from* (8.20) *and* $q^{\uparrow}_{n+k}$ *from* (8.26);
compute $\varepsilon^{\uparrow}_{n+k+1,n} = \Pi_{n+k+1}(hq^{\uparrow}_n)$ *and* $\pi^{\uparrow}_{k,n} = \Pi_{-k-1}(hq^{\uparrow}_n)$;
compute $\varepsilon^{\leftarrow}_{n+k+1,n}$ *from* (7.16) *and* $\pi^{\leftarrow}_{k,n}$ *from* (7.17);
for $j = 0, \ldots, k$
compute $\varepsilon_{n+k,n+j}$, $\pi_{k-j,n+j}$, *and* $\pi_{j-k,n+k}$ *from* (8.14) *and* (8.20);
compute $\varepsilon^{\uparrow}_{n+k+1,n+j}$, $\pi^{\uparrow}_{k-j,n+j}$ $(j \ge 1)$, *and* $\varepsilon^{\uparrow}_{n+j,n+k}$ *from* (8.26);
set $k = k+1$;
set $\mathbf{L}^{(l)} = (\pi_{i-j,n+j})_{i,j=0}^{k-1}$, $\mathbf{L}^{\uparrow(l)} = (\varepsilon^{\uparrow}_{n+i,n+j})_{i,j=0}^{k-1}$, $\sigma_k = \min\{\sigma_{\min}(\mathbf{L}_l), \sigma_{\min}(\mathbf{L}^{\uparrow}_l)\}$;
regular $= (\sigma_k > tol)$;
if not regular
(*use optimal* k): $k = \operatorname{argmax}\{\sigma_j,\ 1 \le j \le k\}$;
if $\sigma_k = 0$;
set $L = n$, *return; matrix is singular;*
column_regular $= (k = 1)$;
if ($n+k \le N$ *and not* column_regular)
(*compute anti-diagonally regular pair, i.e.,* $(-1, n+k)$ *and* $(0, n+k-1)$ *Padé forms of* h)
compute $q^{\leftarrow}_{n+k}$, $\varepsilon^{\leftarrow}_{n+k,n+k}$, $q^{\uparrow}_{n+k}$, *and* $\varepsilon^{\uparrow}_{n+k,n+k}$ *from Theorems* 9.1, 9.2;
compute $\pi^{\uparrow}_{0,n+k} = \Pi_{-1}(hq^{\uparrow}_{n+k})$, *set* $\pi^{\leftarrow}_{0,n+k} = 1$;
set $n = n+k$, $l = l+1$, $\sigma_1 = |\varepsilon^{\uparrow}_{n,n}|$, $\pi_{0,n} = \varepsilon^{\uparrow}_{n,n}$;
compute $\alpha_0^{(n)}, \beta_0^{(n)}$ *from* (7.12) *and* $q_n = q^{\leftarrow}_n \alpha_0^{(n)} + q^{\uparrow}_n \beta_0^{(n)}$ *from* (8.14);
column_regular $= (|\varepsilon^{\uparrow}_{n,n}| > tol)$;
if column_regular
set $\varepsilon_{n,n} = \Pi_{n+1}(hq_n)$;

A new variant of the Schur-type algorithm 7.3, which uses again the normalization (2.40) is

Algorithm 9.2: Look-ahead Schur-type algorithm for adjacent rows in the Padé table using underdetermined Padé forms.
INPUT: $h \in \mathcal{L}$, N, $k_{\max}$;

OUTPUT: *numerator* $p_L^\uparrow$ *and residual* $e_L^\uparrow$ *of anti-diagonally regular* $(-1, L)$ *Padé form of* h *for largest possible* $L \le N$*;*

Set $n = 0,\ l = 0,\ p_0^\uparrow = \Pi_{-\infty:-1}\, h,\ e_0^\uparrow = \Pi_{0:\infty}\, h,\ p_0 = \Pi_{-\infty:0} h,\ e_0 = \Pi_{1:\infty}\, h;$
column_regular $= (|\varepsilon_{n,n}^\uparrow| > tol)$*;*
if not column_regular
    set $p_0^\leftarrow = 1,\ e_0^\leftarrow = -1,\ \sigma_1 = |\varepsilon_{n,n}^\uparrow|;$
while $n < N$
    if column_regular
        set $e_{n+1}^\leftarrow = e_n,\ p_{n+1}^\leftarrow = p_n;$
        compute $\gamma_0^\uparrow = -\pi_{0,n}^\uparrow / \pi_{0,n}$ *and* $\gamma_0 = -\varepsilon_{n,n}/\varepsilon_{n,n}^\uparrow;$
        compute $p_{n+1}^\uparrow = \zeta p_n^\uparrow + p_n \gamma_0^\uparrow$ *and* $e_{n+1}^\uparrow = e_n^\uparrow + e_n \gamma_0^\uparrow;$
        compute $p_{n+1} = \zeta p_n^\uparrow \gamma_0 + p_n$ *and* $e_{n+1} = \zeta^{-1}(e_n^\uparrow \gamma_0 + e_n);$
        set $n = n + 1,\ l = l + 1;$
        column_regular $= (|\varepsilon_{n,n}^\uparrow| > tol),\ \sigma_1 = |\varepsilon_{n,n}^\uparrow|;$
    else
        regular = *false*, $k = 1$,
        while $(k < k_{\max}$ *and* $n + k \le N$ *and not* regular)
            (*compute underdetermined Padé forms*)
            compute $\gamma_k^{(n)}$ *from* (8.21), $\gamma_{k-1}^{\uparrow(n)}$ *from* (8.28)*;*
            compute p_{n+k}, e_{n+k} *from* (8.20) *and* $p_{n+k}^\uparrow, e_{n+k}^\uparrow$ *from* (8.26)*;*
            set $k = k + 1;$
            set $\mathbf{L}^{(l)} = (\pi_{i-j,n+j})_{i,j=0}^{k-1},\ \mathbf{L}^{\uparrow(l)} = (\varepsilon_{n+i,n+j}^\uparrow)_{i,j=0}^{k-1},\ \sigma_k = \min\{\sigma_{\min}(\mathbf{L}_l), \sigma_{\min}(\mathbf{L}_l^\uparrow)\};$
            regular $= (\sigma_k > tol)$*;*
        if not regular
            (*use optimal* k)*:* $k = \operatorname{argmax}\{\sigma_j,\ 1 \le j \le k\};$
            if $\sigma_k = 0;$
                set $L = n$*, return; matrix is singular;*
            column_regular $= (k = 1)$*;*
        if $(n + k \le N$ *and not* column_regular)
            (*compute anti-diagonally regular pair, i.e.,* $(-1, n + k)$ *and* $(0, n + k - 1)$ *Padé forms of* h)
            compute $p_{n+k}^\leftarrow,\ e_{n+k}^\leftarrow,\ p_{n+k}^\uparrow$*, and* $e_{n+k}^\uparrow$ *from Theorems* 9.1, 9.2*;*
            set $n = n + k,\ l = l + 1,\ \sigma_1 = |\varepsilon_{n,n}^\uparrow|;$
            compute $\alpha_0^{(n)}, \beta_0^{(n)}$ *from* (7.12) *and* $e_n,\ p_n$ *from* (8.14)*;*
            column_regular $= (|\varepsilon_{n,n}^\uparrow| > tol)$*;*

In a look-ahead step of a Levinson-type algorithm, we have to compute $q_n^\leftarrow$ and q_{n+j}, $q_{n+j}^\uparrow$ for $j = 0, \ldots, k-1$. Since the recurrences look almost identical to those of the Lanczos process, the operation count is again $2k$ SAXPYs for a computing $q_{n+k}^\leftarrow$ and $q_{n+k}^\uparrow$. We have shown in Section 8.3 how to evaluate the required coefficients of the residuals and the denominators of an anti-diagonally regular pair by computing only $2k$ inner

Operations in a block of size $k > 1$	Levinson-type	Schur-type
inner products	$2k$	–
SAXPYs	$4k - 1$	$8k - 2$

Table 9.1: Operation counts for Algorithms 9.1 and 9.2

products in a step of length k. Inner steps cost one SAXPY for each of the $(k-1)$ inner ROPs and each of the $(k-1)$ inner LOPs. The regular LOP is computed from an anti-diagonally regular pair by using Theorem 8.4 for $k = 0$, as described in Section 8.2. This costs again one SAXPY, if scaling is done implicitly.

For the Schur-type algorithm, we have to compute numerators and residuals, *i.e.*, $p_n^{\leftarrow}$, $e_n^{\leftarrow}$ and p_{n+j}, $p_{n+j}^{\uparrow}$, e_{n+j}, $e_{n+j}^{\uparrow}$, $j = 0, \ldots, k-1$. This requires $4k$ SAXPYs for the anti-diagonally regular pair. As we mentioned before, the block LDU factorization of $\mathbf{T}$ contains only p_{n+j} and $e_{n+j}^{\uparrow}$ but not $p_{n+j}^{\uparrow}$ and e_{n+j}. However, since the underdetermined Padé forms are now used to compute the anti-diagonally regular pairs, we have to compute also $p_{n+j}^{\uparrow}$ and e_{n+j} in this variant. Hence, an inner step of the Schur type algorithm also costs 4 SAXPYs. We summarize the operation counts in Table 9.1. The reader should compare Table 9.1 with the operation counts of the product form of the look-ahead algorithms in Table 7.1.

9.2 Matrix formulation of alternative recurrences

We now want to give the Bareiss-Delosme-Ipsen formulation of the alternative recurrences from the previous section, similar as we did for the product form of our look-ahead algorithms in Section 8.4. Clearly, we do not have to discuss classical steps again, since these are identical in both types of algorithms.

To make things simple, and to profit from what we have done in Section 8.4, we rewrite the alternative recurrences in product form. This means that we eliminate the underdetermined Padé forms from the recurrences (9.4) and (9.7) for the new anti-diagonally regular pair. We could also do this rewriting in terms of matrices, but feel that the presentation is clearer if done in terms of polynomials.

Assume that n and $n+k$ are regular indices, and recall that we can compute left and right underdetermined Padé forms via (8.39), where $u_j^{(n)}$ is defined in (8.18) and $u_j^{\uparrow(n)}$ is defined in (8.24). The coefficients of $u_j^{(n)}$ and $u_j^{\uparrow(n)}$ are used to compute the left and right underdetermined Padé forms in Algorithms 9.1 and 9.2. Hence, they are known. Inserting (8.39) into (9.4) yields

$$\begin{bmatrix} p_{n+k}^{\leftarrow} \\ q_{n+k}^{\leftarrow} \end{bmatrix} = \begin{bmatrix} p_n^{\leftarrow} & p_n^{\uparrow} \\ q_n^{\leftarrow} & q_n^{\uparrow} \end{bmatrix} \sum_{j=0}^{k-1} \begin{bmatrix} u_j^{(n)} \\ \beta_0^{(n)} \end{bmatrix} \zeta^{k-1-j} \theta_j^{\leftarrow}.$$

Comparing this identity with (8.38), the uniqueness of the two-point Padé form $(u_k^{\leftarrow(n)}, v_k^{\leftarrow(n)})$ yields

$$\begin{bmatrix} u_k^{\leftarrow(n)} \\ v_k^{\leftarrow(n)} \end{bmatrix} = \sum_{j=0}^{k-1} \begin{bmatrix} u_j^{(n)} \\ \beta_0^{(n)} \end{bmatrix} \zeta^{k-1-j} \theta_j^{\leftarrow}.$$

Similarly, we insert (8.39) into (9.7) and obtain

$$\begin{bmatrix} p_{n+k}^{\uparrow} \\ q_{n+k}^{\uparrow} \end{bmatrix} = \begin{bmatrix} p_n^{\leftarrow} & p_n^{\uparrow} \\ q_n^{\leftarrow} & q_n^{\uparrow} \end{bmatrix} \left(\zeta \begin{bmatrix} u_{k-1}^{\uparrow(n)} \\ \zeta^{k-1} \end{bmatrix} + \sum_{j=0}^{k-1} \begin{bmatrix} u_j^{\uparrow(n)} \\ \zeta^j \end{bmatrix} \theta_j^{\uparrow} + \begin{bmatrix} \vartheta_{n+k}^{\uparrow} \\ 0 \end{bmatrix} \right),$$

so that

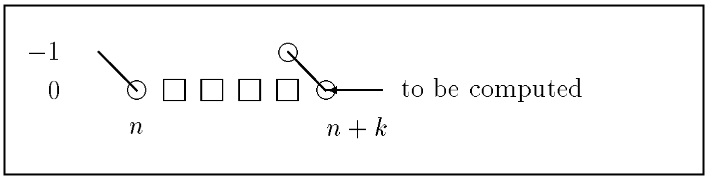
$$\begin{bmatrix} u_k^{\uparrow(n)} \\ v_k^{\uparrow(n)} \end{bmatrix} = \zeta \begin{bmatrix} u_{k-1}^{\uparrow(n)} \\ \zeta^{k-1} \end{bmatrix} + \sum_{j=0}^{k-1} \begin{bmatrix} u_j^{\uparrow(n)} \\ \zeta^j \end{bmatrix} \theta_j^{\uparrow} + \begin{bmatrix} \vartheta_{n+k}^{\uparrow} \\ 0 \end{bmatrix}$$

is just the two-point Padé form $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)})$ used in (8.38). Therefore, we can easily determine the coefficients of the anti-diagonally regular pair of two-point Padé forms $(u_k^{\leftarrow(n)}, v_k^{\leftarrow(n)})$ and $(u_k^{\uparrow(n)}, v_k^{\uparrow(n)})$ from coefficients available in Algorithms 9.1 and 9.2. Together with the recurrence coefficients to compute the underdetermined Padé forms which are known anyway, these coefficients fully determine the matrices $\mathbf{C}_n$ in the matrix formulation (8.46) of the Schur algorithm and (8.47) of the Levinson algorithm.

