

Devilish Tricks for Sequence Acceleration

ROBERT M. CORLESS, Editor-in-Chief, Maple Transactions, Canada

Abstract. The two most famous quotes about divergent series are Abel's "Divergent series are the invention of the devil, and it is shameful to base on them any demonstration whatsoever," and Heaviside's "This series is divergent, therefore we may be able to *do* something with it." Today a lot more is known about divergent series than in either's day, so we can say now that, on balance, Heaviside wins, and we now have plenty of license to use divergent series. This article talks about some "well-known" methods (that is, well-known to experts) to do so, and in particular talks about some of the devilishly good features of evalf/Sum, long one of my favourite tools in Maple. But Abel had a point, too, and we'll see some "shameful" things, which will give the reader some necessary caution to go along with their license.

Additional Key Words and Phrases: divergent series, sequence acceleration, evalf/Sum, Levin's *u*-transform, Euler summation, Euler–Maclaurin sum formula, Zeno's paradoxes, Abel summation, Cesàro summation

Recommended Reference Format:

Robert M. Corless. 2023. Devilish Tricks for Sequence Acceleration. *Maple Trans.* 3, 1, Article 14777 (February 2023), 22 pages. https://doi.org/10.5206/mt.v3i1.14777

1 Historical Paradoxes and the Internet Today

The following was a (mildly) popular source of argument on Twitter and Facebook, at this time of writing:

$$1 - 2 + 3 - 4 + 5 - \dots = 1/4$$
. (1)

This is not at all new. In fact, this is Equation 1.1.2 on p. 1 of the classic book [11], from which we will take a lot of material. One side of the internet argument says that if we use "the" definition of convergence, then "the" meaning of for the series on the left hand side of equation (1) can be deduced as follows. The symbol := here means "is defined to be". Then by definition,

$$\sum_{k\geq 1} a_k := \lim_{N\to\infty} S_N \,, \tag{2}$$

where the *partial sums* S_N are given by

$$S_N = \sum_{k=1}^N a_k \ . \tag{3}$$

This gives "DNE", for "Does Not Exist," as we now show in detail. We use here Cauchy's definition of a limit, which is now conventional: $\lim_{N\to\infty} S_N = L$ if and only if for every $\varepsilon > 0$ there exists an N_{ε} such that $N > N_{\varepsilon} \implies |S_N - L| < \varepsilon$. Here

$$S_N = \sum_{k=1}^{N} (-1)^{k-1} k = \frac{(-1)^{N+1} (N+1)}{2} - \frac{(-1)^{N+1}}{4} + \frac{1}{4}$$
 (4)

Author's address: Robert M. Corless, Rob.Corless@gmail.com, Editor-in-Chief, Maple Transactions, Canada.

Permission to make digital or hard copies of all or part of this work for any use is granted without fee, provided that copies bear this notice and the full citation on the first page. Copyrights for third-party components of this work must be honored. © 2023 Copyright held by the owner/author(s). Publication rights licensed to Maple Transactions, under Creative Commons CC-BY 4.0 License.

https://doi.org/10.5206/mt.v3i1.14777

¹ i.e., the normal first-year calculus meaning

14777:2 RM Corless

which simplifies to -N/2 if N is even and to (N+1)/2 if N is odd, so no such L exists. In the face of that, any computational reasoning that assigned a value 1/4 to that clearly diverging² process would be suspect³. Indeed this conclusion corresponds with our (trained) intuition: start with 1, next partial sum is 1-2=-1; next partial sum is +2, then +3, and so on. Assigning a value to this diverging process would be subject to endless argument. [Have you *met* the modern Internet?]

But the Maple commands below show which side Maple falls on the argument:

> Digits := 15;

$$Digits := 15 \tag{5}$$

 $> Sum((-1)^{k-1} \cdot k, k = 1..infinity) = evalf(Sum((-1)^{k-1} \cdot k, k = 1..infinity))$

Now let us try symbolic summation with a little trick: the use of the keyword formal. $> sum((-1)^{k-1} \cdot k, k = 1..infinity, formal = true);$

$$\frac{1}{4} \tag{7}$$

Aha! So it's not just numerical summation. Here's another way to do it, via an "environment variable":

> *EnvFormal* := *true*;

$$EnvFormal := true$$
 (8)

 $> Sum((-1)^{k-1} \cdot k, k = 1..infinity) = sum((-1)^{k-1} \cdot k, k = 1..infinity)$

$$\sum_{k=1}^{\infty} (-1)^{k-1} k = \frac{1}{4} \tag{9}$$

This usage of the word formal is traditional in this field: a "formal power series" is "formal" in the vernacular sense of "a formality," that is, without any questions being asked or any inconvenience gone to. This is in complete contrast to the use of the word "formal" in the sense of "formal methods" or indeed a "formal investigation" which means serious attention is being paid to the details, where the devil is said to dwell. [Don't ask *me*, I didn't invent this language.] See ?sum, details for more.

All right then. Let's consider another popular choice:

$$1 + 2 + 4 + 8 + \dots = -1. \tag{10}$$

This is Equation 1.1.1.6, again on page 1 of [11]. Again, Maple's evalf/Sum shows its preference: $> evalf(Sum(2^k, k = 0..infinity));$

$$-1.0$$
 (11)

Symbolically, remembering that "formal" is true:

 $> Sum(2^k, k = 0..infinity) = sum(2^k, k = 0..infinity);$

$$\sum_{k=0}^{\infty} 2^k = -1 \tag{12}$$

²Here we use "diverging" in a sense closer to its non-mathematical meaning. A non-mathematician, faced with ever-increasing oscillations of more and more extreme points of view, would be inclined to agree that a "diverging" was what was taking place.

³I am complacently aware that a while ago the youngins would have used the word "sus" here. Now the olds are among us.

The reader's eyebrows may be climbing at this point. Let us now point at an internet example where this *does not* happen:

$$1 + 2 + 3 + 4 + 5 + \dots = -\frac{1}{12}, \tag{13}$$

but Maple's evalf/Sum says:
> evalf(Sum(k, k = 1..infinity));

$$\sum_{k=1}^{\infty} k \tag{14}$$

The reader's eyebrows may or may not actually *lower*, after seeing Maple refuse to answer this question; but possibly some side-eye will be involved, especially after seeing the "formal sum" treatment:

> Sum(k, k = 1..infinity) = sum(k, k = 1..infinity);

$$\sum_{k=1}^{\infty} k = -\frac{1}{12} \,. \tag{15}$$

So, here we seem to have found a place where Maple is ambivalent. It seems curious that the *numerical* summation is refusing to take the hurdle, though.

Other internet chestnuts include $0.999 \cdots = 1$, or

$$\sum_{k>1} 9 \cdot 10^{-k} = 9 \frac{1/10}{1 - 1/10} = 9 \frac{10}{9 \cdot 10} = 1;$$
 (16)

but this is uncontroversially convergent with the normal axioms for the real numbers, and the universally⁴ accepted real value of this sum is 1. The internet argument about this seems to be just the normal process of "getting used to infinity". Now, if hyperreal or surreal numbers, or other nonstandard analysis kinds of things, get involved, then there is room for discussion.

But what I want to talk about here is "just" the real numbers; with a little bit of discussion of floating-point arithmetic and arbitrary-precision floating-point arithmetic, which is meant to mimic the real numbers as closely as possible. As is usual in mathematics, we will occasionally have to move into the complex plane in order to understand what is happening on the real line.

1.1 Even older paradoxes

Before we do that, let's review some even *older* paradoxes, namely some of those famously attributed to Zeno. For background, check out the Stanford Encyclopedia entry on Zeno's paradoxes. There are *nine* paradoxes listed there, which surprised me⁵—I only knew of three, namely the dichotomy, the paradox of the arrow, and the paradox of Achilles and the Tortoise (which are all kind of the same). But it turns out that the *density* paradox, which I hadn't known, has some relevance for the following computation. Furthermore, another one called "the Argument from Finite Size" will *also* be relevant to infinite summation. Again I hadn't known that one.

