When Is 0.999 . . . Equal to 1?

Robin Pemantle and Carsten Schneider

1. INTRODUCTION. The three ellipsis points in the title do not refer to an infinite sequence of 9s but to digits that are increasingly hard to compute. The question is philosophical: How many 9s do we need to see before we start to believe that the constant we are computing is probably equal to 1? In our case, the constant was given by the infinite sum

$$S := \sum_{j,k=1}^{\infty} \frac{H_j(H_{k+1} - 1)}{jk(k+1)(j+k)}, \tag{1}$$

where $H_j := \sum_{i=1}^{j}(1/i)$ are the harmonic numbers.

This question in the title is beyond the scope of a mathematics journal. There are, however, mathematical papers proving identities that were discovered because numerical computation pointed to a simple answer. The anecdotal evidence then accumulates in a misleading manner: when the conjectured identity is false we are less likely ever to know. One purpose of the present note is to document a case in which we were able to evaluate the constant and it turned out not to equal the simple guess (in this case, 1). In fact we will prove:

Theorem 1. *The sum S in* (1) *is given by*

$$S = -4\zeta(2) - 2\zeta(3) + 4\zeta(2)\zeta(3) + 2\zeta(5) = 0.999222\ldots, \tag{2}$$

where $\zeta(n) = \sum_{i=1}^{\infty} i^{-n}$ denotes the Riemann zeta-function.

The second purpose of this note is to demonstrate a piece of software that, with a little human intervention, can find (and prove) this sort of identity.

2. BACKGROUND. The sum (1) arose in a paper giving bounds on the run time of the simplex algorithm on a polytope known as a Klee-Minty cube [**1**]. The Klee-Minty cube is an example of great theoretical importance to analyses of simplex algorithm run times. The derivation of the expression (1) is, however, of no importance here, because S appears in [**1**] only as an upper bound, demonstrably not sharp, for the leading coefficient c of the expected run time. The numerology of S is therefore unrelated to the physical origins of c.

On the other hand, the form of the summation (1) does lead one at least to hope that an exact value might be derived. In principle, any hypergeometric identity, for example, that holds for a finite indefinite or definite sum may be automatically proved via the Wilf-Zeilberger method [**9**], and in fact implementations of WZ-type software often can handle summand expressions of the complexity of (1). Furthermore, in many cases the WZ-machinery will not only prove but also find such an identity, if it exists, given only the left-hand side. This, in general, does not extend to summations over summands involving no extra parameter: if S were to equal 1, that fact would not necessarily be automatically detectable. The relatively simple form of the summand, however, gave us hope that summation tricks more specific to harmonic series might unlock the problem (the identity $\sum 1/(n(n+1)) = 1$ stands as a beacon of hope). Indeed, several telescoping and resummation tricks were initially tried, removing all but one infinite summation in various ways. These identities were useful in improving our numerical bounds on S.

The numerical bounds we had on S were not all that good. It should be noted that the harmonic numbers are themselves sums, so the expression (1) is really a quadruple sum. This makes it perhaps less surprising that our best rigorous bounds were no closer than 10^{-3}. To make a long story short, summing in one variable, then using exact values for thousands of row and column sums and an integral approximation for the remaining terms, led to our best rigorous bounds, namely,

$$0.999197 \le S \le 1.00093.$$

At this point, although the exact value of S was of no use to us, we felt embarrassed to publish numerical bounds on a constant that we suspected was equal to 1. The authors of [**1**] then consulted the experts in harmonic summation, who consulted their computers, and came up with Theorem 1. Later a computer-free proof was given in [**8**]. The remainder of this note proves Theorem 1.

3. SOLVING THE PROBLEM. If a sum such as (1) has a nice value, it does not necessarily follow that a truncated version of the sum has a nice formula. But, if it has a nice closed form, automatic methods might succeed in finding it by first computing a recurrence and afterwards searching for solutions of the recurrence in which the closed form can be represented. Thus we consider a truncated version of the sum, namely,

$$S(a,b) = \sum_{k=1}^{b} \frac{H_{k+1}-1}{k(k+1)} \sum_{j=1}^{a} \frac{H_j}{j(j+k)},$$

that is, the upper limits, instead of being infinite, are taken to be integer variables a and b. In this case, our optimism is rewarded: we are able to simplify the inner sum so that we can sum a second time, provided that we make some alterations that disappear when the upper limit goes to infinity.