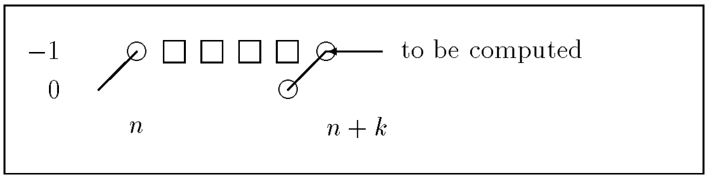
9.3 Related algorithms

In this section we interpret the recurrences of Freund and Zha [42] (Levinson algorithm) and of Freund [38] (Schur algorithm) in the notation we used within this thesis. The statements of the following two corollaries have been proved implicitly in [42] and [38], but we want to give independent proofs here, because they show again the advantage of the Padé approach, where one can use the same argument to derive the Levinson and the Schur recurrences.

We start with pictures for the recurrences again. An illustration of Corollary 9.4 is



and Corollary 9.5 can be visualized by



The two pictures clearly show the symmetry involved in this type of recurrences.

Corollary 9.4: *Let* (p_n, q_n) *be a regular* $(0, n)$ *Padé form of* $h \in \mathcal{L}$ *with residual* e_n*,* (p_{n+j}, q_{n+j}) *be* $(0, n+j)$ *left underdetermined Padé forms with residuals* e_{n+j}*,* $j = 1, \dots, k-1$*, and let* $(p^{\nwarrow}_{n+k}, q^{\nwarrow}_{n+k})$ *be a* $(-1, n+k-1)$ *Padé form of* h *with residual* $e^{\nwarrow}_{n+k}$*. Moreover, let*

$$\vartheta_{n+k} = -e_{n+k-1}(0)/e^{\nwarrow}_{n+k}(0) = -\varepsilon_{n+k-1,n+k-1}/\varepsilon^{\nwarrow}_{n+k,n+k}. \tag{9.8}$$

If a solution of

$$\begin{bmatrix} \pi_{0,n} & \cdots & \pi_{-k+1,n+k-1} \\ \vdots & & \vdots \\ \pi_{k-1,n} & \cdots & \pi_{0,n+k-1} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \vdots \\ \theta_{k-1} \end{bmatrix} = - \begin{bmatrix} 0 \\ \pi_{-k+1,n+k-1} \\ \vdots \\ \pi_{-1,n+k-1} \end{bmatrix} \tag{9.9}$$

exists, then (p_{n+k}, q_{n+k}) *with*

$$\begin{bmatrix} p_{n+k} \\ q_{n+k} \\ e_{n+k} \end{bmatrix} = \begin{bmatrix} p_{n+k-1} \\ q_{n+k-1} \\ e_{n+k-1} \end{bmatrix} + \sum_{j=0}^{k-1} \begin{bmatrix} \zeta^{k-j} p_{n+j} \\ \zeta^{k-j} q_{n+j} \\ e_{n+j} \end{bmatrix} \theta_j + \zeta \begin{bmatrix} p^{\nwarrow}_{n+k} \\ q^{\nwarrow}_{n+k} \\ e^{\nwarrow}_{n+k} \end{bmatrix} \vartheta_{n+k}$$

is a $(0, n+k)$ *Padé form of* h *with monic* $q_{n+k}(0) = 1$ *and residual* e_{n+k}*.*

Proof. We proceed similar to Theorem 9.2. Since by assumption, (p_{n+k}, q_{n+k}) is a regular Padé form, Lemma 2.8 ensures that $e^{\nwarrow}_{n+k}(0) \neq 0$. Clearly, $q_{n+k} \in \mathcal{P}_{n+k}$. From Lemma 8.1 we obtain

$$hq_{n+k} - p_{n+k} = \zeta^{n+k} \left(e_{n+k-1} + e^{\nwarrow}_{n+k} \vartheta_{n+k} + \zeta \sum_{j=0}^{k-1} e_{n+j} \theta_j \right).$$

Hence, the condition $hq_{n+k} - p_{n+k} = O_+(\zeta^{n+k+1})$ is fulfilled for ϑ_{n+k} defined in (9.8). Moreover, $p_{n+k} \in \mathcal{L}_0^*$ if the coefficients θ_j solve the linear system (9.9). □

The normalization used in [42, 38] is the same as ours, namely (2.40). There, the notation was $\varphi_n = q^{\uparrow}_n$, $\psi_n = q^*_n$, $G^{(l)} = (\mathbf{L}^{(l)})^T$, and $F^{(l)} = \mathbf{L}^{\uparrow(l)}$.

To compute the upper neighbor of the regular $(0, n+k)$-Padé form, Freund and Zha proposed the recurrences given in

Corollary 9.5: *Let* $(p^{\uparrow}_n, q^{\uparrow}_n)$ *be an anti-diagonally regular* $(-1, n)$ *Padé form of* $h \in \mathcal{L}$ *with residual* $e^{\uparrow}_n$*,* $(p^{\uparrow}_{n+j}, q^{\uparrow}_{n+j})$ *be* $(-1, n+j)$ *right underdetermined Padé forms with residuals* $e^{\uparrow}_{n+j}$*,* $j = 1, \dots, k-1$*, and* $(p^{\leftarrow}_{n+k}, q^{\leftarrow}_{n+k})$ *be a* $(0, n+k-1)$ *Padé form of* h *with residual* $e^{\leftarrow}_{n+k}$*. Moreover, let*

$$\vartheta^{\uparrow}_{n+k} = -\pi^{\uparrow}_{0,n+k-1}/\pi^{\leftarrow}_{0,n+k}. \tag{9.10}$$

If a solution of

$$\begin{bmatrix} \varepsilon^{\uparrow}_{n,n} & \cdots & \varepsilon^{\uparrow}_{n,n+k-1} \\ \vdots & & \vdots \\ \varepsilon^{\uparrow}_{n+k-1,n} & \cdots & \varepsilon^{\uparrow}_{n+k-1,n+k-1} \end{bmatrix} \begin{bmatrix} \theta^{\uparrow}_0 \\ \vdots \\ \theta^{\uparrow}_{k-1} \end{bmatrix} = - \begin{bmatrix} 0 \\ \varepsilon^{\uparrow}_{n,n+k-1} \\ \vdots \\ \varepsilon^{\uparrow}_{n+k-2,n+k-1} \end{bmatrix} \tag{9.11}$$

exists, then $(p^{\uparrow}_{n+k}, q^{\uparrow}_{n+k})$ *with*

$$\begin{bmatrix} p^{\uparrow}_{n+k} \\ q^{\uparrow}_{n+k} \\ \zeta^k e^{\uparrow}_{n+k} \end{bmatrix} = \zeta \begin{bmatrix} p^{\uparrow}_{n+k-1} \\ q^{\uparrow}_{n+k-1} \\ e^{\uparrow}_{n+k-1} \end{bmatrix} + \sum_{j=0}^{k-1} \begin{bmatrix} p^{\uparrow}_{n+j} \\ q^{\uparrow}_{n+j} \\ e^{\uparrow}_{n+j} \end{bmatrix} \theta^{\uparrow}_j + \begin{bmatrix} p^{\leftarrow}_{n+k} \\ q^{\leftarrow}_{n+k} \\ e^{\leftarrow}_{n+k} \end{bmatrix} \vartheta^{\uparrow}_{n+k}$$

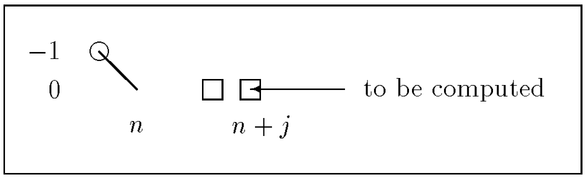
is a $(-1, n+k)$ *Padé form of* h *with monic* $q^{\uparrow}_{n+k}$ *and residual* $e^{\uparrow}_{n+k}$.

Proof. By assumption, $(p^{\uparrow}_{n+k}, q^{\uparrow}_{n+k})$ is an anti-diagonally regular Padé form. Then Lemma 2.9 ensures that $\pi^{\leftarrow}_{0,n+k} \neq 0$. In this case, we obtain from Lemma 8.2

$$hq^{\uparrow}_{n+k} - p^{\uparrow}_{n+k} = \zeta^n \left(\zeta e^{\uparrow}_{n+k-1} + \sum_{j=0}^{k-1} e^{\uparrow}_{n+j} \theta^{\uparrow}_j + \zeta^k e^{\leftarrow}_{n+k} \vartheta^{\uparrow}_{n+k} \right).$$

Hence, the condition $hq^{\uparrow}_{n+k} - p^{\uparrow}_{n+k} = O_+(\zeta^{n+k})$ is equivalent to (9.11). Moreover, $\zeta p^{\uparrow}_{n+k-1} + p^{\leftarrow}_{n+k} \vartheta^{\uparrow}_{n+k} \in \mathcal{L}^*_{-1}$ by (9.10), such that $p^{\uparrow}_{n+k} \in \mathcal{L}^*_{-1}$. □

To apply the recurrences from this corollary in a Levinson algorithm, we first have to compute $q^{\nwarrow}_{n+k}$ *and* $q^{\leftarrow}_{n+k}$. However, from the classical Frobenius identities – given in our notation in Theorem 8.4 (for $k = 0$) – we know that we can compute q_{n+k} from $q^{\leftarrow}_{n+k}$ and $q^{\uparrow}_{n+k}$ by only one SAXPY, if normalization is done implicitly. Hence the expensive recurrence of Corollary 9.4 can be replaced by the inexpensive one from Theorem 8.4, so that we do not need $q^{\nwarrow}_{n+k}$. Inner ROPs are computed exactly the same way as ours. For inner LOPs, $q^{\nwarrow}_n$ instead of $q^{\leftarrow}_n$ is used, which is the recurrences we used in (7.11) in [69]. This results in a block diagonal matrix of the LDU decomposition of $\mathbf{T}$, whose blocks do no longer inherit the Toeplitz structure. An illustration gives



which is the symmetric counterpart of (8.27). If eliminate $q^{\nwarrow}_{n+k}$ from the recurrences given in [42] and [38], then the only difference to our algorithm is that our recurrences involve $q^{\leftarrow}_n$ and the algorithm in [42] uses $q^{\leftarrow}_{n+k}$.

Overhead of SAXPYs for a block of size $k > 1$	Type	Levinson-type	Schur-type
Alg. 7.2, 7.3	last regular pair	$2k-2$	$4k-4$
Huckle [80]	last regular pair	$2k-2$	not proposed
Alg. 9.1, 9.2	complete fact.	$2k-1$	$4k-2$
Alg. 7.2, 7.3 with inner FBOPs	complete fact.	$4k-3$	$6k-5$
Freund/Zha [42], Freund [38]	complete fact.	$4k$	$6k$
Chan/Hansen [26]	complete fact.	$4k-4$	not proposed

Table 9.2: Overhead for different look-ahead algorithms for solving Toeplitz systems.

In Table 9.2, we summarize the overhead of all the variants we proposed in this and the previous chapters. For comparison, we added the overhead of other available methods, namely the Levinson algorithm proposed by Freund and Zha [42], the Schur algorithm of Freund [38], and the Levinson algorithms of Chan and Hansen [26] and Huckle [80]. Since all but the algorithm of Chan and Hansen [26] do not have an overhead of inner products, we list only SAXPYs. The top two lines correspond to algorithms which compute only regular pairs but not the complete (inverse) LDU factorization of the Toeplitz matrix. The bottom part of Table 9.2 summarizes the overhead for methods which compute complete factorizations. For those, our new variant (Algorithms 9.1, 9.2) turns out be the cheapest method known today.

As in all our other variants, overhead occurs only in look-ahead steps. In a regular step ($k = 1$), we do not have to compute $q_n^{\leftarrow}$, $p_n^{\leftarrow}$, and $e_n^{\leftarrow}$, since these are just rescaled versions of q_{n-1}, p_{n-1}, and e_{n-1}. Clearly, this scaling is done only implicitly.

We would like to mention that in a look-ahead step of size $k > 1$, the algorithm of Van Barel and Bultheel [121] uses the same recurrences as our Algorithms 7.2, 7.3, but their algorithm is more expensive in classical steps. Moreover, details on how to implement the algorithm efficiently, *e.g.*, by saving inner products, are not discussed in [121]. Therefore, we have not included this algorithm in Table 9.2.

