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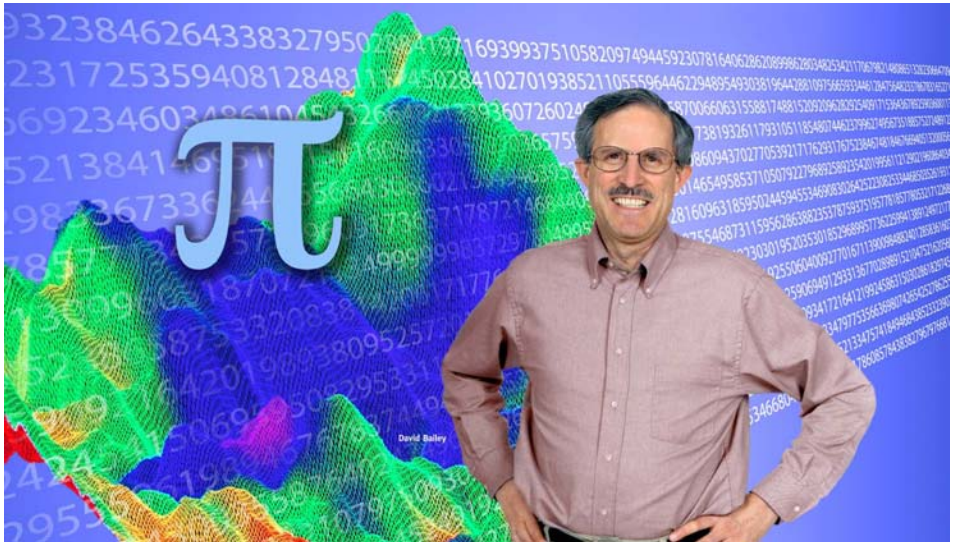
Algorithms for Experimental Mathematics II

David H Bailey

Lawrence Berkeley National Lab



"All truths are easy to understand once they are discovered; the point is to discover them." – Galileo Galilei

Algorithms Used in Experimental Mathematics

- Symbolic computation for algebraic and calculus manipulations.
- Integer-relation methods, especially the “PSLQ” algorithm.
- High-precision integer and floating-point arithmetic.
- High-precision evaluation of integrals and infinite series summations.
- The Wilf-Zeilberger algorithm for proving summation identities.
- Iterative approximations to continuous functions.
- Identification of functions based on graph characteristics.
- Graphics and visualization methods targeted to mathematical objects.

The Wilf-Zeilberger Algorithm for Proving Identities

- A slick, computer-assisted proof scheme to prove certain types of identities.
- Provides a nice complement to PSLQ:
  - PSLQ and the like permit one to discover new identities, but do not constitute rigorous proof, and do not suggest how a rigorous proof may be formulated.
  - W-Z methods permit one to prove certain types of identities, but do not provide any means to discover the identity.

Example Usage of W-Z

Recall these experimentally-discovered identities (from last lecture):

$$\sum_{n=0}^{\infty} \frac{\binom{4n}{2n}\binom{2n}{n}^4}{2^{16n}} \left(120n^2 + 34n + 3\right) = \frac{32}{\pi^2}$$

$$\sum_{n=0}^{\infty} \frac{(-1)^n \binom{2n}{n}^5}{2^{20n}} \left(820n^2 + 180n + 13\right) = \frac{128}{\pi^2}$$

Guillera started by defining

$$G(n,k) = \frac{(-1)^k}{2^{16n}2^{4k}} \left(120n^2 + 84nk + 34n + 10k + 3\right) \frac{\binom{2n}{n}^4 \binom{2k}{k}^3 \binom{4n-2k}{2n-k}}{\binom{2n}{k}\binom{n+k}{n}^2}$$

He then used the EKHAD software package to obtain the companion

$$F(n,k) = \frac{(-1)^k 512}{2^{16n}2^{4k}} \frac{n^3}{4n-2k-1} \frac{\binom{2n}{n}^4 \binom{2k}{k}^3 \binom{4n-2k}{2n-k}}{\binom{2n}{k}\binom{n+k}{n}^2}$$

Example Usage of W-Z, Cont.

When we define

$$H(n,k) \;=\; F(n+1,n+k)+G(n,n+k)$$

Zeilberger's theorem gives the identity

$$\sum_{n=0}^{\infty} G(n,0) \;=\; \sum_{n=0}^{\infty} H(n,0)$$

which when written out is

$$\sum_{n=0}^{\infty} \frac{\binom{2n}{n}^4 \binom{4n}{2n}}{2^{16n}} \left(120n^2+34n+3\right) \;=\; \sum_{n=0}^{\infty} \frac{(-1)^n}{2^{20n+7}} \frac{(n+1)^3}{2n+3} \frac{\binom{2n+2}{n+1}^4 \binom{2n}{n}^3 \binom{2n+4}{n+2}}{\binom{2n+2}{n} \binom{2n+1}{n+1}^2}$$

$$+ \sum_{n=0}^{\infty} \frac{(-1)^n}{2^{20n}} \left(204n^2+44n+3\right) \binom{2n}{n}^5 \;=\; \frac{1}{4} \sum_{n=0}^{\infty} \frac{(-1)^n \binom{2n}{n}^5}{2^{20n}} \left(820n^2+180n+13\right)$$

A limit argument completes the proof of Guillera’s identities.

