WHEN IS 0.999... EQUAL TO 1?

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Abstract. A doubly infinite sum, numerically evaluated at between 0.999 and 1.001, turns out to have a nice value.

1. Introduction

The three dots in the title do not refer to an infinite sequence of 9's, but to digits that are increasingly hard to compute. The question is philosophical: how many 9's 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 when 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:

$$\begin{aligned} S &:= \sum_{j,k=1}^{\infty} \frac{H_j(H_{k+1}-1)}{jk(k+1)(j+k)} \\ &= -4\zeta(2) - 2\zeta(3) + 4\zeta(2)\zeta(3) + 2\zeta(5) \qquad (2) \\ &= 0.999222\ldots \end{aligned}$$

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.

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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 [BP04]. 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 [BP04] 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 [PWZ96], 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 re-summation 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 that 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

$$0.999197 \leq S \leq 1.00093\,.$$

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 [BP04] then consulted the experts in harmonic summation, who consulted their computers, and came up with Theorem 1. 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 will be able to simplify the inner sum so that we can sum a second time if 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 [Sch04] that are inspired by [PWZ96]. 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 which we may then rapidly and rigorously verify.

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

$$k^2\,h(a,k) - (k+1)(2k+1)\,h(a,k+1) + (k+1)(k+2)\,h(a,k+2) = \frac{a(a+k+2)-(a+1)(k+1)H_a}{(k+1)(a+k+1)(a+k+2)} \quad (3)$$

with a variation of Zeilberger's creative telescoping trick.

The way we find this is to guess that there is some r and 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 $k,j \geq 1$. 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 may 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 $H_{j+1} = H_j + \frac{1}{j+1}$. 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 $a,k \geq 1$; here $H_k^{(r)} = \sum_{i=1}^{k}\frac{1}{i^r}$ denotes the generalized harmonic numbers.

We do this by asking Sigma to find solutions to (3) for all $k \geq 1$ 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 [Sch04] 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 proved (5).

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

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

Hence, if we define

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

we have

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

by (5) and (6). Summarizing, problem (2) from above reduces to find and prove 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 n^{th} 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 above. 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

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

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

and

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

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

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

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).

ζ-relations. 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:

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

The first two sums in $C(a,b)$ are available in the literature. Specifically, we find

$$\sum_{i=1}^{\infty} \frac{H_i}{i^2} = 2\zeta(3) \tag{14}$$

$$\sum_{i=1}^{\infty} \frac{H_i^2}{i^3} = -\zeta(2)\zeta(3) + \frac{7}{2}\zeta(5), \tag{15}$$

as a direct consequence of [BBG95]; since this is not available online, we also point out that these can be derived from [FS98, Theorems 2.2,3.1].

In order to obtain the other two sums, we start with the two identities

$$\sum_{i=1}^{b} \frac{H_i^3}{i^2} = \sum_{i=1}^{b} \frac{H_{i-1}^3}{i^2} + H_b^{(5)} - 3\sum_{i=1}^{b} \frac{H_i}{i^4} + 3\sum_{i=1}^{b} \frac{H_i^2}{i^3} \tag{16}$$

$$\sum_{i=1}^{b} \frac{H_i H_i^{(2)}}{i^2} = \sum_{i=1}^{b} \frac{H_{i-1} H_{i-1}^{(2)}}{i^2} - H_b^{(5)} + \sum_{i=1}^{b} \frac{H_i}{i^4} + \sum_{i=1}^{b} \frac{H_i^{(2)}}{i^3}. \tag{17}$$

Then by [BG96, Thm. 2] and [FS98, Cor. 5.2] respectively, we obtain the two identities

$$\sum_{i=1}^{\infty} \frac{H_{i-1} H_{i-1}^{(2)}}{i^2} = -\zeta(2)\zeta(3) + \frac{7}{2}\zeta(5) \tag{18}$$

$$\sum_{i=1}^{\infty} \frac{H_{i-1}^3}{i^2} = \zeta(2)\zeta(3) + \frac{15}{2}\zeta(5). \tag{19}$$

There are two more terms to evaluate, namely $\sum_{i=1}^{\infty} \frac{H_i}{i^4}$ and $\sum_{i=1}^{\infty} \frac{H_i^{(2)}}{i^3}$. By [BBG95] or [FS98, Theorems 2.2,3.1] we arrive at two final identities

$$\sum_{i=1}^{\infty} \frac{H_i}{i^4} = -\zeta(2)\zeta(3) + 3\zeta(5)$$

$$\sum_{i=1}^{\infty} \frac{H_i^{(2)}}{i^3} = 3\zeta(2)\zeta(3) - \frac{9}{2}\zeta(5).$$

Plugging these and (18)–(19) into one half the sum of (16) and (17) proves that

$$\lim_{a,b\to\infty} C(a,b) = -2\zeta(3) + 4\zeta(2)\zeta(3) + 2\zeta(5)$$

and finishes the proof of Theorem 1.

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References

[BP04] J. Balogh and R. Pemantle. The Klee-Minty random edge chain moves with linear speed. *Preprint.*

[BBG95] D. Borwein, J.M. Borwein, and R. Girgensohn. Explicit evaluation of Euler sums. In *Proceedings of the Edinburgh Mathematical Society*, volume 38, pages 277–294, 1995.

[BG96] J.M. Borwein and R. Girgensohn. Evaluation of triple Euler sums. *Electron. J. Combin.*, 3:1–27, 1996.

[FS98] P. Flajolet and B. Salvy. Euler sums and contour integral representations. *Experimental Math.*, 7(1):15–35, 1998.

[PWZ96] M. Petkovšek, H. S. Wilf, and D. Zeilberger. $A = B$. A. K. Peters, Wellesley, MA, 1996.

[Sch04] C. Schneider. The summation package Sigma: Underlying principles and a rhombus tiling application. *Discrete Math. Theor. Comput. Sci.*, 6(2):365–386, 2004.

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