9.4 Isometric Arnoldi algorithm and Padé approximation

Suppose now that a linear operator $A : \mathcal{H} \to \mathcal{H}$ acting on a linear space $\mathcal{H}$ with bilinear form $(\cdot,\cdot) : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ is (formally) isometric, *i.e.*, $(A\mathbf{w}, A\mathbf{v}) = (\mathbf{w}, \mathbf{v})$ for all $\mathbf{v}, \mathbf{w} \in \mathcal{H}$. Then the moment matrix whose (i, j)th entry is

$$(A^i\mathbf{w}, A^j\mathbf{v}) = \begin{cases} (\mathbf{w}, A^{j-i}\mathbf{v}) =: \mu_{j-i}, & i \le j \\ (A^{i-j}\mathbf{w}, \mathbf{v}) =: \mu_{j-i}, & i \ge j \end{cases} \tag{9.12}$$

is a Toeplitz matrix. We could also use a sesquilinear form instead of a bilinear form, but then we would have to conjugate several of our recurrence coefficients. For the sake of readability, we have chosen to work with a bilinear form. If we would use a sesquilinear form which is also an inner product, then the moment matrix would be Hermitian and positive definite for $\mathbf{v} = \mathbf{w}$. This case was studied in detail by Gragg [53]. Here we want to consider the more general situation resulting in a non-Hermitian Toeplitz matrix.

The relation to what we have done so far is made by defining a bilinear form on $\mathcal{P} \times \mathcal{P}$ via

$$\langle s, t\rangle := (s(A)\mathbf{w}, t(A)\mathbf{v}), \qquad s, t \in \mathcal{P} \times \mathcal{P}.$$

Regular and inner formally biorthogonal polynomials with respect to this bilinear form then yield bases of a Krylov space with respect to the operator A and $\mathbf{v}, \mathbf{w} \in \mathcal{H}$:

$$\mathbf{v}_n = q_n^{\uparrow}(A)\mathbf{v} \qquad \text{and} \qquad \mathbf{w}_n = q_n^{*}(A)\mathbf{w}.$$

These bases are characterized by being block biorthogonal to each other with respect to $(\cdot,\cdot)$, because from Theorem 8.8 we know that

$$\mathbf{D} = (\langle q_j^{*}, q_k^{\uparrow}\rangle)_{j,k} = ((\mathbf{w}_j, \mathbf{v}_k))_{j,k}$$

is block diagonal.

From (9.12) we have

$$\mu_j = \begin{cases} (\mathbf{w}, A^j\mathbf{v}) & j \geq 0, \\ (A^{-j}\mathbf{w}, \mathbf{v}) & j \leq 0, \end{cases}$$

so that the formal Laurent series with coefficients μ_j becomes

$$\begin{aligned} h(\zeta) = \sum_{j=-\infty}^{\infty} \mu_j \zeta^j &= \sum_{j=-\infty}^{-1} (A^{-j}\mathbf{w}, \mathbf{v})\zeta^j + \sum_{j=0}^{\infty} (\mathbf{w}, A^j\mathbf{v})\zeta^j \\ &= ((I - \tfrac{1}{\zeta}A)^{-1}\mathbf{w}, \mathbf{v}) + (\mathbf{w}, (I - \zeta A)^{-1}\mathbf{v}) - (\mathbf{w}, \mathbf{v}). \end{aligned}$$

At least in principle, we can now apply one of the variants of the Levinson algorithm to compute the biorthogonal polynomials. However, we run into the same problems as discussed at the end of Section 6.2 for the Lanczos process. Hence we use the recurrences from Algorithm 9.1, because they can be implemented by only two applications of the operator A in each step and do not require multiplications with polynomials of A which are of degree greater than one. Clearly, we again have to replace the moments of the bilinear form by modified moments involving only the bases $\{\mathbf{v}_n\}_n$, $\{\mathbf{w}_n\}_n$ but not the coefficients of LOPs and ROPs.

Assume in the following that $n = n_l$ is an anti-diagonally regular index, and that the next anti-diagonally regular index is $n_{l+1} = n + k$. Let us first collect some properties of LOPs and ROPs from Lemmas 8.1 and 8.2:

$$\begin{aligned} \langle \zeta^i, q_{n+j}^{\uparrow}\rangle &= 0 \quad \text{for} \quad i = 0, \ldots, n-1, \quad j = 0, \ldots, k-1, \\ \langle q_{n+j}^{*}, \zeta^i\rangle &= 0 \quad \text{for} \quad i = 0, \ldots, n-1, \quad j = 0, \ldots, k-1, \\ \langle q_n^{\leftarrow *}, \zeta^i\rangle &= 0 \quad \text{for} \quad i = 0, \ldots, n-2. \end{aligned} \tag{9.13}$$

Since we only want to multiply by polynomials of degree less than or equal to one, we use the recurrences given in Theorems 9.1 and 9.2 and not those from Chapter 7. In terms of the reflected polynomials the recurrence for $q^{\leftarrow}_{n+k}$ reads

$$q^{\leftarrow *}_{n+k} = \sum_{j=0}^{k-1} q^*_{n+j}\theta^{\leftarrow}_j. \tag{9.14}$$

For inner LOPs, we have (8.31) where $\gamma_j^{(n)}$ is given by (8.21). For inner ROPs, we use (8.26) with $\gamma_j^{\uparrow(n)}$ from (8.28).

The normalization remains the same as introduced in (2.40). For the reflected polynomials, this means that q_j^* and $q_j^{\uparrow}$ are monic for every $j \geq 0$, and that by Lemma 8.3 (for $k = 0$ and where n is substituted by $n-1$)

$$\pi^{\leftarrow}_{0,n} = \langle q^{\leftarrow *}_n, \zeta^{n-1}\rangle = \langle q^{\leftarrow *}_n, q^{\uparrow}_{n-1}\rangle = 1 \tag{9.15}$$

for regular indices n. The second equality is a consequence of (9.13) and $q^{\uparrow}_{n-1}$ being monic.

Next we derive linear systems equivalent to (9.3) and (9.6), since these are useless as long as we cannot compute the coefficients of p_{n+j} and $e^{\uparrow}_{n+j}$. Recall that the latter is impossible if we know only the basis vectors $\mathbf{v}_{n+j}, \mathbf{w}_{n+j}$ but not the coefficients of q_{n+j} and $q^{\uparrow}_{n+j}$. The aim is to obtain linear systems which contain only modified moments of the bilinear form (8.1). We give proofs of all statements in order to make clear that this chapter is completely self contained, which means that everything follows *without* using statements from Padé theory. However, we would like to stress that without the help of the Padé table, it would have been very difficult to find the pairs of polynomials which should be used to derive the most efficient recurrences. Moreover, the proofs only lead to a Levinson-type algorithm; a Schur-type algorithm would require further work.

Theorem 9.6: *Let q^*_n be an nth regular LOP, $q^{\uparrow}_n$ be an nth regular ROP, and $q^{\leftarrow *}_n$ be a polynomial satisfying* (9.13) *and* (9.15)*. Moreover, let q^*_{n+j} and $q^{\uparrow}_{n+j}$, $j = 1, \ldots, k-1$ be inner LOPs and ROPs, respectively, and assume $\mathbf{D}^{(l)} = (\langle q^*_{n+i}, q^{\uparrow}_{n+k}\rangle)_{i,j=0}^{k-1}$ to be nonsingular. Then the following statements are valid.*

(i) *If*

$$\vartheta^{\uparrow}_{n+k} = -\frac{\langle 1, \zeta q^{\uparrow}_{n+k-1}\rangle}{\langle 1, q^{\leftarrow}_n\rangle} = -\frac{\langle 1, \zeta q^{\uparrow}_{n+k-1}\rangle}{\langle q^{\leftarrow *}_n, q^{\uparrow}_{n-1}\rangle}, \tag{9.16}$$

and $\mathbf{d}^{\uparrow}_n = [\ \theta^{\uparrow}_0 \ \ \cdots \ \ \theta^{\uparrow}_{k-1}\ ]^T$ *is the unique solution of*

$$\mathbf{D}^{(l)}\mathbf{d}^{\uparrow}_n = -\begin{bmatrix} \langle q^*_n, \zeta q^{\uparrow}_{n+k-1}\rangle \\ \vdots \\ \langle q^*_{n+k-1}, \zeta q^{\uparrow}_{n+k-1}\rangle \end{bmatrix}, \tag{9.17}$$

then $q^{\uparrow}_{n+k}$ defined in (9.7) *is a regular* $(n+k)$*th FOP.*

(ii) *If* $\mathbf{d}_n^{\leftarrow} = [\ \theta_0^{\leftarrow} \ \cdots \ \theta_{k-1}^{\leftarrow}\ ]^T$ *is the unique solution of*

$$(\mathbf{D}^{(l)})^T \mathbf{d}_n^{\leftarrow} = \mathbf{e}_{k-1}, \tag{9.18}$$

then $q_{n+k}^{\leftarrow *}$ *defined in* (9.14) *is left orthogonal to all polynomials of degree less or equal* $n+k-2$ *and normalized by* (9.15).

(iii) *If for* $j = 1, \ldots, k-1$

$$\gamma_j^{(n)} = -\frac{\langle \zeta q_{n+j-1}^*, 1\rangle}{\langle \zeta q_n^{\leftarrow *}, 1\rangle}, \tag{9.19}$$

then q_{n+j}^* *defined in* (8.31) *is an* $(n+j)$*th inner LOP. Moreover, if*

$$\gamma_{j-1}^{\uparrow(n)} = -\frac{\langle 1, \zeta q_{n+j-1}^{\uparrow}\rangle}{\langle 1, q_n^{\leftarrow}\rangle}, \tag{9.20}$$

then $q_{n+j}^{\uparrow}$ *defined in* (8.26) *is an* $(n+j)$*th inner ROP.*

Proof. (i) Recall that inner ROPs are monic and, therefore, $q_{n+k}^{\uparrow}$ defined in (9.7) is monic of degree $n+k$. To prove that it is right orthogonal to every polynomial of degree less than $n+k$, observe that for $\vartheta_{n+k}^{\uparrow}$ given by (9.16)

$$\langle 1, q_{n+k}^{\uparrow}\rangle = \langle 1, \zeta q_{n+k-1}^{\uparrow}\rangle + \langle 1, q_n^{\leftarrow}\rangle \vartheta_{n+k}^{\uparrow} = 0.$$

The second equality in (9.16) follows from (8.12). For $i = 1, \ldots, n-1$, we then have by definition of inner ROPs, (8.32), and (8.12)

$$\begin{aligned}
\langle q_i^*, q_{n+k}^{\uparrow}\rangle &= \langle q_i^* - q_i^*(0), q_{n+k}^{\uparrow}\rangle \\
&= \langle q_i^* - q_i^*(0), \zeta q_{n+k}^{\uparrow}\rangle + \langle q_i^* - q_i^*(0), q_n^{\leftarrow}\rangle \vartheta_{n+k}^{\uparrow} \\
&= \langle \frac{q_i^* - q_i^*(0)}{\zeta}, q_{n+k}^{\uparrow}\rangle + \langle q_n^{\leftarrow *}, \zeta^{n-1-i}(q_i - \rho_{i,i}\zeta^i)\rangle \vartheta_{n+k}^{\uparrow} \\
&= 0,
\end{aligned}$$

because $(q_i^* - q_i^*(0))/\zeta \in \mathcal{P}_{i-1}$, and $\zeta^{n-1-i}(q_i - \rho_{i,i}\zeta^i) \in \mathcal{P}_{n-2}$. For $i = n, \ldots, n+k-1$, we obtain

$$\begin{aligned}
\langle q_i^*, q_{n+k}^{\uparrow}\rangle &= \langle q_i^*, \zeta q_{n+k}^{\uparrow}\rangle + \sum_{j=0}^{k-1} \langle q_i^*, q_{n+j}^{\uparrow}\rangle \theta_j^{\uparrow} + \langle q_i^*, q_n^{\leftarrow}\rangle \vartheta_{n+k} \\
&= \langle q_i^*, \zeta q_{n+k}^{\uparrow}\rangle + \sum_{j=0}^{k-1} \langle q_i^*, q_{n+j}^{\uparrow}\rangle \theta_j^{\uparrow},
\end{aligned}$$

since $q_n^{\leftarrow} \in \mathcal{P}_{n-1}$. Hence $\langle \zeta^i, q_{n+k}^{\uparrow}\rangle = 0$ for $i = 0, \ldots, n+k-1$ for $\theta_j^{\uparrow}$ taken from (9.17) and $\vartheta_{n+k}^{\uparrow}$ from (9.16).

(ii) Clearly, $q_{n+k}^{\leftarrow *}$ defined in (9.14) is in $\mathcal{P}_{n+k-1}$ since it is a linear combination of polynomials in $\mathcal{P}_{n+k-1}$. For $i = 0, \ldots, n-1$ we have from Lemma 8.2

$$\langle q_{n+k}^{\leftarrow *}, q_i^{\uparrow} \rangle = \sum_{j=0}^{k-1} \langle q_{n+j}^{*}, q_i^{\uparrow} \rangle \theta_j^{\uparrow} = 0.$$

The conditions $\langle q_{n+k}^{\leftarrow *}, q_i^{\uparrow} \rangle = 0$ for $i = n, \ldots, n+k-2$ and $\langle q_{n+k}^{\leftarrow *}, q_{n+k-1}^{\uparrow} \rangle = 1$ are equivalent to (9.18).

