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Comparing a series to an integral

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Comparing a series to an integral

Leon Siegel

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We consider the difference between the definite integral $\int_0^\infty u^x e^{-u}\,\mathrm{d}u$, where x is a real parameter, and the approximating sum $\sum_{k=1}^\infty k^x e^{-k}$. We use properties of Bernoulli numbers to show that this difference is unbounded and has infinitely many zeros. We also conjecture that the sign of the difference at any positive integer n is determined by the sign of $\cos\bigl((n+1)\arctan(2\pi)\bigr)$.

1. Introduction

There are a variety of situations where it is necessary to examine differences of sums and integrals. The Euler–Maclaurin summation formula is the usual tool for estimating $\int_{u\le Y} g(u)\,\mathrm{d}u - \sum_{n\le Y} g(n)$ [Abramowitz and Stegun 1964, p. 806], but it can also be interesting to develop exact formulas for particular choices of $g(u)$. For instance, the Euler–Mascheroni constant arises if we set $g(u)=1/u$ and consider the limit as $Y\to\infty$ [Wells 1986, p. 12]. The purpose of this paper is to examine the function

$$f(x) := \sum_{k=1}^{\infty} k^x e^{-k} - \int_0^\infty t^x e^{-t}\,\mathrm{d}t.$$

The integral on the right equals $\Gamma(x+1)$, where $\Gamma(x)$ is the gamma function, and the infinite series converges absolutely for all values of x. We can obtain an exact expression for $f(n)$ when $n\ge 1$ by using classical formulas for polylogarithms of negative order [Weisstein 2013]:

$$f(n) = -n! + \sum_{k=0}^{n} \frac{1}{(e-1)^{k+1}} \sum_{j=0}^{k} (-1)^j \binom{k}{j} (k+1-j)^n. \tag{1}$$

The main goal of this paper is to prove that $f(x)$ has infinitely many positive real zeros, and that the function becomes unbounded as $x\to\infty$. Further, in Conjecture 1 we hypothesize that $f(n)$ has the same sign as $\cos\bigl((n+1)\arctan(2\pi)\bigr)$ whenever

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n is a positive integer. We prove that the conjecture is true with finitely many exceptions, provided that $\arctan(2\pi)/\pi$ has finite irrationality measure. If we expand $\cos\bigl((n+1)\arctan(2\pi)\bigr)$ using trigonometric identities, then we obtain the equivalent conjecture that the following identity holds for all positive integers n:

$$\operatorname{sign}\left[\sum_{j=0}^{n+1}(-1)^j\binom{n+1}{2j}(2\pi)^{2j}\right] = \operatorname{sign}\left[-(e-1)^{n+1}n! + \sum_{k=0}^{n}(e-1)^{n-k}\sum_{j=0}^{k}(-1)^j\binom{k}{j}(k+1-j)^n\right]. \tag{2}$$

The left-hand side of (2) is a polynomial in π, while the right-hand side is a polynomial in e. Based on numerical experiments, we conjecture that (π, e) is the unique, nontrivial (i.e., $\neq (0, 1)$) tuple of real numbers which makes (2) valid for all positive integers n. When we choose values close to π and e respectively, we notice that (2) is false for some n in all considered cases. Surprisingly, (2) is valid for $n \le 128$ if you insert $(\pi + 0.015, e)$, but only for $n \le 2$ in the case of $(\pi, e + 0.015)$. So the equation seems to be a lot more sensitive to small modifications in the argument on the right-hand side. Also, choosing various random tuples (x, y) further away from (π, e), we always found an n such that (2) was wrong.

2. Elementary properties of $f(x)$

In this section we prove that $f(x)$ is an unbounded function by showing that the sequence $\{f(n)\}_{n=1}^{\infty}$ is unbounded as $n \to \infty$. Our proof uses properties of Bernoulli numbers. The n-th Bernoulli number is defined by

$$\frac{x}{e^x - 1} = \sum_{n=0}^{\infty} B_n \frac{x^n}{n!}, \tag{3}$$

and the generating series converges for $|x| < 2\pi$. It is known that Bernoulli numbers are always rational, and that $B_n = 0$ if $n > 1$ is odd. Bernoulli numbers have many interesting combinatorial properties [Abramowitz and Stegun 1964], and the following asymptotic holds for large values of n:

$$|B_{2n}| \sim \frac{n^{2n}}{(\pi e)^{2n}}. \tag{4}$$

This property will be used later. We begin by deriving a new formula for B_n. Then in Theorem 1, we use our formula to prove that $f(x)$ is unbounded.

