

Ten Problems in Experimental Mathematics

David H. Bailey, Jonathan M. Borwein, Vishaal Kapoor, and Eric W. Weisstein

March 9, 2006

1. INTRODUCTION. This article was stimulated by the recent SIAM “100 Digit Challenge” of Nick Trefethen, beautifully described in [12] (see also [13]). Indeed, these ten numeric challenge problems are also listed in [15, pp. 22–26], where they are followed by the ten symbolic/numeric challenge problems that are discussed in this article. Our intent in [15] was to present ten problems that are characteristic of the sorts of problems that commonly arise in “experimental mathematics” [15][16]. The challenge in each case is to obtain a high precision numeric evaluation of the quantity, and then, if possible, to obtain a symbolic answer, ideally one with proof. Our goal in this article is to provide solutions to these ten problems, and at the same time, to present a concise account of how one combines symbolic and numeric computation, which may be termed “hybrid computation,” in the process of mathematical discovery.

The passage from object α to answer ω often relies on being able to compute the object to sufficiently high precision, for example, to determine numerically whether α is algebraic or is a rational combination of known constants. While some of this is now automated in mathematical computing software such as *Maple* and *Mathematica*, in most cases intelligence is needed, say in choosing the search space and in deciding the degree of polynomial to hunt for. In a similar sense, using symbolic computing tools such as those incorporated in *Maple* and *Mathematica* often requires significant human interaction to produce material results. Such matters are discussed in greater detail in [15] and [16].

Integer relation detection. Several of these solutions involve the usage of integer relation detection schemes to find experimentally a likely relationship. For a given real vector (x_1, x_2, \dots, x_n) an integer relation algorithm is a computational scheme that either finds the n -tuple of integers (a_1, a_2, \dots, a_n) , not all zero, such that $a_1x_1 + a_2x_2 + \dots + a_nx_n = 0$ or else establishes that there is no such integer vector within a ball of some radius about the origin, where the metric is the Euclidean norm $(a_1^2 + a_2^2 + \dots + a_n^2)^{1/2}$.

At the present time, the best known integer relation algorithm is the PSLQ algorithm [25] of Helaman Ferguson, who is well known in the community for his mathematical sculptures. Simple formulations of the PSLQ algorithm and several variants are given in [7]. Another widely used integer relation detection scheme involves the Lenstra-Lenstra-Lovasz (LLL) algorithm. The PSLQ algorithm, together with related lattice reduction schemes such as LLL, was recently named one of ten “algorithms of the century” by the publication *Computing in Science and Engineering* [3].

Perhaps the best-known application of PSLQ is the 1995 discovery, by means of a PSLQ computation, of the “BBP” formula for π :

$$\pi = \sum_{k=0}^{\infty} \frac{1}{16^k} \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right).$$

This formula permits one to calculate directly binary or hexadecimal digits beginning at the n th digit, without the need to calculate any of the first $n-1$ digits [6]. This result has, in turn, led to more recent results that suggest a possible route to a proof that π and some other mathematical constants are 2-normal (i.e., that every m -long binary string occurs in the binary expansion with limiting frequency b^{-m} [8][9]). The BBP formula even has some practical applications: it is used, for example, in the g95 compiler for transcendental function evaluations [34].

All integer relation schemes require very high precision arithmetic, both in the input data and in the operation of the algorithms. Simple reckoning shows that if an integer relation solution vector (a_1, a_2, \dots, a_n) has Euclidean norm 10^d , then the input data must be specified to at least dn digits, lest the true solution be lost in a sea of numerical artifacts. In some cases, including one mentioned at the end of the next section, thousands of digits are required before a solution can be found with these methods. This is the principal reason for the great interest in high-precision numerical evaluations in experimental mathematics research. It is also the motivation behind this set of ten challenge problems.

2. THE BIFURCATION POINT B_3 .

Problem 1. *Compute the value of r for which the chaotic iteration $x_{n+1} = rx_n(1 - x_n)$, starting with some x_0 in $(0, 1)$, exhibits a bifurcation between four-way periodicity and eight-way periodicity. Extra credit: This constant is an algebraic number of degree not exceeding twenty. Find the minimal polynomial with integer coefficients that it satisfies.*

History and context. The chaotic iteration $x_{n+1} = rx_n(1 - x_n)$ has been studied since the early days of chaos theory in the 1950s. It is often called the “logistic iteration,” since it mimics the behavior of an ecological population that, if its growth one year outstrips its food supply, often falls back in numbers for the following year, thus continuing to vary in a highly irregular fashion. When r is less than one iterates of the logistic iteration converge to zero. For r in the range $1 < r < B_1 = 3$ iterates converge to some nonzero limit. If $B_1 < r < B_2 = 1 + \sqrt{6} = 3.449489\dots$, the limiting behavior bifurcates—every other iterate converges to a distinct limit point. For r with $B_2 < r < B_3$ iterates hop between a set of four distinct limit points; when $B_3 < r < B_4$, they select between a set of eight distinct limit points; this pattern repeats until $r > B_\infty = 3.569945672\dots$, when the iteration is completely chaotic (see Figure 1). The limiting ratio $\lim_n (B_n - B_{n-1}) / (B_{n+1} - B_n) = 4.669201\dots$ is known as *Feigenbaum’s delta constant*.

A very readable description of the logistic iteration and its role in modern chaos theory are given in Gleick’s book [26]. Indeed, John von Neumann had suggested using the logistic map as a random number generator in the late 1940s. Work by W. Ricker in

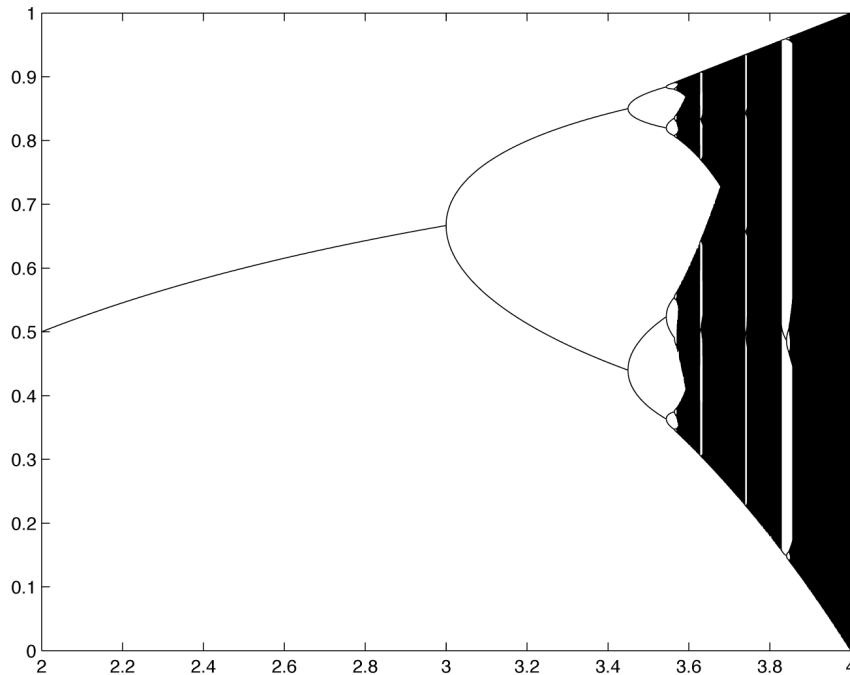


Figure 1: Bifurcation in the logistic iteration.

1954 and detailed analytic studies of logistic maps beginning in the 1950s with Paul Stein and Stanislaw Ulam showed the existence of complicated properties of this type of map beyond simple oscillatory behavior [35, pp. 918-919].

Solution. We first describe how to obtain a highly accurate numerical value of B_3 using a relatively straightforward search scheme. Other schemes could be used to find B_3 ; we present this one to underscore the fact that computational results sufficient for the purposes of experimental mathematics can often be obtained without resorting to highly sophisticated techniques.

Let $f_8(r, x)$ be the eight-times iterated evaluation of $rx(1 - x)$, and let $g_8(r, x) = f_8(r, x) - x$. Imagine a three-dimensional graph, where r ranges from left to right and x ranges from bottom to top (as in Figure 1), and where $g_8(r, x)$ is plotted in the vertical (out-of-plane) dimension. Given some initial r slightly less than B_3 , we compute a “comb” of function values at n evenly spaced x values (with spacing h_x) near the limit of the iteration $x_{n+1} = f_8(r, x_n)$. In our implementation, we use $n = 12$, and we start with $r = 3.544$, $x = 0.364$, $h_r = 10^{-4}$, and $h_x = 5 \times 10^{-4}$. With this construction, the comb has $n/2$ negative function values, followed by $n/2$ positive function values. We then increment r by h_r and reevaluate the “comb,” continuing in this fashion until two sign changes are observed among the n function values of the “comb.” This means that a bifurcation occurred just prior to the current value of r , so we restore r to its previous value (by subtracting h_r), reduce h_r , say by a factor of four, and also reduce the h_x roughly by a factor of 2.5. We continue in this fashion, moving the value of r and its associated

“comb” back and forth near the bifurcation point with progressively smaller intervals h_r . The center of the comb in the x -direction must be adjusted periodically to ensure that $n/2$ negative function values are followed by $n/2$ positive function values, and the spacing parameter h_x must be adjusted as well to ensure that two sign changes are disclosed when this occurs. We quit when the smallest of the n function values is within two or three orders of magnitude of the “epsilon” of the arithmetic (e.g., for 2000-digit working precision, “epsilon” is 10^{-2000}). The final value of r is then the desired value B_3 , accurate to within a tolerance given by the final value of r_h . With 2000-digit working precision, our implementation of this scheme finds B_3 to 1330-digit accuracy in about five minutes on a 2004-era computer. The first hundred digits are as follows:

$$B_3 = 3.544090359551922853615965986604804540583099845444573675457812530 \\ 3058429428588630122562585664248917999626 \dots$$

With even a moderately accurate value of r in hand (at least two hundred digits or so), one can use a PSLQ program (such as the PSLQ programs available at the URL <http://crd.lbl.gov/~dhbailey/mpdist>) to check whether r is an algebraic constant. This is done by computing the vector $(1, r, r^2, \dots, r^n)$ for various n , beginning with a small value such as two or three, and then searching for integer relations among these $n+1$ real numbers. When $n \geq 12$, the relation

$$0 = r^{12} - 12r^{11} + 48r^{10} - 40r^9 - 193r^8 + 392r^7 + 44r^6 + 8r^5 - 977r^4 \\ - 604r^3 + 2108r^2 + 4913 \tag{1}$$

can be recovered.

A symbolic solution that explicitly produces the polynomial (1) can be obtained as follows. We seek a sequence x_1, x_2, \dots, x_4 that satisfies the equations

$$x_2 = rx_1(1 - x_1), x_3 = rx_2(1 - x_2), x_4 = rx_3(1 - x_3), x_1 = rx_4(1 - x_4),$$

and

$$1 = \left| \prod_{i=1}^4 r(1 - 2x_i) \right|.$$

The first four conditions represent a period-4 sequence in the logistic equation $x_{n+1} = rx_n(1 - x_n)$, and the last condition represents the stability of the cycle, which must be 1 or -1 for a bifurcation point (see [33] for details).