Ok, what's the Density Paradox? Reading Zeno's words at the link above, we digest them to mean—talking about numerical quantities and not physical bodies—that between every two numbers there must be another. Certainly this is true for rational numbers: between a/b and c/d we have (for instance) (a + c)/(b + d).

This is not a problem when talking about numbers; we are quite happy to have an infinite number of numbers, even between very tightly spaced rationals. And we are happy to have even more real numbers, although somehow the rationals are dense in the reals while having measure

⁴Well, almost universally.

⁵Even though my friend Nic Fillion had long ago told me that there were a lot of them.

14777:4 RM Corless

zero (we suspect that Zeno, Cantor, and Lebesgue all would have got along fine). We'll leave talking about physical particles, though, to the physicists.

But this density is an innate property of rational and real numbers; also of complex numbers of course. What about floating point numbers? No. No floating-point system that we know of preserves this property⁶. For IEEE double precision floats, which are represented in a 64 bit word, not only are there gaps between consecutive floating-point numbers, there is also a minimum positive real number (about 10^{-309}) and a maximum positive real number (about 10^{308}). In Maple it's more complicated, but still true: the NextAfter function gives the next float. With Digits := 15, the command NextAfter(1.0, infinity) gives 1.0000000000001, which is $1 + 10^{-14}$. With this as a clue, we rephrase Zeno's Dichotomy paradox as follows, and implement it in Maple.

Suppose Atalanta (who was famous for her running speed) had to travel from x = 1 to x = 2. Zeno notes that before Atalanta gets to 2, she first has to get to 1 + 1/2. Before she gets *there*, she first has to get to 1 + 1/4. Continuing in this way, Zeno arrived at the paradox that Atalanta couldn't even get started, because there were an infinite number of things she had to do before getting anywhere.

Nice to know that there were internet arguments even before there was an internet. Anyway, consider the following Maple code:

```
Digits := 15:
    one := 1.0:
    s := 1.0:
    zeno := 0:
    while one+s > one do
        s := s/2;
        zeno := zeno + 1;
    end do:
    "Loop_terminated,_after_", zeno, "_halvings_";
    "Atalanta's_step:", evalf[3](s),
    "_or_2_to_the_", round( log[2](s) );
```

"Loop terminated, after ", 48, " halvings " "Atalanta's step:",
$$3.55 \times 10^{-15}$$
, " or 2 to the ", -48 (17)

Not only does this loop terminate (which would have confounded Zeno, although he might gleefully have pointed out that Atalanta *still* can't get anywhere because adding a step of size $s = 2^{-48}$ to 1 apparently results in her staying in exactly the same place), it terminates in exactly 48 iterations. A comparable code in Python takes 53 iterations, by the way, and has $s = 2^{-53} \approx 10^{-16}$. Explaining those numbers requires us to know more about floating-point arithmetic⁷ than maybe we want to.

All I need here, however, is to point out that floats are not a perfect mirror of the real numbers, and they cannot be. They are not associative (take the resulting s from the above loop; compute -1 + 1 + s in two ways, one as (-1 + 1) + s and the other as -1 + (1 + s). The first way you get s, the second way you get s. Aristotle himself observed something which predicts that floats *cannot* be perfect: in "On the Heavens" he says "Admit, for instance, the existence of a minimum magnitude,

⁶This is certainly true of fixed-width floating-point systems. For variable-width systems such as Maple's, this property could be preserved if one's computer had infinite memory, infinite speed, and Digits was varied during the computation. In practice, one runs out of memory or patience. And, *whatever* the setting of Digits, there will be numbers between 1 and NextAfter(1) which cannot be represented. Probably Zeno could have made something of this argument.

⁷And maybe about programming languages. The version of the code shown here is thanks to Paul DeMarco at Maplesoft; the original version, which looked plausible, would behave differently in different Maple environments owing to code transformations that could change the behaviour. Zeno would have been pleased at the subtlety, I think.

and you will find that the minimum which you have introduced, small as it is, causes the greatest truths of mathematics to totter."

We remark that the *machine epsilon* (which is sort of what *s* is behaving like here, except with convert-to-decimal magic thrown into the mix as well) is not at all the minimum magnitude even in double precision floats: that's typically called something like realmin and it is, for IEEE double precision normalized numbers, about 10⁻³⁰⁸. Maple's minimum magnitude is ridiculously smaller than that, but still causes "great truths" to totter. Anyway, back to series.

Let's consider one more Zenoism: the Argument from Finite Size, as discussed in the Stanford Encyclopedia. The reader thereof will notice the occurrence of the sum

$$1 - 1 + 1 - 1 + 1 - \cdots$$
 (18)

which Euler famously summed to 1/2 (we will see how, later). But as Christopher Long (@octonion on Twitter) points out, this infinite sum therefore cannot be associative⁸:

$$(1-1) + (1-1) + (1-1) + \dots = 0$$
 (19)

pretty clearly, because even Zeno would agree that adding nothing gets you nothing, even if you do it infinitely many times (this is part of the Argument from Finite Size); but then

$$1 + (-1 + 1) + (-1 + 1) + \dots = 1$$
 (20)

just as clearly. One wonders if other arrangements could produce yet different answers (yes, if you allow commutativity as well).

Of course we are only adding *countably* many things here; adding uncountably many nonzero things always gives you infinity, according to the accepted model of the real numbers (I remember my real analysis professor, C. W. Lamb, proving this in class; that would have been in Autumn of 1978, I believe. Maybe I could reproduce that proof now...yes, I think I can. Accumulation points come into it.).

In the rest of this paper, we are going to be looking at the numerical evaluation of limits, especially of limits of finite sums. This tends to push the capacity of floating-point to *its* limit, so to speak. Nonetheless we're going to see some remarkable successes.

2 Convergence and its uses

claim to be the first to have noticed it.

The biggest problem with solving equations is the *existence* of solutions. This is "Moler's Law": the hardest thing to compute is something that doesn't exist. One of my friends, George Corliss, once got paid a nice consulting fee for informing an engineering firm that the linear system they were trying to solve was inconsistent and had no solutions; this information is worth money. [Sometimes a lot more than money, of course.] The best thing that a convergent series gives you is a *proof of existence* of a solution. This is still the main use of series. What, you say? Can't we use them to compute things? Sometimes, no!

As an example, consider the very simple differential equation $\dot{y}(t) = -1000y(t)$, together with the initial condition y(0) = 1. You might roll your eyes as I tell you that the solution is given by the convergent series

$$y(t) = \sum_{k \ge 0} \frac{(-1000)^k}{k!} t^k \tag{21}$$

but really the mathematical meaning of this is quite clear. There is a limit for the sum, it is unique, and it solves the differential equation.

If you want to use the series to compute $\exp(-1000t)$, say at t = 1, that's a different matter.

⁸He has several very interesting points, some of which we will take up later; this one is of course classical and he does not

14777:6 RM Corless

$$> evalf(Sum(\frac{(-1000)^k}{k!}, k = 0..infinity));$$
 Float(∞) (22)

That might make you scratch your head, if you don't know about the *condition number* of a sum, or the basic principle that a good numerical method gives you the exact result for a slightly different input. Maple's apparently nonsensical result above is perfectly understandable and arguably what it should be returning (I certainly expected something like this answer, although it's actually better for my purpose than I had hoped). If it makes you feel better, using sum and exact arithmetic first gets the comforting symbolic answer e^{-1000} , although it suggestively writes this as $1/e^{1000}$:

$$> sum(\frac{(-1000)^k}{k!}, k = 0...infinity);$$

$$\frac{1}{z_1000}$$
(23)

Numerical evaluation of this symbolic result⁹ gives us the correct answer near $5 \cdot 10^{-435}$.

So why is Maple returning $Float(\infty)$ for something that should be ridiculously tiny? And in what world is that acceptable?

To get this series to converge, we have to take enough terms that the remainder is smaller than the error we want. If we want error less than 10^{-15} , we have to have $1000^k/k! < 10^{-15}$ (the series is an alternating series and so the error will be less than the first term neglected). Solving this numerically in Maple we find that k > 2748; so we have to take more than 2748 terms¹⁰. So what?