The inner sum. In a first step we compute a closed form evaluation of the inner sum

$$h(a,k) := \sum_{j=1}^{a} f(k,j)$$

with $f(k,j) := \frac{H_j}{j(j+k)}$. Here we follow the summation principles given in [**10**] that are inspired by [**9**]. Note that all the computations are carried out with the summation package Sigma in the computer algebra system Mathematica. The role of the computer here is to produce equations that we can then rapidly and rigorously verify.

Our first step is to compute for the definite sum $h(a,k)$ the recurrence relation

$$\begin{aligned} k^2\, h(a,k) - (k+1)(2k+1)\, h(a,k+1) \\ + (k+1)(k+2)\, h(a,k+2) = \frac{a(a+k+2)-(a+1)(k+1)H_a}{(k+1)(a+k+1)(a+k+2)} \end{aligned} \tag{3}$$

with a variation of Zeilberger's creative telescoping trick. The way we find this is to guess that there is some r, some constants $c_0, \dots, c_r$ depending on k but not j, and some function $g(k, j)$, which we assume to have a relatively simple form, such that a relation

$$\sum_{s=0}^{r} c_s f(k+s, j) = g(k, j+1) - g(k, j)$$

holds for all k and j. We ask Sigma to find such a relation for various classes of functions g and for $r = 1, 2, \dots,$ until we achieve success with $r = 2$, $c_0(k) = k^2$, $c_1(k) = -(k+1)(2k+1)$, $c_2(k) = (k+1)(k+2)$, and

$$g(k, j) = -\frac{jH_j + k + j}{(k+j)(k+j+1)}.$$

We can then verify the relation

$$c_0(k) f(k, j) + c_1(k) f(k+1, j) + c_2(k) f(k+2, j) = g(k, j+1) - g(k, j) \quad (4)$$

by polynomial arithmetic and by using the relation $H_{j+1} = H_j + 1/(j+1)$. Summing (4) over k in the interval $\{1, \dots, a\}$ proves (3).

Next we are in the position to discover and prove that

$$h(a, k) = \frac{kH_k^2 - 2H_k + kH_k^{(2)} + 2kH_a^{(2)}}{2k^2} - \frac{(kH_a - 1)}{k^2} \sum_{i=1}^{k} \frac{1}{a+i} - \frac{1}{k} \sum_{i=1}^{k} \frac{1}{i} \sum_{j=1}^{i} \frac{1}{a+j} \quad (5)$$

holds for all positive integers a and k. Here the $H_k^{(r)} = \sum_{i=1}^{k} i^{-r}$ denote the *generalized harmonic numbers*. We do this by asking Sigma to find solutions to (3) for all k and then to plug in the initial conditions, which in this case are to match the values of $h(a, k)$ for $k = 1, 2$ (see [**10**] for further details). Once Sigma has found the expression on the right-hand side of (5), it is again a finite exercise in polynomial arithmetic to verify that it satisfies (3) and that it satisfies the two initial conditions. Since r initial conditions uniquely determine the solution, we have established (5).

Some terms vanish in the limit. At some point, if we do not winnow out some terms that disappear in the limit, our computer will begin to balk. Luckily it is easy to identify certain terms that contribute $o(1)$ to the definite sum as a and b go to infinity and can therefore be ignored in the evaluation of S. We have, for example, the elementary estimates

$$\lim_{a\to\infty} \frac{1}{k^2} \sum_{i=1}^{k} \frac{1}{a+i} = 0, \quad \lim_{a\to\infty} \frac{H_a}{k} \sum_{i=1}^{k} \frac{1}{a+i} = 0, \quad \lim_{a\to\infty} \frac{1}{k} \sum_{i=1}^{k} \frac{1}{i} \sum_{j=1}^{i} \frac{1}{a+j} = 0. \quad (6)$$

Hence, if

$$S'(a, b) := \sum_{k=1}^{b} \frac{H_{k+1} - 1}{k(k+1)} \frac{kH_k^2 - 2H_k + kH_k^{(2)} + 2kH_a^{(2)}}{2k^2}, \quad (7)$$

we have

$$\lim_{a,b\to\infty} S'(a,b) = S$$

by (5) and (6). To summarize: problem (2) reduces to the problem of discovering and then proving the identity

$$\lim_{a,b\to\infty} S'(a,b) = -4\zeta(2) - 2\zeta(3) + 4\zeta(2)\zeta(3) + 2\zeta(5). \tag{8}$$