(iii) Similar to (i). $\gamma_j^{(n)}$ is chosen such that $\langle q_{n+j}^{*}, 1 \rangle = 0$. Then for $i = 1, \ldots, n-1$,

$$\begin{aligned} \langle q_{n+j}^{*}, q_i^{\uparrow} \rangle &= \langle q_{n+j}^{*}, q_i^{\uparrow} - q_i^{\uparrow}(0) \rangle \\ &= \langle q_{n+j-1}^{*} + q_n^{\leftarrow *}, \frac{q_i^{\uparrow} - q_i^{\uparrow}(0)}{\zeta} \rangle \\ &= 0. \end{aligned}$$

Finally, $\gamma_j^{\uparrow(n)}$ is chosen such that $\langle 1, q_{n+j}^{\uparrow} \rangle = 0$. Then for $i = 1, \ldots, n-1$,

$$\begin{aligned} \langle q_i^{*}, q_{n+j}^{\uparrow} \rangle &= \langle q_i^{*} - q_i^{*}(0), q_{n+j}^{\uparrow} \rangle \\ &= \langle \frac{q_i^{\uparrow} - q_i^{\uparrow}(0)}{\zeta}, q_{n+j-1}^{\uparrow} \rangle + \langle q_i^{\uparrow} - q_i^{\uparrow}(0), q_n^{\leftarrow} \rangle \\ &= 0, \end{aligned}$$

where the last equality was already proved in (i). □

The only recurrence which is missing in the previous theorem is the one to compute a regular LOP from an anti-diagonally regular pair.

Corollary 9.7: *Let $q_n^{\uparrow}$ be an nth regular ROP and $q_n^{\leftarrow *}$ be a polynomial satisfying* (9.13) *and* (9.15). *Then*

$$q_n^{*} = \zeta q_n^{\leftarrow *} \alpha_n + q_n^{\uparrow *} \beta_n,$$

where

$$\begin{bmatrix} \alpha_n \\ \beta_n \end{bmatrix} = \frac{1}{\langle 1, q_n^{\leftarrow} \rangle} \begin{bmatrix} \langle q_n^{*}, q_n^{\uparrow} \rangle \\ -\langle \zeta q_n^{\leftarrow *}, 1 \rangle \end{bmatrix} \tag{9.21}$$

is a monic nth regular LOP.

Proof. For $i = 1, \ldots, n-1$ we have

$$\begin{aligned} \langle q_n^{*}, \zeta^i \rangle &= \langle \zeta q_n^{\leftarrow *}, \zeta^i \rangle \alpha_n + \langle q_n^{\uparrow *}, \zeta^i \rangle \beta_n \\ &= \langle q_n^{\leftarrow *}, \zeta^{i-1} \rangle \alpha_n + \langle \zeta^{n-i} q_n^{\uparrow} \rangle \beta_n \\ &= 0 \end{aligned}$$

for all $\alpha_n, \beta_n \in \mathbb{C}$ and

$$\langle q_n^{*}, 1 \rangle = \langle \zeta q_n^{\leftarrow *}, 1 \rangle \alpha_n + \langle \zeta^n q_n^{\uparrow} \rangle \beta_n = 0$$

for α_n, β_n satisfying (9.21). Finally, $q_n(0) = 1$ is equivalent to

$$\langle 1, q_n^{\leftarrow} \rangle = q_n^{\leftarrow}(0)\langle q_n^*, q_n^{\uparrow} \rangle - q_n^{\uparrow}(0)\langle \zeta q_n^{\leftarrow *}, 1 \rangle$$

which follows from

$$\begin{aligned} q_n^{\leftarrow}(0)\langle q_n^*, q_n^{\uparrow}\rangle &= \langle \zeta q_n^{\leftarrow *}, q_n^{\uparrow}\rangle \\ &= \langle \zeta q_n^{\leftarrow *}, \zeta^n + q_n^{\uparrow}(0)\rangle \\ &= \langle q_n^{\leftarrow *}, \zeta^{n-1}\rangle + q_n^{\uparrow}(0)\langle \zeta q_n^{\leftarrow *}, 1\rangle \\ &= \langle 1, q_n^{\leftarrow}\rangle + q_n^{\uparrow}(0)\langle \zeta q_n^{\leftarrow *}, 1\rangle. \end{aligned}$$

□

The following Lemma gives equivalent expressions for (9.16), (9.19), and (9.20).

Lemma 9.8: *Let the assumption of Theorem* 9.6 *be valid. Then, for* $j = 0, \ldots, k-1$ *the following equalities hold*

$$\begin{aligned} q_n^*(0)\,\langle 1, \zeta q_{n+j}^{\uparrow}\rangle &= \langle q_n^*, \zeta q_{n+j}^{\uparrow}\rangle, \\ q_n^{\uparrow}(0)\,\langle \zeta q_{n+j}^*, 1\rangle &= \langle \zeta q_{n+j}^*, q_n^{\uparrow}\rangle, \\ q_{n-1}^{\uparrow}(0)\,\langle \zeta q_n^{\leftarrow *}, 1\rangle &= \langle 1, q_n^{\leftarrow}\rangle. \end{aligned}$$

Proof. For $i = 1, \ldots, n$ we have from (8.32),

$$\begin{aligned} \langle \zeta^i, \zeta q_{n+j}^{\uparrow}\rangle &= \langle \zeta^{i-1}, q_{n+j}^{\uparrow}\rangle = 0, \\ \langle \zeta q_{n+j}^*, \zeta^i\rangle &= \langle q_{n+j}^*, \zeta^{i-1}\rangle = 0. \end{aligned}$$

Similar, for $i = 1, \ldots, n-1$, it holds

$$\langle \zeta q_n^{\leftarrow *}, \zeta^i\rangle = \langle q_n^{\leftarrow *}, \zeta^{i-1}\rangle = 0.$$

Hence, in all the bilinear forms, only the constant terms play a role. This proves the Lemma. □

Recall that a desirable feature of look-ahead Levinson-type is to avoid an overhead of inner products. We have shown how this can be accomplished for our Levinson-type algorithms 7.2 and 9.1. Next we show, that the same is possible for an implementation based on the recurrences of the previous theorem.

We suggest to compute the inner products $\langle q_n^*, q_n^{\uparrow}\rangle$, $\langle \zeta q_n^{\leftarrow *}, 1\rangle$, and $\langle 1, \zeta q_{n+j-1}^{\uparrow}\rangle$, $\langle \zeta q_{n+j-1}^*, 1\rangle$ for $j = 1, \ldots, k-1$, *i.e.*, in total $2k$ inner products, explicitly.

From Theorem 8.8, it is known that the blocks $\mathbf{D}^{(l)}$ of the block diagonal matrix $\mathbf{D}$ have Toeplitz structure. Hence it is sufficient to compute the first row and column of $\mathbf{D}^{(l)}$. For the first row we obtain from Lemma 9.8,

$$\langle q_n^*, q_{n+j}^{\uparrow}\rangle = \langle q_n^*, \zeta q_{n+j-1}^{\uparrow}\rangle = q_n^*(0)\langle 1, \zeta q_{n+j-1}^{\uparrow}\rangle, \quad j \geq 1.$$

The first column is treated similarly,

$$\begin{aligned}\langle q_{n+j}^*, q_n^\uparrow\rangle &= \langle \zeta q_{n+j-1}^*, q_n^\uparrow\rangle + \langle \zeta q_n^{\leftarrow *}\gamma_j^{(n)}, q_n^\uparrow\rangle \\ &= q_n^\uparrow(0)\langle \zeta q_{n+j-1}^*, 1\rangle + \gamma_j^{(n)} q_n^{\leftarrow *}(0)\langle q_n^*, q_n^\uparrow\rangle, \quad j \geq 1.\end{aligned}$$

Here, the last equality follows from q_n^* being monic of degree n. Therefore, $\mathbf{D}^{(l)}$ can be updated from inner products we computed explicitly.

For the right-hand side in (9.17), we have shown in the proof of Theorem 8.8, that for $k \geq 2$, *i.e.*, in a look-ahead step,

$$\langle q_{n+j}^*, \zeta q_{n+k-1}^\uparrow\rangle = \langle q_{n+j-1}^*, q_{n+k-1}^\uparrow\rangle, \qquad \text{for} \quad j = 1, \ldots, k-1.$$

This means that the last $k-1$ entries of the right-hand side in (9.17) are elements from $\mathbf{D}^{(l)}$. For the first one, $\langle q_n^*, \zeta q_{n+k-1}^\uparrow\rangle$, we apply the recurrence (9.7) and obtain

$$\langle q_n^*, \zeta q_{n+k-1}^\uparrow\rangle = \sum_{j=0}^{k-1}\langle q_n^*, q_{n+j}^\uparrow\rangle\theta_j^\uparrow.$$

It remains to show how one can obtain the denominators in (9.16), which are the same as in (9.20). If the last step was a look-ahead step, then $\langle 1, q_n^{\leftarrow}\rangle = 1$ by our normalization, and if the last step was a step of length one, then

$$\langle 1, q_n^{\leftarrow}\rangle = \langle 1, q_{n-1}\rangle = \langle q_{n-1}^*, \zeta^{n-1}\rangle = \langle q_{n-1}^*, q_{n-1}^\uparrow\rangle,$$

which has been computed already.

In summary, the $2k$ inner products we suggested to compute explicitly are sufficient to update any other inner product which appears in Theorem 9.6 and Corollary 9.7.

The new Levinson algorithm can be obtained directly from Algorithm 9.1 if one writes all the recurrences involving (underdetermined) Padé forms in the 0th row in terms of the reflected polynomials and replaces the linear systems by those of this section. We therefore omit the details.

10. EXTRAPOLATION

In this chapter, we exploit the close relation between general extrapolation algorithms and Padé approximation to extend some well known extrapolation algorithms for application to nonnormal Padé tables. This connection is discussed *e.g.*, by Gragg [52], Baker and Graves-Morris [5] and Brezinski and Redivo-Zaglia [16].

We will first explain this relation and then show that with the background we have from Chapters 4–6, where we developed recurrences for computing Padé forms on a certain diagonal of the Padé table, it is in fact a very simple task to generalize extrapolation algorithms.

A different look-ahead extrapolation algorithm was proposed recently by Brezinski and Redivo-Zaglia [17]. The derivation of our algorithm, which exploits one more time the Padé connection, turns out to simplify matters considerably.

10.1 Extrapolation and Padé approximation

Using Cramer's rule to solve (2.30) and the expansion of a determinant in its first row one can easily show that the denominator $q_{m,n}$ of a regular (m, n) PF $(p_{m,n}, q_{m,n})$ normalized by $q_{m,n}(0) = 1$ of a formal power series h with coefficients (2.5) can be expressed as

$$q_{m,n}(\zeta) = \det \begin{bmatrix} 1 & \zeta & \cdots & \zeta^n \\ \mu_{m+1} & \mu_m & \cdots & \mu_{m-n+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{m+n} & \mu_{m+n-1} & \cdots & \mu_m \end{bmatrix}. \tag{10.1}$$

Further, we conclude that in view of $p_{m,n} = \Pi_{0:m}\,(hq_{m,n})$,

$$p_{m,n}(\zeta) = \det \begin{bmatrix} h_m(\zeta) & \zeta h_{m-1}(\zeta) & \cdots & \zeta^n h_{m-n}(\zeta) \\ \mu_{m+1} & \mu_m & \cdots & \mu_{m-n+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{m+n} & \mu_{m+n-1} & \cdots & \mu_m \end{bmatrix}, \tag{10.2}$$

where

$$h_m(\zeta) \equiv \Pi_{0:m}\, h = \sum_{k=0}^{m} \mu_k \zeta^k.$$

Let $\{\nu_j\}_{j\geq 0}$ be an arbitrary sequence, then the general G-transformation [57] is defined as

$$G_n^{(m)} = \frac{\det \begin{bmatrix} \nu_{m+n} & \nu_{m+n-1} & \cdots & \nu_m \\ \mu_{m+n} & \mu_{m+n-1} & \cdots & \mu_m \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{m+2n-1} & \mu_{m+2n-2} & \cdots & \mu_{m+n-1} \end{bmatrix}}{\det \begin{bmatrix} 1 & 1 & \cdots & 1 \\ \mu_{m+n} & \mu_{m+n-1} & \cdots & \mu_m \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{m+2n-1} & \mu_{m+2n-2} & \cdots & \mu_{m+n-1} \end{bmatrix}}.$$

This transformation is quite general; see *e.g.*, [11]. For instance, if

$$\mu_0 = \nu_0 \qquad \text{and} \qquad \mu_j = \nu_j - \nu_{j-1}, \quad j \geq 1, \tag{10.3}$$

then it is just Shanks transformation [110]. Note that in this particular case, we have $h_m(1) = \nu_m$ and thus from (10.1) and (10.2)

$$G_n^{(m)} = \frac{p_{m+n-1,n}(1)}{q_{m+n-1,n}(1)}. \tag{10.4}$$

Clearly, $G_n^{(m)}$ exists if and only if $q_{m+n-1,n}(1) \neq 0$.

Because of (10.4), computing the G-transformations corresponds to evaluating Padé approximants at one. Recursive algorithms for computing the G-transformations in its general form can be found in [104]. For the special case (10.3), the probably best known algorithm is the epsilon algorithm by Wynn [122]. Wynn's epsilon algorithm computes the epsilon table by a rhombus rule: to obtain $r_{m+n,n}(1)$ it computes recursively $r_{m+j,k}(1)$ for $j + k \leq 2n$ besides some auxiliary quantities which are not of interest here. It is well known that the mth entry of the $2n$th column of the epsilon table is just $r_{m+n,n}(1)$, where $r_{m+n,n}$ is the $(m+n, n)$ Padé form of h; see *e.g.*, [51].