Computation of the Pi Function
[Pi(x) = number of primes less than x]

x	$\pi(x)$	$\int_2^x dt/\log t$	Difference
10^1	4	5	1
10^2	25	29	4
10^3	168	177	9
10^4	1229	1245	16
10^5	9592	9629	37
10^6	78498	78627	129
10^7	6 64579	6 64917	338
10^8	57 61455	57 62208	753
10^9	508 47534	508 49234	1700
10^{10}	4550 52511	4550 55614	3103
10^{11}	41180 54813	41180 66400	11587

x	$\pi(x)$	$\int_2^x dt/\log t$	Difference
10^{12}	3 76079 12018	3 76079 50280	38262
10^{13}	34 60655 36839	34 60656 45809	1 08970
10^{14}	320 49417 50802	320 49420 65691	3 14889
10^{15}	2984 45704 22669	2984 45714 75287	10 52618
10^{16}	27923 83410 33925	27923 83442 48556	32 14631
10^{17}	2 62355 71576 54233	2 62355 71656 10821	79 56588
10^{18}	24 73995 42877 40860	24 73995 43096 90414	219 49554
10^{19}	234 05766 72763 44607	234 05766 73762 22381	998 77774
10^{20}	2220 81960 25609 18840	2220 81960 27836 63483	2227 44643
10^{21}	21127 26948 60187 31928	21127 26948 66161 26181	5973 94253
10^{22}	2 01467 28668 93159 06290	2 01467 28669 12482 61497	19323 55207

Computation of the Pi Function

The most efficient currently known algorithms for computing the Pi function are based on numerically integrating the Riemann zeta function with complex arguments, to sufficiently high precision that one can round to obtain the correct result.

- Current state-of-the-art methods are given in Richard Crandall and Carl Pomerance, *Prime Numbers: A Computational Perspective*.
- This and numerous other examples in experimental mathematics emphasize the importance of high-precision numerical integration (i.e., quadrature).

Newton Iteration Methods

Newton iterations arise frequently in experimental math, such as to iteratively solve an equation p(x) = 0:

$$x_{k+1} = x_k - \frac{p(x)}{p'(x)}$$

Numerous applications include:

- Performing division and square roots using high-precision arithmetic.
- Computing exp to high precision, given a fast scheme for log.
- Finding polynomial roots and roots of more general functions.

Potential pitfalls:

- Numerous evaluations may need to be computed to locate the root.
- Derivative of function may be zero at a zero of the function.

See companion book for ways to deal with such problems.

History of Numerical Quadrature

- 1670: Newton devises Newton-Coates integration.
- 1740: Thomas Simpson develops Simpson's rule.
- 1820: Gauss develops Gaussian quadrature.
- 1950-1980: Adaptive quadrature, Romberg integration, Clenshaw-Curtis integration, others.
- 1985-1990: Maple and Mathematica feature built-in numerical quadrature facilities.
- 2000: Very high-precision quadrature (1000+ digits).

With these high-precision values, we can now use PSLQ to obtain analytical evaluations of integrals.