The outer sum. Our next step is guided by the fact that we know a few infinite sums in which the nth summand is of the form n^{-c} times a monomial in the harmonic and generalized harmonic numbers H_n and $H_n^{(p)}$. While we cannot solve the general problem of summing all such univariate series, it makes sense to attempt to manipulate things into this form. Thus we ask Sigma to try to write the summand of the right-hand side of (7) in the form $g(a,k) - g(a,k-1)$, where the only infinite sums that appear in g are of the form described earlier. The program obligingly produces the function $g(a,k) = A(a,k) + B(a,k) + C(a,k)$, where A, B, and C are given by

$$\begin{aligned} A(a,b) = {} & \frac{1}{2(b+1)^2}\Big(6H_b + 4bH_b + 4H_b^2 + 3bH_b^2 + H_b^3 + bH_b^3 - 6bH_a^{(2)} \\ & + 2H_bH_a^{(2)} + 2bH_bH_a^{(2)} - 2H_b^{(2)} - 7bH_b^{(2)} + H_bH_b^{(2)} + bH_bH_b^{(2)}\Big), \end{aligned} \tag{9}$$

$$B(a,b) = -\frac{2b^2}{(b+1)^2}\Big(H_a^{(2)} + H_b^{(2)}\Big) \tag{10}$$

and

$$C(a,b) = (H_a^{(2)} - 1)\sum_{i=1}^{b}\frac{H_i}{i^2} - \sum_{i=1}^{b}\frac{H_i^2}{i^3} + \frac{1}{2}\sum_{i=1}^{b}\frac{H_i^3}{i^2} + \frac{1}{2}\sum_{i=1}^{b}\frac{H_iH_i^{(2)}}{i^2}. \tag{11}$$

This time the correctness of the result supplied by Sigma is verified by polynomial arithmetic and the definition of H_k without need to appeal to any uniqueness results for solutions to recurrences. Summing the relation

$$g(a,k) - g(a,k-1) = \frac{H_{k+1} - 1}{k(k+1)}\,\frac{kH_k^2 - 2H_k + kH_k^{(2)} + 2kH_a^{(2)}}{2k^2}$$

over k in the interval $\{1, \ldots, b\}$ proves that

$$S'(a,b) = A(a,b) + B(a,b) + C(a,b), \tag{12}$$

where A, B, and C are as in (9)–(11).

Euler sums and multiple ζ-values. Now we must make good on our supposition that the form of $g(a,k)$ leads to sums we can evaluate in terms of the zeta-function. The limits of $A(a,b)$ and $B(a,b)$ are obvious:

$$\lim_{a,b\to\infty} A(a,b) = 0, \qquad \lim_{a,b\to\infty} B(a,b) = -4\zeta(2). \tag{13}$$

The sums in $C(a, b)$ are handled in two steps, the first being to reduce them to multiple ζ-values, which can be done for any Euler sum.

The *Euler sum* of index $(p_1 \le \cdots \le p_k; q)$, named after [**4**] (see also [**2**]), is defined by

$$S_{p_1,\dots,p_k;q} = \sum_{n=1}^{\infty} \frac{H_n^{(p_1)} H_n^{(p_2)} \cdots H_n^{(p_k)}}{n^q}. \tag{14}$$

Repeated indices $p_i = p_{i+1}$ are allowed, so the summand may have powers of generalized harmonic numbers in the numerator. Each of the summands in $C := \lim_{a,b\to\infty} C(a, b)$ is an Euler sum. Define the *multiple ζ-values* by

$$\zeta(a_1, \dots, a_k) = \sum_{n_1 > \cdots > n_k} \frac{1}{n_1^{a_1} \cdots n_k^{a_k}}.$$

The number k is called the *multiplicity* of the multiple ζ-value and $a_1 + \cdots + a_k$ is known as its *weight*. The numbers $a_1, \dots, a_k$ need not be increasing, but it is required that $a_1 \ge 2$, because this is the condition for the sum to be finite.

One may expand each $H_n^{(p_j)}$ of (14), and in this way the general Euler sum becomes the sum of $j_1^{-p_1} \cdots j_k^{-p_k} n^{-q}$ over all $(k+1)$-tuples satisfying $n \ge j_1, \dots, j_k$. Decomposing according to the set of distinct values among $j_1, \dots, j_k, n$ produces an expression for $S_{p_1,\dots,p_k;q}$ that is a linear combination of multiple ζ-values with weight $q + p_1 + \cdots + p_k$ and multiplicity at most $k+1$. In the same way, one sees that any product of Euler sums or multiple ζ-values is itself a linear combination of multiple ζ-values.