What is the maximum term in that collection? This occurs at k = 1000 (and at k = 999), and the value is about 10^{432} . Now we see the issue. Double-precision floating-point arithmetic *overflows* at about 10^{308} . Overflow gives Float(∞) in Maple.

We should be able to fix this, by using *Stoutemyer's Rule of Thumb*:

"In my experience, it is often wise to use more than n decimal digits of precision when summing n terms of a series, computing nth degree regressions, computing the zeros of an nth degree polynomial, etc."

—David R. Stoutemyer

Indeed, setting Digits to 883 should work. Sadly, not with evalf/Sum; I have reported the bug (it's not properly paying attention to the setting of Digits). But it's a convergent series!

Now, if instead we compute exp(1000) by this series, and reciprocate it, we get a good answer. But who wants to add up thousands of terms in a series anyway? That's way too much work. This is inherent in the first year notion of convergence, mind: we are always taking the limit as the number of terms goes to infinity (and therefore the amount of work goes to infinity).

Patient: "Doctor, it hurts when I do this:" (raises their arm).

Doctor: "Well, don't do that, then."

-Anonymous

Even if your series converges, you almost always want it to converge faster. This leads us to *sequence acceleration methods*. There have been many different developments, here. It turns out that some of these methods are so good that they can even give good answers for *divergent* series.

⁹Maybe raising the question of how it does so: I suspect the answer is a combination of "argument reduction" by squaring, and use of a fine approximation on a small interval.

 $^{^{10}}$ This is not enough terms for an accurate answer, of course. We need the term to be less than $10^{-15} \cdot 10^{-432}$ and for that 3611 terms are needed.

Divergence is a consequence of your definitions

"... consider two series that have the following general term:

$$\frac{1000^n}{1 \cdot 2 \cdot 3 \cdots n} \text{ and } \frac{1 \cdot 2 \cdot 3 \cdots n}{1000^n}.$$

Pure mathematicians would say that the first series converges and even that it converges rapidly since the millionth term is much smaller than the 999999th; however, they will consider the second series to be divergent since the general term is able to grow beyond all bounds.

Conversely, astronomers will consider the first series to be divergent since the first thousand terms increase; they will call the second series convergent since the first thousand terms decrease and since this decrease is rapid at first."

-Henri Poincaré, [14, Ch. 8, p. 317]

>
$$evalf(Sum(\frac{(-1)^k \cdot k!}{1000^k}, k = 0..infinity));$$

$$0.999001994023881$$
(24)

Aha! We have identified the issue. Maple is really an *astronomer*!

Indeed, consider

$$F(x) := \int_{0}^{\infty} \frac{e^{-t}}{1 + xt} dt \tag{25}$$

 $F(x) := \int_0^\infty \frac{\mathrm{e}^{-t}}{1+xt} dt$ (25) and expand $1/(1+xt) = 1-xt+x^2t^2-x^3t^3+\cdots$ in a geometric series; integrate term-by-term¹¹ and one gets

$$\sum_{k\geq 0} (-1)^k k! \, x^k \tag{26}$$

and putting x = 1/1000 gives us the series above. Evaluating the (convergent) integral definition of F(x) numerically when x = 0.001, we get 0.999001994023878, which differs by about $3 \cdot 10^{-15}$ from the evalf/Sum above. According to Hardy, it was Euler who did this first.

What really annoys (some) mathematicians is that the answer obtained by (accelerating) this divergent series is quite correct¹². So we have the seemingly paradoxical situation where we cannot (easily) numerically evaluate a convergent series, but instead we can easily and correctly use a divergent series to get our answer. This really does annoy some people, but doubtless Oliver Heaviside could have put "I told you so." on his tombstone 13. But, if we are careful to define our terms well, and in particular to be careful which limit we are taking, everything will turn out to be completely logical. Hardy makes this distinction, that it is the habit of definition that truly marks logical rigour.

¹¹The step in this computation that annoys people is the previous one: the series is convergent only if xt < 1, but we integrate from t = 0 to $t = \infty$, well outside the radius of convergence. The resulting series is therefore divergent.

¹²Maybe my favourite "howler" (meaning an incorrect manipulation that nevertheless gets the right answer) is the computation of 16/64: cancel the sixes, to get 1/4, which is correct! Not convinced? Try 19/95 and cancel the nines. The moral of this footnote is just because you get the right answer sometimes doesn't mean your technique will always work. By the way, some students really hate this example. Yes, it gets some discussion on the internet, as well.

¹³The historical remarks in [11] show this is rather unfair; Hardy points out that even when Heaviside was happily using divergent series, some mathematicians had already explained why this worked. But it does make a good story.

14777:8 RM Corless

And, in the face of the paradoxes we began with, we really do need the support of logic, as Charles Dodgson would have emphatically advocated:

"When I use a word," Humpty Dumpty said, in rather a scornful tone, "it means just what I choose it to mean—neither more nor less."

"The question is," said Alice, "whether you can make words mean so many different things."

"The question is," said Humpty Dumpty, "which is to be master—that's all."

-Charles Dodgson, writing as Lewis Carroll, Through the Looking Glass

4 Why divergent series are sometimes useful

The real answer is that *infinity is just a model*, for some real situations. That might not be so clear as a bald statement; let's flesh that out a bit. Suppose we want to compute F(x) from equation (25) above, for some small x. We have several methods at our disposal. Let's look at the series

$$1 - x + 2x^2 + O(x^3). (27)$$

That $O(x^3)$ symbol really means something: it means that if you take the *limit as* $x \to 0$, the bits denoted by the $O(x^3)$ symbol will behave like x^3 , times a constant; mathematically, there exists a constant K so that this term is smaller than Kx^3 . This vanishes, compared to $1 - x + 2x^2$, as x gets closer to zero. Now, we don't really know what the constant is (a little bigger than 6 will work, but pretend we don't know that). But we are sure that for *small enough* x, the first three terms are going to give us an accurate answer. And so it does.

What if we want *more* accuracy? Well, in this model, that means you have to take x *closer* to zero. This somehow is less satisfactory than the notion of "convergence" where one can always do more work (take more terms) and get more accuracy, for a given x. But in practice we are *often satisfied* with the accuracy we have. In fact for this example one can take quite a few more terms (a thousand terms, before things start to get worse). But the principle stands: this interpretation of a series is not about $n \to \infty$ but rather $x \to 0$. That's all! As Hardy notes dryly in [11], this has been known for quite some time, now. Yet somehow not everyone knows this.

5 Some popular acceleration methods

The general field is called sequence acceleration because finding the limit of a series is the same as finding the limit of a sequence ¹⁴ of its partial sums. So, any method for the numerical evaluation of a limit of a sequence is likely to be interesting for series as well.

5.1 Aitken's Λ^2 method

Alexander Aitken was a very remarkable man. He had a powerful memory, and was an excellent mental calculator. This talent might seem quaint nowadays when anyone can ask their phone to compute whatever arithmetical question they like; but it was very useful in Aitken's day. He played the violin, as well, and took a violin with him when he served in the First World War; his stories of how he had to sneak this unofficial baggage with him as he travelled is a very human point in his memoirs *From Gallipoli to the Somme* (he served in both places). He was elected to the Royal Society for Literature for that work, by the way—as I said, a remarkable man.

He comes into this story because he invented a useful method for accelerating the convergence of many sequences. The method is simple to state: if the sequence one wishes to accelerate is

¹⁴You will notice that the Wikipedia link above used "series acceleration." This is another case where ordinary English and mathematical English don't match: to a non-mathematician, a sequence is just another word for series; but for math, we reserve the word series for, well, a sequence of partial sums. There's those shifty eyes again.

denoted by λ_n , then the accelerated sequence is

$$\mu_n = \lambda_{n+2} - \frac{(\lambda_{n+2} - \lambda_{n+1})^2}{(\lambda_{n+2} - \lambda_{n+1}) - (\lambda_{n+1} - \lambda_n)},$$
(28)

which is written in a deliberately unsimplified way to improve numerical stability of the iteration.