First, we deal with the system corresponding to $1 + \prod_{i=1}^4 r(1 - 2x_i) = 0$. We compute the lexicographic Groebner basis in *Maple*:

```
with(Groebner):
L := [x2 - r*x1*(1-x1), x3 - r*x2*(1-x2), x4 - r*x3*(1-x3),
      x1 - r*x4*(1-x4), r^4*(1-2*x1)*(1-2*x2)*(1-2*x3)*(1-2*x4)+1];
gbasis(L, plex(x1, x2, x3, x4, r));
```

After a cup of coffee, we discover the univariate element

$$(r^4 + 1)(r^4 - 8r^3 + 24r^2 - 32r + 17) \times (r^4 - 4r^3 - 4r^2 + 16r + 17) \times \\ (r^{12} - 12r^{11} + 48r^{10} - 40r^9 - 193r^8 + 392r^7 + 44r^6 + 8r^5 - 977r^4 \\ - 604r^3 + 2108r^2 + 4913)$$

in the Groebner basis, in which the monomial ordering is lexicographical with r last.

The first three of these polynomials have no real roots, and the fourth has four real roots. Using trial and error, it is easy to determine that B_3 is the root of the minimal polynomial

$$r^{12} - 12r^{11} + 48r^{10} - 40r^9 - 193r^8 + 392r^7 + 44r^6 + 8r^5 - 977r^4 \\ - 604r^3 + 2108r^2 + 4913,$$

which has the numerical value stated earlier. The corresponding *Mathematica* code reads:

```
GroebnerBasis[{x2 - r x1(1 - x1), x3 - r x2(1 - x2),
  x4 - r x3(1 - x3), x1 - r x4(1 - x4),
  r^4(1 - 2x1)(1 - 2x2)(1 - 2x3)(1 - 2x4) + 1},
  r,
  {x1, x2, x3, x4}, MonomialOrder -> EliminationOrder] // Timing
```

This requires only 1.2 seconds on a 3 GHz computer. These computations can also be recreated very quickly in *Magma*, an algebraic package available at <http://magma.maths.usyd.edu.au/magma>:

```
Q := RationalField(); P<x,y,z,w,r> := PolynomialRing(Q,5);
I:= ideal< P| y - r*x*(1-x), z - r*y*(1-y), w - r*z*(1-z),
  x - r*w*(1-w), r^4*(1-2*x)*(1-2*y)*(1-2*z)*(1-2*w)+1>;
time B := GroebnerBasis(I);
```

This took 0.050 seconds on a 2.4Ghz Pentium 4.

The significantly more challenging problem of computing and analyzing the constant $B_4 = 3.564407266095\dots$ is discussed in [7]. In this study, conjectural reasoning suggested that B_4 might satisfy a 240-degree polynomial, and, in addition, that $\alpha = -B_4(B_4 - 2)$ might satisfy a 120-degree polynomial. The constant α was then computed to over 10,000-digit accuracy, and an advanced three-level multi-pair PSLQ program was employed, running on a parallel computer system, to find an integer relation for the vector $(1, \alpha, \alpha^2, \dots, \alpha^{120})$. A numerically significant solution was obtained, with integer coefficients descending monotonically from 257^{30} , which is a 73-digit integer, to the final value, which is one (a striking result that is exceedingly unlikely to be a numerical artifact). This experimentally discovered polynomial was recently confirmed in a large symbolic computation [30].

Additional information on the Logistic Map is available at <http://mathworld.wolfram.com/LogisticMap.html>.

3. MADELUNG'S CONSTANT.

Problem 2. Evaluate

$$\sum_{(m,n,p) \neq 0} \frac{(-1)^{m+n+p}}{\sqrt{m^2 + n^2 + p^2}}, \quad (2)$$

where convergence means the limit of sums over the integer lattice points enclosed in increasingly large cubes surrounding the origin. Extra credit: Usefully identify this constant.

History and context. Highly conditionally convergent sums like this are very common in physical chemistry, where they are usually written down with no thought of convergence. The sum in question arises as an idealization of the electrochemical stability of NaCl. One computes the total potential at the origin when placing a positive or negative charge at each nonzero point of the cubic lattice [16, chap. 4].

Solution. It is important to realize that this sum must be viewed as the limit of the sum in successively larger cubes. The sum diverges when spheres are used instead. To clarify this consider, for complex s , the series

$$b_2(s) = \sum_{(m,n) \neq 0} \frac{(-1)^{m+n}}{(m^2 + n^2)^{s/2}}, \quad b_3(s) = \sum_{(m,n,p) \neq 0} \frac{(-1)^{m+n+p}}{(m^2 + n^2 + p^2)^{s/2}}. \quad (3)$$

These converges in two and three dimensions, respectively, over increasing “cubes,” provided that $\operatorname{Re} s > 0$. When $s = 1$, one *may* sum over circles in the plane but not spheres in three-space, and one may *not* sum over diamonds in dimension two. Many chemists do not know that $b_3(1) \neq \sum_n (-1)^n r_3(n)/\sqrt{n}$, a series that arises by summing over increasing spheres but that diverges. Indeed, the number $r_3(n)$ of representations of n as a sum of three squares is quite irregular—no number of the form $8n + 7$ has such a representation—and is not $O(n^{1/2})$. This matter is somewhat neglected in the discussion of Madelung’s constant in Julian Havil’s deservedly popular recent book *Gamma: Exploring Euler’s Constant*, [27], which contains a wealth of information related to each of our problems in which Euler had a hand.

Straightforward methods to compute (3) are extremely unproductive. Such techniques produce at most three digits—indeed, the physical model should have a solar-system sized salt crystal to justify ignoring the boundary. Thus, we are led to using more sophisticated methods. We note

$$b_3(s) = \sum' \frac{(-1)^{i+j+k}}{(i^2 + j^2 + k^2)^{s/2}},$$

where \sum' signifies a sum over $\mathbb{Z}^3 \setminus \{(0, 0, 0)\}$, and let $M_s(f)$ denote the Mellin transform

$$M_s(f) = \int_0^\infty f(x)x^{s-1}dx.$$

The quantity that we wish to compute is $b_3(1)$. It follows by symmetry that

$$\begin{aligned} b_3(1) &= \sum' \frac{(-1)^{i+j+k}(i^2 + j^2 + k^2)}{(i^2 + j^2 + k^2)^{3/2}} \\ &= 3 \sum' \frac{(-1)^i(i^2)(-1)^{j+k}}{(i^2 + j^2 + k^2)^{3/2}}. \end{aligned} \quad (4)$$

We note that $M_s(e^{-t}) = \Gamma(s)$, so

$$M_{3/2}\left(q^{n^2+j^2+k^2}\right) = \Gamma\left(\frac{3}{2}\right)(n^2 + j^2 + k^2)^{-3/2},$$

where n, j , and k are arbitrary integers and $q = e^{-t}$. Continuing, we rewrite equation (4) as

$$\Gamma\left(\frac{3}{2}\right)b_3(1) = 3M_{3/2}\left[\sum_{n=-\infty}^{\infty} (-1)^n n^2 q^{n^2} \theta_4^2(x)\right],$$

where $\theta_4(x) = \sum_{n=-\infty}^{\infty} (-1)^n x^{n^2}$ is the usual Jacobi theta-function. Since the *theta transform*—a form of Poisson summation—yields $\theta_4(e^{-\pi/s}) = \sqrt{s}\theta_2(e^{-s\pi})$, it follows that

$$\Gamma\left(\frac{3}{2}\right)b_3(1) = 3 \sum_{n=-\infty}^{\infty} n^2 M_{3/2}\left(\sum (-1)^n n^2 q^{n^2} \frac{\pi}{x} \theta_2^2\left(\frac{\pi}{x}\right)\right).$$

Also, $\Gamma\left(\frac{3}{2}\right) = \sqrt{\pi}/2$, so

$$b_3(1) = 12\sqrt{\pi} \sum_{n=1}^{\infty} (-1)^n n^2 \sum_{(j,k) \text{ odd}} \int_0^{\infty} [e^{-n^2x - (\pi^2/4x)(j^2+k^2)}] x^{-1/2} dx.$$

The integral is evaluated in [19, Exercise 4, sec. 2.2] and is $(\pi/n^2)^{1/2} e^{-\pi n\sqrt{j^2+k^2}}$, whence

$$b_3(1) = 48\pi \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \sum_{n=1}^{\infty} (-1)^n n e^{-\pi n\sqrt{(2j+1)^2+(2k+1)^2}}.$$

Finally, when $a > 0$,

$$4 \sum_{n=1}^{\infty} (-1)^{n+1} n e^{-an} = \frac{4e^{-a}}{(1 + e^{-a})^2} = \operatorname{sech}^2\left(\frac{a}{2}\right),$$

from which we obtain

$$b_3(1) = 12\pi \sum_{\substack{m,n \geq 1 \\ m,n \text{ odd}}} \operatorname{sech}^2\left(\frac{\pi}{2}(m^2 + n^2)^{1/2}\right). \quad (5)$$

Summing m and n from 1 up to 81 in (5) gives

$$\begin{aligned} b_3(1) &= 1.74756459463318219063621203554439740348516143662474175 \\ &\quad 8152825350765040623532761179890758362694607891 \dots \end{aligned}$$

It is possible to accelerate the convergence further still. Details can be found in [19],[16].

There are closed forms for sums with an even number of variables, up to 24 and beyond. For example, $b_2(2s) = -4\alpha(s)\beta(s)$, where

$$\alpha(s) = \sum_{n \geq 0} (-1)^n / (n+1)^s$$

and

$$\beta(s) = \sum_{n \geq 0} (-1)^n / (2n+1)^s.$$

In particular, $b_2(2) = -\pi \log 2$. No such closed form for b_3 is known, while much work has been expended looking for one. The formula for b_2 is due to Lorenz (1879). It was rediscovered by G. H. Hardy and is equivalent to Jacobi's Lambert series formula for $\theta_3^2(q)$:

$$\theta_3^2(q) - 1 = 4 \sum_{n \geq 0} (-1)^n \frac{q^{2n+1}}{1 - q^{2n+1}}.$$

This, in turn, is equivalent to the formula for the number $r_2(n)$ of representations of n as a sum of two squares, counting order and sign,

$$r_2(n) = 4(d_1(n) - d_3(n)),$$

where d_k is the number of divisors of n congruent to k modulo four. The analysis of three squares is notoriously harder.

Additional information on Madelung's constant and lattice sums is available at <http://mathworld.wolfram.com/MadelungConstants.html> and <http://mathworld.wolfram.com/LatticeSum.html>.