As in Chapters 4–6, from now on we will keep the index m fixed and index Padé forms according to their denominator degree n.

In the general case, G-transformations are still related to Padé approximation, since for the denominator q_n of an $(m + n - 1, n)$ Padé form of h, it holds from (10.2)

$$G_n^{(m)} = \left(\sum_{j=0}^{n} \rho_{n-j,n} \nu_{m+j} \right) / q_n(1), \tag{10.5}$$

where $\rho_{j,n}$ are the coefficients of q_n as defined in (2.25). Note that the numerator of the $(m+n-1, n)$ Padé form no longer occurs in (10.5), and recall that q_n^* can be interpreted as a formally orthogonal polynomial with respect to a linear form (5.1). This makes it possible to apply algorithms which recursively compute FOPs, *e.g.*, those described in Chapters 4–6.

However, the recursive algorithms [104, 122] can break down if the Padé table is not normal. Recently, Brezinski and Redivo-Zaglia [17] proposed look-ahead algorithms for higher order G-transformations to overcome the difficulties arising with nonnormal Padé tables. Their algorithms compute FOPs with respect to the linear form (5.1), which are normalized to be one at one. The basic idea is to introduce a second sequence of FOPs with respect to the linear functional Φ' defined by

$$\Phi'(\zeta^i) = \Phi(\zeta^i(\zeta - 1))$$

and give coupled recurrences between the two sequences of FOPs. Theoretical properties of "adjacent" FOPs are given by Draux [36]. The coupling is needed solely to enforce the specific normalization of the FOPs at one. However, the coupling turns out to be unnecessary if one does not enforce this normalization. Moreover, it is not clear that the algorithms [17] perform look-ahead steps of minimal length.

10.2 Look-ahead extrapolation algorithms

Here we intend to present two algorithms which provide an alternative way to compute the Padé approximations $r_{m+n,n}(1)$ for $n = 0, 1, \ldots$ for general Padé tables. The recurrences proceed directly along only one diagonal, *i.e.*, they do not compute the Padé approximants $r_{m+j,k}$ in a complete sector $j + k \leq 2n$.

Our algorithms work with one linear functional only instead of two as the algorithm in [17]. The key point is that Algorithms 4.2 and 4.3 can easily be modified such that they additionally evaluate each diagonal Padé form at a fixed value a. This is due to the fact that residuals, numerators, and denominators of Padé forms satisfy the same recurrence relations. We could benefit from this fundamental result many times in this thesis already. The computation of the corresponding $(m + n, n)$ Padé approximant at a from the computed Padé form is then trivial. We first check, whether the denominator $q_n(a)$ is different from zero (or not too close to zero in finite precision arithmetic). If it is, then we compute the Padé approximant as $p_n(a)/q_n(a)$, but if it is not, we nevertheless use the values of the Padé form $(p_n(a), q_n(a))$ to advance the recursion. The main difference to the epsilon algorithm is that $p_n(a)$ and $q_n(a)$ are updated independently, and from these updates, $r_n(a)$ is computed. The epsilon algorithm works instead directly with $r_n(a)$. Using recurrences for evaluating Padé forms allows us to avoid a normalization of q_n at a as was used in [17]. Hence our algorithm performs look-ahead steps of minimal size.

For extrapolation algorithms, we set $a = 1$. Due to the block structure of the Padé table, these values are the same in a whole block of the Padé table, hence no inner polynomials are required for extrapolation algorithms. They may be useful to save operations, as was shown in Chapter 6.

We first describe the Levinson-type algorithm.

Algorithm 10.1: Look-ahead Levinson-type algorithm for evaluating Padé approximants on a diagonal of the Padé table.

INPUT: $h \in \mathcal{L}$, m, N;

OUTPUT: $r_{m+N,N}(a)$ *of a regular* $(m+L, L)$ *Padé approximant of* h; *for largest possible* $L \leq N$;

Set $n = 0$, $q_0 = 1$, $q_0^{\nwarrow} = 0$, $\varepsilon_{0,0}^{\nwarrow} = -1$, $\varepsilon_{1,0}^{\nwarrow} = 0$;

Set $p_0(a) = \Pi_{0:m} h(a)$, $q_0(a) = 1$, $e_0^{\nwarrow}(a) = -1$, $p_0^{\nwarrow}(a) = a^{m-1}$, $q_0^{\nwarrow}(a) = 0$;

while $n < N$

  set $k = 1$; *compute* $\varepsilon_{n,n} = \Pi_{m+2n+1}(hq_n)$, $\varepsilon_{n+1,n} = \Pi_{m+2n+2}(hq_n)$;

  while $\sigma_{\min}(\mathbf{S}_{k,n}) < tol$ *and* $n + k < N$

    set $k = k + 1$;

    set $\varepsilon_{n+2k-2,n} = \Pi_{m+2n+2k-1}(hq_n)$, $\varepsilon_{n+2k-1,n} = \Pi_{m+2n+2k}(hq_n)$;

    compute $\varepsilon_{n+2k-2,n}^{\nwarrow}$, $\varepsilon_{n+2k-1}^{\nwarrow}$ *from* (4.5);

  solve (4.2) *for the coefficients of* $u_k \in \mathcal{P}_{k-1}$ *and* $v_k \in \mathcal{P}_k$;

  compute $q_{n+k} = \zeta^2 q_n^{\nwarrow} u_k + q_n v_k$ (*Corollary* 4.1);

  compute Padé form at a:

$$\begin{bmatrix} p_{n+k}(a) \\ q_{n+k}(a) \end{bmatrix} = \begin{bmatrix} a^2 p_n^{\nwarrow}(a) & p_n(a) \\ a^2 q_n^{\nwarrow}(a) & q_n(a) \end{bmatrix} \begin{bmatrix} u_k(a) \\ v_k(a) \end{bmatrix}$$

  if $|q_{n+k}(a)| > tol$, *then set* $r_{n+k}(a) = p_{n+k}(a)/q_{n+k}(a)$;

  if $n + k < N$

    if $k = 1$

      set $q_{n+1}^{\nwarrow} = q_n$, $\varepsilon_{n+1,n+1}^{\nwarrow} = \varepsilon_{n,n}$, $\varepsilon_{n+2,n+1}^{\nwarrow} = \varepsilon_{n+1,n}$;

      set $q_{n+1}^{\nwarrow}(a) = q_n(a)$, $p_{n+1}^{\nwarrow}(a) = p_n^{\nwarrow}(a)$;

    else

      solve (4.3) *for the coefficients of* $u_k^{\nwarrow} \in \mathcal{P}_{k-2}$ *and* $v_k^{\nwarrow} \in \mathcal{P}_{k-1}$;

      compute $q_{n+k}^{\nwarrow} = \zeta^2 q_n^{\nwarrow} u_k^{\nwarrow} + q_n v_k^{\nwarrow}$ (*Corollary* 4.1);

      set $\varepsilon_{n+k,n+k}^{\nwarrow} = 1$ *and compute* $\varepsilon_{n+k+1,n+k}^{\nwarrow} = \Pi_{2k-1}(e_n^{\nwarrow} u_k^{\nwarrow} + e_n v_k^{\nwarrow})$,

      where $e_n^{\nwarrow} = \sum_{j=0}^{2k-1} \varepsilon_{n+j,n}^{\nwarrow} \zeta^j$ *and* $e_n = \sum_{j=0}^{2k-1} \varepsilon_{n+j,n} \zeta^j$;

      compute Padé form at a:

$$\begin{bmatrix} p_{n+k}^{\nwarrow}(a) \\ q_{n+k}^{\nwarrow}(a) \end{bmatrix} = \begin{bmatrix} a^2 p_n^{\nwarrow}(a) & p_n(a) \\ a^2 q_n^{\nwarrow}(a) & q_n(a) \end{bmatrix} \begin{bmatrix} u_k^{\nwarrow}(a) \\ v_k^{\nwarrow}(a) \end{bmatrix}$$

  else

    set $L = n$;

  set $n = n + k$;

This algorithm is a simple extension of Algorithm 4.2. Similarly, one could extend Algorithm 6.1.

Note that we have updated $q_{n+k}(a)$ separately from q_{n+k}. This is much less expensive than evaluating $q_{n+k}(a)$ explicitly, since we only have to evaluate the polynomials u_k, v_k of low degree at a but not higher degree polynomials. Nevertheless, we need all the coefficients of q_{n+k} to proceed in the recursion.

For the general higher order G-transformation, the Padé approximant is not evaluated at a certain prescribed value. Here, one has to compute the coefficients of the denominators of the diagonal Padé forms explicitly and then compute the transformations via (10.5). Hence one can apply Algorithm 4.2 directly instead of the variant given above. The additional evaluations of the Padé forms at a are unnecessary then.

The following Schur type algorithm does not compute the denominators of Padé forms but only residuals. If denominators are required, one can of course update them with the recurrences from Corollary 4.1, but this will in general be more expensive then computing them directly with the Levinson type algorithm. Since the Schur type algorithm does not involve any inner products, it may be an attractive variant on computer architectures where inner products involve a bottleneck in the computation due to the global communication involved.

We present an extension of Algorithm 4.3, but, oviously, one could also extend Algorithm 6.2.

Algorithm 10.2: Look-ahead Schur-type algorithm for evaluating Padé approximants on a diagonal of the Padé table.
INPUT: $h \in \mathcal{L}$, m, N;
OUTPUT: *residual* e_N *of regular* $(m+L, L)$ *Padé form of* h *for largest possible* $L \leq N$;
Set $n = 0$, $e_0 = \Pi_{m+1:\infty} h$, $e_0^{\nwarrow} = -1$;
Set $p_0(a) = \Pi_{0:m} h(a)$, $q_0(a) = 1$, $p_0^{\nwarrow}(a) = a^{m-1}$, $q_0^{\nwarrow}(a) = 0$;
while $n < N$
  set $k = 1$;
  while $\sigma_{\min}(\mathbf{S}_{k,n}) < tol$ *and* $n + k < N$
    set $k = k + 1$;
  solve (4.2) *for the coefficients of* $u_k \in \mathcal{P}_{k-1}$ *and* $v_k \in \mathcal{P}_k$;
  compute $e_{n+k} = \zeta^{-2k}(e_n^{\nwarrow} u_k + e_n v_k)$ (*Corollary* 4.1);
  compute Padé form at a:

$$\begin{bmatrix} p_{n+k}(a) \\ q_{n+k}(a) \end{bmatrix} = \begin{bmatrix} a^2 p_n^{\nwarrow}(a) & p_n(a) \\ a^2 q_n^{\nwarrow}(a) & q_n(a) \end{bmatrix} \begin{bmatrix} u_k(a) \\ v_k(a) \end{bmatrix}$$

  if $|q_{n+k}(a)| > tol$, *then set* $r_{n+k}(a) = p_{n+k}(a)/q_{n+k}(a)$;
  if $n + k < N$
    if $k = 1$
      set $e_{n+1}^{\nwarrow} = e_n$, $q_{n+1}^{\nwarrow}(a) = q_n(a)$, $p_{n+1}^{\nwarrow}(a) = p_n^{\nwarrow}(a)$;

else

solve (4.3) *for the coefficients of* $u_k^{\nwarrow} \in \mathcal{P}_{k-2}$ *and* $v_k^{\nwarrow} \in \mathcal{P}_{k-1}$*;*

compute $e_{n+k}^{\nwarrow} = \zeta^{-2k+2}(e_n^{\nwarrow} u_k^{\nwarrow} + e_n v_k^{\nwarrow})$*;*

compute Padé form at a*:*

$$\begin{bmatrix} p_{n+k}^{\nwarrow}(a) \\ q_{n+k}^{\nwarrow}(a) \end{bmatrix} = \begin{bmatrix} a^2 p_n^{\nwarrow}(a) & p_n(a) \\ a^2 q_n^{\nwarrow}(a) & q_n(a) \end{bmatrix} \begin{bmatrix} u_k^{\nwarrow}(a) \\ v_k^{\nwarrow}(a) \end{bmatrix}$$

else

set $L = n$*;*

set $n = n + k$*;*

Both algorithms require $O(N^2)$ arithmetic operations, as the epsilon algorithm by Wynn. However, Wynn's algorithm computes the complete sector of the Padé table while we compute only a certain diagonal.

11. NUMERICAL EXPERIMENTS

In this chapter we present numerical experiments for the different versions of look-ahead row-algorithms presented in this thesis. The application on which we want to compare the algorithms is the solution of linear systems with Toeplitz coefficient matrices. The comparison covers the algorithms discussed in Chapter 7–9. Our intention was to show the impact of different look-ahead strategies, different types of recurrences, and different options for solving Toeplitz systems on the relative accuracy of the computed solution. Since our numerical experiments with the codes for the diagonal recurrences from Chapter 4–6 gave similar results, we decided to concentrate on row recurrences, *i.e.*, on the Toeplitz case.

In the following, we consider only well-conditioned linear systems and we assume that the length of the look-ahead steps as well as the total number of such steps are bounded independently of N. This justifies to consider all computations of order at most $O(k_{\max}^3)$ as negligible, where $k_{\max}$ is the maximal length of look-ahead steps if N is large; see Figure 11.2 below.