The reason it works is that *if* the convergence is of the form $\lambda_n = \mu + \alpha r^n$ for some r with |r| < 1 (and the smaller the better) then that combination of λ_n , λ_{n+1} , and λ_{n+2} eliminates everything but the μ (try to prove it yourself—my derivation took less than a page, and I found it rather fun). In practice, if the error has multiple geometric terms (e.g. $\mu + \alpha r^n + \beta s^n$ with |s| < |r| < 1) then this process will only eliminate the largest error. Nonetheless the process can be helpful (and, after all, you can do it again, as well).

Now let's consider some example routine kind of computation from Aitken's day—perhaps the computation of the largest eigenvalue of the following symmetric matrix.

$$\mathbf{A} = \begin{bmatrix} 152 & -24 & 55 & 159 & 70 \\ -24 & -122 & -98 & 89 & 0 \\ 55 & -98 & -160 & 41 & -25 \\ 159 & 89 & 41 & 100 & -12 \\ 70 & 0 & -25 & -12 & 90 \end{bmatrix} . \tag{29}$$

One common method then was *power iteration* together with the Rayleigh quotient. One chose a random vector \mathbf{u} and normalized it by taking $\mathbf{v}_0 = \mathbf{u}/\|\mathbf{u}\|_2$ so $\|\mathbf{v}_0\|_2 = 1$. When I asked for a random vector, Maple gave me

$$\mathbf{u} = \begin{bmatrix} -4 \\ 5 \\ -91 \\ -44 \\ -38 \end{bmatrix}$$
 (30)

but I won't bore you with the floating-point normalized vector. Then we iterate:

$$\lambda_n = \mathbf{v}_n^T \mathbf{A} \mathbf{v}_n \tag{31}$$

and put $\mathbf{u} = \mathbf{A}\mathbf{v}_n$ and normalize to get $\mathbf{v}_{n+1} = \mathbf{u}/\|\mathbf{u}\|_2$ so $\|\mathbf{v}_{n+1}\|_2 = 1$. I was somewhat unlucky in my choice of initial vector, but after 50 iterations the sequence λ_n is visibly converging, and the error in λ_{50} is about $-2.3 \cdot 10^{-4}$.

Aitken's accelerated sequence, however, achieves better error than that already by μ_{25} (which needs λ_{27}); and by μ_{48} the error is $1.6 \cdot 10^{-10}$.

Aitken acceleration is altogether a practical tool; and it can be used for acceleration of series convergence, too. It is connected to other extrapolation methods such as Padé methods [8, 7].

5.2 Stirling and averaging two estimates

Let's consider Stirling's formula for factorial, a famous and famously divergent series. Let us also consider its lesser-known cousin, which is beginning to be called DeMoivre's formula¹⁵.

Stirling's formula (that is, the formula popularly attributed to Stirling, even though it was DeMoivre who invented it) is

$$\ln z! \sim \ln\left(\sqrt{2}\,\sqrt{\pi}\right) + \left(z + \frac{1}{2}\right)\ln(z) - z + z\left(\sum_{n=1}^{\infty} \frac{B_{2n}}{2n\,(2n-1)\,z^{2n}}\right) \tag{32}$$

¹⁵I find it deeply amusing that Stirling invented equation (33) which is now beginning to be called DeMoivre's formula, and DeMoivre invented equation (32), which is called Stirling's formula. See [3, 6].

14777:10 RM Corless

where the B_{2n} are the *Bernoulli* numbers, named after Daniel Bernoulli (he says without checking—there were lots of Bernoullis, and lots of opportunity to get this wrong)¹⁶. To be fair to DeMoivre, he was the one who connected this formula to the Bernoulli numbers, and deserves some credit.

Stirling's *original* formula is below (he had a method for constructing it, and did not notice the Bernoulli numbers in it):

$$\ln z! \sim \ln\left(\sqrt{2}\sqrt{\pi}\right) + \left(z + \frac{1}{2}\right)\ln\left(z + \frac{1}{2}\right) - z - \frac{1}{2} - \left(z + \frac{1}{2}\right)\left(\sum_{n=1}^{\infty} \frac{\left(1 - 2^{1-2n}\right)B_{2n}}{2n\left(2n - 1\right)\left(z + \frac{1}{2}\right)^{2n}}\right) \tag{33}$$

Now, equation (33), which (to be redundant for certainty) is Stirling's *original* formula, is about twice as accurate as equation (32), which is the "formula popularly known as Stirling's formula." Moreover, the error is typically the opposite sign, which suggests something interesting: let's take a weighted average of the two. Let's take z = 6 and use just the terms up to but not including the sums, in each:

$$\ln 6! \sim \left(\sqrt{2}\sqrt{\pi}\right) + \left(6 + \frac{1}{2}\right)\ln(6) - 6$$

$$\approx 6.56537508318698, \tag{34}$$

which has error about $-1.4 \cdot 10^{-2}$, and

$$\ln 6! \sim \ln\left(\sqrt{2}\sqrt{\pi}\right) + \left(6 + \frac{1}{2}\right)\ln\left(6 + \frac{1}{2}\right) - 6 - \frac{1}{2}$$

$$\approx 6.58565268306498, \tag{35}$$

which has error about $6.4 \cdot 10^{-3}$. Now we take 2/3 times the last one and add 1/3 times the first one, weighting the average more heavily on the more better estimate: We get

$$ln 6! \approx 6.57889348310565$$
(36)

which has error about $-3.5 \cdot 10^{-4}$.

Voilá: a sequence acceleration method! Take *two* methods and combine them so that the leading error terms of each are eliminated. For z = 15, the errors are $-5.5 \cdot 10^{-3}$, $2.68 \cdot 10^{-3}$, and $-6 \cdot 10^{-5}$ (substantially better).

5.3 Richardson Extrapolation

Lewis Fry Richardson was a Quaker and a pacifist "conscientious objector". In the time of the First World War, pacifists were not treated well, and frequently accused of cowardice. Richardson himself wondered if his pacifism was principled or not, so he volunteered as a member of the Friends Ambulance Unit and served without weapons, but not without danger. Indeed, courage marked his character rather strongly; after the war, rather than continue to work in the Meteorological Service when it was taken over by the Defence Department (and the only people interested in his numerical weather prediction were "the poison gas people") he quit his job. He quit his job *in the Depression*.

He wrote an extremely influential book [16] which was the first to quantify war (by counting deaths on a logarithmic scale).

His presence here, however, is because of the "averaging" idea of the previous section. If we know that an approximation A_n of n terms to a quantity Q has an error expansion of the form

$$Q = A_n + \frac{c_2}{n^2} + \frac{c_4}{n^4} + \frac{c_6}{n^6} + \cdots$$
 (37)

 $^{^{16}\}mathrm{I}$ was wrong! $\textit{\it Jacob}$ Bernoulli. And also Seki Takakazu at very nearly the same time.

(and it turns out that whether that series for the error converges or not doesn't matter) then we have a very simple averaging process that we can use to eliminate those leading error terms.

Suppose we use n = N terms to estimate our quantity Q. Maybe N = 10, but let's just leave it symbolic for the moment. Then

$$Q = A_N + \frac{c_2}{N^2} + \frac{c_4}{N^4} + \frac{c_6}{N^6} + \cdots . (38)$$

Now use n = 2N terms and get another estimate

$$Q = A_{2N} + \frac{c_2}{4N^2} + \frac{c_4}{16N^4} + \frac{c_6}{64N^6} + \cdots$$
 (39)

This estimate is a better one; its error is about four times smaller. So, consider the average (-Q+4Q)/3 (yes, it's an average, even if one of the terms is negative).

$$Q = \frac{-Q + 4Q}{3} = \frac{-A_N + 4A_{2N}}{3} + \frac{-c_2/N^2 + 4c_2/(4N^2)}{3} + \frac{-c_4/N^4 + 4c_4/(16N^4)}{3} + \cdots$$

$$= \frac{4A_{2N} - A_N}{3} - \frac{3c_4/4}{N^4} + \cdots$$
(41)

and we have eliminated the $O(1/N^2)$ term, notably without even computing c_2 .

This is already helpful, but consider the triangular array below:

The first column is our basic approximation using n = N terms (first row), then n = 2N terms (second row), and so on. Going down the column, each new A_n takes twice as much work as the one above it.