4. DOUBLE EULER SUMS.

Problem 3. Evaluate the sum

$$C = \sum_{k=1}^{\infty} \left(1 - \frac{1}{2} + \cdots + (-1)^{k+1} \frac{1}{k}\right)^2 \frac{1}{(k+1)^3}. \quad (6)$$

Extra credit: Evaluate this constant as a multiterm expression involving well-known mathematical constants. This expression has seven terms and involves π , $\log 2$, $\zeta(3)$, and $\text{Li}_5(1/2)$, where $\text{Li}_n(x) = \sum_{k>0} x^k/k^n$ is the n th polylogarithm. (Hint: The expression is "homogenous," in the sense that each term has the same total "degree." The degrees of π and $\log 2$ are each 1, the degree of $\zeta(3)$ is 3, the degree of $\text{Li}_5(1/2)$ is 5, and the degree of α^n is n times the degree of α .)

History and context. In April 1993, Enrico Au-Yeung, an undergraduate at the University of Waterloo, brought to the attention of one of us (Borwein) the curious result

$$\sum_{k=1}^{\infty} \left(1 + \frac{1}{2} + \cdots + \frac{1}{k}\right)^2 k^{-2} = 4.59987\dots \approx \frac{17}{4}\zeta(4) = \frac{17\pi^4}{360}. \quad (7)$$

The function $\zeta(s)$ in (7) is the classical *Riemann zeta-function*:

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}.$$

Euler had solved Bernoulli's *Basel problem* when he showed that, for each positive integer n , $\zeta(2n)$ is an explicit rational multiple of π^{2n} [16, sec. 3.2].

Au-Yeung had computed the sum in (7) to 500,000 terms, giving an accuracy of five or six decimal digits. Suspecting that his discovery was merely a modest numerical coincidence, Borwein sought to compute the sum to a higher level of precision. Using Fourier analysis and Parseval's equation, he obtained

$$\frac{1}{2\pi} \int_0^\pi (\pi - t)^2 \log^2(2 \sin \frac{t}{2}) dt = \sum_{n=1}^{\infty} \frac{(\sum_{k=1}^n \frac{1}{k})^2}{(n+1)^2}. \quad (8)$$

The idea here is that the series on the right of (8) permits one to evaluate (7), while the integral on the left can be computed using the numerical quadrature facility of *Mathematica* or *Maple*. When he did this, Borwein was surprised to find that the conjectured identity holds to more than thirty digits. We should add here that, by good fortune, $17/360 = 0.047222\dots$ has period one and thus can plausibly be recognized from its first six digits, so that Au-Yeung's numerical discovery was not entirely far-fetched.

Solution. We define the multivariate zeta-function by

$$\zeta(s_1, s_2, \dots, s_k) = \sum_{n_1 > n_2 > \dots > n_k > 0} \prod_{j=1}^k n_j^{-|s_j|} \sigma_j^{-n_j},$$

where the s_1, s_2, \dots, s_k are nonzero integers and $\sigma_j = \text{signum}(s_j)$. A fast method for computing such sums based on Hölder convolution is discussed in [20] and implemented in the EZFace+ interface, which is available as an online tool at the URL

<http://www.cecm.sfu.ca/projects/ezface+>. Expanding the squared term in (6), we have

$$C = \sum_{0 < i, j < k} \frac{(-1)^{i+j}}{ijk^3} = 2\zeta(3, -1, -1) + \zeta(3, 2). \quad (9)$$

Evaluating this in EZFace+ we quickly obtain

$$C = 0.156166933381176915881035909687988193685776709840303872957529354497075037440295791455205653709358147578\dots$$

Given this numerical value, PSLQ or some other integer-relation-finding tool can be used to see if this constant satisfies a rational linear relation with the following constants (as suggested in the hint): $\pi^5, \pi^4 \log(2), \pi^3 \log^2(2), \pi^2 \log^3(2), \pi \log^4(2), \log^5(2), \pi^2 \zeta(3), \pi \log(2) \zeta(3), \log^2(2) \zeta(3), \zeta(5), \text{Li}_5(1/2)$. The result is quickly found to be

$$C = 4 \text{Li}_5\left(\frac{1}{2}\right) - \frac{1}{30} \log^5(2) - \frac{17}{32} \zeta(5) - \frac{11}{720} \pi^4 \log(2) + \frac{7}{4} \zeta(3) \log^2(2) + \frac{1}{18} \pi^2 \log^3(2) - \frac{1}{8} \pi^2 \zeta(3).$$

This result has been proved in various ways, both analytic and algebraic. Indeed, all evaluations of sums of the form $\zeta(\pm a_1, \pm a_2, \dots, \pm a_m)$ with *weight* $w = \sum_k a_m, (k < 8)$, as in (9) have been established.

Further history and context. What Borwein did not know at the time was that Au-Yeung's suspected identity follows directly from a related result proved by De Doelder in 1991. In fact, it had cropped up even earlier as a problem in this MONTHLY, but the story goes back further still. Some historical research showed that Euler considered these summations. In response to a letter from Goldbach, he examined sums that are equivalent to

$$\sum_{k=1}^{\infty} \left(1 + \frac{1}{2^m} + \dots + \frac{1}{k^m}\right) \frac{1}{(k+1)^n}. \quad (10)$$

The great Swiss mathematician was able to give explicit values for certain of these sums in terms of the Riemann zeta-function.

Starting from where we left off in the previous section provides some insight into evaluating related sums. Recall that the Taylor expansion of $f(x) = -\frac{1}{2} \log(1-x) \log(1+x)$ takes the form

$$f(x) = \sum_{k=1}^{\infty} \left(1 - \frac{1}{2} + \frac{1}{3} - \dots + \frac{1}{2k-1}\right) \frac{x^{2k}}{2k}.$$

Applying Parseval's identity to $f(e^{it})$, we have an effective way of computing

$$\sum_{k=1}^{\infty} \frac{\left(1 - \frac{1}{2} + \frac{1}{3} - \dots + \frac{1}{2k-1}\right)^2}{(2k)^2}$$

in terms of an integral that can be rapidly evaluated in *Maple* or *Mathematica*.

Alternatively, we may compute

$$\sum_{k=1}^{\infty} \frac{\left(1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{k}\right)^2}{k^2}.$$

The Fourier expansions of $(\pi - t)/2$ and $-\log|2 \sin(t/2)|$ are

$$\sum_{n=1}^{\infty} \frac{\sin(nt)}{n} = \frac{\pi - t}{2}, \quad (0 < t < 2\pi)$$

and

$$\sum_{n=1}^{\infty} \frac{\cos(nt)}{n} = -\log|2 \sin(t/2)|, \quad (0 < t < 2\pi), \quad (11)$$

respectively. Multiplying these together, simplifying, and doing a partial fraction decomposition gives

$$-\log|2 \sin(t/2)| \cdot \frac{\pi - t}{2} = \sum_{n=1}^{\infty} \frac{1}{n} \sum_{k=1}^{n-1} \frac{1}{k} \sin(nt)$$

on $(0, 2\pi)$. Applying Parseval's identity results in

$$\frac{1}{4\pi} \int_0^{2\pi} (\pi - t)^2 \log^2(2 \sin(t/2)) dt = \sum_{n=1}^{\infty} \frac{\left(1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n}\right)^2}{(n+1)^2}.$$

The integral may be computed numerically in *Maple* or *Mathematica*, delivering an approximation to the sum.

The *Clausen functions* defined by

$$\text{Cl}_2(\theta) = \sum_{n=1}^{\infty} \frac{\sin(n\theta)}{n^2}, \quad \text{Cl}_3(\theta) = \sum_{n=1}^{\infty} \frac{\cos(n\theta)}{n^3}, \quad \text{Cl}_4(\theta) = \sum_{n=1}^{\infty} \frac{\sin(n\theta)}{n^4}, \dots$$

arise as repeated antiderivatives of (11). They are useful throughout harmonic analysis and elsewhere. For example, with $\alpha = 2 \arctan \sqrt{7}$, one discovers with the aid of PSLQ that

$$6\text{Cl}_2(\alpha) - 6\text{Cl}_2(2\alpha) + 2\text{Cl}_2(3\alpha) \stackrel{?}{=} 7\text{Cl}_2\left(\frac{2\pi}{7}\right) + 7\text{Cl}_2\left(\frac{4\pi}{7}\right) - 7\text{Cl}_2\left(\frac{6\pi}{7}\right) \quad (12)$$

(here the question mark is used because no proof is yet known) or, in what can be shown to be equivalent, that

$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log\left(\left|\frac{\tan(t) + \sqrt{7}}{\tan(t) - \sqrt{7}}\right|\right) dt \stackrel{?}{=} L_{-7}(2) = 1.151925470\dots \quad (13)$$

This arises from the volume of an ideal tetrahedron in hyperbolic space [15, pp. 90–91]. (Here $L_{-7}(s) = \sum_{n>0} \chi_{-7}(n)n^{-s}$ is the primitive L -series modulo seven, whose character pattern is 1, 1, -1, 1, -1, -1, 0, which is given by

$$\chi_{-7}(k) = 2(\sin(k\tau) + \sin(2k\tau) - \sin(3k\tau))/\sqrt{7}$$

with $\tau = 2\pi/7$.)

Although (13) has been checked to twenty thousand decimal digits, by using a numerical integration scheme we shall describe in section 8, and although it is known for K -theoretic reasons that the ratio of the left- and right-hand sides of (12) is rational [14], to the best of our knowledge there is no proof of either (12) or (13). We might add that recently two additional conjectured identities related to (13) have been discovered by PSLQ computations. Let I_n be the definite integral of (13), except with limits $n\pi/24$ and $(n+1)\pi/24$. Then

$$\begin{aligned} -2I_2 - 2I_3 - 2I_4 - 2I_5 + I_8 + I_9 - I_{10} - I_{11} &\stackrel{?}{=} 0, \\ I_2 + 3I_3 + 3I_4 + 3I_5 + 2I_6 + 2I_7 - 3I_8 - I_9 &\stackrel{?}{=} 0. \end{aligned} \quad (14)$$

Readers who attempt to calculate numerical values for either the integral in (13) or the integral I_9 in (14) should note that the integrand has a nasty singularity at $t = \arctan \sqrt{7}$.

In retrospect, perhaps it was for the better that Borwein had not known of De Doelder's and Euler's results, because Au-Yeung's intriguing numerical discovery launched a fruitful

line of research by a number of researchers that has continued until the present day. Sums of this general form are known nowadays as “Euler sums” or “Euler-Zagier sums.” Euler sums can be studied through a profusion of methods: combinatorial, analytic, and algebraic. The reader is referred to [16, chap. 3] for an overview of Euler sums and their applications. We take up the story again in Problem 9.

Additional information on Euler sums is available at <http://mathworld.wolfram.com/EulerSum.html>.

5. KHINTCHINE’S CONSTANT.

Problem 4. Evaluate

$$K_0 = \prod_{k=1}^{\infty} \left[1 + \frac{1}{k(k+2)} \right]^{\log_2 k} = \prod_{k=1}^{\infty} k^{\left[\log_2 \left(1 + \frac{1}{k(k+2)} \right) \right]}. \quad (15)$$

Extra credit: Evaluate this constant in terms of a less-well-known mathematical constant.