Lemma 1. $$B_n = \sum_{k=n}^{\infty} \frac{f(k) - kf(k-1)}{(k-n)!} \quad \textit{for } n \ge 2.$$

Proof. Consider the generating function of the Bernoulli numbers,

$$g(x) := \frac{x}{e^x - 1},$$

whose Taylor series at $x = -1$ is

$$g(x) = \frac{e}{e-1} - \frac{e(e-2)}{(e-1)^2}(x+1) + \sum_{n=2}^{\infty} \frac{f(n) - nf(n-1)}{n!}(x+1)^n. \tag{5}$$

The Taylor coefficients at $n = 0$ and $n = 1$ are calculated directly. To obtain the coefficients when $n \geq 2$, we use

$$\begin{aligned} g^{(n)}(-1) =& \frac{\mathrm{d}^n}{\mathrm{d}x^n}\left[\frac{-x}{1-e^x}\right]_{x=-1} = \frac{\mathrm{d}^n}{\mathrm{d}x^n}\left[-x\sum_{m=0}^{\infty} e^{mx}\right]_{x=-1} \\ =& \sum_{m=1}^{\infty} m^n e^{-m} - n\sum_{m=1}^{\infty} m^{n-1}e^{-m} \\ =& \left(\sum_{m=1}^{\infty} m^n e^{-m} - n!\right) - n\left(\sum_{m=1}^{\infty} m^{n-1}e^{-m} - (n-1)!\right) \\ =& f(n) - nf(n-1). \end{aligned} \tag{6}$$

Since formula (3) is also valid when x lies in a neighborhood of -1, we can equate the two results:

$$\begin{aligned} g(x) = \sum_{n=0}^{\infty} \frac{B_n}{n!}x^n &= \sum_{n=0}^{\infty} \frac{g^{(n)}(-1)}{n!}(x+1)^n \\ &= \sum_{n=0}^{\infty} \frac{g^{(n)}(-1)}{n!}\sum_{k=0}^{n}\binom{n}{k}x^k = \sum_{n=0}^{\infty}\left[\sum_{k=n}^{\infty}\frac{g^{(k)}(-1)}{(k-n)!}\right]\frac{x^n}{n!}. \end{aligned}$$

Comparing coefficients and then applying (6), we find that for $n \geq 2$,

$$B_n = \sum_{k=n}^{\infty} \frac{g^{(k)}(-1)}{(k-n)!} = \sum_{k=n}^{\infty} \frac{f(k) - kf(k-1)}{(k-n)!}. \qquad \square$$

Theorem 1. *The sequence $\{f(n)\}_{n=1}^{\infty}$ is unbounded.*

Proof. We construct a proof by contradiction. Assume that $|f(n)| < C$ for some $C > 0$ and every $n \in \mathbb{N}$. By Lemma 1 and the triangle inequality, we have

$$|B_n| \leq \sum_{k=n}^{\infty} \frac{|f(k) - kf(k-1)|}{(k-n)!} \leq \sum_{k=n}^{\infty} \frac{C(1+k)}{(k-n)!} \leq Ce(n+2).$$

This contradicts the asymptotic $|B_{2n}| \sim n^{2n}/(\pi e)^{2n}$, which holds for n sufficiently large. $\square$

Remark. Despite the fact that $f(n)$ is unbounded as $n \to \infty$, the ratio $f(n)/n!$ converges to zero. To prove this, we can use residue calculus to show that

$$\frac{f(n)}{n!} = \frac{1}{2\pi i} \oint_\gamma \frac{z^{-n-1}}{1 - e^{z-1}} \, \mathrm{d}z,$$

where $\gamma = \{z \in \mathbb{C} \colon |z| = 2\}$. We then employ the triangle inequality and numerical integration to obtain the crude upper bound $|f(n)|/n! \le 0.82 \times 2^{-n}$. In fact, it is possible to develop a much sharper upper bound using formula (12) below.