In the second column, put the averages $R_{1,2n} = (4A_{2n} - A_n)/3$ using the entry to the left and above left; each of these entries costs only a single multiplication by 4, a subtraction, and a division by 3; this is generally trivial cost. But the error in this second column decreases not like $O(1/n^2)$ as we go down the column, but like $O(1/n^4)$.

If it worked once, do it again! The third column is the average $R_{2,2n} = (16R_{1,2n} - R_{1,n})/15$, which removes the $O(1/n^4)$ error term, leaving $O(1/n^6)$. Again production of this column requires only trivial arithmetic cost (in comparison with the first column of A_n 's). The fourth column is built using the average $R_{3,2n} = (2^6R_{2,2n} - R_{2,n})/(2^6 - 1)$, and the fifth using $R_{4,2n} = (2^8R_{3,2n} - R_{3,n})/(2^8 - 1)$, and so on.

The diagonal entries in the triangular array will converge to Q faster than any power of 1/N. When used for numerical integration starting with the trapezoidal rule or the midpoint rule, this technique is called "Romberg Integration" after Werner Romberg. His history, involving the Second World War, is worth reading, as well, but let's stick with Richardson here.

Here is an example of Richardson extrapolation to compute a (moderately) difficult sum. Consider

$$A_n = -\ln(n) - \frac{1}{2n} + \sum_{k=1}^n \frac{1}{k} \,. \tag{43}$$

Then Maple's asympt command says that $\gamma = A_n + c_2/n^2 + c_4/n^4 + \cdots$, where γ is the Euler–Mascheroni constant. Indeed, Euler knew this asymptotic expansion. This suggests that Richardson extrapolation is a decent method for computing this constant; in fact this constant is one of the harder ones to compute. In 1977 Richard Brent held the record, at just over 20,000 digits; as of May

14777:12 RM Corless

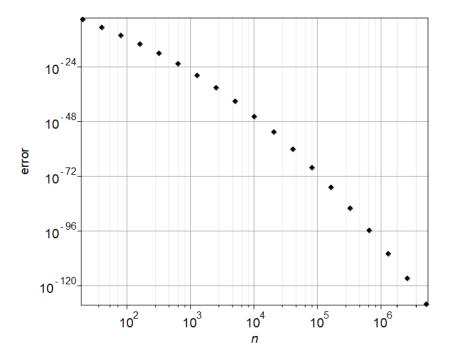


Fig. 1. Errors in Richardson extrapolation (diagonal entries in the table) for the computation of the Euler–Mascheroni constant by the sum (43). Notice the downward curve of the error on the log-log plot. If the error were $\varepsilon = K/n^p$ then plotting $\ln(\varepsilon) = -p \ln(n) + \ln K$ would be a straight line with slope -p.

2020 the record is now more than six hundred billion digits. When we make a table of A_n for n = 10, $20, \ldots, 2^{18} \cdot 10 = 2,621,440$, the computer takes 15 seconds to compute the first column. I worked in 150 Digit arithmetic.

The triangular table takes only milliseconds once the first column is done, however. And then the diagonal entries have the errors seen in Figure 1. The best error in the first column was about 10^{-11} ; but the best error in the triangular table is about 10^{-128} . Notice that we are combining estimates in such a way as to *cancel the errors*: we have to have all figures accurately enough in the sums in the first column, and use high enough precision arithmetic in our "trivial" recombinations, to accurately eliminate the error.

5.4 Euler summation

Euler¹⁷ had little patience with technicalities. He knew perfectly well what convergence was (so did Newton) but he was more interested in changing the rules (or, more properly, finding out which sets of rules gave interesting results). So for him, a sum like

$$1 - 1 + 1 - 1 + \cdots$$
 (44)

 $^{^{17}}I$ wanted to type the math in this paper in "euler" font, designed by Hermann Zapf for Donald Knuth, and used in my favourite discrete mathematics textbook, namely [10]. But for some reason the Δ symbol, which I need later, becomes a weird little backtick. I don't know whether to blame ACM or the euler package.

was more a challenge to his imagination than anything else. What *could* this mean? One method of solving problems is to try to generalize them, so Euler put in a parameter; we'll call it *z*.

$$1-z+z^2-z^3+\cdots \tag{45}$$

which reduces to the previous when we put z=1. Now, if |z|<1, this is a geometric series, and converges to 1/(1+z). Now we say "obviously what we *meant* to say with our $1-1+1-1+\cdots$ was to sum this geometric series and then let $z\to 1$." In which case, the answer is 1/2. This kind of makes sense because with one set of brackets it's 1 and another set it's 0 and this is sort of the average of the two. This method is often called *Abel* summation; in view of Abel's well-known condemnation of divergent series, it might seem surprising. But there it is. The location of the nearest pole in the complex plane becomes directly relevant.

The idea of Euler (Abel) summation can be used for the sum Maple "failed" at: Write

$$\zeta(s) = \sum_{k \ge 1} \frac{1}{k^s} \,, \tag{46}$$

the sum defining the Riemann zeta function if $\Re s > 1$. This is not a power series, though (it is a prototypical Dirichlet series) and so summation by this series is a little different. This function can be analytically continued around the pole at s = 1, by a reflection formula which (according to Hardy) Euler knew a hundred years before Riemann did; and $\zeta(-1) = -1/12$. We therefore write

$$\sum_{k>1} k = -\frac{1}{12} \tag{47}$$

and the joke in the cartoon linked above was born.

Going back to the geometric power series (45), we can be bolder (Euler was nothing if not bold) and differentiate with respect to *z*:

$$0 - 1 + 2z - 3z^{2} + \dots = -\frac{1}{(1+z)^{2}}$$
 (48)

and now when we set z = 1 we get the sum in equation (1), or rather, its negative.

This might make you uneasy—but all it's doing is changing the meaning that we ascribe to an infinite sum. Humpty Dumpty would approve.

Some questions might occur to you, though. Is this method at all consistent? Does it produce the "right" answer when the series converges? Or can we choose power series in two different ways for the same numerical sum and get two different answers? And if this method is so great, why don't we teach this instead of all those nasty ratio tests and things?

We'll leave those questions for the moment, but we remark that in Maple one can turn all those nasty convergence tests *off* by asking for "formal" treatment, as we have seen. If we turn formal treatment off, we can use assumptions:

> EnvFormal := false;

$$EnvFormal := false$$
 (49)

 $> sum(\frac{1}{n^s}, n = 1..infinity)$ assuming $\Re(s) > 1$;

$$\zeta(s)$$
 (50)

14777:14 RM Corless

5.5 The Euler-Maclaurin sum formula

Consider the (convergent) sum

$$\sum_{k>1} \frac{1}{k^2} \,. \tag{51}$$

Euler (through a truly magical method, with a terrifying disregard for convergence issues) identified this as $\pi^2/6$. But can we use it to compute $\pi^2/6$? The conventional way winds up being ridiculously slow: to get six digits of accuracy seems to require about a million terms, as can be seen by using the integral test to estimate the remainder after summing N terms.

Euler (and Maclaurin) turned that on its head: if we can estimate the error with an integral, why don't we use that to improve our sum?

$$\sum_{k>1} \frac{1}{k^2} = \sum_{k=1}^{N} \frac{1}{k^2} + \sum_{k>N+1} \frac{1}{k^2}$$
 (52)

and we can, using the left-hand and right-hand Riemann sums for the monotonically decreasing function $1/x^2$, say that

$$\int_{t=N+1}^{\infty} \frac{1}{t^2} dt < \sum_{k=N+1}^{\infty} \frac{1}{k^2} < \int_{t=N}^{\infty} \frac{1}{t^2} dt.$$
 (53)

You can use Student:-Calculus1:-RiemannSum with output=plot to draw pictures that will convince you of that. But the integrals are 1/(N+1) and 1/N, respectively; which gives us the "million terms" estimate.