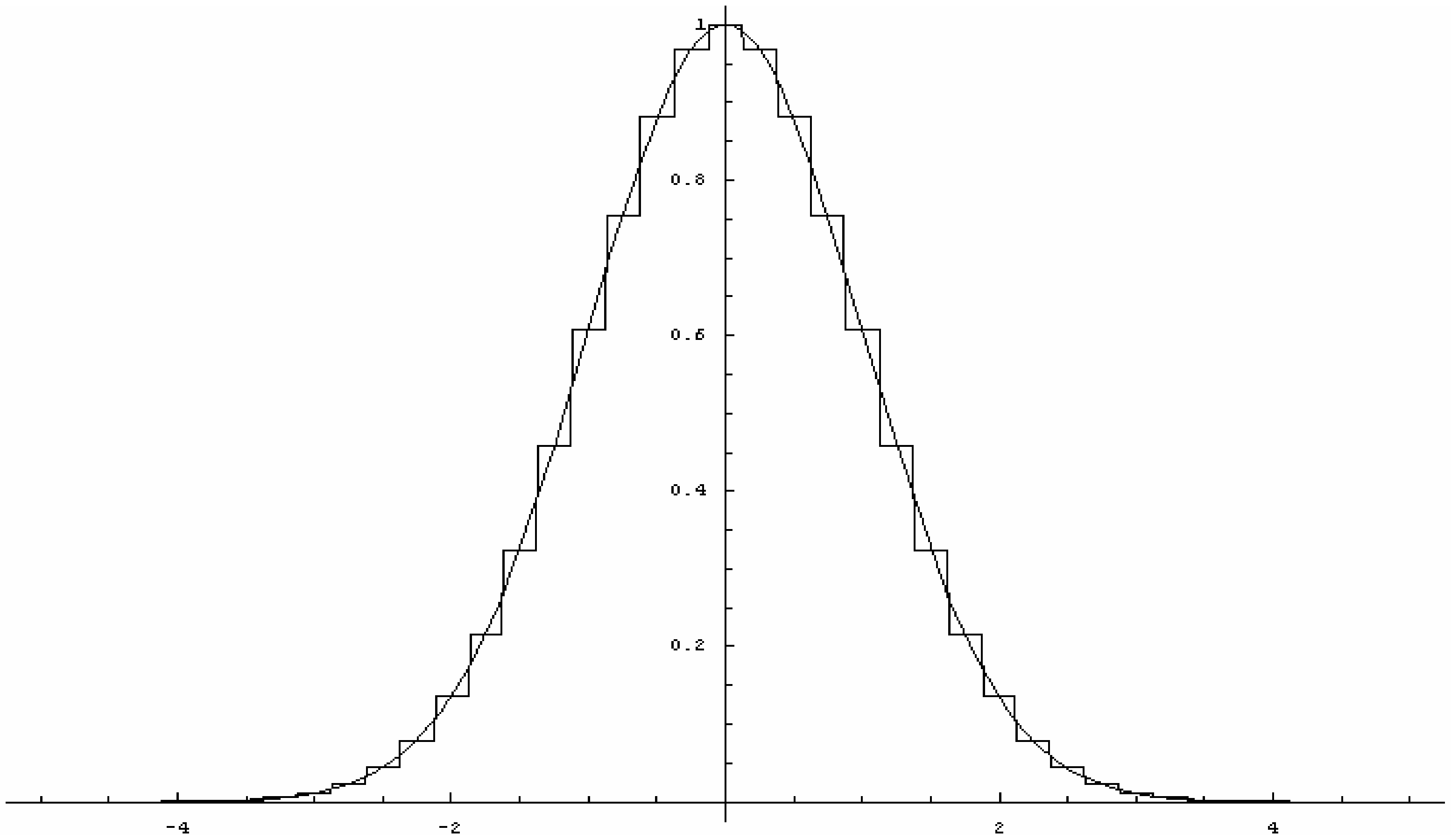
The Euler-Maclaurin Formula

$$\int_a^b f(x)\,dx = h\sum_{j=0}^{n} f(x_j) - \frac{h}{2}(f(a)+f(b))$$
$$- \sum_{i=1}^{m} \frac{h^{2i}B_{2i}}{(2i)!}\left(D^{2i-1}f(b) - D^{2i-1}f(a)\right) - E(h)$$
$$|E(h)| \le 2(b-a)[h/(2\pi)]^{2m+2} \max_{a\le x\le b} |D^{2m+2}f(x)|$$

[Here h = (b - a)/n and x_j = a + j h. D^m f(x) means m-th derivative of f(x).]

Note when f(t) and all of its derivatives are zero at a and b, the error E(h) of a simple block-function approximation to the integral goes to zero more rapidly than any power of h.

Block-Function Approximation to the Integral of a Bell-Shaped Function



Quadrature and the Euler-Maclaurin Formula

Given f(x) defined on (-1,1), employ a function g(t) such that g(t) goes from -1 to 1 over the real line, with g'(t) going to zero for large |t|. Then substituting x = g(t) yields

$$\begin{aligned}\int_{-1}^{1} f(x)\,dx &= \int_{-\infty}^{\infty} f(g(t))g'(t)\,dt \\ &\approx h\sum_{-N}^{N} g'(hj)f(g(hj)) = h\sum_{-N}^{N} w_j f(x_j)\end{aligned}$$

[Here x_j = g(hj) and w_j = g'(hj).]

If g'(t) goes to zero rapidly enough for large t, then even if f(x) has an infinite derivative or blow-up singularity at an endpoint, the product f(g(t)) g'(t) often is a nice bell-shaped function for which the E-M formula applies.

Four Suitable ‘g’ Functions

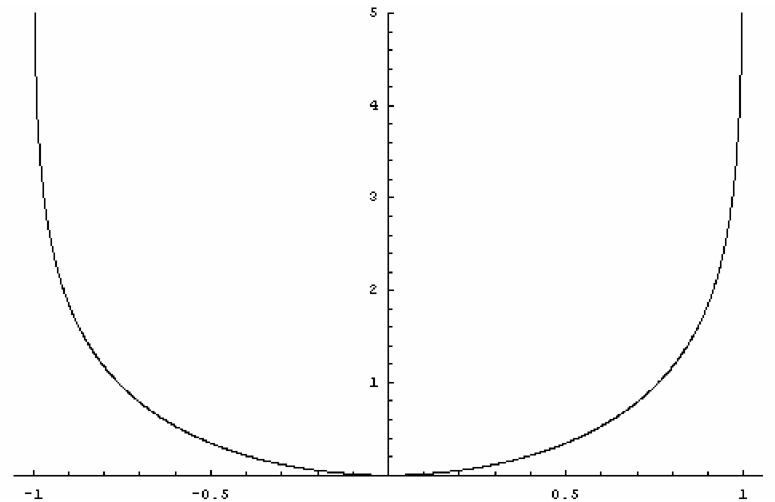
$$
\begin{aligned}
g(t) &= \mathrm{erf}(t) & g'(t) &= \frac{2}{\sqrt{\pi}} e^{-t^2} \\
g(t) &= \tanh t & g'(t) &= \frac{1}{\cosh^2 t} \\
g(t) &= \tanh(\pi/2 \cdot \sinh t) & g'(t) &= \frac{\pi/2 \cdot \sinh t}{\cosh^2(\pi/2 \cdot \sinh t)} \\
g(t) &= \tanh(\sinh t) & g'(t) &= \frac{\sinh t}{\cosh^2(\sinh t)}
\end{aligned}
$$

The third and fourth are known as “tanh-sinh” quadrature.

Original and Transformed Integrand Function

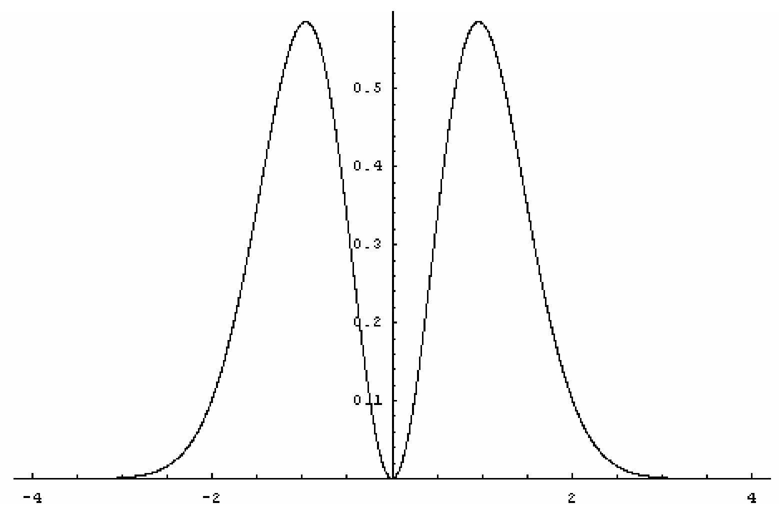
Original function (on [-1,1]):

$$f(t) \;=\; -\log\cos\left(\frac{\pi t}{2}\right)$$



Transformed function using g(t) = erf t:

$$f(g(t))g'(t) \;=\; -\frac{2}{\sqrt{\pi}}\log\cos\left(\frac{\pi \mathrm{erf} t}{2}\right)\exp(-t^2)$$