History and context. Given some particular continued fraction expansion $\alpha = [a_0, a_1, \dots]$, consider forming the limit

$$K_0(\alpha) = \lim_{n \rightarrow \infty} (a_0 a_1 \cdots a_n)^{1/n}.$$

Based on the *Gauss-Kuzmin distribution*, which establishes that the digit distribution of a random continued fraction satisfies $\text{Prob}\{a_k = n\} = \log_2(1 + (k(k+2))^{-1})$, Khintchine showed that the limit exists for almost all continued fractions and is a certain constant, which we now denote K_0 . This circle of ideas is accessibly developed in [27]. As such a constant has an interesting interpretation, computation seems like the next step.

Taking logarithms of both sides of (15) and simplifying, we have

$$\log 2 \cdot \log K_0 = \sum_{n=1}^{\infty} \log n \cdot \log \left(1 + \frac{1}{n(n+2)} \right).$$

Such a series converges extremely slowly. Computing the sum of the first 10000 terms gives only two digits of $\log 2 \cdot \log K_0$. Thus, direct computation again proves to be quite difficult.

Solution. Rewriting $\log n$ as the telescoping sum

$$\log n = (\log n - \log(n-1)) + \cdots + (\log 2 - \log 1) = \sum_{k=2}^n \log \left(\frac{k}{k-1} \right),$$

we see that

$$\log 2 \cdot \log K_0 = \sum_{n=2}^{\infty} \sum_{k=2}^n \log \frac{k}{k-1} \cdot \log \frac{(n+1)^2}{n(n+2)}.$$

We interchange the order of summation to obtain

$$\log 2 \cdot \log K_0 = \sum_{k=2}^{\infty} \sum_{n=k}^{\infty} \log \frac{(n+1)^2}{n(n+2)} \log \frac{k}{k-1}. \quad (16)$$

But

$$\sum_{n=k}^{\infty} \log \frac{(n+1)^2}{n(n+2)} = \log \frac{(k+1)}{k} = \log \left(1 + \frac{1}{k}\right),$$

so (16) transforms into

$$\log 2 \cdot \log K_0 = - \sum_{k=2}^{\infty} \log \left(1 - \frac{1}{k}\right) \log \left(1 + \frac{1}{k}\right). \quad (17)$$

The Maclaurin series for $-\log(1-x)\log(1+x)$ is

$$\sum_{k=1}^{\infty} \left(1 - \frac{1}{2} + \frac{1}{3} - \dots + \frac{1}{2k-1}\right) \frac{x^{2k}}{k}.$$

This allows us to rewrite $\log 2 \cdot \log K_0$ as

$$\begin{aligned} \log 2 \log K_0 &= \sum_{k=1}^{\infty} \left(1 - \frac{1}{2} + \frac{1}{3} - \dots + \frac{1}{2k-1}\right) \frac{1}{k} \sum_{n=2}^{\infty} n^{-2k} \\ &= \sum_{k=1}^{\infty} \left(1 - \frac{1}{2} + \frac{1}{3} - \dots + \frac{1}{2k-1}\right) \frac{1}{k} (\zeta(2k) - 1). \end{aligned}$$

Appealing to either *Maple* or *Mathematica*, we can easily compute this sum. Taking the first 161 terms, we obtain one hundred digits of K_0 :

$$\begin{aligned} K_0 &= 2.68545200106530644530971483548179569382038229399446295 \\ &\quad 3051152345557218859537152002801141174931847709 \dots \end{aligned}$$

However, faster convergence is possible, and the constant has now been computed to more than seven thousand places. Moreover, the harmonic and other averages are similarly treated. It appears to satisfy its own predicted behavior (for details, see [5],[32]). Correspondingly, using 10^8 terms one can obtain the approximation $K_0(\pi) \approx 2.675 \dots$. Note however that $K_0(e) = \infty = \lim_{n \rightarrow \infty} \sqrt[3n]{(2n)!}$, since e is a member of the measure zero set of exceptions not having $K_0(\alpha) = K_0$, as a result of the non-Gauss-Kuzmin distribution of terms in the continued fraction $e = [2, 1, 2, 1, 1, 4, 1, 1, 6, \dots]$.

We emphasize that while it is known that almost all numbers α have limits $K_0(\alpha)$ that equal K_0 , this has not been exhibited for any explicit number α , excluding artificial examples constructed using their continued fractions [5].

6. RAMANUJAN'S AGM CONTINUED FRACTION.

Problem 5. For positive real numbers a, b , and η define $R_\eta(a, b)$ by

$$R_\eta(a, b) = \frac{a}{\eta + \frac{b^2}{\eta + \frac{4a^2}{\eta + \frac{9b^2}{\eta + \dots}}}}.$$

Calculate $R_1(2, 2)$. Extra credit: Evaluate this constant as a two-term expression involving a well-known mathematical constant.

History and context. This continued fraction arises in Ramanujan's *Notebooks*. He discovered the beautiful fact that

$$\frac{R_\eta(a, b) + R_\eta(b, a)}{2} = R_\eta\left(\frac{a+b}{2}, \sqrt{ab}\right).$$

The authors wished to record this in [15] and to check the identity computationally. A first attempt to find $R_1(1, 1)$ by direct numerical computation failed miserably, and with some effort only three reliable digits were obtained: $0.693\dots$. With hindsight, it was realized that the slowest convergence of the fraction occurs in the mathematically simplest case, namely, when $a = b$. Indeed, $R_1(1, 1) = \log 2$ as the first primitive numerics had tantalizingly suggested.

Solution. Attempting a direct computation of $R_1(2, 2)$ using a depth of twenty thousand gives only two digits. Thus we must seek more sophisticated methods. From [16, (1.11.70)] we learn that when $0 < b < a$,

$$\mathcal{R}_1(a, b) = \frac{\pi}{2} \sum_{n \in \mathbb{Z}} \frac{aK(k)}{K^2(k) + a^2n^2\pi^2} \operatorname{sech}\left(n\pi \frac{K(k')}{K(k)}\right), \quad (18)$$

where $k = b/a = \theta_2^2/\theta_3^2$ and $k' = \sqrt{1 - k^2}$. Here θ_2 and θ_3 are Jacobian theta-functions, and K is a complete elliptic integral of the first kind.

Writing (18) as a Riemann sum, we find that

$$\mathcal{R}(a) = \mathcal{R}_1(a, a) = \int_0^\infty \frac{\operatorname{sech}(\pi x/(2a))}{1+x^2} dx = 2a \sum_{k=1}^\infty \frac{(-1)^{k+1}}{1+(2k-1)a}, \quad (19)$$

where the final equality follows from the Cauchy-Lindelöf theorem. This sum may also be written as

$$\mathcal{R}(a) = \frac{2a}{1+a} {}_2F_1\left(\frac{1}{2a} + \frac{1}{2}, 1; \frac{1}{2a} + \frac{3}{2}; -1\right),$$

where ${}_2F_1(\cdot)$ denotes the hypergeometric function [1, p. 556]. The latter form is what we use in *Maple* or *Mathematica* to determine

$$\begin{aligned} \mathcal{R}(2) = & 0.97499098879872209671990033452921084400592021999471060574526825 \\ & 1285877387455708594352325320911129362\dots \end{aligned}$$

This constant, as written, is a bit difficult to recognize, but if one first divides by $\sqrt{2}$ and exploits the *Inverse Symbolic Calculator*, an online tool available at the URL <http://www.cecm.sfu.ca/projects/ISC/ISCmain.html>, it becomes apparent that the quotient is $\pi/2 - \log(1 + \sqrt{2})$. Thus we conclude, experimentally, that

$$\mathcal{R}(2) = \sqrt{2}[\pi/2 - \log(1 + \sqrt{2})].$$

Indeed, it follows (see [18]) that

$$\mathcal{R}(a) = 2 \int_0^1 \frac{t^{1/a}}{1+t^2} dt.$$

Note that $\mathcal{R}(1) = \log 2$. No nontrivial closed-form expression is known for $\mathcal{R}(a, b)$ when $a \neq b$, although

$$\mathcal{R}_1 \left(\frac{1}{4\pi} \beta \left(\frac{1}{4}, \frac{1}{4} \right), \frac{\sqrt{2}}{8\pi} \beta \left(\frac{1}{4}, \frac{1}{4} \right) \right) = \frac{1}{2} \sum_{n \in \mathbf{Z}} \frac{\operatorname{sech}(n\pi)}{1+n^2}$$

is almost closed. It would be pleasant to find a direct proof of (19). Further details are to be found in [18],[17], and [16].

7. EXPECTED DISTANCE ON A UNIT SQUARE.

Problem 6. Calculate the expected distance E_2 between two random points on different sides of the unit square:

$$E_2 = \frac{2}{3} \int_0^1 \int_0^1 \sqrt{x^2 + y^2} dx dy + \frac{1}{3} \int_0^1 \int_0^1 \sqrt{1 + (u - v)^2} du dv. \quad (20)$$

Extra credit: Express this constant as a three-term expression involving algebraic constants and an evaluation of the natural logarithm with an algebraic argument.

History and context. This evaluation and the next were discovered, in slightly more complicated form, by James D. Klein [16, p. 66]. He computed the numerical integral and compared it with the result of a Monte Carlo simulation. Indeed, a straightforward approach to a quick numerical value for an arbitrary iterated integral is to use a Monte-Carlo simulation, which entails approximating the integral by a sum of function values taken at pseudo-randomly generated points within the region. It is important to use a good pseudo-random number generator for this purpose. We tried doing a Monte Carlo evaluation for this problem, using a pseudo-random number generator based on the recently discovered class of provably normal numbers [9],[15, pp. 169–70]. The results we obtained for the two integrals in question, with 10^8 pseudo-random pairs, are 0.765203... and 1.076643..., respectively, yielding an expected distance of 0.869017.... Unfortunately, none of these three values immediately suggests a closed form, and they are not sufficiently accurate (because of statistical limitations) to be suitable for PSLQ or other constant recognition tools. More digits are needed.

Solution. It is possible to calculate high-precision numerical values for these two integrals using a two-dimensional quadrature (numerical integration) program. In our program, we employed a two-dimensional version of the “tanh-sinh” quadrature algorithm, which we will discuss in more detail in Problem 8. Two-dimensional quadrature is usually much more expensive than one-dimensional quadrature, at a given precision level, because many more function evaluations must be performed. Often a highly parallel computer system must be used to obtain a high-precision result in reasonable run time [11]. Nonetheless,

in this case we were able to evaluate the first of the two integrals to 108-digit accuracy in twenty-one minutes runtime on a 2004-era computer, and the second to 118-digit accuracy in just twenty seconds. The first is more difficult due to nondifferentiability of the integrand at the origin.