But what if we averaged these? This would give us a trapezoidal rule estimate for the integral, which (because the function $1/t^2$ is convex up, is an upper bound). Then the midpoint rule estimate would give us a lower bound. Indeed this is what happened with Stirling's method earlier. Explicitly, if the midpoint rule estimate is (note the lower limit)

$$M_N = \sum_{k=N+1}^{\infty} \frac{1}{k^2}$$
 (54)

$$<\int_{t=N+1/2}^{\infty} \frac{1}{t^2} dt = \frac{1}{N+1/2}$$
 (55)

and the trapezoidal rule estimate is (with its different lower limit)

$$T_N = -\frac{1}{2(N+1)^2} + \sum_{k=N+1}^{\infty} \frac{1}{k^2}$$
 (56)

$$> \int_{t=N+1}^{\infty} \frac{1}{t^2} dt = \frac{1}{N+1} \,, \tag{57}$$

then we trap the sum between two bounds:

$$\frac{1}{N+1} + \frac{1}{2(N+1)^2} < \sum_{k=N+1}^{\infty} \frac{1}{k^2} < \frac{1}{N+1/2}$$
 (58)

which means

$$\sum_{k=1}^{N} \frac{1}{k^2} + \frac{1}{N+1} + \frac{1}{2(N+1)^2} < \sum_{k=1}^{\infty} \frac{1}{k^2} < \sum_{k=1}^{N} \frac{1}{k^2} + \frac{1}{N+1/2}$$
 (59)

and moreover the difference between those bounds, the width of the interval, is $1/(2(2N+1)(N+1)^2)$. If N=100 this width is less than $0.25 \cdot 10^{-6}$ so we don't need a million terms to get this accuracy, we only need N=100. Writing these sums concisely, the sum in the middle is 1.64493_{390}^{415} where we have used a common notation from interval arithmetic to show the lower and upper bounds.

Even better, we know the sum is closer to the right endpoint (because the midpoint rule is twice as accurate) so the average—weighted 2/3 on the right to 1/3 on the left—would give us an even better estimate.

Taking this to its asymptotic extreme by using better and better quadrature rules that use more and more derivative information at either end (the formulas are classical but not taught much anymore) gives us in the end the The Euler–Maclaurin Sum Formula:

$$\sum_{k=L}^{U} f(k) = \int_{t=L}^{U} f(t) dt - \sum_{j=1}^{\ell} \frac{B_j}{j!} \left(f^{(j-1)}(U) - f^{(j-1)}(L) \right) + R_{\ell}$$
 (60)

The remainder term R_{ℓ} can be bounded, if one likes; there is a formula at that Wikipedia link. Honestly, I can't remember the last time I ever bounded the remainder; nice to know that it's there if we need it, though.

For our example, Maple has eulermac, one of the oldest pieces of code in Maple; I believe it was written originally by Greg Fee, probably in about 1982. The call eulermac($1/k^2$, k=N+1..infinity) gets

$$\int_{N+1}^{\infty} \frac{1}{k^2} dk + \frac{1}{2(N+1)^2} + \frac{1}{6(N+1)^3} - \frac{1}{30(N+1)^5} + \frac{1}{42(N+1)^7} - O\left(\frac{1}{(N+1)^9}\right)$$
 (61)

(the integral isn't evaluated because we haven't told Maple that N > -1). Once we do, Maple tells us the integral is 1/(N+1), which, well, we knew.

Requiring six digit accuracy suggests that N = 10 or so; much better than a million terms! It is important to remember, though, to use the Euler–Maclaurin formula on the tail of the series, not the head (or the whole series).

For our example, here are the results using 10 terms.

$$\sum_{k=1}^{10} \frac{1}{k^2} = \frac{1968329}{1270080} \tag{62}$$

The Euler-Maclaurin correction in equation (61) gives

$$\frac{64908293}{682050985} \tag{63}$$

and adding equations (62) and (63) gives

$$\frac{40712555943643}{24750266143680} \approx 1.644934066862 \tag{64}$$

whereas $\pi^2/6 \approx 1.644934066848$, which is different only by about $1.4 \cdot 10^{-11}$.

The series on the right from the Euler–Maclaurin method in equation (61) is divergent, by the way, as one takes the number of Euler–Maclaurin terms ℓ to infinity. It is asymptotically correct as $N \to \infty$, however, and that turns out to be what is important. What is especially nice about this, though, is that N = 10 is big enough for this "limit to infinity" to be relevant.

This method is absolutely a workhorse of sequence acceleration, and can be used in many different ways. But, Maple has other tools: more simply, evalf/Sum(1/k^2, k=1..infinity) takes only 15ms to give 100 Digits of $\pi^2/6$. It could not do that without some kind of sequence acceleration. Let's look at how evalf/Sum does it.

14777:16 RM Corless

5.6 Levin's *u*-transform

Maple's evalf/Sum uses Levin's *u*-transform [13]. This method was actually invented over thirty years previous to that paper, and published by Bickley and Miller [2]; but Stigler's Law of Eponymy—namely, that no scientific discovery is named after its discoverer—is true more often than not. There is also a nice post on Stack Exchange about it.

Whoever it's named for, it is a kind of *weighted averaging* method. It works quite well—according to [17] it's one of the more effective methods—and has the advantage that it is simple to program.

How does it work? It assumes that the partial sums $s_n = \sum_{k=1}^n a_k$ have been computed, and that they satisfy an asymptotic error formula of the somewhat unexpected (but apparently commonly encountered) form

$$\frac{s-s_n}{a_n} = \alpha_{-1}n + \alpha_0 + \frac{\alpha_1}{n} + \cdots, \tag{65}$$

which is expressed as an asymptotic series *in powers of n* starting with 1 and decreasing. This is equation (19) in [2]. Then, multiplying by n^r for some r, and taking the (r + 2)nd difference, all the terms up to and including α_r on the right are eliminated:

$$\Delta^{(r+2)} \left(n^r \frac{s - s_n}{a_n} \right) \approx 0 \tag{66}$$

if we ignore terms α_{r+1} and higher. Solving for s, we get (if the denominator is not zero)

$$s = \frac{\Delta^{(r+2)}(n^r s_n/a_n)}{\Delta^{(r+2)}(n^r/a_n)} . \tag{67}$$

This is equation (20) in [2]. Later authors realized that one could equally well multiply by $(n + \beta)^r$ as n^r and sometimes this parameter improves matters (Maple apparently always uses $\beta = 1$). One can expand the forward differences, and we get binomial coefficients: e.g. $\Delta^3(f) = f_{n+3} - 3f_{n+2} + 3f_{n+1} - f_n$.

5.6.1 An example that works. Consider the Theodorus constant [5, 9], defined as

$$T = \sum_{k > 1} \frac{1}{k^{3/2} + k^{1/2}} \,. \tag{68}$$

Writing this as

 $> Sum(\frac{1}{k^{\frac{3}{2}} + k^{\frac{1}{2}}}, k = 1..infinity)$

$$\sum_{k=1}^{\infty} \frac{1}{k^{\frac{3}{2}} + \sqrt{k}} \tag{69}$$

and applying evalf to this inert Sum (with Digits=20) gives > evalf(%);

$$1.8600250792211903072$$
 (70)

In comparison, the Euler–Maclaurin sum approach, where we add up the first 100 terms and use an asymptotic series of order 15 for the tail, gives the same digits, apart from ending in 5 instead of ending in 2. The first method is certainly more convenient! There are many other examples of the success of evalf/Sum in [5], as well. See [6] for its use for Stirling's original series; it also works well for the formula popularly known as Stirling's.

In the Theodorus case, when we compute the asymptotics of $(s - s_N)/a_N$ we get

$$\frac{s - s_N}{a_N} \sim 2N + \frac{5}{6} - \frac{17}{120N} + \frac{13}{420N^2} + O\left(\frac{1}{N^3}\right)$$
 (71)

which is clearly of the correct form for Levin's *u*-transform.