Theorem 2. *The function $f(x)$ has infinitely many zeros.*

Proof. First notice that $f(2) \approx -0.0077$ and $f(3) \approx 0.0065$, so by continuity $f(x)$ has at least one zero in the interval $(2, 3)$. To prove that the function has infinitely many zeros, we proceed by contradiction.

Assume that f has only finitely many zeros. Then for any sufficiently large integer m, the elements of the set $\{f(m), f(m+1), f(m+2), \dots\}$ all have the same sign. Now consider the function

$$h(x) := \frac{1}{x} - \frac{1}{e^x - 1},$$

which has the Taylor series

$$h(x) = \frac{1}{e-1} + \sum_{k=1}^{\infty} \frac{f(k)}{k!} (x+1)^k. \tag{7}$$

Differentiating m times gives

$$h^{(m)}(x) = \sum_{k=m}^{\infty} \frac{f(k)}{(k-m)!} (x+1)^{k-m}. \tag{8}$$

If the elements of the set $\{f(m), f(m+1), \dots\}$ are strictly positive, then (8) becomes a sum over positive numbers whenever $x \in (-1, 0)$, and it follows that $h^{(m)}(x)$ is strictly positive. If we notice that

$$h(x) = \frac{1}{x} - \frac{1}{x} \frac{x}{e^x - 1} = -\sum_{n=1}^{\infty} \frac{B_n}{n!} x^{n-1},$$

then we also have

$$h^{(m)}(x) = -\sum_{n=m+1}^{\infty} \frac{B_n}{n!} \frac{(n-1)!}{(n-m-1)!} x^{n-m-1}. \tag{9}$$

The key observation is that formulas (8) and (9) have overlapping domains of convergence on the negative real axis near the origin. If x is a sufficiently small negative real number, then (9) implies

$$h^{(m)}(x) \approx -\frac{B_{m+1}}{m+1},$$

but (8) guarantees

$$h^{(m)}(x) > 0.$$

This is a contradiction, because Bernoulli numbers assume both positive and negative values as m increases. We can deal with the case where $\{f(m), f(m+1), \dots\}$ are strictly negative in a similar manner. □

In Theorem 2 we proved that $f(x)$ has infinitely many real zeros. In fact, we can be much more precise about the locations of the zeros. If x_j denotes the j-th positive real zero of $f(x)$ such that $f(x_j) = 0$, then we expect that

$$x_j \approx -1 + \frac{\pi(2j+1)}{2\arctan(2\pi)}. \tag{10}$$

The first approximation gives $x_1 \approx 2.335\dots$, and this is reasonably close to the true value $x_1 = 2.306\dots$. We have observed numerically that the approximations become more accurate for large values of j. To derive (10), consider an identity which is valid for $\mathrm{Re}(x) > 0$ and $\mathrm{Re}(\mu) > 0$:

$$\frac{1}{\Gamma(x+1)} \sum_{k=1}^{\infty} k^x e^{-\mu k} = \sum_{k=-\infty}^{\infty} \frac{1}{(\mu + 2\pi i k)^{x+1}}. \tag{11}$$

Formula (11) is a special case of an identity due to Lipschitz [Rademacher 1973, p. 77], and follows from the Poisson summation formula. Set $\mu = 1$ and take the real part of both sides to obtain

$$\frac{f(x)}{\Gamma(x+1)} = 2\sum_{k=1}^{\infty} \frac{\cos\big((x+1)\arctan(2\pi k)\big)}{(1+4\pi^2k^2)^{(x+1)/2}}. \tag{12}$$

Equation (12) converges rapidly, and we can approximate $f(x)$ by truncating the series. The first term gives

$$\frac{f(x)}{\Gamma(x+1)} \approx 2\,\frac{\cos\big((x+1)\arctan(2\pi)\big)}{(1+4\pi^2)^{(x+1)/2}}, \tag{13}$$

and we immediately recover (10). It is somewhat subtle to determine how often (13) actually provides a good approximation of $f(x)$, and we touch on this point in the next section.