Test Integrals

$$1: \int_0^1 t \log(1+t)\, dt = 1/4$$

$$2: \int_0^1 t^2 \arctan t\, dt = (\pi - 2 + 2\log 2)/12$$

$$3: \int_0^{\pi/2} e^t \cos t\, dt = (e^{\pi/2} - 1)/2$$

$$4: \int_0^1 \frac{\arctan(\sqrt{2+t^2})}{(1+t^2)\sqrt{2+t^2}}\, dt = 5\pi^2/96$$

$$5: \int_0^1 \sqrt{t} \log t\, dt = -4/9$$

$$6: \int_0^1 \sqrt{1-t^2}\, dt = \pi/4$$

$$7: \int_0^1 \frac{t}{\sqrt{1-t^2}} dt = 1$$

$$8: \int_0^1 \log t^2\, dt = 2$$

$$9: \int_0^{\pi/2} \log(\cos t)\, dt = -\pi \log(2)/2$$

$$10: \int_0^{\pi/2} \sqrt{\tan t}\, dt = \pi\sqrt{2}/2$$

$$11: \int_0^{\infty} \frac{1}{1+t^2}\, dt = \pi/2$$

$$12: \int_0^{\infty} \frac{e^{-t}}{\sqrt{t}}\, dt = \sqrt{\pi}$$

$$13: \int_0^{\infty} e^{-t^2/2}\, dt = \sqrt{\pi/2}$$

$$14: \int_0^{\infty} e^{-t} \cos t\, dt = 1/2$$

Quadratic Convergence with Tanh-Sinh Quadrature

Level	Prob. 1	Prob. 2	Prob. 3	Prob. 4	Prob. 5	Prob. 6	Prob. 7
1	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-5}	10^{-5}	10^{-6}
2	10^{-11}	10^{-11}	10^{-9}	10^{-9}	10^{-12}	10^{-12}	10^{-12}
3	10^{-24}	10^{-19}	10^{-21}	10^{-18}	10^{-28}	10^{-25}	10^{-26}
4	10^{-51}	10^{-38}	10^{-49}	10^{-36}	10^{-62}	10^{-50}	10^{-49}
5	10^{-98}	10^{-74}	10^{-106}	10^{-73}	10^{-129}	10^{-99}	10^{-98}
6	10^{-195}	10^{-147}	10^{-225}	10^{-145}	10^{-265}	10^{-196}	10^{-194}
7	10^{-390}	10^{-293}	10^{-471}	10^{-290}	10^{-539}	10^{-391}	10^{-388}
8	10^{-777}	10^{-584}	10^{-974}	10^{-582}		10^{-779}	10^{-777}

Level	Prob. 8	Prob. 9	Prob. 10	Prob. 11	Prob. 12	Prob. 13	Prob. 14
1	10^{-5}	10^{-4}	10^{-6}	10^{-2}	10^{-2}	10^{-1}	10^{-1}
2	10^{-12}	10^{-11}	10^{-12}	10^{-5}	10^{-4}	10^{-3}	10^{-2}
3	10^{-29}	10^{-24}	10^{-25}	10^{-11}	10^{-9}	10^{-6}	10^{-5}
4	10^{-62}	10^{-50}	10^{-48}	10^{-22}	10^{-15}	10^{-9}	10^{-8}
5	10^{-130}	10^{-97}	10^{-98}	10^{-45}	10^{-28}	10^{-19}	10^{-14}
6	10^{-266}	10^{-195}	10^{-194}	10^{-91}	10^{-50}	10^{-37}	10^{-26}
7	10^{-540}	10^{-389}	10^{-388}	10^{-182}	10^{-92}	10^{-66}	10^{-48}
8		10^{-777}	10^{-777}	10^{-365}	10^{-170}	10^{-126}	10^{-88}
9				10^{-731}	10^{-315}	10^{-240}	10^{-164}
10					10^{-584}	10^{-457}	10^{-304}
11						10^{-870}	10^{-564}

At level k, $h = 2^{-k}$. I.e., each level halves h and doubles N, the # of abscissas.

Error Estimation in Tanh-Sinh Quadrature

Let F(t) be the desired integrand function on [a,b]. Define f(t) = F(g(t)) g'(t), where g(t) = tanh (sinh t) (or one of the other g functions above). Then an estimate of the error of the quadrature result, with interval h, is:

$$E_2(h,m) \;=\; h(-1)^{m-1}\left(\frac{h}{2\pi}\right)^{2m}\sum_{j=a/h}^{b/h} D^{2m} f(jh)$$

First order (m = 1) estimates are remarkably accurate. Higher-order estimates (m > 1) can be used to obtain “certificates” on the accuracy of a tanh-sinh quadrature result.

This formula was originally discovered due to a “bug” in our computer program – by mistake we implemented this formula and found it to be extremely accurate.

Error Estimation Results

Results for using tanh-sinh quadrature to integrate the function

$$F(t) \;=\; 1/(1+t^2+t^4+t^6) \quad \text{on} \quad [-1,1]$$

h	$E(h)$	$\lvert E(h) - E_2(h,1)\rvert$	$\lvert E(h) - E_2(h,2)\rvert$
$1/1$	5.34967×10^{-3}	9.81980×10^{-4}	4.77454×10^{-3}
$1/2$	-3.36641×10^{-4}	1.12000×10^{-7}	5.60084×10^{-7}
$1/4$	-3.73280×10^{-8}	1.67517×10^{-16}	8.37583×10^{-16}
$1/8$	5.58389×10^{-17}	2.29357×10^{-32}	1.14679×10^{-31}
$1/16$	-7.64525×10^{-33}	2.07256×10^{-64}	1.03628×10^{-63}
$1/32$	-6.90852×10^{-65}	7.23441×10^{-129}	3.61721×10^{-128}
$1/64$	$-2.41147 \times 10^{-129}$	9.08805×10^{-259}	4.54403×10^{-258}