To illustrate, these ideas, we write C as a sum of products of Euler sums and then change these term-by-term into multiple ζ-values. From the definitions,

$$C = S_{\emptyset;2} S_{1;2} - S_{1;2} - S_{1,1;3} + \frac{1}{2} S_{1,1,1;2} + \frac{1}{2} S_{1,2;2}.$$

Of course $S_{\emptyset;2} = \zeta(2)$. Next,

$$S_{1;2} = \sum_{n \ge j \ge 1} n^{-2} j^{-1} = \sum_{n \ge 1} n^{-3} + \sum_{n > j \ge 1} n^{-2} j^{-1} = \zeta(3) + \zeta(2, 1).$$

The remaining values are

$$\begin{aligned} S_{1,1;3} &= 2\zeta(3, 1, 1) + \zeta(3, 2) + 2\zeta(4, 1) + \zeta(5), \\ S_{1,1,1;2} &= 6\zeta(2, 1, 1, 1) + 3\zeta(2, 2, 1) + 3\zeta(2, 1, 2) \\ &\quad + 6\zeta(3, 1, 1) + 3\zeta(3, 2) + 3\zeta(4, 1) + \zeta(5), \\ S_{1,2;2} &= \zeta(2, 2, 1) + \zeta(2, 1, 2) + \zeta(3, 2) + \zeta(4, 1) + \zeta(5). \end{aligned}$$

These are derived in the same way as $S_{1;2}$. For example,

$$S_{1,1;3} = \sum_{n \ge j, k \ge 1} n^{-3} j^{-1} k^{-1},$$

where the triples decompose into $n = j = k$, $n = j \geq k$, $n = k \geq j$, $n > j = k$, $n > j > k$, and $n > k > j$. Putting this all together gives

$$C = (\zeta(2) - 1)(\zeta(3) + \zeta(2, 1)) + \zeta(3, 1, 1) + \zeta(3, 2) + 3\zeta(2, 1, 1, 1) \\ + 2\zeta(2, 2, 1) + 2\zeta(2, 1, 2) + \zeta(2, 3). \tag{15}$$

The decomposition of products of ζ-values and multiple ζ-values into linear combinations of multiple ζ-values is entirely analogous. For instance,

$$\zeta(2)\zeta(3) = \zeta(2, 3) + \zeta(3, 2) + \zeta(5). \tag{16}$$

Reducing to ordinary ζ-values. Theorem 1 indicates that reduction to single ζ-values is possible. This is worthwhile, because the single ζ-values may be more easily and accurately obtained than multiple ζ-values. For example, Maple computes five-hundred digits of $\zeta(5)$ in under ten seconds.

As it happens, some Euler sums and multiple ζ-values can be represented as sums of products of single ζ-values. Others, it appears, cannot, though this is not proved and no algorithm is known for determining which Euler sums or which multiple ζ-values can be represented in this way. For large k the number of $\mathbb{Q}$-linearly independent multiple ζ-values of weight k is conjectured by Zagier to grow like 1.32^k [**5**, p.17], which outstrips the dimension $e^{O(\sqrt{k})}$ of the monomials $\zeta(k_1) \cdots \zeta(k_m)$ in single ζ-values of total degree $k = k_1 + \cdots + k_m$. However, when $k = 3, 4, 5, 6, 7$, or 9 the dimensions are known to be equal, hence every multiple ζ-value of these weights is a polynomial over $\mathbb{Q}$ in single ζ-values.

Among the known relations, two classes suffice for our problem, namely, the sum and duality relations. The sum relation of degree k says that the sum of all multiple ζ-values of fixed multiplicity m and weight k is equal to $\zeta(k)$. For $k = 3, 5$ and $m = 2$, these are

$$\zeta(3) = \zeta(2, 1), \qquad \zeta(5) = \zeta(4, 1) + \zeta(3, 2) + \zeta(2, 3).$$

The sum relations were conjectured by Moen [**7**, sec. 3], known in special cases to Euler [**4**], and proved by Granville [**6**].

