SOME OBSERVATIONS ON COMPUTER AIDED ANALYSIS

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Preamble: Over the last quarter Century and especially during the last decade, a dramatic 're- experimentalization' of Mathematics has begun to take place. In this process, fueled by advances in hardware, software and theory, the computer plays a laboratory role for pure and applied mathematicians; a role which in the eighteenth and nineteenth centuries the physical sciences played much more fully than in our century.

Operations previously viewed as non-algorithmic, such as indefinite integration, may now be performed within powerful symbolic manipulation packages like Maple, Mathematica, Macsyma, Scratchpad to name a few. Similarly, calculations previously viewed as "practically" non-algorithmic or certainly not worth the effort, such as large symbolic Taylor expansions are computable with very little programming effort.

New subjects such as computational geometry, fractal geometry, turbulence, and chaotic dynamical systems have sprung up. Indeed many second-order phenomena only become apparent after considerable computational experimentation. Classical subjects like number theory, group theory and logic have received new infusions. The boundaries between mathematical physics, knot theory, topology and other pure mathematical disciplines are more blurred than in many generations. Computer assisted proofs of "big" theorems are more and more common: witness the 1976 proof of the Four Colour theorem and the more recent 1989 proof of the non-existence of a projective plane of order ten (by C. Lam et al at Concordia).

There is also a cascading profusion of sophisticated computational and graphical tools. Many mathematicians use them but there are still many who do not. More importantly, expertise is highly focused: researchers in partial differential equations may be at home with numerical finite element packages, or with the NAG or IMSL Software Libraries, but may have little experience with symbolic or graphic languages. Similarly, optimizers may be at home with non-linear programming packages or with Matlab. The learning curve for many of these tools is very steep and researchers and students tend to stay with outdated but familiar resources long after these have been superceded by newer software. Also, there is very little methodology for the use of the computer as a general adjunct to research rather than as a means of solving highly particular problems.

We are currently structuring "The Simon Fraser Centre for Experimental and Constructive Mathematics" to provide a focal point for Mathematical research on such questions as

"How does one use the computer
- to build intuition?
- to generate hypotheses?
- to validate conjectures or prove theorems?
- to discover nontrivial examples and counter-examples?"

(Since we will be offering a number of graduate student, post-doctoral and visiting fellowhips we are keen to hear from interested people.)

0. INTRODUCTION. Our intention is to display three sets of analytic results which we have obtained over the past few years entirely or principally through directed computer experimentation. While each set in some way involves Pi, our main interest is in the role of directed discovery in the analysis. The results we display either could not or would not have been obtained without access to high level symbolic computation. In our case we primarily used Maple, but the precise vehicle is not the point. We intend to focus on the pitfalls and promises of what Lakatos called "quasi-inductive" mathematics.

1. CUBIC SERIES FOR PI.

The Mathematical Component. Ramanujan [10] produced a number of remarkable series for $1/\pi$ including

$$\frac{1}{\pi} = \frac{2\sqrt{2}}{9801}\sum_{n=0}^{\infty}\frac{(4n)!}{4^{4n}(n!)^4}\frac{[1103+26390n]}{99^{4n}}. \tag{1.1}$$

This series adds roughly eight digits per term and was used by Gosper in 1985 to compute 17 million terms of the continued fraction for π. Such series exist because various modular invariants are rational (which is more-or-less equivalent to identifying those imaginary quadratic fields with class number 1) see [3]. The larger the discriminant of such a field the greater the rate of convergence. Thus with $d = -163$ we have the largest of the class number 1 examples

$$\frac{1}{\pi} = 12\sum_{n=0}^{\infty}(-1)^n \frac{(6n)!}{(n!)^3(3n)!}\frac{13591409 + n545140134}{(640320^3)^{n+1/2}}, \tag{1.2}$$

a series first displayed by the Chudnovskys [10]. The underlying approximation also produces

$$\pi \sim 3\log(640320)/\sqrt{163}$$

and is correct to 16 places.