But that's not all. We can subtract one divergent sum from another in order to get a very large *finite* sum very quickly. Consider the following Theodorus sum, from [5]:

> theta :=
$$n \rightarrow evalf(Sum(\arctan(\frac{1}{\operatorname{sqrt}(k)}), k = 1..n - 1));$$

$$\theta := n \mapsto evalf\left(\sum_{k=1}^{n-1} \arctan\left(\frac{1}{\sqrt{k}}\right)\right)$$
 (72)

> Digits := 30;

$$Digits := 30 \tag{73}$$

> CodeTools:-Usage(theta(10¹²));

$$1.99999784221717000722044572919 \times 10^{6} \tag{74}$$

Adding up one trillion terms to do that directly is not really possible; and the sum is divergent. This raises the question: *can* one write a finite sum as a difference of two divergent ones? Apparently, the answer is yes. Adding a trillion-and-one terms, and subtracting the two answers, gets an accurate arctan of $1/\sqrt{10^{12}}$. Blink, blink.

5.6.2 Examples that fail.

Khinchin's constant: The partial quotients a_n of the continued fraction

$$x = \frac{1}{a_1 + \frac{1}{a_2 + \frac{1}{a_3 + \frac{1}{$$

for almost every $x \in (0, 1)$, will have *geometric mean* given by *Khinchin's constant*:

$$\lim_{n \to \infty} \left(\prod_{k=1}^{n} a_n \right)^{1/n} = K = \prod_{k=1}^{\infty} \left(1 + \frac{1}{k(k+2)} \right)^{\log_2 k} . \tag{76}$$

These infinite products are convergent, although only just. Equivalently, the infinite sum

$$\ln K = \sum_{k>1} \log_2(k) \ln \left(1 + \frac{1}{k(k+2)} \right) \tag{77}$$

is also convergent. Since the terms decay like $\ln k/k^2$ one might think that Maple's evalf/Sum wouldn't have much more trouble with this than it did with Euler's sum for $\pi^2/6$. Sadly, this is not the case: applying evalf/Sum to the above returns unevaluated.

Evidently the error model

$$\frac{s-s_n}{a_n} = \alpha_{-1}n + \alpha_0 + \cdots \tag{78}$$

14777:18 **RM Corless**

does not hold true for this sum, and indeed when we check we see that there are logarithmic terms present, which we discover when we try the Euler-Maclaurin formula. The Euler-Maclaurin approach can be made to work, yielding (apart from the ln 2 factor)

$$s - s_N = \sum_{k > N+1} \ln k \ln \left(1 + \frac{1}{k(k+2)} \right) = \frac{1 + \ln N}{N} - \frac{1 + 3\ln N}{N^2} + \cdots$$
 (79)

so

$$\frac{s - s_N}{\ln N \ln(1 + 1/(N(N+2)))} \sim \frac{N}{\ln N} + \cdots$$
 (80)

and not $\alpha_{-1}N + \cdots$. This shows that Levin's *u*-transform can't work for this series.

Using the Euler–Maclaurin series to $O(N^{-13})$ and a thousand terms (which ought to have been overkill) and working in 30 Digit precision I managed to get K = 2.6854520010653064453097148404; the last three digits should have been 354. But there are faster ways to compute this constant, anyway: see [1].

A sum containing a Möbius function

The following is a much harder example, which I take from [4, p. 7]. Consider the following code.

```
P := s -> evalf(Sum(NumberTheory:-Moebius(k)*ln(Zeta(k*s))/k,
                    k = 1 .. infinity);
for n in [seq(combinat[fibonacci](k), k = 7 .. 14)] do
    Digits := n;
    (1 - P(2.0))^2 + 1 - P(4.0);
end do;
```

This computes a certain quantity with increasing precision but not, as it turns out, increasing accuracy. At every stage, it is wrong from the seventh decimal place on. This is the worst kind of computer output: wrong, but plausible. For the correct value, see Richard Brent's paper (cited above).

Let's look at a simpler example,

$$\sum_{k\geq 1} \frac{\mu(k)}{k^2} \,. \tag{81}$$

Here $\mu(k)$ is the Möbius function: it is 0 if the square of a prime divides k, it is -1 if k has an odd number of prime factors, and it is +1 if k has an even number of prime factors. Thus the tail of the series satisifies

$$\left| \sum_{k>N+1} \frac{\mu(k)}{k^2} \right| \le \sum_{k>N+1} \frac{1}{k^2} < \frac{1}{N}$$
 (82)

by use of the upper bound provided by the integral $\int_{x=N}^{\infty} dx/x^2$. We now ask Maple's evalf/Sum to evaluate the infinite sum in (81).

> alias(mu = NumberTheory:-Moebius):

$$> S := Sum(\frac{\operatorname{mu}(k)}{k^2}, k = 1..\operatorname{infinity});$$

$$S := \sum_{k=1}^{\infty} \frac{\mu(k)}{k^2} \tag{83}$$

> evalf(S);

> evalf[20](S);

$$0.60625850340136054422$$
 (85)

> evalf[150](evalf[50](S) - evalf[100](S))

$$-3.4013605442176870748299319727891156462585034013605 \times 10^{-51}$$
 (86)

The agreement of all of those sums, at all those different settings of Digits, suggests emphatically that the value of this (convergent) sum is 0.606258.... But the true value is 0.6079.

How do we know the correct answer? Slow, unaccelerated addition using exact arithmetic. Since the error when truncating at N terms is less than 1/N, then for error less than $5 \cdot 10^{-5}$ we have to take $N > 2 \cdot 10^4$. I took $N = 5 \cdot 10^5$ just to be even more sure; the sum took 30 seconds or so.

 $> slow := n \rightarrow add(\frac{mu(k)}{k^2}, k = 1..n)$: I removed a pointless warning message there about k becoming a local variable.

 $> s4 := slow(5 \cdot 10^5)$:

>
$$e4 := \frac{1}{5.0 \cdot 10^5} :$$

> $evalf[10](s4);$

> evalf[15](S);

The evalf/Sum result is wrong from the third decimal on. The difficulty here is the Möbius function. Here is what Richard Brent had to say, from an email to me about this:

By the way, I would be suspicious of any series acceleration method applied to a series whose signs depend on the Möbius function, since to all appearances these signs are random (The Riemann Hypothesis implies that they are "close" to random).

Right now, Maple's evalf/Sum will not warn you that it cannot handle the Möbius function. Levin's *u*-transform is an "irregular" summation method, which means it does not guarantee to always compute convergent sums correctly. But it is a *power tool*: use it with care.

A Maple Worksheet with these computations.

6 Concluding remarks

Maple can do more than just accelerate numerical sums, of course. Cesàro summation [11, Ch. 1] (also sometimes called Féjer summation, because Féjer used it for Fourier series) consists of taking the limit of averaged sums:

$$C := \lim_{u \to \infty} \frac{1}{u - \ell + 1} \sum_{n = \ell}^{u} s_n . \tag{89}$$

This will frequently work symbolically in Maple. It can give peculiar results, however: $\operatorname{try} \sum_{k=1}^n (-1)^{k+1} k$, which gives (as we saw earlier) $s_n = \frac{(-1)^{n+1}(n+1)}{2} - \frac{(-1)^{n+1}}{4} + \frac{1}{4}$ and $\lim_{N \to \infty} (\sum_{n=1..N} s_n)/N$ as -i/4..1/2 + i/4. Blink, again. Maple will sometimes return interval limits, but it was not even clear to me what that set of symbols means together; thanks to Preben Alsholm for enlightening me on that, on the Maple betatest forum. Notice the straight evalf/Sum result is 1/4, which agrees with Abel's method. It turns out that what Maple means by -i/4..1/2 + i/4 is the complex rectangle with lower left corner at 0 - i/4 and upper right corner at 1/2 + i/4. This rectangle contains the circle centred at 1/4 + 0i and of radius 1/4, which if you don't know N is an integer is the complete set $1/4 + e^{i\pi N}/4$ which you get when you write $(-1)^N = e^{i\pi N}$; this foray into the complex plane was unexpected.

This points out that our earlier worries about *consistency* of summation methods do need some attention. It turns out, though, that except for "dilution" of a series, we are mostly ok (as

14777:20 RM Corless

Euler was sure we would be). What is "dilution"? Write for example $1 - 1 + 1 - 1 + \cdots$ as the $1 - 1 + 0 + 1 - 1 + 0 + 1 - 1 + 0 + \cdots$, inserting an infinite amount of nothing into the series, and use Abel summation as follows:

$$\left(\sum_{k=0}^{\infty} x^{3k}\right) - \left(\sum_{k=0}^{\infty} x^{3k+1}\right) + 0 \cdot \left(\sum_{k=0}^{\infty} x^{3k+2}\right) = \frac{1}{x^2 + x + 1}$$
 (90)

which gives 1/3 as $x \to 1^-$, not 1/2. Note that similar reasoning makes $1 + 0 - 1 + 1 + 0 - 1 + \cdots = 2/3$, which is again different. Christopher Long was also having fun with this kind of thing (math Twitter was rather interesting, once upon a time).