Second, one has the duality theorem, conjectured by Hoffman [**7**] and proved by Zagier [**11**]. These imply equality between $\zeta(p_1, \ldots, p_k)$ and $\zeta(q_1, \ldots, q_l)$ of equal weights when the index sequences are related by an operation akin to transposing a partition. The exact definition is given, for example, in [**5**, p. 29], but all we need to do here is to represent the multiple ζ-values of weight five and multiplicities three and four in terms of those of multiplicity two:

$$\begin{aligned} \zeta(2, 2, 1) &= \zeta(3, 2), \\ \zeta(2, 1, 2) &= \zeta(2, 3), \\ \zeta(3, 1, 1) &= \zeta(4, 1), \\ \zeta(2, 1, 1, 1) &= \zeta(5). \end{aligned}$$

Using the duality relations to eliminate all terms of multiplicity greater than two from (15) and then using (16) gives

$$C = (\zeta(2) - 1)(\zeta(3) + \zeta(2, 1)) + \zeta(4, 1) + 3\zeta(2)\zeta(3).$$

The sum relations now yield

$$C = 4\zeta(2)\zeta(3) - 2\zeta(3) + 2\zeta(5),$$

which finishes the proof of Theorem 1.

We remark that one more relation is needed to reduce all multiple ζ-values of weight five to polynomials in single ζ-values, namely,

$$\zeta(3, 2) = 3\zeta(2)\zeta(3) - \frac{11}{2}\zeta(5), \tag{17}$$

but that our expression for C can be simplified in terms of single ζ-values without (17). This identity (17) can be produced by a formula in [**3**] that can transform any double ζ-value with odd weight to a polynomial in single ζ-values.

ACKNOWLEDGMENTS. The authors are grateful to Doron Zeilberger for routing the problem from its originator to Sigma and Sigma's human operator. The reduction of the Euler sum to the form in the conclusion of Theorem 1 was accomplished in a very ad hoc manner in a previous draft, and we are indebted to an anonymous referee for leading us to the Euler sum literature and elucidating the more methodical approach taken in the present manuscript.

The first author was supported in part by NSF grant DMS-0103635 and by a Research Experiences for Undergraduates supplement from NSF. The second author was supported by the SFB-grant F1305 of the Austrian FWF and by grant P16613-N12 of the Austrian FWF.

REFERENCES

1. J. Balogh and R. Pemantle, The Klee-Minty random edge chain moves with linear speed (2006, preprint).
2. B. Berndt, *Ramanujan's Notebooks, I*, Springer-Verlag, New York, 1985.
3. D. Borwein, J. M. Borwein, and R. Girgensohn, Explicit evaluation of Euler sums, *Proc. Edinb. Math. Soc. (2)* **38** (1995) 277–294.
4. L. Euler, Meditationes circa singulare serierum genus, in *Opera Omnia*, ser. I, vol. 15. B. G. Teubner, Berlin, 1927, pp. 217–267.
5. P. Flajolet and B. Salvy, Euler sums and contour integral representations, *Experimental Math.* **7** (1998) 15–35.
6. A. Granville, A decomposition of Riemann's zeta-function, in *Analytic Number Theory*, London Mathematical Society Lecture Note Series, no. 247, Y. Motohashi, ed., Cambridge University Press, Cambridge, 1997, pp. 95–101.
7. M. Hoffman, Multiple harmonic series, *Pacific J. Math.* **152** (1992) 275–290.
8. A. Panholzer and H. Prodinger. Computer-free evaluation of an infinite double sum, *Sém. Lothar. Combin.* **55** (2005) 1–3.
9. M. Petkovšek, H. S. Wilf, and D. Zeilberger, $A = B$, A K Peters, Wellesley, MA, 1996.
10. C. Schneider, The summation package Sigma: Underlying principles and a rhombus tiling application, *Discrete Math. Theor. Comput. Sci.* **6** (2004) 365–386.
11. D. Zagier, Values of zeta functions and their applications, in *First European Congress of Mathematics (Paris 1992)*, vol. 2., Birkhäuser, Boston, 1994, pp. 497–512.

Department of Mathematics, University of Pennsylvania, 209 South 33rd Street, Philadelphia, PA 19096, USA
pemantle@math.upenn.edu

Research Institute for Symbolic Computation, Johannes Kepler University Linz, Altenberger Str. 69, A–4040 Linz, Austria
Carsten.Schneider@risc.uni-linz.ac.at