Quadratic versions of these series correspond to class number two imaginary quadratic fields. The most spectacular and largest example has $d = -427$ and

$$\frac{1}{\pi} = 12\sum_{n=0}^{\infty}\frac{(-1)^n(6n)!}{(n!)^3(3n)!}\frac{(A+nB)}{C^{n+1/2}} \tag{1.3}$$

where

$$\begin{aligned} A &:= 212175710912\sqrt{61} + 1657145277365 \\ B &:= 13773980892672\sqrt{61} + 107578229802750 \\ C &:= [5280(236674 + 30303\sqrt{61})]^3. \end{aligned}$$

This series adds roughly twenty-five digits per term, $\sqrt{C}/(12A)$ already agrees with pi to twenty-five places [3]. The last two series are of the form

$$\sum_{n=0}^{\infty}(a(t) + nb(t))\frac{(6n)!}{(3n)!(n!)^3}\frac{1}{(j(t))^n} = \frac{\sqrt{-j(t)}}{\pi} \tag{$*$}$$

where

$$\begin{aligned} b(t) &= (t(1728 - j(t)))^{1/2} \\ a(t) &= \frac{b(t)}{6}\left(1 - \frac{E_4(t)}{E_6(t)}\left(E_2(t) - \frac{6}{\pi\sqrt{t}}\right)\right) \\ j(t) &= \frac{1728E_4^3(t)}{E_4^3(t) - E_6^2(t)} \end{aligned}$$

Here t is the appropriate discriminant, j is the "absolute invariant", and E_2, E_4 and E_6 are Eisenstein series.

For a further discussion of these see [2] where many such quadratic examples are considered. Various of the recent record setting calculations of pi have been based on these series. In particular the Chudnovskys computed over two billion digits of π using the second series above.

There is an unlimited number of such series with increasingly more rapid convergence. The price one pays is that one must deal with more complicated algebraic irrationalities. Thus a class number p field will involve p^{th} degree algebraic integers as the constants $A = a(t)$, $B = b(t)$ and $C = c(t)$ in the series. The largest class number three example of $(*)$ corresponds to $d = -907$ and gives 37 or 38 digits per term. It is

$$\frac{\sqrt{-C^3}}{\pi} = \sum_{n=0}^{\infty}\frac{(6n)!}{(3n)!(n!)^3}\frac{A+nB}{C^{3n}} \tag{1.4}$$

where

$$\begin{aligned}
C =& 4320 * 2^{2/3} * 3^{1/3}(-4711544446661617873062970863 + 52735595419633 * 2721^{1/2})^{1/3} \\
&- 4320 * 2^{2/3} * 3^{1/3}(4711544446661617873062970863 + 52735595419633 * 2721^{1/2})^{1/3} \\
&- 16580537033280
\end{aligned}$$

$$\begin{aligned}
A =& 27136 \ (2581002591670714650084289323501202067163298721 \\
&+ 9978043250154204170701650 0 * 2721^{1/2})^{1/3} \\
&- 27136 \ (-2581002591670714650084289323501202067163298721 \\
&+ 99780432501542041707016500 * 2721^{1/2})^{1/3} + 37222766169818947772
\end{aligned}$$

$$\begin{aligned}
B =& 193019904 * 907^{1/3} \\
&(669688603151350564827513538409197361 2 + 22970050316722125 * 2721^{1/2})^{1/3} \\
&- 193019904 * 907^{1/3} \\
&(-6696886031513505648275135384091973612 + 22970050316722125 * 2721^{1/2})^{1/3} \\
&+ 3521779493604002065512
\end{aligned}$$