Indeed, in this case both *Maple* and *Mathematica* are able to evaluate each of these integrals numerically, as is, to more than one hundred decimal digit accuracy in just a few minutes run time, either by evaluating the inner integral symbolically and the outer integral numerically or else by performing full two-dimensional numerical quadrature. *Maple*, *Mathematica*, and the two-dimensional quadrature program all agreed on the following numerical value for the expected distance:

$$\alpha = 0.86900905527453446388497059434540662485671927963168056 \\ 9660350864584179822174693053113213554875435754 \dots$$

Using PSLQ, with the basis elements α , $\sqrt{2}$, $\log(\sqrt{2} + 1)$, and 1, we obtain

$$\alpha = \frac{1}{9}\sqrt{2} + \frac{5}{9}\log(\sqrt{2} + 1) + \frac{2}{9}. \quad (21)$$

An alternate solution is to attempt to evaluate the integrals symbolically! In fact, in this case Version 5.1 of *Mathematica* can do both the integrals “out of the box,” whereas in the first case *Maple* appears to need coaxing, for instance, by converting to polar coordinates:

$$2 \int_0^{\pi/4} \int_0^{\sec\theta} r^2 dr d\theta = \frac{2}{3} \int_0^{\pi/4} \sec^3 \theta d\theta = \frac{1}{3}\sqrt{2} - \frac{1}{6}\log(2) + \frac{1}{3}\log(2 + \sqrt{2}),$$

since the radius for a given θ is $1/\cos\theta$. As for the second integral, *Maple* and *Mathematica* both give

$$-\frac{1}{3}\sqrt{2} - \frac{1}{2}\log(\sqrt{2} - 1) + \frac{1}{2}\log(1 + \sqrt{2}) + \frac{2}{3}.$$

To obtain the second integral analytically, write it as $2 \int_0^1 \int_0^u \sqrt{1 + (u - v)^2} dv du$. Now change variables (set $t = u - v$) to obtain $1/2 \int_0^1 \{u\sqrt{1 + u^2} + \operatorname{arcsinh} u\} du$. Thus, the expected distance is

$$\frac{1}{9}\sqrt{2} - \frac{1}{9}\log(2) + \frac{2}{9}\log(2 + \sqrt{2}) - \frac{1}{6}\log(\sqrt{2} - 1) + \frac{1}{6}\log(1 + \sqrt{2}) + \frac{2}{9},$$

which can be simplified to the formula (21) above.

Additional information on the problem is available at <http://mathworld.wolfram.com/SquareLinePicking.html>.

8. EXPECTED DISTANCE ON A UNIT CUBE.

Problem 7. Calculate the expected distance between two random points on different faces of the unit cube. (Hint: This can be expressed in terms of integrals as

$$E_3 : = \frac{4}{5} \int_0^1 \int_0^1 \int_0^1 \int_0^1 \sqrt{x^2 + y^2 + (z - w)^2} dw dx dy dz \\ + \frac{1}{5} \int_0^1 \int_0^1 \int_0^1 \int_0^1 \sqrt{1 + (y - u)^2 + (z - w)^2} du dw dy dz.)$$

Extra credit: Express this constant as a six-term expression involving algebraic constants and two evaluations of the natural logarithm with algebraic arguments.

History and context. As we noted earlier, this evaluation was discovered, in essentially the same form, by Klein [16, p. 66]. As with Problem 6, a Monte Carlo integration scheme can be used to obtain a quick approximation to the integrals. The values we obtained were 0.870792... and 1.148859..., respectively, yielding an expected distance of 0.926406.... Once again, however, these numerical values do not immediately suggest a closed-form evaluation, yet the accuracy is too low to apply PSLQ or other constant recognition schemes. What's more, in this case, unlike Problem 6, neither *Maple* nor *Mathematica* are able to evaluate these four-fold integrals directly—though *Mathematica* comes close. As in most cases “help” is needed, in the form of mathematical manipulation to render these integrals in a form where mathematical computing software can evaluate them—numerically or symbolically.

Solution. Let ${}_2F_1(\cdot)$ again denote the hypergeometric function [1, p. 556]. One may show that the first integral evaluates to

$$\frac{\sqrt{2\pi}}{5} \sum_{n=2}^{\infty} \frac{{}_2F_1(1/2, -n+2; 3/2; 1/2)}{(2n+1)\Gamma(n+2)\Gamma(5/2-n)} + \frac{4}{15} \sqrt{2} + \frac{2}{5} \log(\sqrt{2}+1) - \frac{1}{75} \pi$$

and the second generalized hypergeometric function formally evaluates to

$$\frac{\sqrt{\pi}}{10} \sum_{n=0}^{\infty} \frac{{}_4F_3(1, 1/2, -1/2-n, -n-1; 2, 1/2-n, 3/2; -1)}{(2n+1)\Gamma(n+2)\Gamma(3/2-n)} \\ - \frac{2}{25} + \frac{\sqrt{2}}{50} + \frac{1}{10} \log(\sqrt{2}+1).$$

(Although the second diverges as a Riemann sum, both *Maple* and *Mathematica* can handle it, with some human help, producing numerical values of the corresponding Borel sum.) Both expressions are consequences of the binomial theorem, modulo an initial integration with respect to z in the first case. These expansions allow one to compute the expectation to high precision numerically and to express both of the individual integrals in terms of the same set of constants. The numerical value of the desired expectation is

$$0.926390055174046729218163586547779014444960190107335046732521921271418 \\ 504594036683829313473075349968212\dots$$

An integer relation search in the span of $\{1, \pi, \sqrt{2}, \sqrt{3}, \log(1 + \sqrt{2}), \log(2 + \sqrt{3})\}$ produces

$$\frac{4}{75} + \frac{17}{75} \sqrt{2} - \frac{2}{25} \sqrt{3} - \frac{7}{75} \pi + \frac{7}{25} \log(1 + \sqrt{2}) + \frac{7}{25} \log(7 + 4\sqrt{3}).$$

With substantial effort we were able to nurse the symbolic integral out of *Maple*. We started, as in the previous problem, by integrating with respect to w over $[0, z]$, doubling, and continuing in this fashion until we reduced the problem to showing that

$$\begin{aligned} & 3 \int_0^1 \frac{-(x^2 + 1) \ln(\sqrt{2 + x^2} - 1) + \ln(\sqrt{2} - 1)}{x^2(x^2 + 1)} dx \\ & - \int_0^1 (2x^3 + 6x^2 + 3) \ln(\sqrt{2 + x^2} - 1) dx = \\ & -\frac{5}{3} \pi + \frac{7}{6} \sqrt{2} + \frac{7}{2} \ln(1 + \sqrt{2}) - \frac{3}{2} \ln(2) + \ln(1 + \sqrt{3}) + \frac{37}{24} + \frac{3}{4} \ln(1 + \sqrt{2}) \pi, \end{aligned}$$

which we leave to the reader to establish.

Mathematica was more helpful: consider

```
4/5 Integrate[Sqrt[x^2 + y^2 + (z - w)^2], {x, 0, 1}, {y, 0, 1},
  {w, 0, 1}, {z, 0, 1}] // Timing
{52.483021*Second, (168*Sqrt[2] - 24*Sqrt[3] - 44*Pi + 72*ArcSinh[1] +
  162*ArcSinh[1/Sqrt[2]] + 24*Log[2] - 240*Log[-1 + Sqrt[3]] +
  192*Log[1 + Sqrt[3]] + 20*Log[26 + 15*Sqrt[3]] + 3*Log[70226 +
  40545*Sqrt[3]])/900}
```

This form is what the shipping version of *Mathematica* 5.1 returns on a 3.0 GHz Pentium 4. It evaluates the first integral directly, while the second one can be done with a little help. The combined outcomes can then be simplified symbolically to the result shown.

There is also an ingenious method due to Michael Trott using a Laplace transform to reduce the four-dimensional integrals to integrals over one-dimensional integrands. It proceeds by eliminating the square roots (which cause most of the difficulty in symbolic evaluation of the multiple integrals) at the expense of introducing one additional (but “easy”) integral. The original problem can then be written in terms of the *single* integral

$$\int_0^\infty \left[-\frac{14}{25} e^{-z^2} \sqrt{\pi} \operatorname{erf}^2(z) + \frac{28e^{-2z^2} \operatorname{erf}(z)}{25z} + \frac{7e^{-z^2} \operatorname{erf}(z)}{25z} - \frac{12e^{-3z^2}}{25\sqrt{\pi}} + \frac{68e^{-2z^2}}{75\sqrt{\pi}} + \frac{8e^{-z^2}}{75\sqrt{\pi}} \right] dz,$$

which can be evaluated directly in *Mathematica* to produce the symbolic expression for E_3 .

Nonetheless, we must emphasize that (i) one needs to proceed with confidence, since such symbolic computations can take several minutes, and (ii) phrases like “*Maple* can not” or “*Mathematica* can” are release-specific and may also depend on the skill of the human user to make use of expert knowledge in mathematics, symbolic computation, or both, in order to produce a form of the problem that is most amenable to computation in a given software system. This explains our desire to illustrate various solution paths here and elsewhere.

Additional information on this problem is available at <http://mathworld.wolfram.com/CubeLinePicking.html>. For more information about the Laplace transform trick applied to the related problem of expected distance in a unit hypercube, see <http://mathworld.wolfram.com/HypercubeLinePicking.html>.

9. AN INFINITE COSINE PRODUCT.

Problem 8. Calculate

$$\pi_2 = \int_0^\infty \cos(2x) \prod_{n=1}^\infty \cos\left(\frac{x}{n}\right) dx.$$

History and context. The challenge of showing that $\pi_2 < \pi/8$ was posed by Bernard Mares, Jr., along with the problem of demonstrating that

$$\pi_1 = \int_0^\infty \prod_{n=1}^\infty \cos\left(\frac{x}{n}\right) dx < \frac{\pi}{4}.$$

This is indeed true, although the error is remarkably small, as we shall see.

Solution. The computation of a high-precision numerical value for this integral is rather challenging, owing in part to the oscillatory behavior of $\prod_{n \geq 1} \cos(x/n)$ (see Figure 2) but mostly because of the difficulty of computing high-precision evaluations of the integrand. Note that evaluating thousands of terms of the infinite product would produce only a few correct digits. Thus it is necessary to rewrite the integrand in a form more suitable for computation.