This chapter starts with a discussion about look-ahead criteria. It continues with a survey on various options for solving Toeplitz systems from the output we obtain from look-ahead Levinson and Schur algorithms. Finally we present numerical examples with our C implementation of all the different algorithms.

11.1 Look-ahead strategies

A crucial point in designing look-ahead algorithms is a criterion for determining the length of a look-ahead step. The main purpose of this criterion is to determine the well-conditioned submatrices of $\mathbf{T}$ in order to compute the column-regular or anti-diagonally regular pairs used in our algorithms. From the operation counts we gave for the algorithms, it becomes clear that look-ahead steps are more expensive than classical steps, so the aim of the criterion is also to avoid look-ahead steps whenever possible.

Since all our algorithms involve the solution of one or two small linear systems, mostly of dimension one, the weakest criterion one has to ensure is to guarantee that the coefficient matrices of all the linear systems which arise are nonsingular. In practice, when the computations are done in finite precision arithmetic, we will require that these matrices are well-conditioned. To achieve this task, we propose to keep the smallest singular value of these coefficient matrices above some tolerance, as we sketched in the algorithms. For the algorithms of Chapter 7, we check

$$\sigma_{\min}(\mathbf{M}_{k,n}) > \operatorname{tol}(n), \tag{11.1}$$

and for the algorithms of Chapter 9 we test on

$$\min\{\sigma_{\min}(\mathbf{L}^{\uparrow(l)}), \sigma_{\min}(\mathbf{L}^{(l)})\} > \operatorname{tol}(n) \tag{11.2}$$

or

$$\sigma_{\min}(\mathbf{D}^{(l)}) > \operatorname{tol}(n). \tag{11.3}$$

where $n = n_l$ is the index of the last anti-diagonally well-conditioned pair. Note that at this point we allow the tolerances to depend on the index n. If we check if $n+k$ is an anti-diagonally regular index, then $\mathbf{M}_{k,n}$ is a $(2k-1)\times(2k-1)$ matrix and $\mathbf{L}^{\uparrow(l)}, \mathbf{L}^{(l)}$, and $\mathbf{D}^{(l)}$ are $k \times k$ matrices.

Numerical experiments with the look-ahead Lanczos algorithms [39] showed that in this application, the check (11.3) is not sufficient to get a reliable implementation. In fact, it was shown that the algorithm performs best if one sets $\operatorname{tol}(n)$ equal to machine precision ϵ and then applies some other heuristic criterion. Parlett [100] suggests to set $\operatorname{tol}(n)$ to $\epsilon^{1/3}$ or $\epsilon^{1/4}$, because this would imply that the Lanczos vectors remain linearly independent; see [100, Theorem 10.1].

For the solution of Toeplitz systems, we implemented the checks (11.1)–(11.3) for different tolerances $\operatorname{tol}(n)$ and found out that a value of the order 0.1 gives satisfactory results for this application. However, the check (11.2) seems to give better results. Additionally, we restricted the length of a look-ahead step to $k_{\max}$. If the checks failed for each $1 \le k \le k_{\max}$, we set k to the value for which the left-hand side of (11.1), (11.2), or (11.3) attained its maximum. Only if this maximum is below a tolerance which is of the order of machine precision, the algorithm fails and should be restarted with a larger value of $k_{\max}$.

A heuristic explanation is the following: From the inversion formulas (2.42) and (2.43) we have the upper bounds

$$\|\mathbf{T}_n^{-1}\| \le \|\mathbf{T}_n^{-1}\|_F \le 2n\,\|\mathbf{q}_n^{\leftarrow}\|\,\|\mathbf{q}_n^{\uparrow}\| \tag{11.4}$$

and

$$\max\{\|\mathbf{T}_n^{-1}\|,\, \|\mathbf{T}_{n+1}^{-1}\|\} \le \max\{\|\mathbf{T}_n^{-1}\|_F,\, \|\mathbf{T}_{n+1}^{-1}\|_F\} \le \frac{2n}{|\pi_{0,n}|}\|\mathbf{q}_n\|\,\|\mathbf{q}_n^{\uparrow}\|. \tag{11.5}$$

Therefore, $|\pi_{0,n}|$ and the norms of $\mathbf{q}_n$, $\mathbf{q}_n^{\uparrow}$ in a generic step and the norms of $\mathbf{q}_n^{\leftarrow}$ and $\mathbf{q}_n^{\uparrow}$ in a look-ahead step yield explicit upper bounds on the inverse of the principal submatrix $\mathbf{T}_n$. Since the linear systems with coefficient matrices $\mathbf{M}_{k,n}$, $\mathbf{L}^{\uparrow(l)}$, and $\mathbf{L}^{(l)}$ we have to solve in the various algorithms contain in its right-hand sides coefficients of residuals and numerators of Padé forms, we can conclude that these right-hand sides are small if the norms of the coefficient vectors $\mathbf{q}_n^{\leftarrow}$ and $\mathbf{q}_n^{\uparrow}$ are sufficiently small, because we assumed that $\mathbf{T}_N$ itself is well conditioned. Then the checks (11.1) and (11.2) guarantee that the solutions of these linear systems cannot be large. From the triangle inequality we then obtain that $\mathbf{q}_{n+k}^{\leftarrow}$ and $\mathbf{q}_{n+k}^{\uparrow}$ cannot grow too much. Recall that for $n = n_l$ and $k = 1$ we have $\pi_0 = \mathbf{L}^{(l)} = \mathbf{L}^{\uparrow(l)} = \mathbf{D}^{(l)}$.

Hence, a possible strategy to decide whether a pair of $(0, n)$ and $(-1, n)$ Padé forms is column well-conditioned could be based on the two inequalities

$$|\pi_0| > \mathrm{tol}(n) \qquad \text{and} \qquad \max\{\|\mathbf{q}_n\|, \|\mathbf{q}_n^{\uparrow}\|\} \leq \mathrm{Tol}(n).$$

This would guarantee that

$$\max\{\|\mathbf{T}_n^{-1}\|, \|\mathbf{T}_{n+1}^{-1}\|\} \leq 2n \, \frac{[\mathrm{Tol}(n)]^2}{\mathrm{tol}(n)}. \tag{11.6}$$

For an anti-diagonally well-conditioned pair one would require

$$\max\{\|\mathbf{q}_n^{\leftarrow}\|, \|\mathbf{q}_n^{\uparrow}\|\} \leq \mathrm{Tol}(n),$$

which yields the upper bound

$$\|\mathbf{T}_n^{-1}\| \leq 2n \, [\mathrm{Tol}(n)]^2. \tag{11.7}$$

However, computing the norms is quite expensive and the bounds (11.6) and (11.7) turned out to be fairly pessimistic in practice. Extensive numerical tests have shown that the heuristic argument we explained above is justified in practice and that the cheap tests are sufficient to achieve good accuracy.

In order to manifest this statement, we created a random Toeplitz matrix of dimension 150 with a very ill-conditioned leading principal submatrix of dimension 50. Examples with an ill-conditioned principal submatrix of dimension n can be constructed from a random Toeplitz matrix by first computing the eigenvalues of the nth principal submatrix and then subtracting a suitable scalar multiple of the identity from the original Toeplitz matrix. For the test example of dimension 150, we monitor for each column well-conditioned index the upper bound (11.4) versus n. For all n which are not column well-conditioned, we computed the pair $\mathbf{q}_n^{\leftarrow}$, $\mathbf{q}_n^{\uparrow}$, no matter whether it was anti-diagonally well-conditioned or not. Of course, we used only the well-conditioned pairs to proceed in the algorithm. Figure 11.1 shows the true spectral norms of $\mathbf{T}_n^{-1}$ versus n in a logarithmic plot (dotted line), the upper bound (11.4) if n is column well-conditioned and the upper bound (11.5) otherwise (solid line). The + marks indicate that a look-ahead step was performed at this index. The picture clearly shows that the simple check on the smallest singular correctly detects ill-conditioned submatrices.

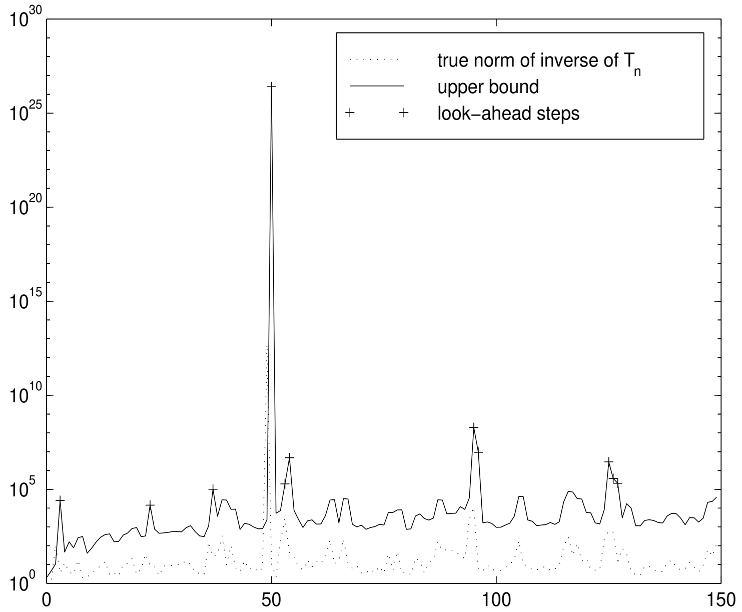


Figure 11.1: $\|\mathbf{T}_n^{-1}\|$ versus n, upper bounds (11.4) and (11.5).

A different look-ahead strategy was proposed by Freund and Zha [42]. It is based on the Schur complement of $\mathbf{T}_{n+k}$. In a number of numerical tests we found no significant difference in the numerical behavior of our algorithms when implementing the tests from [42]. We therefore omit the details here and refer the reader to the original paper [42].

If one does not want to set the tolerances before starting the algorithm, then one could determine the singular values of all matrices which arise in the linear systems for the recurrence coefficients for steps of length $1 \leq k \leq k_{\max}$ and then setting the tolerance to the optimal value within these initial steps. A similar choice was proposed by Van Barel and Bultheel [121].

11.2 Options for solving Toeplitz systems

We have seen that look-ahead Levinson and Schur algorithms yield block LDU decompositions of $\mathbf{T}^{-1}$ and $\mathbf{T}$, respectively, at least if we compute additionally inner formally biorthogonal polynomials or numerators and denominators of underdetermined Padé forms and the block diagonal matrix $\mathbf{D}$. Clearly, when one of these LDU decompositions is known, it is easy to solve a Toeplitz system

$$\mathbf{Tx} = \mathbf{b} \tag{11.8}$$

in roughly N^2 additions and multiplications. However, this is just one way of applying the outcome of our algorithms to this task. There are several other options, which we want to compare here with these two.

Inverse block LDU decomposition

All our look-ahead Levinson algorithms generate directly an inverse block LDU decomposition

$$\mathbf{T}^{-1} = \mathbf{R}^{\uparrow}\mathbf{D}^{-1}\mathbf{R}^T$$

and in intermediate steps, inverse LDU decompositions of all the well conditioned submatrices of $\mathbf{T}$, if we compute not only regular formally biorthogonal polynomials but also fill the gaps with inner FBOPs. This was shown in Theorem 8.8. These decompositions can be used to update the solutions of a nested sequence of Toeplitz systems of order n, $n = 1, 2, \ldots, N$:

$$\mathbf{T}_n\mathbf{x}_n = \mathbf{b}_n. \tag{11.9}$$

Clearly, a solution of the subsystem of order n is only computed if $\mathbf{T}_n$ is well conditioned, which is equivalent to n being a well-conditioned index which corresponds to a well-conditioned Padé form. Let us assume that $n = n_l$ and $n+k = n_{l+1}$ are well conditioned indices and denote the $(n+k)\times(n+k)$ principal submatrices $\mathbf{R}_{n+k}$ and $\mathbf{R}^{\uparrow}_{n+k}$ of $\mathbf{R}$ and $\mathbf{R}^{\uparrow}$, respectively, by

$$\mathbf{R}_{n+k} = \begin{bmatrix} \mathbf{R}_n & \mathbf{B} \\ \mathbf{0} & \mathbf{R}^{(l)} \end{bmatrix} \qquad \mathbf{R}^{\uparrow}_{n+k} = \begin{bmatrix} \mathbf{R}^{\uparrow}_n & \mathbf{B}^{\uparrow} \\ \mathbf{0} & \mathbf{R}^{\uparrow(l)} \end{bmatrix},$$

where l denotes the index of the block starting with the regular index $n = n_l$. The $(n+k)$th principal submatrix of the block diagonal matrix $\mathbf{D}$ is written as

$$\mathbf{D}_{n+k} = \begin{bmatrix} \mathbf{D}_n & \mathbf{0} \\ \mathbf{0} & \mathbf{D}^{(l)} \end{bmatrix},$$

so that $\mathbf{T}_n^{-1} = \mathbf{R}^{\uparrow}_n\mathbf{D}_n^{-1}\mathbf{R}_n^T$. If $\mathbf{x}_n$ is the solution of (11.9), and if we write

$$\mathbf{b}_{n+k} = \begin{bmatrix} \mathbf{b}_n \\ \mathbf{c} \end{bmatrix},$$

then a solution of

$$\mathbf{T}_{n+k}\mathbf{x}_{n+k} = \mathbf{b}_{n+k}$$

is given by

$$\begin{aligned} \mathbf{x}_{n+k} &= \begin{bmatrix} \mathbf{R}^{\uparrow}_n & \mathbf{B}^{\uparrow} \\ \mathbf{0} & \mathbf{R}^{\uparrow(l)} \end{bmatrix} \begin{bmatrix} \mathbf{D}_n^{-1} & \mathbf{0} \\ \mathbf{0} & (\mathbf{D}^{(l)})^{-1} \end{bmatrix} \begin{bmatrix} \mathbf{R}_n^T & \mathbf{0} \\ \mathbf{B}^T & (\mathbf{R}^{(l)})^T \end{bmatrix} \begin{bmatrix} \mathbf{b}_n \\ \mathbf{c} \end{bmatrix} \\ &= \begin{bmatrix} \mathbf{x}_n \\ \mathbf{0} \end{bmatrix} + \begin{bmatrix} \mathbf{B}^{\uparrow} \\ \mathbf{R}^{\uparrow(l)} \end{bmatrix} \mathbf{y}, \end{aligned} \tag{11.10}$$

where

$$\mathbf{y} = (\mathbf{D}^{(l)})^{-1}(\mathbf{B}^T\mathbf{b}_n + (\mathbf{R}^{(l)})^T\mathbf{c}).$$

Therefore, $\mathbf{x}_{n+k}$ can be updated from $\mathbf{x}_n$ by using only those columns of $\mathbf{R}$ and $\mathbf{R}^\uparrow$ which belong to the current block. This update procedure costs k inner products for computing $\mathbf{B}^T\mathbf{b}_n$ plus k SAXPYs for the update, if we consider all computations of order at most $O(k^3)$ as negligible. The most important advantage of applying a procedure which uses only quantities available from the current block is that we do not have to store the complete factorization. Hence, the storage requirement is only $O(N)$.