For full details, see paper by DHB and Jonathan Borwein, “Effective Error Estimates in Euler-Maclaurin Based Quadrature Schemes,” available at **`http://crd.lbl.gov/~dhbailey/dhbpapers/em-error.pdf`**

Experimental Result Using PSLQ and Tanh-Sinh Quadrature - Example 1

Let

$$C(a) = \int_0^1 \frac{\arctan\sqrt{x^2+a^2}}{(x^2+1)\sqrt{x^2+a^2}}dx$$

Then PSLQ yields

$$\begin{aligned} C(0) &= (\pi \log 2)/8 + G/2 \\ C(1) &= \pi/4 - \pi\sqrt{2}/2 + 3\sqrt{2}/2 \cdot \arctan\sqrt{2} \\ C(\sqrt{2}) &= 5\pi^2/96 \end{aligned}$$

Several general results have now been proven, including

$$\int_0^\infty \frac{\arctan\sqrt{x^2+a^2}\,dx}{(x^2+1)\sqrt{x^2+a^2}} = \frac{\pi}{2\sqrt{a^2-1}}\left(2\arctan\sqrt{a^2-1} - \arctan\sqrt{a^4-1}\right)$$

Example 2

$$\frac{2}{\sqrt{3}}\int_0^1 \frac{\log^6 x \arctan[x\sqrt{3}/(x-2)]}{x+1}\,dx \;=$$

$$\frac{1}{81648}\big(-229635L_3(8)+29852550L_3(7)\log 3$$

$$-1632960L_3(6)\pi^2+27760320L_3(5)\zeta(3)$$

$$-275184L_3(4)\pi^4+36288000L_3(3)\zeta(5)$$

$$-30008L_3(2)\pi^6-57030120L_3(1)\zeta(7)\big)$$

where

$$L_{-3}(s) \;=\; \sum_{n=1}^{\infty}\left[1/(3n-2)^s-1/(3n-1)^s\right]$$

is the Dirichlet series.

Example 3

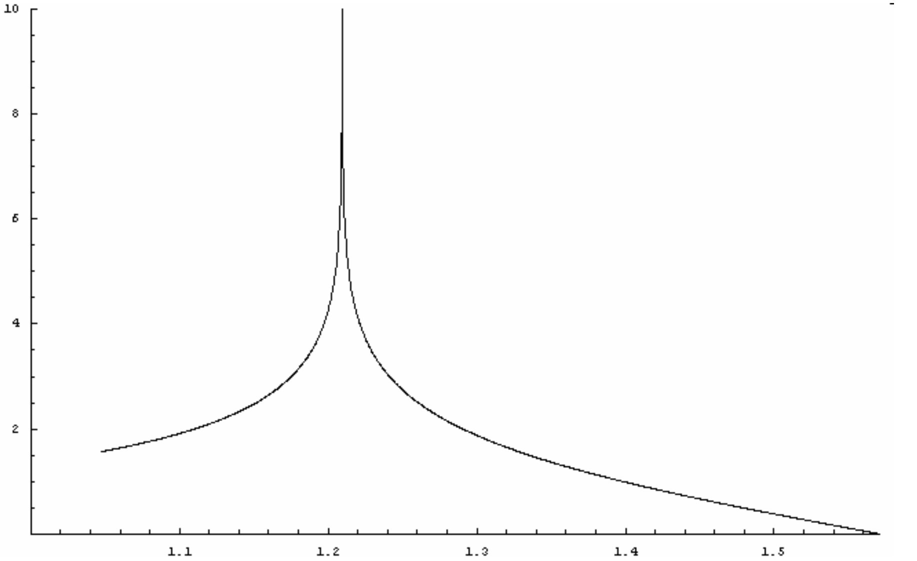
$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| dt$$

$$\stackrel{?}{=} \sum_{n=0}^{\infty} \left[\frac{1}{(7n+1)^2} + \frac{1}{(7n+2)^2} - \frac{1}{(7n+3)^2} + \frac{1}{(7n+4)^2} - \frac{1}{(7n+5)^2} - \frac{1}{(7n+6)^2} \right]$$

This arises in mathematical physics, from analysis of the volumes of ideal tetrahedra in hyperbolic space.

This "identity" has now been verified numerically to 20,000 digits, but no proof is known.

Note that the integrand function has a nasty singularity.



Example 4

Define

$$J_n = \int_{n\pi/60}^{(n+1)\pi/60} \log\left|\frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}}\right| dt$$

Then

$$\begin{aligned} 0 \stackrel{?}{=} & -2J_2 - 2J_3 - 2J_4 + 2J_{10} + 2J_{11} + 3J_{12} \\ & +3J_{13} + J_{14} - J_{15} - J_{16} - J_{17} - J_{18} \\ & -J_{19} + J_{20} + J_{21} - J_{22} - J_{23} + 2J_{25} \end{aligned}$$

This has been verified to over 1000 digits. The interval in J_{23} includes the singularity.

Example 5 (Jan 2006)

The following integrals arise from Ising theory in mathematical physics:

$$C_n = \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

We first showed that this can be transformed to a 1-D integral:

$$C_n = \frac{2^n}{n!}\int_0^\infty t K_0^n(t)\; dt$$

where K_0 is a modified Bessel function. We then computed 500-digit numerical values, from which we found these results (now proven):

$$C_3 = L_{-3}(2) = \sum_{n \ge 0}\left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2}\right)$$

$$C_4 = 14\zeta(3)$$

$$\lim_{n\to\infty} C_n = 2e^{-2\gamma}$$

Cautionary Example

These constants agree to 42 decimal digit accuracy, but are NOT equal:

$$\int_0^\infty \cos(2x) \prod_{n=0}^{\infty} \cos(x/n)\, dx \quad = \quad 0.39269908169872415480783042290993786052464543418723\ldots$$

$$\frac{\pi}{8} \quad = \quad 0.39269908169872415480783042290993786052464617492189\ldots$$

Computing this integral is nontrivial, due to difficulty in evaluating the integrand function to high precision.