Let $f(x)$ signify the integrand. We can express $f(x)$ as

$$f(x) = \cos(2x) \left[\prod_{k=1}^m \cos(x/k) \right] \exp(f_m(x)), \quad (22)$$

where we choose m greater than x and where

$$f_m(x) = \sum_{k=m+1}^\infty \log \cos\left(\frac{x}{k}\right). \quad (23)$$

The k th summand can be expanded in a Taylor series [1, p. 75], as follows:

$$\log \cos\left(\frac{x}{k}\right) = \sum_{j=1}^\infty \frac{(-1)^j 2^{2j-1} (2^{2j} - 1) B_{2j}}{j(2j)!} \left(\frac{x}{k}\right)^{2j},$$

in which B_{2j} are Bernoulli numbers. Observe that since $k > m > x$ in (23), this series converges. We can then write

$$f_m(x) = \sum_{k=m+1}^\infty \sum_{j=1}^\infty \frac{(-1)^j 2^{2j-1} (2^{2j} - 1) B_{2j}}{j(2j)!} \left(\frac{x}{k}\right)^{2j}. \quad (24)$$

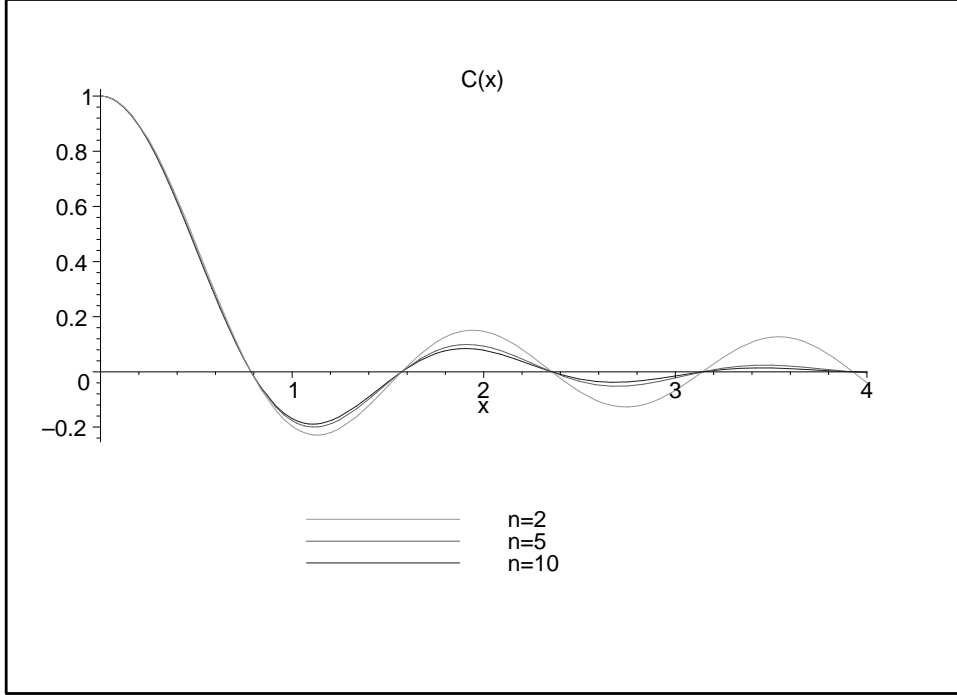


Figure 2: Approximations to $\prod_{n \geq 1} \cos(x/n)$.

After applying the identity [1, p. 807]

$$B_{2j} = \frac{(-1)^{j+1} 2(2j)! \zeta(2j)}{(2\pi)^{2j}}$$

and interchanging the sums, we obtain

$$f_m(x) = - \sum_{j=1}^{\infty} \frac{(2^{2j} - 1) \zeta(2j)}{j \pi^{2j}} \left[\sum_{k=m+1}^{\infty} \frac{1}{k^{2j}} \right] x^{2j}.$$

Note that the inner sum can also be written in terms of the zeta-function, as follows:

$$f_m(x) = - \sum_{j=1}^{\infty} \frac{(2^{2j} - 1) \zeta(2j)}{j \pi^{2j}} \left[\zeta(2j) - \sum_{k=1}^m \frac{1}{k^{2j}} \right] x^{2j}.$$

This can now be reduced to a compact form for purposes of computation as

$$f_m(x) = - \sum_{j=1}^{\infty} a_j b_{j,m} x^{2j}, \quad (25)$$

where

$$a_j = \frac{(2^{2j} - 1) \zeta(2j)}{j \pi^{2j}}, \quad (26)$$

$$b_{j,m} = \zeta(2j) - \sum_{k=1}^m \frac{1}{k^{2j}}. \quad (27)$$

We remark that $\zeta(2j)$, a_j , and $b_{j,m}$ can all be precomputed, say for j up to some specified limit and for a variety of m . In our program, which computes this integral to 120-digit accuracy, we precompute $b_{j,m}$ for $m = 1, 2, 4, 8, 16, \dots, 256$ and for j up to 300. During the quadrature computation, the function evaluation program picks m to be the first power of two greater than the argument x , and then applies formulas (22) and (25). It is not necessary to compute $f(x)$ for x larger than 200, since for these large arguments $|f(x)| < 10^{-120}$ and thus may be presumed to be zero.

The computation of values of the Riemann zeta-function can be done using a simple algorithm due to Peter Borwein [21] or, since what we really require is the entire set of values $\{\zeta(2j) : 1 \leq j \leq n\}$ for some n , by a convolution scheme described in [5]. It is important to note that the computation of both the zeta values and the $b_{j,m}$ must be done with a much higher working precision (in our program, we use 1600-digit precision) than the 120-digit precision required for the quadrature results, since the two terms being subtracted in formula (27) are very nearly equal. These values need to be calculated to a *relative* precision of 120 digits.

With this evaluation scheme for $f(x)$ in hand, the integral (22) can be computed using, for instance, the tanh-sinh quadrature algorithm, which can be implemented fairly easily on a personal computer or workstation and is also well suited to highly parallel processing [10],[11],[16, p. 312]. This algorithm approximates an integral $f(x)$ on $[-1, 1]$ by transforming it to an integral on $(-\infty, \infty)$ via the change of variable $x = g(t)$, where $g(t) = \tanh(\pi/2 \cdot \sinh t)$:

$$\int_{-1}^1 f(x) dx = \int_{-\infty}^{\infty} f(g(t))g'(t) dt = h \sum_{j=-\infty}^{\infty} w_j f(x_j) + E(h). \quad (28)$$

Here $x_j = g(hj)$ and $w_j = g'(hj)$ are abscissas and weights for the tanh-sinh quadrature scheme (which can be precomputed), and $E(h)$ is the error in this approximation.

The function $g'(t) = \pi/2 \cdot \cosh t \cdot \operatorname{sech}^2(\pi/2 \cdot \sinh t)$ and its derivatives tend to zero very rapidly for large $|t|$. Thus, even if the function $f(t)$ has an infinite derivative, a blow-up discontinuity, or oscillatory behavior at an endpoint, the product function $f(g(t))g'(t)$ is in many cases quite well behaved, going rapidly to zero (together with all of its derivatives) for large $|t|$. In such cases, the Euler-Maclaurin summation formula [2, p. 180] can be invoked to conclude that the error $E(h)$ in the approximation (28) decreases very rapidly—faster than any power of h . In many applications, the tanh-sinh algorithm achieves quadratic convergence (i.e., reducing the size h of the interval in half produces twice as many correct digits in the result).

The tanh-sinh quadrature algorithm is designed for a finite integration interval. In this problem, where the interval of integration is $[0, \infty)$, it is necessary to convert the integral to a problem on a finite interval. This can be done with the simple substitution $s = 1/(x + 1)$, which yields an integral from 0 to 1.

In spite of the substantial computation required to construct the zeta- and b -arrays, as well as the abscissas x_j and weights w_j needed for tanh-sinh quadrature, the entire calculation requires only about one minute on a 2004-era computer, using the ARPREC

arbitrary precision software package available at <http://crd.lbl.gov/~dhbailey/mpdist>. The first hundred digits of the result are the following:

0.392699081698724154807830422909937860524645434187231595926812285162
093247139938546179016512747455366777....

A *Mathematica* program capable of producing 100 digits of this constant is available on Michael Trott's website:

http://www.mathematicaguidebooks.org/downloads/N_2_01_Evaluated.nb.

Using the Inverse Symbolic Calculator, for instance, one finds that this constant is likely to be $\pi/8$. But a careful comparison with a high-precision value of $\pi/8$, namely,

0.392699081698724154807830422909937860524646174921888227621868074038
477050785776124828504353167764633497...,

reveals that they are *not* equal—the two values differ by approximately 7.407×10^{-43} . Indeed, these two values are provably distinct. This follows from the fact that

$$\sum_{n=1}^{55} 1/(2n+1) > 2 > \sum_{n=1}^{54} 1/(2n+1).$$

See [16, chap. 2] for additional details. We do not know a concise closed-form expression for this constant.

Further history and context. Recall the *sinc* function

$$\operatorname{sinc} x = \frac{\sin x}{x},$$

and consider, the seven highly oscillatory integrals:

$$\begin{aligned} I_1 &= \int_0^\infty \operatorname{sinc} x \, dx = \frac{\pi}{2}, \\ I_2 &= \int_0^\infty \operatorname{sinc} x \operatorname{sinc} \left(\frac{x}{3}\right) \, dx = \frac{\pi}{2}, \\ I_3 &= \int_0^\infty \operatorname{sinc} x \operatorname{sinc} \left(\frac{x}{3}\right) \operatorname{sinc} \left(\frac{x}{5}\right) \, dx = \frac{\pi}{2}, \\ &\vdots \\ I_6 &= \int_0^\infty \operatorname{sinc} x \operatorname{sinc} \left(\frac{x}{3}\right) \cdots \operatorname{sinc} \left(\frac{x}{11}\right) \, dx = \frac{\pi}{2}, \\ I_7 &= \int_0^\infty \operatorname{sinc} x \operatorname{sinc} \left(\frac{x}{3}\right) \cdots \operatorname{sinc} \left(\frac{x}{13}\right) \, dx = \frac{\pi}{2}. \end{aligned}$$

It comes as something of a surprise, therefore, that

$$\begin{aligned} I_8 &= \int_0^\infty \operatorname{sinc} x \operatorname{sinc} \left(\frac{x}{3}\right) \cdots \operatorname{sinc} \left(\frac{x}{15}\right) \, dx \\ &= \frac{467807924713440738696537864469}{935615849440640907310521750000} \pi \approx 0.49999999992646\pi. \end{aligned}$$

When this was first discovered by a researcher, using a well-known computer algebra package, both he and the software vendor concluded there was a “bug” in the software. Not so! It is fairly easy to see that the limit of the sequence of such integrals is $2\pi_1$. Our analysis, via Parseval’s theorem, links the integral

$$I_N = \int_0^\infty \operatorname{sinc}(a_1x) \operatorname{sinc}(a_2x) \cdots \operatorname{sinc}(a_Nx) dx$$

with the volume of the polyhedron P_N described by

$$P_N = \{x : |\sum_{k=2}^N a_k x_k| \leq a_1, |x_k| \leq 1, 2 \leq k \leq N\},$$

for $x = (x_2, x_3, \dots, x_N)$. If we let

$$C_N = \{(x_2, x_3, \dots, x_N) : -1 \leq x_k \leq 1, 2 \leq k \leq N\},$$

then

$$I_N = \frac{\pi \operatorname{Vol}(P_N)}{2a_1 \operatorname{Vol}(C_N)}.$$

Thus, the value drops precisely when the constraint $\sum_{k=2}^N a_k x_k \leq a_1$ becomes *active* and bites the hypercube C_N . That occurs when $\sum_{k=2}^N a_k > a_1$. In the foregoing,

$$\frac{1}{3} + \frac{1}{5} + \cdots + \frac{1}{13} < 1,$$

but on addition of the term $1/15$, the sum exceeds 1, the volume drops, and $I_N = \pi/2$ no longer holds. A similar analysis applies to π_2 . Moreover, it is fortunate that we began with π_1 or the falsehood of $\pi_2 = 1/8$ would have been much harder to see.

Additional information on this problem is available at <http://mathworld.wolfram.com/InfiniteCosineProductIntegral.html> and <http://mathworld.wolfram.com/BorweinIntegrals.html>.