The series we computed of largest discriminant was the class number four example with $d = -1555$. Then

$$\begin{aligned}
C =& -214772995063512240 - 96049403338648032 * 5^{1/2} \\
&- 1296 * 5^{1/2}(10985234579463550323713318473 \\
&+ 4912746253692362754607395912 * 5^{1/2})^{1/2}
\end{aligned}$$

$$\begin{aligned}
A =& 63365028312971999585426220 + 28337702140800842046825600 * 5^{1/2} \\
&+ 384 * 5^{1/2}(10891728551171178200467436212395209160385656017 \\
&+ 4870929086578810225077338534541688721351255040 * 5^{1/2})^{1/2}
\end{aligned}$$

$$\begin{aligned}
B =& 7849910453496627210289749000 + 3510586678260932028965606400 * 5^{1/2} \\
&+ 2515968 * 3110^{1/2} \ (6260208323789001636993322654444020882161 \\
&+ 2799650273060444296577206890718825190235 * 5^{1/2})^{1/2}
\end{aligned}$$

The series (1.4) with these constants gives 50 additional digits per term.

The Computational Component. The absolute invariant, and so the coefficients A, B, and C satisfy polynomial equations of known degree and height. Thus the problem of determining the coefficients of each series reduces to algebra and can be entirely automated. This is really the dream case for computer aided analysis. Indeed from the expressions for $j(t)$, $a(t)$, $b(t)$ we straightforwardly computed their values to several hundred digits. The lattice basis reduction algorithm, as implemented in Maple, now provides the minimal polynomials for each quantity. In addition, a higher precision calculation actually provides a proof of the claimed identity. This last step requires knowing a priori bounds on the degrees and heights of the invariants. While somewhat mathematically sophisticated, the computation required is fairly easy though a little slow.

2. FRAUDS AND IDENTITIES.

2a. The Mathematical Component. Gregory's series for π, truncated at $500,000$ terms gives to forty places

$$4 \sum_{k=1}^{500,000} \frac{(-1)^{k-1}}{2k-1} = 3.14159\underline{0}6535897932\underline{40}4626433832\underline{6}9502884197. \tag{2.1}$$

To one's initial surprise only the underlined digits are wrong. This is explained, ex post facto, by setting N equal to one million in the result below:

Theorem 1. *For integer N divisible by 4 the following asymptotic expansion holds:*

$$\frac{\pi}{2} - 2\sum_{k=1}^{N/2} \frac{(-1)^{k-1}}{2k-1} \sim \sum_{m=0}^{\infty} \frac{E_{2m}}{N^{2m+1}} = \frac{1}{N} - \frac{1}{N^3} + \frac{5}{N^5} - \frac{61}{N^7} + \cdots \tag{2.2}$$

where the coefficients are the even Euler numbers 1, −1, 5, −61, 1385, −50521....

The Computational Component. The observation (2.1) arrived in the mail from Roy North. After verifying its truth numerically, it was an easy matter to generate a large number of the "errors" to high precision. We then recognized the sequence of errors in (2.2) as the Euler numbers — with the help of Sloane's 'Handbook of Integer Sequences'. The presumption that (2.2) is a form of Euler-Maclaurin summation is now formally verifiable for any fixed N in Maple. This allowed us to determine that (2.2) is equivalent to a set of identities between Bernoulli and Euler numbers that could with effort have been established. Secure in the knowledge that (2.2) holds it is easier, however, to use the Boole Summation formula which applies directly to alternating series and Euler numbers (see [5]).

This is a good example of a phenomenon which really does not become apparent without working to reasonably high precision (who recognizes 2, −2, 10 ?), and which highlights the role of pattern recognition and hypothesis validation in experimental mathematics. It was an amusing additional exercise to compute Pi to 5,000 digits from (2.2). Indeed, with $N = 200,000$ and correcting using the first thousand even Euler numbers, we obtained 5,263 digits of Pi (plus 12 guard digits).

2b. The Mathematical Component. The following evaluations are correct to the precision indicated.

Sum 1 (correct to all digits)

$$\sum_{n=1}^{\infty} \frac{o(2^n)}{2^n} = \frac{1}{9}$$

where $o(n)$ counts the <u>odd</u> digits in n: $o(901) = 2$, $o(811) = 2$, $o(406) = 0$.
By comparison

Sum 2 (correct to 30 digits)

$$\sum_{n=1}^{\infty} \frac{e(2^n)}{2^n} = \frac{3166}{3069}$$

where $e(n)$ counts the even digits in n.