Infinite Series Summation

How can we obtain high-precision of slowly converging infinite series, e.g.:

$$\pi = 1 - 1/3 + 1/5 - 1/7 + \cdots$$
$$G = 1 - 1/3^2 + 1/5^2 - 1/7^2 + \cdots$$

One fairly general method is to apply a technique we have already seen: the Euler-Maclaurin formula (in a slightly different form):

$$\sum_{j=a}^{\infty} f(j) = \int_a^{\infty} f(x)\,dx + \frac{1}{2} f(a) - \sum_{i=1}^{m} \frac{B_{2i}}{(2i)!} f^{(2i-1)}(a) + E$$

The usual strategy is to manually compute the first 10^5 or 10^6 terms, then use this formula to obtain an accurate estimate of the "tail."

Typically each additional term of the summation adds several more digits of accuracy to the result. All calculations must be done using the target precision.

Example: Computing Catalan

Let f(x) = (2x+1) / [(4x+1)^2 (4x+3)^2]. Then we can write

$$
\begin{aligned}
G &= (1 - 1/3^2) + (1/5^2 - 1/7^2) + (1/9^2 - 1/11^2) + \cdots \\
&= 8 \sum_{k=0}^{\infty} \frac{2k+1}{(4k+1)^2(4k+3)^2} \\
&= 8 \sum_{k=0}^{n} \frac{2k+1}{(4k+1)^2(4k+3)^2} + 8 \sum_{k=n+1}^{\infty} \frac{2k+1}{(4k+1)^2(4k+3)^2} \\
&= 8 \sum_{k=0}^{n} \frac{2k+1}{(4k+1)^2(4k+3)^2} + 8 \int_{n+1}^{\infty} f(x)\, dx + 4 f(n+1) \\
&\quad -8 \sum_{i=1}^{m} \frac{B_{2i}}{(2i)!} f^{(2i-1)}(n+1) + 8E,
\end{aligned}
$$

Some details for practical usage, such as how to compute Bernoulli numbers, are given in the companion book and *Experimentation in Mathematics*.

Apery-Like Summations

The following formulas for zeta(n) have been known for many years:

$$\zeta(2) = 3\sum_{k=1}^{\infty}\frac{1}{k^2\binom{2k}{k}},$$

$$\zeta(3) = \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}},$$

$$\zeta(4) = \frac{36}{17}\sum_{k=1}^{\infty}\frac{1}{k^4\binom{2k}{k}}.$$

These results have led some to speculate that

$$Q_5 := \zeta(5)/\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}}$$

might be some nice rational or algebraic value.

Sadly, PSLQ calculations have established that if Q_5 satisfies a polynomial with degree at most 25, then at least one coefficient has 380 digits.

Apery-Like Relations Found Using Integer Relation Methods

$$\zeta(5) = 2\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}} - \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^2},$$

$$\zeta(7) = \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^7\binom{2k}{k}} + \frac{25}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}$$

$$\begin{aligned}\zeta(9) = {} & \frac{9}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^9\binom{2k}{k}} - \frac{5}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^7\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^2} + 5\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4} \\ & + \frac{45}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^6} - \frac{25}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}\sum_{j=1}^{k-1}\frac{1}{j^2},\end{aligned}$$

$$\begin{aligned}\zeta(11) = {} & \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^{11}\binom{2k}{k}} + \frac{25}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^7\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4} \\ & - \frac{75}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^8} + \frac{125}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}\sum_{i=1}^{k-1}\frac{1}{i^4}\end{aligned}$$

Formulas for 7 and 11 were found by Jonathan Borwein and David Bradley; 5 and 9 are due to Koecher. This general formula was found by Koecher:

$$\sum_{k=1}^{\infty}\frac{1}{k(k^2-x^2)} = \frac{1}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\frac{5k^2-x^2}{k^2-x^2}\prod_{m=1}^{k-1}\left(1-\frac{x^2}{m^2}\right)$$

Newer Results

Using bootstrapping and an application of the “Pade” function, Borwein and Bradley produced the following remarkable result:

$$\sum_{k=1}^{\infty} \frac{1}{k^3(1 - x^4/k^4)} = \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k} (1 - x^4/k^4)} \prod_{m=1}^{k-1} \left(\frac{1 + 4x^4/m^4}{1 - x^4/m^4} \right)$$

Following an analogous – but more deliberate – experimental-based procedure, DHB, Borwein and Bradley obtained a similar general formula for zeta(2n+2) that is pleasingly parallel to above:

$$\sum_{k=1}^{\infty} \frac{1}{k^2 - x^2} = 3 \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k} \left(1 - x^2/k^2\right)} \prod_{m=1}^{k-1} \left(\frac{1 - 4\, x^2/m^2}{1 - x^2/m^2} \right)$$

Note that this gives an Apery-like formula for zeta(2n), since the LHS equals

$$\sum_{n=0}^{\infty} \zeta(2n+2) x^{2n} = \frac{1 - \pi x \cot(\pi x)}{2x^2}$$

This experimental discovery will be sketched in the new few slides.

The Experimental Scheme

We first conjectured that zeta(2n+2) is a rational combination of terms of the form:

$$\sigma(2r; [2a_1, \cdots, 2a_N]) \;:=\; \sum_{k=1}^{\infty} \frac{1}{k^{2r}\binom{2k}{k}} \prod_{i=1}^{N} \sum_{n_i=1}^{k-1} \frac{1}{n_i^{2a_i}}$$

where $r + a_1 + a_2 + \ldots + a_N = n + 1$ and a_i are listed in nonincreasing order. We can then write:

$$\sum_{n=0}^{\infty} \zeta(2n+2)\, x^{2n} \;\stackrel{?}{=}\; \sum_{n=0}^{\infty} \sum_{r=1}^{n+1} \sum_{\pi \in \Pi(n+1-r)} \alpha(\pi)\, \sigma(2r; 2\pi)\, x^{2n}$$

where $\Pi(m)$ denotes the additive partitions of m. We can then deduce that

$$\sum_{n=0}^{\infty} \zeta(2n+2)\, x^{2n} \;=\; \sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}(k^2 - x^2)} P_k(x)$$

where $P_k(x)$ are polynomials whose general form we hope to discover.