10. A MULTIVARIATE ZETA-FUNCTION.

Problem 9. Calculate

$$\sum_{i>j>k>l>0} \frac{1}{i^3 j k^3 l}.$$

Extra credit: Express this constant as a single-term expression involving a well-known mathematical constant.

History and context. We resume the discussion from Problem 3. In the notation introduced there, we ask for the value of $\zeta(3, 1, 3, 1)$. The study of such sums in two variables, as we noted, originates with Euler. These investigations were apparently due to a serendipitous mistake. Goldbach wrote to Euler [15, pp. 99–100]:

When I recently considered further the indicated sums of the last two series in my previous letter, I realized immediately that the same series arose due to a mere writing error, from which indeed the saying goes, “Had one not erred, one would have achieved less [*Si non errasset, fecerat ille minus*].”

Euler’s *reduction formula* is

$$\zeta(s, 1) = \frac{s}{2} \zeta(s+1) - \frac{1}{2} \sum_{k=1}^{s-2} \zeta(k+1) \zeta(s+1-k),$$

which *reduces* the given double Euler sums to a sum of products of classical ζ -values. Euler also noted the first *reflection formulas*

$$\zeta(a, b) + \zeta(b, a) = \zeta(a) \zeta(b) - \zeta(a+b),$$

certainly valid when $a > 1$ and $b > 1$. This is an easy algebraic consequence of adding the double sums. Another marvelous fact is the *sum formula*

$$\sum_{\Sigma a_i = n, a_i \geq 0} \zeta(a_1 + 2, a_2 + 1, \dots, a_r + 1) = \zeta(n + r + 1) \quad (29)$$

for nonnegative integers n and r . This, as David Bradley observes, is equivalent to the generating function identity

$$\sum_{n > 0} \frac{1}{n^r (n-x)} = \sum_{k_1 > k_2 > \dots > k_r > 0} \prod_{j=1}^r \frac{1}{k_j - x}.$$

The first three nontrivial cases of (29) are $\zeta(3) = \zeta(2, 1)$, $\zeta(4) = \zeta(3, 1) + \zeta(2, 2)$, and $\zeta(2, 1, 1) = \zeta(4)$.

Solution. We notice that such a function is a generalization of the zeta-function. Similar to the definition in section 4, we define

$$\zeta(s_1, s_2, \dots, s_k; x) = \sum_{n_1 > n_2 > \dots > n_k > 0} \frac{x^n}{n_1^{s_1} n_2^{s_2} \dots n_r^{s_r}}, \quad (30)$$

for s_1, s_2, \dots, s_k nonnegative integers. We see that we are asked to compute $\zeta(3, 1, 3, 1; 1)$. Such a sum can be evaluated directly using the EZFace+ interface at

<http://www.cecm.sfu.ca/projects/ezface+>, which employs the Hölder convolution, giving us the numerical value

$$\begin{aligned} &0.005229569563530960100930652283899231589890420784634635522547448 \\ &97214886954466015007497545432485610401627 \dots \end{aligned} \quad (31)$$

Alternatively, we may proceed using differential equations. It is fairly easy to see [16, sec. 3.7] that

$$\frac{d}{dx} \zeta(n_1, n_2, \dots, n_r; x) = \frac{1}{x} \zeta(n_1 - 1, n_2, \dots, n_r; x), \quad (n_1 > 1), \quad (32)$$

$$\frac{d}{dx} \zeta(n_1, n_2, \dots, n_r; x) = \frac{1}{1-x} \zeta(n_2, \dots, n_r; x), \quad (n_1 = 1), \quad (33)$$

with initial conditions $\zeta(n_1; 0) = \zeta(n_1, n_2; 0) = \cdots = \zeta(n_1, \dots, n_r; 0) = 0$, and $\zeta(\cdot; x) \equiv 1$. Solving

```
> dsys1 =
> diff(y3131(x), x) = y2131(x)/x,
> diff(y2131(x), x) = y1131(x)/x,
> diff(y1131(x), x) = 1/(1-x)*y131(x),
> diff(y131(x), x) = 1/(1-x)*y31(x),
> diff(y31(x), x) = y21(x)/x,
> diff(y21(x), x) = y11(x)/x,
> diff(y11(x), x) = y1(x)/(1-x),
> diff(y1(x), x) = 1/(1-x);
> init1 = y3131(0) = 0, y2131(0) = 0, y1131(0) = 0,
> y131(0)=0, y31(0)=0, y21(0)=0, y11(0)=0, y1(0)=0;
```

in *Maple*, we obtain 0.005229569563518039612830536519667669502942 (this is valid to thirteen decimal places). Maple's `identify` command is unable to identify portions of *this* number, and the inverse symbolic calculator does not return a result. It should be mentioned that both *Maple* and the ISC identified the constant $\zeta(3, 1)$ (see the remark under the "history and context" heading). From the hint for this question, we know this is a single-term expression. Suspecting a form similar to $\zeta(3, 1)$, we search for constants c and d such that $\zeta(3, 1, 3, 1) = c\pi^d$. This leads to $c = 1/81440 = 2/10!$ and $d = 8$.

Further history and context. We start with the simpler value, $\zeta(3, 1)$. Notice that

$$-\log(1-x) = x + \frac{1}{2}x^2 + \frac{1}{3}x^3 + \cdots,$$

so

$$\begin{aligned} f(x) &= -\log(1-x)/(1-x) = x + \left(1 + \frac{1}{2}\right)x^2 + \left(1 + \frac{1}{2} + \frac{1}{3}\right)x^3 + \cdots \\ &= \sum_{n \geq m > 0} \frac{x^n}{m}. \end{aligned}$$

As noted in the section on double Euler sums,

$$\frac{(-1)^{m+1}}{\Gamma(m)} \int_0^1 x^n \log^{m-1} x \, dx = \frac{1}{(n+1)^m},$$

so integrating f using this transform for $m = 3$, we obtain

$$\begin{aligned} \zeta(3, 1) &= \frac{1}{2} \int_0^1 f(x) \log^2 x \, dx \\ &= 0.270580808427784547879000924 \dots \end{aligned}$$

The corresponding generating function is

$$\sum_{n \geq 0} \zeta(\{3, 1\}_n) x^{4n} = \frac{\cosh(\pi x) - \cos(\pi x)}{\pi^2 x^2},$$

equivalent to Zagier's conjectured identity

$$\zeta(\{3, 1\}_n) = \frac{2\pi^{4n}}{(4n+2)}.$$

Here $\{3, 1\}_n$ denotes n -fold concatenation of $\{3, 1\}$.

The proof of this identity (see [16, p. 160]) derives from a remarkable factorization of the generating function in terms of hypergeometric functions:

$$\sum_{n \geq 0} \zeta(\{3, 1\}_n) x^{4n} = {}_2F_1\left(x\frac{(1+i)}{2}, -x\frac{(1+i)}{2}; 1; 1\right) {}_2F_1\left(x\frac{(1-i)}{2}, -x\frac{(1-i)}{2}; 1; 1\right).$$

Finally, it can be shown in various ways that

$$\zeta(\{3\}_n) = \zeta(\{2, 1\}_n)$$

for all n , while a proof of the numerically-confirmed conjecture

$$\zeta(\{2, 1\}_n) \stackrel{?}{=} 2^{3n} \zeta(\{-2, 1\}_n) \tag{34}$$

remains elusive. Only the first case of (34), namely,

$$\sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{m=1}^{n-1} \frac{1}{m} = 8 \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \sum_{m=1}^{n-1} \frac{1}{m} \quad (= \zeta(3))$$

has a self-contained proof [16]. Indeed, the only other established case is

$$\sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{m=1}^{n-1} \frac{1}{m} \sum_{p=1}^{m-1} \frac{1}{p^2} \sum_{q=1}^{p-1} \frac{1}{q} = 64 \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \sum_{m=1}^{n-1} \frac{1}{m} \sum_{p=1}^{m-1} \frac{(-1)^p}{p^2} \sum_{q=1}^{p-1} \frac{1}{q} \quad (= \zeta(3, 3)).$$

This is an outcome of a complete set of equations for multivariate zeta functions of depth four.

There has been abundant evidence amassed to support identity (34) since it was found in 1996. For example, very recently Petr Lisonek checked the first eighty-five cases to one thousand places in about forty-one hours with only the *expected roundoff error*. And he checked $n = 163$ in ten hours. This is the *only* identification of its type of an Euler sum with a distinct multivariate zeta-function.

11. A WATSON INTEGRAL.

Problem 10. *Evaluate*

$$W = \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{1}{3 - \cos x - \cos y - \cos z} dx dy dz. \tag{35}$$

History and context. The integral arises in Gaussian and spherical models of ferromagnetism and in the theory of random walks. It leads to one of the most impressive closed-form evaluations of an equivalent multiple integral due to G. N. Watson:

$$\begin{aligned}\widehat{W} &= \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{1}{3 - \cos x - \cos y - \cos z} dx dy dz \\ &= \frac{1}{96} (\sqrt{3} - 1) \Gamma^2\left(\frac{1}{24}\right) \Gamma^2\left(\frac{11}{24}\right) \\ &= 4\pi \left(18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6}\right) K^2(k_6),\end{aligned}\tag{36}$$

where $k_6 = (2 - \sqrt{3})(\sqrt{3} - \sqrt{2})$ is the sixth singular value. The most self-contained derivation of this very subtle result is due to Joyce and Zucker in [28] and [29], where more background can also be found.

Solution. In [31], it is shown that a simplification can be obtained by applying the formula

$$\frac{1}{\lambda} = \int_0^{\infty} e^{-\lambda t} dt \quad (\operatorname{Re}\lambda > 0)\tag{37}$$

to W_3 . The three-dimension integral is then reducible to a single integral by using the identity

$$\frac{1}{\pi} \int_0^{\infty} \exp(t \cos \theta) d\theta = I_0(t),\tag{38}$$

in which $I_0(t)$ is the modified Bessel function of the first kind. It follows from this that $W = \int_0^{\infty} \exp(-3t) I_0^3(t) dt$. This integral can be evaluated to one hundred digits in *Maple*, giving

$$\begin{aligned}W_3 &= 0.50546201971732600605200405322714025998512901481742089 \\ &\quad 21889934878860287734511738168005372470698960380 \dots\end{aligned}\tag{39}$$

Finally, an integer relation hunt to express $\log W$ in terms of $\log \pi$, $\log 2$, $\log \Gamma(k/24)$, and $\log(\sqrt{3} - 1)$ will produce (36).

We may also write W_3 as a product solely of values of the gamma function. This is what our *Mathematician's Toolkit* returned:

$$\begin{aligned}0 = & -1.*\log[w3] + -1.*\log[\text{gamma}[1/24]] + 4.*\log[\text{gamma}[3/24]] + \\ & -8.*\log[\text{gamma}[5/24]] + 1.*\log[\text{gamma}[7/24]] + 14.*\log[\text{gamma}[9/24]] + \\ & -6.*\log[\text{gamma}[11/24]] + -9.*\log[\text{gamma}[13/24]] + 18.*\log[\text{gamma}[15/24]] + \\ & -2.*\log[\text{gamma}[17/24]] + -7.*\log[\text{gamma}[19/24]]\end{aligned}$$

Proving this is achieved by comparing the result with (36) and establishing the implicit gamma representation of $(\sqrt{3} - 1)^2/96$.