Sum 3 (correct to 267 digits)

$$\sum_{n=1}^{\infty} \frac{\lfloor n \tanh \pi \rfloor}{10^n} = \frac{1}{81}$$

where $\lfloor \ \rfloor$ is the greatest integer function: $\lfloor 3.7 \rfloor = 3$.

Sum 4 (correct to in excess of 500 million digits)

$$\sum_{n=1}^{\infty} \frac{\lfloor n e^{\sqrt{163\pi/9}} \rfloor}{2^n} = 1280640$$

Sum 5 (correct to in excess of 42 billion digits)

$$\left(\frac{1}{10^5} \sum_{n=-\infty}^{\infty} e^{-\frac{n^2}{10^{10}}} \right)^2 = \pi.$$

The Computational Component. Analysis of these and other seemingly rational evaluations may be found in [6]. Sum 1 occured as a problem proposed by Levine, *College Math J.*, **19**, #5, (1989) and

Bowman and White, *MAA Monthly*, **96** (1989), 745. Sum 2 relates to a problem of Diamond's in the *MAA Monthly*, **96** (1989), 838. Sums 2,3,4 all have transcendental values and are explained by a lovely continued fraction expansion originally studied by Mahler. Computer assisted analysis lead us to a similar more subtle expansion for the generating function of $\lfloor n\alpha + \beta \rfloor$:

$$\sum_{n=0}^{\infty} \lfloor n\alpha + \beta \rfloor x^n.$$

Sum 5 arises from an application of Poisson summation or equivalently as a modular transformation of a theta function. While asymptotically rapid, this series is initially very slow and virtually impossible for high-precision explicit computation.

These evaluations ask the question of how one develops appropriate intuition to be persuaded by say Sum 1 but not by Sum 2 or Sum 3? They also underline that no level of digit agreement is really conclusive of anything. Ten digits of coincidence is persuasive in some contexts while ten billion is misleading in others. In our experience, symbolic coincidence is much more impressive than undigested numeric coincidence.

3. THE CUBIC ARITHMETIC GEOMETRIC MEAN.

The Mathematical Component. For $0 < s < 1$, let $a_0 := 1$ and $b_0 := s$ and define the cubic AGM by

$$a_{n+1} := \frac{a_n + 2b_n}{3}$$

$(AG3)$

$$b_{n+1} := \sqrt[3]{\frac{(a_n^2 + a_n b_n + b_n^2) b_n}{3}}$$

which converge cubically to a common limit

(3.1) $$AG_3(1, s) = \frac{1}{{}_2F_1 J(1/3, 2/3; 1; 1 - s^3)}$$

where the hypergeometric function $F(s) := {}_2F_1(1/3, 2/3; 1; s) = \sum_{n=0}^{\infty} \frac{(3n!)}{(n!)^3 3^{3n}} s^n$. In particular, the hypergeometric function possesses the simple cubic functional equation

$${}_2F_1\left(\frac{1}{3}, \frac{2}{3}; 1; 1 - x^3\right) = \frac{3}{1+2x}\ {}_2F_1\left(\frac{1}{3}; \frac{2}{3}; 1, \left(\frac{1-x}{1+2x}\right)^3\right).$$

This can be validated symbolically once known! As an example

$$AG_3(1, 1/100) = \frac{1}{{}_2F_1(1/3, 2/3; 1; 1 - 100^{-3})}$$

and 4 iterations of $(AG3)$ will compute the hypergeometric function at 0.999999 to 25 significant digits. Any direct computation so near the radius of convergence is doomed.

Continuing, we let

(3.2) $$L(q) := \sum_{n,m=-\infty}^{\infty} q^{n^2+nm+m^2}$$

and

$$M(q) := (3L(q^3) - L(q))/2.$$

Theorem 2. *The functions $L(q)$ and $M(q)$ "parametrize" the cubic AGM in the sense that if $a := L(q)$ and $b := M(q)$ then*

$$L(q^3) = \frac{a + 2b}{3}$$

and

$$M(q^3) = \sqrt[3]{\frac{(a^2+ab+b^2)b}{3}}$$

while $AG_3(1, M(q)/L(q)) = L(q)$.