The Bootstrap Process

$$\zeta(2) = 3\sum_{k=1}^{\infty}\frac{1}{\binom{2k}{k}k^2} = 3\sigma(2,[0]),$$

$$\zeta(4) = \mathbf{3}\sum_{k=1}^{\infty}\frac{1}{\binom{2k}{k}k^4} - 9\sum_{k=1}^{\infty}\frac{\sum_{j=1}^{k-1} j^{-2}}{\binom{2k}{k}k^2} = \mathbf{3}\sigma(4,[0]) - 9\sigma(2,[2])$$

$$\begin{aligned}
\zeta(6) &= \mathbf{3}\sum_{k=1}^{\infty}\frac{1}{\binom{2k}{k}k^6} - \mathbf{9}\sum_{k=1}^{\infty}\frac{\sum_{j=1}^{k-1} j^{-2}}{\binom{2k}{k}k^4} - \frac{45}{2}\sum_{k=1}^{\infty}\frac{\sum_{j=1}^{k-1} j^{-4}}{\binom{2k}{k}k^2} \\
&\quad + \frac{27}{2}\sum_{k=1}^{\infty}\sum_{j=1}^{k-1}\frac{\sum_{i=1}^{k-1} i^{-2}}{j^2\binom{2k}{k}k^2}, \\
&= \mathbf{3}\sigma(6,[]) - \mathbf{9}\sigma(4,[2]) - \frac{45}{2}\sigma(2,[4]) + \frac{27}{2}\sigma(2,[2,2]) \\
\zeta(8) &= \mathbf{3}\sigma(8,[]) - \mathbf{9}\sigma(6,[2]) - \frac{45}{2}\sigma(4,[4]) + \frac{27}{2}\sigma(4,[2,2]) - 63\sigma(2,[6]) \\
&\quad + \frac{135}{2}\sigma(2,[4,2]) - \frac{27}{2}\sigma(2,[2,2,2]) \\
\zeta(10) &= \mathbf{3}\sigma(10,[]) - \mathbf{9}\sigma(8,[2]) - \frac{45}{2}\sigma(6,[4]) + \frac{27}{2}\sigma(6,[2,2]) - \mathbf{63}\sigma(4,[6]) \\
&\quad + \frac{135}{2}\sigma(4,[4,2]) - \frac{27}{2}\sigma(4,[2,2,2]) - \frac{765}{4}\sigma(2,[8]) + 189\sigma(2,[6,2]) \\
&\quad + \frac{675}{8}\sigma(2,[4,4]) - \frac{405}{4}\sigma(2,[4,2,2]) + \frac{81}{8}\sigma(2,[2,2,2,2])
\end{aligned}$$

Coefficients Obtained

Partition	Alpha	Partition	Alpha	Partition	Alpha
[empty]	3/1	1	-9/1	2	-45/2
1,1	27/2	3	-63/1	2,1	135/2
1,1,1	-27/2	4	-765/4	3,1	189/1
2,2	675/8	2,1,1	-405/4	1,1,1,1	81/8
5	-3069/5	4,1	2295/4	3,2	945/2
3,1,1	-567/2	2,2,1	-2025/8	2,1,1,1	405/4
1,1,1,1,1	-243/40	6	-4095/2	5,1	9207/5
4,2	11475/8	4,1,1	-6885/8	3,3	1323/2
3,2,1	-2835/2	3,1,1,1	567/2	2,2,2	-3375/16
2,2,1,1	6075/16	2,1,1,1,1	-1215/16	1,1,1,1,1,1	243/80
7	-49149/7	6,1	49140/8	5,2	36828/8

Partition	Alpha	Partition	Alpha	Partition	Alpha
5,1,1	-27621/10	4,3	32130/8	4,2,1	-34425/8
4,1,1,1	6885/8	3,3,1	-15876/8	3,2,2	-14175/8
3,2,1,1	17010/8	3,1,1,1,1	-1701/8	2,2,2,1	10125/16
2,2,1,1,1	-6075/16	2,1,1,1,1,1	729/16	1,1,1,1,1,1,1	-729/560
8	-1376235/56	7,1	1179576/56	6,2	859950/56
6,1,1	-515970/56	5,3	902286/70	5,2,1	-773388/56
5,1,1,1	193347/70	4,4	390150/64	4,3,1	-674730/56
4,2,2	-344250/64	4,2,1,1	413100/64	4,1,1,1,1	-41310/64
3,3,2	-277830/56	3,3,1,1	166698/56	3,2,2,1	297675/56
3,2,1,1,1	-119070/56	3,1,1,1,1,1	10206/80	2,2,2,2	50625/128
2,2,2,1,1	-60750/64	2,2,1,1,1,1	18225/64	2,1,1,1,1,1,1	-1458/64
1,1,1,1,1,1,1,1	2187/4480				