3. A conjecture on the sign of $f(n)$

A second observation from (13) is that the sign of $f(n)$ should always equal the sign of $\cos\big((n+1)\arctan(2\pi)\big)$. We have verified this numerically for $n \le 5000$ in Maple, and as a result we have the following conjecture:

Conjecture 1. *For all positive integers n,*

$$\operatorname{sign} f(n) = \operatorname{sign}\cos\big((n+1)\arctan(2\pi)\big). \tag{14}$$

Equivalently, for every positive integer n,

$$\begin{aligned}\operatorname{sign}&\left[\sum_{j=0}^{n+1}(-1)^j\binom{n+1}{2j}(2\pi)^{2j}\right]\\ &= \operatorname{sign}\left[-(e-1)^{n+1}n! + \sum_{k=0}^{n}(e-1)^{n-k}\sum_{j=0}^{k}(-1)^j\binom{k}{j}(k+1-j)^n\right]. \end{aligned}\tag{15}$$

Conjecture 1 is easy to check numerically. The main difficulty in actually proving the conjecture is to determine how often (13) leads to a good approximation of $f(n)$. The reason that (14) might fail is because $(n+1)\arctan(2\pi)$ is unreasonably close to a half-integer multiple of π. This would cause the first term of the infinite series in (12) to nearly vanish, in which case higher-order terms would dominate and the estimate in (13) would fail. Thus we need to rule out the possibility that $(n+1)\arctan(2\pi)$ is unreasonably close to a half-integer multiple of π. This is equivalent to ruling out the possibility that $\arctan(2\pi)/\pi$ is unreasonably well approximated by rational numbers. Before proceeding, we note that $\arctan(2\pi)/\pi$ is trivially irrational, because otherwise we would have an identity of the form $2\pi = \tan(p\pi/q)$ for some $(p,q) \in \mathbb{Z}^2$, contradicting the transcendence of π.

Lemma 2. *Equation* (14) *is true for any positive integer n which satisfies*

$$\big|\cos\big((n+1)\arctan(2\pi)\big)\big| > \frac{2.6}{1.98^{n+1}}. \tag{16}$$

Proof. First, rewrite (12) as

$$\frac{f(n)}{n!} = 2\frac{\cos\big((n+1)\arctan(2\pi)\big)}{(1+4\pi^2)^{(n+1)/2}} + 2\sum_{k=2}^{\infty}\frac{\cos\big((n+1)\arctan(2\pi k)\big)}{(1+4\pi^2k^2)^{(n+1)/2}}.$$

If the first term on the right dominates, then it follows easily that

$$\operatorname{sign}\frac{f(n)}{n!} = \operatorname{sign}\frac{2\cos\big((n+1)\arctan(2\pi)\big)}{(1+4\pi^2)^{(n+1)/2}},$$

and this is equivalent to Conjecture 1. Thus we need to prove

$$\left|2\frac{\cos\bigl((n+1)\arctan(2\pi)\bigr)}{(1+4\pi^2)^{(n+1)/2}}\right| > \left|2\sum_{k=2}^{\infty}\frac{\cos\bigl((n+1)\arctan(2\pi k)\bigr)}{(1+4\pi^2k^2)^{(n+1)/2}}\right|. \tag{17}$$

Equation (16) easily implies that

$$\left|2\frac{\cos\bigl((n+1)\arctan(2\pi)\bigr)}{(1+4\pi^2)^{(n+1)/2}}\right| > \frac{5.2}{1.98^{n+1}(1+4\pi^2)^{(n+1)/2}} > \frac{5.2}{12.59^{n+1}}. \tag{18}$$

On the other hand, by the triangle inequality

$$\begin{aligned}\left|2\sum_{k=2}^{\infty}\frac{\cos\bigl((n+1)\arctan(2\pi k)\bigr)}{(1+4\pi^2k^2)^{(n+1)/2}}\right| &\le 2\sum_{k=2}^{\infty}\frac{1}{(1+4\pi^2k^2)^{(n+1)/2}}\\ &< \frac{2}{(1+16\pi^2)^{(n-1)/2}}\sum_{k=2}^{\infty}\frac{1}{1+4\pi^2k^2}\\ &< \frac{5.2}{(1+16\pi^2)^{(n+1)/2}} < \frac{5.2}{12.6^{n+1}}. \end{aligned}\tag{19}$$