Similar searches suggest there is no similar four-dimensional closed form—the relevant Bessel integral is $W_4 = \int_0^\infty \exp(-4t)I_0^4(t) dt$. (N.B. $\int_0^\infty \exp(-2t)I_0^2(t) dt = \infty$.) In this case it is necessary to compute $\exp(-t)I_0(t)$ carefully, using a combination of the formula

$$\exp(-t)I_0(t) = \exp(-t) \sum_{n=0}^{\infty} \frac{t^{2n}}{2^{2n}(n!)^2}$$

for t up to roughly $1.2 \cdot d$, where d is the number of significant digits desired for the result, and

$$\exp(-t)I_0(t) \approx \frac{1}{\sqrt{2\pi t}} \sum_{n=0}^N \frac{\prod_{k=1}^n (2k-1)^2}{(8t)^n n!}$$

for large t , where the upper limit N of the summation is chosen to be the first index n such that the summand is less than 10^{-d} (since this is an asymptotic expansion, taking more terms than N may increase, not decrease the error). We have implemented this as ‘bessel-exp’ in our *Mathematician’s Toolkit*, available at <http://crd.lbl.gov/~dhbailey/mpdist>. Using this software, which includes a PSLQ facility, we found that W_4 is not expressible as a product of powers of $\Gamma(k/120)$ ($0 < k < 120$) with coefficients having fewer than 80 digits. This result does not, of course, rule out the possibility of a larger relation, but it does cast some doubt, in an experimental sense, that such a relation exists. Enough to stop looking.

Additional information on this problem is available at <http://mathworld.wolfram.com/WatsonsTripleIntegrals.html>.

12. CONCLUSION. While all the problems described herein were studied with a great deal of experimental computation, clean proofs are known for the final results given (except for Problem 7), and in most cases a lot more has by now been proved. Nonetheless, in each case the underlying object suggests plausible generalizations that are still open.

The “hybrid computations” involved in these solutions are quite typical of modern experimental mathematics. Numerical computations by themselves produce no insight, and symbolic computations frequently fail to produce full-fledged, closed-form solutions. But when used together, with significant human interaction, they are often successful in discovering new facts of mathematics and in suggesting routes to formal proof.

ACKNOWLEDGMENTS. Bailey’s work was supported by the Director, Office of Computational and Technology Research, Division of Mathematical, Information, and Computational Sciences of the U.S. Department of Energy, under contract number DE-AC02-05CH11231; also by the NSF, under Grant DMS-0342255. Borwein’s work was supported in part by NSERC and the Canada Research Chair Programme. Kapoor’s work was performed as part of an independent study project at the University of British Columbia. Weisstein’s work on *MathWorld* is supported by Wolfram Research as a free service to the world mathematics and Internet communities.

References

- [1] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions*, Dover, New York, 1970.

- [2] K. E. Atkinson, *An Introduction to Numerical Analysis*, John Wiley & Sons, New York, 1989.
- [3] D. H. Bailey, Integer relation detection, *Comp. Sci. & Eng.* **2** (2000) 24–28.
- [4] D. H. Bailey and J. M. Borwein, Sample problems of experimental mathematics (2003), available at <http://www.experimentalmath.info/expmath-probs.pdf>.
- [5] D. H. Bailey, J. M. Borwein, and R. E. Crandall, On the Khintchine constant, *Math. Comp.* **66** (1997) 417–431.
- [6] D. H. Bailey, P. B. Borwein, and S. Plouffe, On the rapid computation of various polylogarithmic constants, *Math. Comp.* **66** (1997) 903–913.
- [7] D. H. Bailey and D. J. Broadhurst, Parallel integer relation detection: Techniques and applications, *Math. Comp.* **70** (2000) 1719–1736.
- [8] D. H. Bailey and R. E. Crandall, On the random character of fundamental constant expansions, *Experiment. Math.* **10** (2001) 175–190.
- [9] _____, Random generators and normal numbers, *Experiment. Math.* **11** (2002) 527–546.
- [10] D. H. Bailey, X. S. Li and K. Jeyabalan, A comparison of three high-precision quadrature schemes, *Experiment. Math.* **14** (2005) 317–329.
- [11] D. H. Bailey and J. M. Borwein, Highly parallel, high-precision numerical integration (2004), available at <http://crd.lbl.gov/~dhbailey/dhbpapers/quadparallel.pdf>.
- [12] F. Bornemann, D. Laurie, S. Wagon, and J. Waldvogel, *The SIAM 100 Digit Challenge: A Study in High-Accuracy Numerical Computing*, SIAM, Philadelphia, 2004.
- [13] J. M. Borwein, The 100 digit challenge: An extended review, *Math Intelligencer* **27** (2005) 40–48.
- [14] J. M. Borwein and D. J. Broadhurst, Determinations of rational Dedekind-zeta invariants of hyperbolic manifolds and Feynman knots and links (1998), available at <http://arxiv.org/abs/hep-th/9811173>.
- [15] J. M. Borwein and D. H. Bailey, *Mathematics by Experiment*, A K Peters, Natick, MA, 2004.
- [16] J. M. Borwein, D. H. Bailey, and R. Girgensohn, *Experimentation in Mathematics: Computational Paths to Discovery*, A K Peters, Natick, MA, 2004.
- [17] J. Borwein and R. Crandall, On the Ramanujan AGM fraction. Part II: The complex-parameter case, *Experiment. Math.* **13** (2004) 287–295.
- [18] J. Borwein, R. Crandall, and Greg Fee, On the Ramanujan AGM fraction. Part I: The real-parameter case, *Experiment. Math.* **13** (2004) 275–285.

- [19] J. M. Borwein and P. B. Borwein, *Pi and the AGM*, Canadian Mathematical Society Series of Monographs and Advanced Texts, no. 4, John Wiley & Sons, New York, 1998.
- [20] J. M. Borwein, D. M. Bradley, D. J. Broadhurst, and P. Lisoněk, Special values of multiple polylogarithms, *Trans. Amer. Math. Soc.* **353** (2001) 907–941.
- [21] P. Borwein, An Efficient Algorithm for the Riemann zeta function (1995), available at <http://www.cecm.sfu.ca/personal/pborwein/PAPERS/P155.pdf>.
- [22] R. E. Crandall, *Topics in Advanced Scientific Computation*, Springer-Verlag, New York, 1996.
- [23] R. E. Crandall, New representations for the Madelung constant, *Experiment. Math.* **8** (1999) 367–379.
- [24] R. E. Crandall and J. P. Buhler, Elementary function expansions for Madelung constants, *J. Phys. A* **20** (1987) 5497–5510.
- [25] H. R. P. Ferguson, D. H. Bailey, and S. Arno, Analysis of PSLQ, an integer relation finding algorithm, *Mathematics of Computation* **68** (1999) 351–369.
- [26] James Gleick, *Chaos: The Making of a New Science*, Penguin Books, New York, 1987.
- [27] Julian Havel, *Gamma: Exploring Euler's Constant*, Princeton University Press, Princeton, 2003.
- [28] G. S. Joyce and I. J. Zucker, Evaluation of the Watson integral and associated logarithmic integral for the d -dimensional hypercubic lattice, *J. Phys. A* **34** (2001) 7349–7354.
- [29] _____, On the evaluation of generalized Watson integrals, *Proc. Amer. Math. Soc.* **133** (2005) 71–81.
- [30] I. Kotsireas and K. Karamanos, Exact computation of the bifurcation point B_4 of the logistic map and the Bailey-Broadhurst conjectures, *Intl. J. Bifurcation and Chaos* **14** (2004) 2417–2423.
- [31] A. A. Maradudin, E. W. Montroll, G. H. Weiss, R. Herman, and H. W. Milnes, *Green's Functions for Monatomic Simple Cubic Lattices*, Academie Royale de Belgique, Memories XIV, **7** (1960).
- [32] D. Shanks and J. W. Wrench Jr., Khintchine's constant, *Amer. Math. Monthly* **66** (1959) 276–279.
- [33] S. H. Strogatz, *Nonlinear Dynamics and Chaos: With Applications to Physics, Biology, Chemistry and Engineering*, Perseus Book Group, Philadelphia, 2001.
- [34] A. Vaught, personal communication (2004).
- [35] S. Wolfram, *A New Kind of Science*, Wolfram Media, Champaign, IL, 2002.

DAVID H. BAILEY received his B.S. at Brigham Young University and received his Ph.D. (1976) from Stanford University. He worked for the Department of Defense and for SRI International, before spending fourteen years at NASA's Ames Research Center in California. Since 1997 he has been the chief technologist of the Computational Research Department at the Lawrence Berkeley National Laboratory. In 1993, he was a corecipient of the Chauvenet Prize from the MAA, and in that year was also awarded the Sidney Fernbach Award from the IEEE Computer Society. His research spans computational mathematics and high-performance computing. He is the author (with Jonathan Borwein and, for volume two, Roland Girgensohn) of two recent books on experimental mathematics.

Lawrence Berkeley National Laboratory, Berkeley, CA 94720
dhbailey@lbl.gov

JONATHAN M. BORWEIN received his DPhil from Oxford (1974) as a Rhodes Scholar. He taught at Dalhousie, Carnegie-Mellon, and Waterloo, before becoming the Shrum Professor of Science and a Canada Research Chair in Information Technology at Simon Fraser University. At SFU he was founding director of the Centre for Experimental and Constructive Mathematics. In 2004, he rejoined Dalhousie University in the Faculty of Computer Science. Jonathan has received several awards, including the 1993 Chauvenet Prize of the MAA, Fellowship in the Royal Society of Canada, and Fellowship in the American Association for the Advancement of Science. His research spans computational number theory and optimization theory, as well as numerous topics in computer science. He is the author of ten books, and is cofounder of Math Resources, Inc., an educational software firm.

Faculty of Computer Science, Dalhousie University, Halifax, NS, B3H 2W5
jmborwein@cs.dal.ca

VISHAAL KAPOOR graduated from Simon Fraser University with a B.S. degree in mathematics and is currently completing his M.S. at the University of British Columbia under the supervision of Greg Martin.

Department of Mathematics, University of BC, Vancouver, BC, V6T 1Z2
vkapoor@math.ubc.ca

ERIC W. WEISSTEIN graduated from Cornell University, with a B.A. degree in physics, and from the California Institute of Technology (M.S., 1993; Ph.D., 1996) with degrees in planetary astronomy. Upon completion of his doctoral thesis, Weisstein became a research scientist in the Department of Astronomy at the University of Virginia in Charlottesville. Since 1999 he has been a member of the Scientific Information group at Wolfram Research, where he holds the official title "Encyclopedist." Eric is best known as the author of the *MathWorld* website (<http://mathworld.wolfram.com>), an online compendium of mathematical knowledge, as well as the author of the *CRC Concise Encyclopedia of Mathematics*.

Wolfram Research Inc., Champaign, IL 61820
eww@wolfram.com