Resulting Polynomials

$$
\begin{aligned}
P_3(x) \approx\;& 3-\frac{45}{4}x^2-\frac{45}{16}x^4-\frac{45}{64}x^6-\frac{45}{256}x^8-\frac{45}{1024}x^{10}-\frac{45}{4096}x^{12}-\frac{45}{16384}x^{14}\\
&-\frac{45}{65536}x^{16}\\
P_4(x) \approx\;& 3-\frac{49}{4}x^2+\frac{119}{144}x^4+\frac{3311}{5184}x^4+\frac{38759}{186624}x^6+\frac{384671}{6718464}x^8\\
&+\frac{3605399}{241864704}x^{10}+\frac{33022031}{8707129344}x^{12}+\frac{299492039}{313456656384}x^{14}\\
P_5(x) \approx\;& 3-\frac{205}{16}x^2+\frac{7115}{2304}x^4+\frac{207395}{331776}x^6+\frac{4160315}{47775744}x^8+\frac{74142995}{6879707136}x^{10}\\
&+\frac{1254489515}{990677827584}x^{12}+\frac{20685646595}{142657607172096}x^{14}+\frac{336494674715}{20542695432781824}x^{16}\\
P_6(x) \approx\;& 3-\frac{5269}{400}x^2+\frac{6640139}{1440000}x^4+\frac{1635326891}{5184000000}x^6-\frac{5944880821}{18662400000000}x^8\\
&-\frac{21287425229134 9}{67184640000000000}x^{10}-\frac{14143638495690738 1}{24186470400000000000}x^{12}\\
&-\frac{7052426027485911598 9}{8707129344000000000000000}x^{14}-\frac{31533457168819214655541}{31345665638400000000000000000}x^{16}\\
P_7(x) \approx\;& 3-\frac{5369}{400}x^2+\frac{8210839}{1440000}x^4-\frac{199644809}{5184000000}x^6-\frac{680040118121}{18662400000000}x^8\\
&-\frac{27850031177504 9}{67184640000000000}x^{10}-\frac{841367152178726 81}{24186470400000000000}x^{12}\\
&-\frac{2236337781388343168 9}{8707129344000000000000000}x^{14}-\frac{5560090840263911428841}{31345665638400000000000000000}x^{16}
\end{aligned}
$$

After Using "Pade" Function in Mathematica

$$
\begin{aligned}
P_1(x) &\stackrel{?}{=} 3 \\
P_2(x) &\stackrel{?}{=} \frac{3(4x^2-1)}{(x^2-1)} \\
P_3(x) &\stackrel{?}{=} \frac{12(4x^2-1)}{(x^2-4)} \\
P_4(x) &\stackrel{?}{=} \frac{12(4x^2-1)(4x^2-9)}{(x^2-4)(x^2-9)} \\
P_5(x) &\stackrel{?}{=} \frac{48(4x^2-1)(4x^2-9)}{(x^2-9)(x^2-16)} \\
P_6(x) &\stackrel{?}{=} \frac{48(4x^2-1)(4x^2-9)(4x^2-25)}{(x^2-9)(x^2-16)(x^2-25)} \\
P_7(x) &\stackrel{?}{=} \frac{192(4x^2-1)(4x^2-9)(4x^2-25)}{(x^2-16)(x^2-25)(x^2-36)}
\end{aligned}
$$

which immediately suggests the general form:

$$\sum_{n=0}^{\infty} \zeta(2n+2)x^{2n} \stackrel{?}{=} 3\sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}(k^2-x^2)} \prod_{m=1}^{k-1} \frac{4x^2-m^2}{x^2-m^2}$$

Confirmations of Zeta(2n+2) Formula

- We symbolically computed the power series coefficients of the LHS and the RHS , and have verified that they agree up to the term with x^{100}.
- We verified that Z(1/6), Z(1/2), Z(1/3), Z(1/4), where Z(x) is the RHS, give numerically correct values (analytic values are known for LHS, using the cot formula).
- We then affirmed that the formula gives numerical values with LHS=RHS (to available 400-digit) for 100 pseudorandomly chosen arguments x.
- We subsequently proved this formula two different ways, including using the Wilf-Zeilberger method.

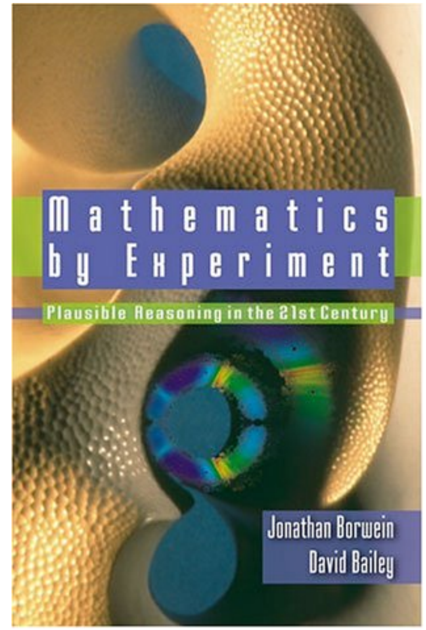
Full details are available in paper by DHB, Jonathan Borwein and David Bradley, “Experimental Determination of Apery-Like Identities for Zeta(2n+2),“ available at

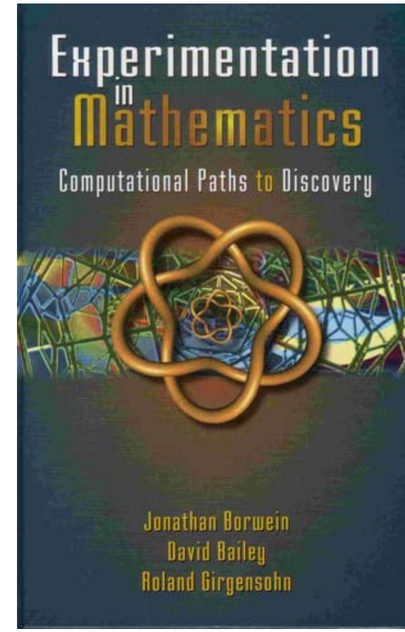
`http://crd.lbl.gov/~dhbailey/dhbpapers/apery.pdf`

Summary

New techniques now permit integrals, infinite series sums and other entities to be evaluated to high precision (hundreds or thousands of digits), thus permitting PSLQ-based schemes to discover new identities.

These methods typically do not suggest proofs, but often it is much easier to find a proof when one “knows” the answer is right.





Full details are available in companion book for this course, or in one of the two books recently published by Jonathan M. Borwein, DHB and (for vol 2) Roland Girgensohn. A “Reader’s Digest” condensed version of these two books is available FREE at

`http://www.experimentalmath.info`