An equivalent equation for $\mathbf{y}$ can be obtained from the equality $\mathbf{D}^{(l)} = (\mathbf{R}^{(l)})^T\mathbf{L}^{\uparrow(l)}$, cf. (8.35). From the Toeplitz structure we have

$$\mathbf{T}_{n+k} = \begin{bmatrix} \mathbf{T}_n & \mathbf{U} \\ \mathbf{V} & \mathbf{T}_k \end{bmatrix},$$

which yields

$$\begin{aligned} \mathbf{y} &= (\mathbf{L}^{\uparrow(l)})^{-1}\left((\mathbf{R}^{(l)})^{-T}\mathbf{B}^T\mathbf{b}_n + \mathbf{c}\right) \\ &= (\mathbf{L}^{\uparrow(l)})^{-1}\left((\mathbf{R}^{(l)})^{-T}\left[\ \mathbf{B}^T \quad (\mathbf{R}^{(l)})^T\ \right]\mathbf{T}_{n+k}\begin{bmatrix} \mathbf{x}_n \\ \mathbf{0} \end{bmatrix} - \mathbf{V}\mathbf{x}_n + \mathbf{c}\right) \\ &= (\mathbf{L}^{\uparrow(l)})^{-1}(\mathbf{c} - \mathbf{V}\mathbf{x}_n), \end{aligned} \tag{11.11}$$

because the first n columns of the product $[\ \mathbf{B}^T \quad (\mathbf{R}^{(l)})^T\ ]\mathbf{T}_{n+k}$ are zero since $\mathbf{R}^T\mathbf{T} = \mathbf{L}^T$ is block upper triangular by Theorem 8.9. For the symmetric positive definite case, (11.11) is well-known; see [49, Section 4.7.3]. In the look-ahead case, the formula was derived differently in [42, Section 6.1].

The inverse block LDU decomposition can also be generated as a byproduct of the look-ahead Schur algorithm, but, unless these columns are used anyway to control the look-ahead step size, this increases the costs by about 50%, namely for applying the Levinson recursion (without computation of the inner products). Here, the key point is that the recurrence coefficients are identical for Levinson and for Schur-type algorithms.

Block LDU decomposition

The primary output of our look-ahead Schur algorithms are the matrices $\mathbf{L}$ and $\mathbf{L}^\uparrow$ of the LDU decomposition

$$\mathbf{T} = \mathbf{L}^\uparrow\mathbf{D}^{-1}\mathbf{L}^T \tag{11.12}$$

of $\mathbf{T}$. Again, the full decomposition requires to compute underdetermined Padé forms. Due to the Toeplitz structure of the blocks of $\mathbf{D}$, this matrix also contains only quantities from $\mathbf{L}$ and $\mathbf{L}^\uparrow$. We refer to Section 8.3 for details. The inverse of $\mathbf{D}$ is not needed for solving (11.8).

When using the LDU decomposition (11.12) for computing the solution of the linear system (11.8) one can perform the forward elimination for the first linear system in

$$\mathbf{L}^{\uparrow}\mathbf{y} = \mathbf{b}, \quad \text{where } \mathbf{L}^{T}\mathbf{x} = \mathbf{D}\mathbf{y}, \tag{11.13}$$

with $O(N)$ storage. This involves solving linear systems with the diagonal blocks $\mathbf{L}^{\uparrow(l)}$, which are just scalars in generic steps. If we use the Schur-type algorithm 9.2, where we have computed an anti-diagonally regular pair from a previous anti-diagonally regular pair and underdetermined Padé forms, then the QR or LU decomposition of $\mathbf{L}^{\uparrow(l)}$ is available anyway, because $\mathbf{L}^{\uparrow(l)}$ is just the coefficient matrix in (9.6). But one still has to store the complete triangular part of $\mathbf{L}$ for solving the second system in (11.13) by backsubstitution. However, for solving (11.8) with the Schur algorithm there are also more efficient ways that we will discuss below.

Inversion formulas

In Section 2.6, we collected several inversion formulas which gave explicit expressions for the inverse of a Toeplitz matrix in terms of a pair of denominators of Padé forms. The look-ahead Levinson algorithm produces this last pair directly. If $N-1$ is a column-regular index, *i.e.*, if $\mathbf{T}_{N-1}$ and $\mathbf{T}_{N}$ are regular (or well conditioned), we can apply the Gohberg-Semencul formula (2.43) for $m = 0$ and $n = N-1$. If this is not the case, then by assumption, N is an anti-diagonally regular index. We then have to compute the denominators of the anti-diagonally regular pair of $(-1, N)$ and $(0, N-1)$ Padé forms in order to apply Heinig's inversion formula (2.42) for $m = 0$ and $n = N$.

In a Schur-type algorithm, the denominators are usually not computed, but as mentioned above, we could compute them additionally at the cost of some extra work.

Applying the inversion formula is an $O(N \log N)$ process, if we use fast Fourier transformation techniques.

Another approach complementing the Schur algorithm

Since $\mathbf{T} = \mathbf{L}^{\uparrow}(\mathbf{R}^{\uparrow})^{-1}$, we can write (11.8) as

$$\mathbf{L}^{\uparrow}\mathbf{y} = \mathbf{b}, \quad \text{where } \mathbf{x} = \mathbf{R}^{\uparrow}\mathbf{y}. \tag{11.14}$$

As we have explained above, the first, block lower triangular system for $\mathbf{y}$ can be solved by forward substitution without storing $\mathbf{L}^{\uparrow}$. Moreover, in the look-ahead Schur-type algorithm 7.3, which computes anti-diagonally regular pairs from anti-diagonally regular pairs without using underdetermined Padé forms, it is sufficient to compute the numerators of right underdetermined Padé forms, *i.e.*, columns of $\mathbf{L}^{\uparrow}$. There is no need for computing left underdetermined Padé forms and residuals of right underdetermined Padé forms.

If we have run the recurrences for the Levinson algorithm additionally, then the solution $\mathbf{x}$ is obtained by just multiplying the temporary vector $\mathbf{y}$ by the upper triangular matrix $\mathbf{R}^{\uparrow}$. Since this involves only quantities from the current block, the storage requirement is only $O(N)$ again.

If $\mathbf{R}^{\uparrow}$ has not been computed, then this simple technique is not applicable. Using the matrix formulation (8.46) of the Levinson algorithm, we find $\mathbf{x}$ according to $\mathbf{R}^{\uparrow}\mathbf{y} = \mathbf{J}\mathbf{R}^{\uparrow(J)}(\mathbf{J}\mathbf{y})$ via

$$\mathbf{x} = \mathbf{J}\left[\ \mathbf{R} \mid \mathbf{R}^{\uparrow(J)}\ \right]\left[\frac{\mathbf{0}}{\mathbf{J}\mathbf{y}}\right] = \left[\ \mathbf{J} \mid \mathbf{J}\ \right]\prod_{j=0}^{J-1}\mathbf{C}_{n_j}\ \left[\frac{\mathbf{0}}{\mathbf{J}\mathbf{y}}\right] \tag{11.15}$$

Again, the storage requirement is only $O(N)$. We have to store all the coefficients of the small two-point Padé forms we used for updating one column-regular or anti-diagonally regular pair from the previous one. Moreover, we need the recurrence coefficients for left and right underdetermined Padé forms.

For the Bareiss algorithm applied to a symmetric positive definite $\mathbf{T}$, Delosme and Ipsen [32, 81] derived a formula that is similar to (11.15). They made use of the fact that in this case the matrices $\mathbf{C}_n$ are hyperbolic rotations, and thus the inverse of their product is equal to a diagonally scaled transpose of the product. Thus, both the forward elimination and the backsubstitution can be performed by applying a product of hyperbolic rotations.

11.3 Operation counts: Schur versus Levinson algorithms

The main difference between a Levinson and a Schur algorithms is that the Levinson algorithm spends about half of the operations on computing inner products but the Schur algorithm requires only SAXPYs. This makes the Schur algorithm highly attractive on parallel computers, in particular on those, where inner products represent a bottleneck of the computation due to the global communication involved.

To summarize the various options for solving the linear systems, the Levinson and the Schur algorithm both require $2N^2+O(N)$ operations to compute the LDU or inverse LDU factorization of a Toeplitz matrix, because the overhead of our look-ahead algorithms is only of order N by the assumptions made in the prefix of this Chapter. They are satisfied when $\mathbf{T}$ has only a few ill-conditioned principal submatrices, a situation which often happens in practice.

For the Schur algorithm, one still has the option of computing the LDU decomposition, *i.e.*, running the Levinson recurrences additionally. This costs another $N^2+O(N)$ operations, so that computing the LDU and the inverse LDU decomposition simultaneously does not double the cost, but can be done in $3N^2+O(N)$ flops.

The cheapest way of solving the linear system with the Levinson algorithm is to apply a suitable inversion formula by exploiting fast Fourier transformation techniques.

This is an $O(N \log N)$ process, in total, we need $2N^2 + O(N \log N)$ flops to get the solution. Updating the solution from the inverse LDU decomposition via (11.10) costs $N^2+O(N)$ flops, hence we can get the solution with this technique in $3N^2+O(N)$ flops.

For the Schur algorithm, the cheapest solution method is using the LDU decomposition (11.13). The solution process costs again $N^2+O(N)$ flops, hence the overall process can be done in $3N^2 + O(N)$ flops. However, using the LDU decomposition is only possible if we can store one complete block lower triangular factor of this decomposition. If N is large, this becomes prohibitive. One then has the option to run the Levinson algorithm additionally and use (11.14). The price for this procedure is $4N^2 + O(N)$ flops, since the solution costs again $N^2 + O(N)$ flops. Another option is again to apply an inversion formula, which costs $3N^2 + O(N \log N)$ flops. A cheaper variant stems from the matrix formulation (11.15), where one uses the second equation in (11.14) only implicitly by essentially running the Levinson algorithm backwards. Since the matrices $\mathbf{C}_n$ are of size $2N \times 2N$, computing $\mathbf{x}$ from (11.15) costs $N^2 + O(N)$ flops. Hence, this variant costs $3.5N^2 + O(N)$ flops.

11.4 Numerical examples

We have implemented all our algorithms in MATLAB and in C, but present only the results from the C implementation. The C code is available from the author. It uses the Basic Linear Algebra Subroutines (BLAS) and LAPACK routines [2] for computing the smallest singular value and for solving the linear systems which arise in look-ahead steps. For the examples we present here, the linear systems have been solved by Gaussian elimination with partial pivoting. Optionally, the code can solve the linear systems by QR factorization. All our numerical examples were done on an SGI Power Indigo 2 with machine precision $1.11 \cdot 10^{-16}$.

We compare our algorithms with the FORTRAN implementation of the look-ahead Levinson algorithm [26], written by Hansen and Chan [70], which is – to the best of the authors knowledge – the only available implementation of a look-ahead algorithm; see also [45]. Unfortunately, the implementation of Freund and Zha's look-ahead Levinson algorithm announced in [42, Section 9] was not available at the time of this writing. Hence we were not able to add comparisons with this code also. In [45], yet another high performance library is announced, which will be developed for distributed memory machines. This library will mainly contain algorithms based on transforming the original Toeplitz matrix to some other structured matrix where pivoting can be applied. It was also not finished yet.