Thus combining (19) and (18) shows that

$$\begin{aligned}&\left|\frac{2\cos\bigl((n+1)\arctan(2\pi)\bigr)}{(1+4\pi^2)^{(n+1)/2}}\right| - \left|2\sum_{k=2}^{\infty}\frac{\cos\bigl((n+1)\arctan(2\pi k)\bigr)}{(1+4\pi^2k^2)^{(n+1)/2}}\right|\\ &\qquad > \frac{5.2}{12.59^{n+1}} - \frac{5.2}{12.6^{n+1}} > 0,\end{aligned}$$

and (17) follows immediately. Therefore Conjecture 1 is true whenever n is a positive integer for which (16) holds. □

It is typically very tricky to determine how well a particular number θ can be approximated by rational numbers. We say that θ has irrationality measure μ if μ is the smallest real number such that

$$\left|\theta - \frac{p}{q}\right| > \frac{1}{q^{\mu}}$$

for all but finitely many pairs $(p, q) \in \mathbb{Z}^2$ with $q > 0$. The Thue–Roth–Siegel theorem guarantees that $\mu = 2$ whenever θ is algebraic and irrational [Roth 1955]. An easy consequence of this theorem is that θ can never be algebraic and have irrationality measure greater than 2. The typical method for proving that particular numbers are *transcendental* is to construct infinite sequences of rational numbers which approximate them too well. Liouville gave the first examples of transcendental numbers in 1851 [Niven 1956, p. 93]. He proved that numbers like

$$\theta_0 = \sum_{n=1}^{\infty} \frac{1}{10^{n!}}$$

are always transcendental. Notice that if we set $p_N = \sum_{n=1}^{N} 10^{N!-n!}$ and $q_N = 10^{N!}$, then it is easy to show that

$$\left|\theta_0 - \frac{p_N}{q_N}\right| \le \frac{2}{q_N^{N+1}}.$$

Given any $k > 0$, this allows us to construct infinite sequences of rational numbers so that $|\theta_0 - p/q| < 1/q^k$. Numbers with this property are called *Liouville numbers* and are said to have infinite irrationality measure. While a simple counting argument shows that almost all numbers are irrational, the set of Liouville numbers has measure zero inside the irrational numbers. Irrational numbers typically have finite irrationality measures; it is known that π has irrationality measure at most 7.6063 [Salikhov 2008], and $\log 2$ has irrationality measure at most 3.57455391 [Marcovecchio 2009].

Theorem 3. *Assume that* $\arctan(2\pi)/\pi$ *has finite irrationality measure. Then Conjecture 1 is true for n sufficiently large.*

Proof. Assume that (16) fails for some integer n. Then we have

$$\frac{2.6}{1.98^{n+1}} \ge \left|\cos\big((n+1)\arctan(2\pi)\big)\right| = \left|\sin\big((n+1)\arctan(2\pi) - \tfrac{\pi}{2} - \pi j\big)\right|$$

for any integer j. Select j so that $z \in [-\pi/2, \pi/2]$, where z is the argument of the sine function. Elementary estimates show that $|\sin z| \ge 2|z|/\pi$. Thus

$$\frac{2.6}{1.98^{n+1}} \ge \frac{2}{\pi}\left|(n+1)\arctan(2\pi) - \frac{\pi}{2} - \pi j\right|,$$

and rearranging gives

$$\frac{1.3}{(n+1)1.98^{n+1}} \ge \left|\frac{\arctan(2\pi)}{\pi} - \frac{2j+1}{2(n+1)}\right|. \tag{20}$$

If $\arctan(2\pi)/\pi$ has finite irrationality measure, then (20) can only hold for finitely many values of n. We conclude that (16) holds for n sufficiently large, which implies that Conjecture 1 is also true for n sufficiently large. □

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