Thus a step of the iteration has the effect of sending q to q^3. From this, one is led to an easy to state but hard to derive

Cubic iteration for π. *Let* $a_0 := 1/3$, $s_0 := (\sqrt{3}-1)/2$ *and set*

$$(1+2s_n)(1+2s^*_{n-1}) = 3 \quad \textit{where} \quad s* := \sqrt[3]{1-s^3}$$
$$a_n := (1+2s_n)^2 a_{n-1} - 3^{n-1}[(1+2s_n)^2 - 1],$$

then $1/a_n$ *converges cubically to* π.

This iteration gives 1, 5, 21, 70, $\cdots$ digits correct and more than triples accuracy at each step.

The Computational Component. This is the most challenging and most satisfying of our three examples for computer assisted analysis. We began with one of Ramanujan's typically enigmatic entries in Chapter 20 of his notebook, now decoded in [1]. It told us that a "quadratic modular equation" relating to F was

$$(1-u^3)(1-v^3) = (1-uv)^3. \tag{3.3}$$

¿From this we gleaned that some function R should exist so that $u := R(q)$ and $v := R(q^2)$ would solve (3.3). We formally solved for the coefficents of R and learned nothing. Motivated by the analogy with the classical theory of the AGM iteration [2] we looked at $F(1-R(q)^3)$ which produced

$$F(1-R(q)^3) = 1 + 6q + 6q^3 + 6q^4 + 12q^7 + 6q^9 + 6q^{12} + 12q^{13} + 6q^{16} + 12q^{19} + 12q^{21} + 6q^{25} + \cdots.$$

This was "pay-dirt" since the coefficients were sparse and very regular. Some analysis suggested that they related to the number of representations of the form $m^2 + 3n^2$. From this we looked at theta function representations and were rewarded immediately by the apparent identity $F(1-R(q)^3) = L(q)$. Given the truth of this it was relatively easy to determine that $R(q) = M(q)/L(q)$ with M and L as in (3.2).

It was now clear that the behaviour as q goes to q^3 should be at least as interesting as (3.3). Indeed, motivated by the modular properties of L we observed symbolically that

$$1 = R(q)^3 + \left[\frac{(1-R(q))}{(1+2R(q))}\right]^3. \tag{3.4}$$

At this stage in [4] we resorted rather unsatisfactorily to a classical modular function proof of (3.4) and so to a proof of Theorem 2. Later we returned with Frank Garvan [8] to a search for an elementary proof. This proved successful. By searching for product expansions for M we were lead to an entirely natural computer-guided proof — albeit with human insight along the way.

It is actually possible, as described in [8], to search for, discover and prove all modular identities of the type of (3.3) and (3.4) in an entirely automated fashion. Again, this is possible because we have ultimately reduced most of the analytic questions to algebra through the machinery of modular forms.

As a final symbolic challenge we observe that (3.1) may be recast as saying that

$$I(a_n, b_n) = I(a_{n+1}, b_{n+1})$$

where

$$I(a,b) = \int_0^\infty \frac{t\,dt}{\sqrt[3]{(t^3+a^3)(t^3+b^3)^2}}.$$

This invariance should be susceptible to a direct — hopefully experimentally guided — proof.

4. CONCLUSIONS. The sort of experiences we have had doing mathematics interactively has persuaded us of several conclusions. It is necessary to develop good context dependent intuition. It is useful to take advantage of the computer to do the easy — many unimaginable hand-calculations are trivial to code. (So trivial, in fact, that one has to resist the temptation to compute mindlessly.) The skill is to recognize when to try speculative variations on a theme and to know when one has actually learnt something from them. The mathematical opportunities are virtually unlimited but only in a relatively painless to use high level and multi-faceted environment.

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