Let us first compare the execution times of the different algorithms. Figure 11.2 shows the execution times for a FORTRAN implementation of the classical Levinson algorithm [3] available from NETLIB, the FORTRAN implementation of the look-ahead Levinson algorithm from Hansen and Chan [70], our C imple-

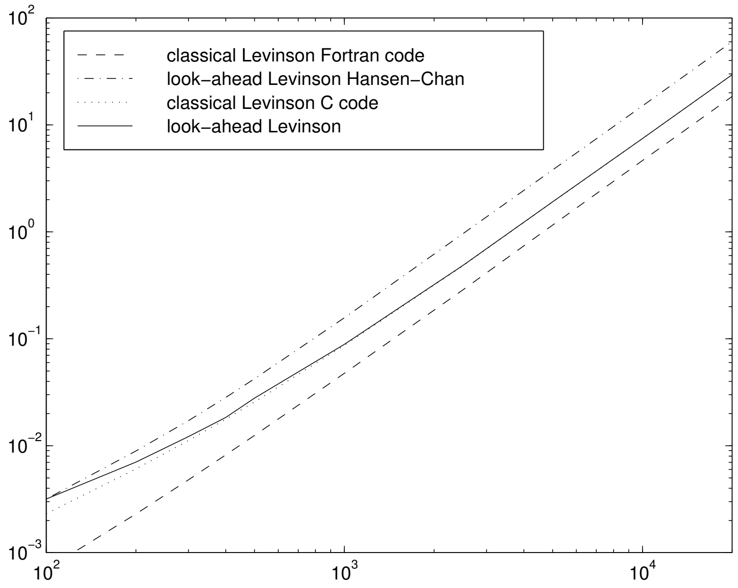


Figure 11.2: Execution times in seconds versus the dimension of the C implementation of the classical and the look-ahead Levinson algorithm compared with execution times of the FORTRAN implementation of the classical and the look-ahead Levinson algorithm from Hansen and Chan.

mentation of the classical Levinson algorithm and of our look-ahead Levinson algorithm 9.1, which uses inner FBOPs for computing anti-diagonally regular pairs. The execution times have been computed for random Toeplitz matrices of dimensions $N = 100, 200, 300, 400, 500, 1000, 2500, 5000, 10000, 20000$ with an ill-conditioned principal submatrix of dimension 50. The plot is in a double logarithmic scale, where the x-axis shows the dimensions and the y-axis shows the execution times in seconds.

The figure shows that the C implementation is slower than the FORTRAN code from the Argonne package [3]. The main reason is that our C implementation uses the Basic Linear Algebra Subroutines (BLAS) and the FORTRAN code does not. For the Toeplitz solvers, this turns out to be more expensive on our machine because most of the copy operations for long vectors could be done simultaneously to computations if we would implement them by hand. We nevertheless decided to use the BLAS and hope that it is available in an optimized form on most of the machines. The interesting observation from this figure is that the execution times of the FORTRAN implementation by Hansen and Chan are pretty larger than those of the classical Levinson algorithm although Hansen and Chan also do not use the BLAS copy function. However, for the C implementation you cannot even distinguish the two lines for the classical and the Levinson algorithm for dimensions larger than about 1000. Note that both classical algorithms gave wrong

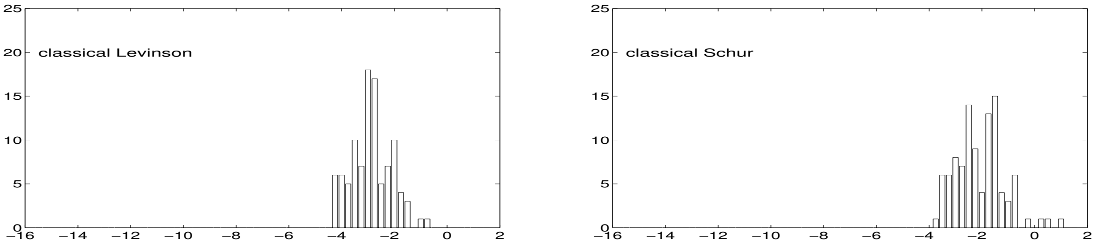


Figure 11.3: Histograms of relative errors of the C implementation of the classical Levinson and Schur algorithm.

results because of the ill-conditioned principal submatrix.

For comparing the accuracy of the algorithms we created a set of 100 random test examples of dimension 500 with a very ill-conditioned principal submatrix of dimension 50. We used this test set for all examples. The right-hand sides of the linear systems were computed such that a given random vector was the exact solution. This allowed us to compare the different algorithms by computing the relative errors

$$\frac{\|\mathbf{x}_{exact} - \mathbf{x}_{comput.}\|}{\|\mathbf{x}_{exact}\|}.$$

For our algorithms, we used a tolerance of 0.1 for checking if a regular Padé form is also column-regular, *i.e.*, we enforce $|\pi_{0,n}| > 0.1$. The tolerance for the smallest singular values in (11.1) or (11.2) was 0.3. We present the results in form of histograms, where the x-axis shows the logarithm of the achieved relative error and where the y-axis contains the number of examples which achieved an accuracy in a given interval of length 0.25 in a logarithmic scale. Note that some of the Toeplitz matrices may itself be ill-conditioned, so that we cannot expect to get full accuracy for all of the 100 test examples. In fact, our algorithm produced warnings that the results may be inaccurate for two of the 100 examples.

Figure 11.3 shows the performance of different algorithms when the solution is computed by one of the (inverse) LDU decompositions for our C implementation of the classical Levinson and Schur algorithm. Clearly, the accuracy is poor because of the very ill-conditioned principal submatrix of dimension 50.

Figure 11.4 shows the achieved accuracies for the FORTRAN implementations of the classical Levinson algorithm [3] and the look-ahead Levinson algorithm [70], where we have set the maximal block size to 6.

In Figure 11.5 we compare our look-ahead Levinson algorithms 7.2 and 9.1. For solving the linear systems we used the update formula (11.10). Here and in the following we will call Algorithm 7.2 the product form of our look-ahead Levinson algorithm, because it is based on products of Padé forms with little two-point Padé forms. Recall that Algorithm 9.1, which uses inner FBOPs, has less overhead when we compute the

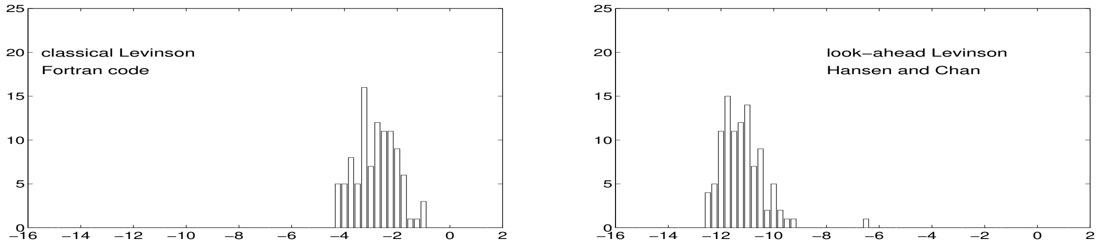


Figure 11.4: Histograms of relative errors of FORTRAN implementation of the classical Levinson and the look-ahead Levinson algorithm of Hansen and Chan.

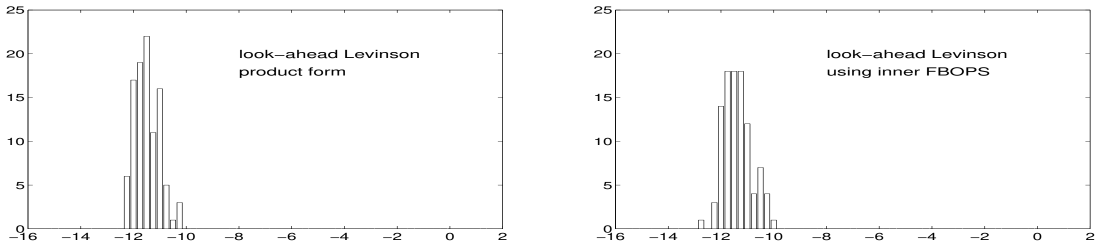


Figure 11.5: Histograms of relative errors of our C implementation of the look-ahead Levinson algorithms 7.2 and 9.1.

complete LDU decomposition, as we did in all our experiments here. This most efficient look-ahead algorithm gave slightly better results than the Hansen and Chan algorithm. However, as we have seen before, it has much less overhead and shorter execution times. We therefore recommend to use the Levinson algorithm 9.1.

Figure 11.6 shows the analogous results for our Schur algorithms 7.3 (product form) and 9.2 (using underdetermined Padé forms). For solving the linear systems we used the LDU decomposition (11.13). Since the denominators of the Padé forms have not been computed the algorithms required $O(N^2)$ storage. The results are very similar to those of our look-ahead Levinson algorithms. Again, we recommend to use the Schur algorithm 9.2 since it has less overhead then the product form 7.3.

Finally, Figure 11.7 shows accuracies for the Schur algorithms where additionally the inverse LDU decomposition is computed. The solutions were obtained from (11.14).

Figure 11.8 shows the performance of different algorithms when the solution is computed by one of the inversion formulas from Section 2.6. As we mentioned before, this solution technique is only applicable when we have run the Levinson algorithm, either alone or combined with the Schur algorithm.

For these algorithms, one can also compute the solution from an LDU decomposition and then apply an inversion formula in order to improve the accuracy by one step of iterative refinement. These accuracies are presented in Figure 11.9, where the intervals

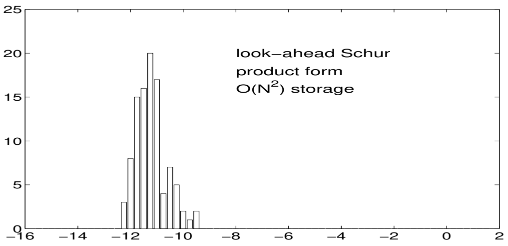


Figure 11.6: Histograms of relative errors of our C implementation of the look-ahead Schur algorithms 7.3 and 9.2.

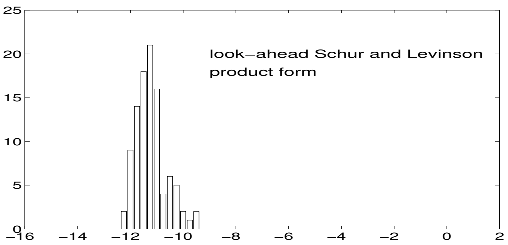


Figure 11.7: Histograms of relative errors of our C implementation of the look-ahead Schur algorithms 7.3 and 9.2 both combined with the corresponding recurrences of the Levinson algorithms.

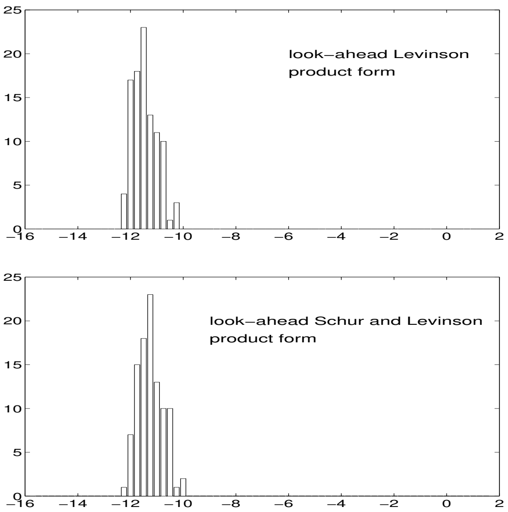


Figure 11.8: Histograms of relative errors of our look-ahead algorithms where the solutions are obtained by applying an inversion formula.

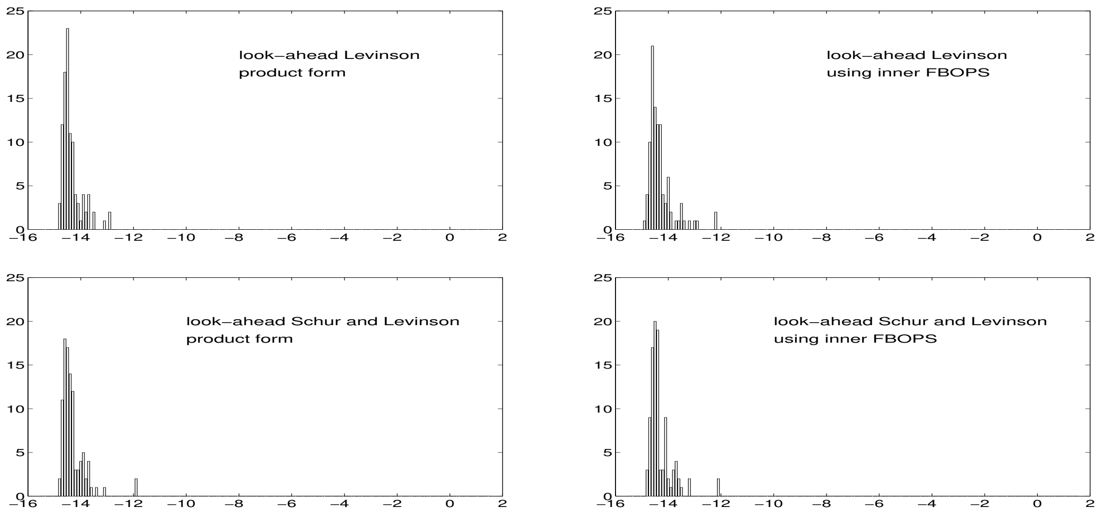


Figure 11.9: Histograms of relative errors where the solutions are obtained from an (inverse) LDU decomposition and are improved by one step of iterative refinement.

for the histograms now have length 0.1 to leave the scale of the y-axis identical to the other examples. They are pretty close to machine precision. Clearly, one could do more than one refinement steps to further improve the accuracy.

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