Of course there is more. Borel summation is a kind of weighted average summation: instead of weighting each partial sum s_n the same, weight it by $z^n/n!$, and then take the limit as $z \to \infty$: so

$$B := \lim_{z \to \infty} \frac{\sum_{n \ge 0} s_n z^n / n!}{\sum_{n \ge 0} z^n / n!}$$
(91)

and the sum in the denominator is, of course, e^z . Borel summation is 'more powerful' than Abel summation or Cesàro summation are: consider $\sum_{k\geq 0} t^k$. Cesàro summation demands

$$C = \lim_{N \to \infty} \frac{1}{1 - t} + \frac{t^{N+2} - t}{(t - 1)^2 (N + 1)}$$
(92)

which exists if $|t| \le 1$ but $t \ne 1$, whilst the Borel sum is

$$B = \lim_{z \to \infty} \frac{1 - t e^{z(t-1)}}{1 - t} . \tag{93}$$

[Maple walked through some incomplete Gamma functions to get this far.] This limit exists so long as $\Re(t) < 1$ and in particular sums the series for all negative t.

We now return to Christopher Long's remarks about the failure of associativity and commutativity for divergent infinite sums. He also notes that this fails for some *convergent* sums, too: if a sum is *conditionally* but not *absolutely* convergent, that is, $\sum_{k\geq \ell} a_k$ converges but $\sum_{k\geq \ell} |a_k|$ does not, then simply by taking the terms in a different order we may make the sum turn out any way we please [15, Part I, Ch. 3, Sec. 5]. Consider the alternating harmonic sum $\sum_{k\geq 1} (-1)^k/k$. To make this come out to be, say, π instead of its "natural" sum $-\ln 2$, take first some positive terms 1/2, 1/4, and so on. Add them in that order until the sum is greater than π . Because the harmonic sum is divergent, we will eventually be able to do so. Now take the negative terms -1, -1/3, and so on, and add them to our previous sum until the sum is less than π . Now take from the remaining pile of positive terms and add until the sum is greater than π . Now take from the remaining pile of negative terms until the sum is less than π . Continue in this way and one may make the final sum as close as we please to π .

This conclusion is quite ridiculous. It is also true. Try programming it in Maple and see how many terms you need to get π to three place accuracy this way! (To get an error of less than 0.1 we need over ten thousand positive terms, but only six negative terms; an error of less than 0.05 takes more than twenty-one thousand positive terms and eleven negative terms; that's as far as I went).

For still more fun with series, see [15, Chapter 4]. There are some very interesting puzzles there! As a final note, floating-point summation can depend on the order you take the sums in. Generally speaking, it is better to start with the smallest terms. See [12], of course, for a discussion of "compensated summation" and "doubly compensated summation," but see also [19] and [18] for new developments. And, for a very interesting discussion of Euler–Maclaurin summation for hypergeometric functions, see Fredrik Johansson's blog.

Acknowledgments

I thank Richard Brent for some very useful observations on Levin's *u*-transform. Discussions with Paul DeMarco, Erik Postma, and Jürgen Gerhard of Maplesoft were interesting and helpful. Allan Wittkopf, also of Maplesoft, gave comments on an early draft. Annie Cuyt reminded me of Richardson extrapolation, which I certainly should not have forgotten. Preben Alsholm cleared up a question of mine about the return of the "complex interval" from the Cesàro sum.

David W. Boyd at UBC first taught me Euler–Maclaurin summation (and to use it on the tail of the series, not the head) in a memorable reading course in number theory, almost forty-five years ago. Thank you!

Partially supported by NSERC grant RGPIN-2020-06438, and partially supported by the grant PID2020-113192GB-I00 (Mathematical Visualization: Foundations, Algorithms and Applications) from the Spanish MICINN.

7 Links given earlier in the paper, gathered together

- (1) https://youtu.be/XFDM1ip5HdU: What does it feel like to invent math? 3Blue1Brown
- (2) https://twitter.com/pickover/status/1470554018942529541?s=20&t=cgyNKRYzjkDN4a0A_eXVrw: a math meme about divergent series
- (3) https://plato.stanford.edu/entries/paradox-zeno/: Stanford Encyclopedia entry on Zeno's paradoxes
- (4) https://en.wikipedia.org/wiki/Atalanta Atalanta
- (5) https://en.wikipedia.org/wiki/Leonhard_Euler: Euler
- (6) https://en.wikipedia.org/wiki/Series_acceleration: sequence acceleration
- (7) https://en.wikipedia.org/wiki/Alexander_Aitken: Alexander Aitken
- (8) https://en.wikipedia.org/wiki/Aitken's_delta-squared_process: Aitken's Δ^2 process
- (9) https://encyclopediaofmath.org/wiki/Extrapolation_algorithm: list of extrapolation methods
- (10) https://en.wikipedia.org/wiki/Seki_Takakazu: Seki Takakazu
- (11) https://en.wikipedia.org/wiki/Lewis_Fry_Richardson: Lewis Fry Richardson, of *Richardson extrapolation* (also Richardson iteration, which is a different thing).
- (12) https://en.wikipedia.org/wiki/Friends'_Ambulance_Unit the Ambulance unit Richardson served in in WWI
- (13) https://en.wikipedia.org/wiki/Werner_Romberg: Werner Romberg, of "Romberg integration", aka an application of Richardson iteration to quadrature.
- (14) https://en.wikipedia.org/wiki/Lorenzo_Mascheroni: Lorenzo Mascheroni, of the Euler–Mascheroni constant
- (15) https://en.wikipedia.org/wiki/Dirichlet_series: Dirichlet series
- (16) https://en.wikipedia.org/wiki/Basel_problem Euler's way of summing $\sum 1/k^2$
- (17) https://en.wikipedia.org/wiki/Euler\T1\textendashMaclaurin_formula: The Euler–Maclaurin Sum Formula
- (18) https://en.wikipedia.org/wiki/Stigler's_law_of_eponymy: Stigler's Law of Eponymy
- (19) https://math.stackexchange.com/questions/6625/levins-u-transformation: a nice post on Stack Exchange about Levin's *u*-transform
- (20) https://twitter.com/octonion/status/1481083645687472129?s=20&t=_APRJzu98At1NM66LVy85Q: Christopher Long on Twitter
- (21) https://fredrikj.net/blog/2010/07/Euler--Maclaurin-summation-of-hypergeometric-series/: Fredrik Johansson's blog
- (22) https://maple.cloud/app/6715514771734528/Sequence+Acceleration+Support+Material?key=85FCF504EDA
 The Maple worksheet with the computations reported in this paper.

14777:22 RM Corless

References

[1] David Bailey, Jonathan Borwein, and Richard Crandall. "On the Khintchine constant". In: *Mathematics of Computation* 66.217 (1997), pp. 417–431 (cit. on p. 18).

- [2] WG Bickley and JCP Miller. "The numerical summation of slowly convergent series of positive terms". In: *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science* 22.149 (1936), pp. 754–767 (cit. on p. 16).
- [3] Jonathan M. Borwein and Robert M. Corless. "Gamma and Factorial in the Monthly". In: *The American Mathematical Monthly* 125.5 (Apr. 2018), pp. 400–424. DOI: 10.1080/00029890.2018. 1420983 (cit. on p. 9).
- [4] Richard Brent. "Some Instructive Mathematical Errors". In: *Maple Transactions* 1.1 (Oct. 2021). DOI: 10.5206/mt.v1i1.14069. URL: https://doi.org/10.5206/mt.v1i1.14069 (cit. on p. 18).
- [5] Ewan Brinkman, Robert Corless, and Veselin Jungic. "The Theodorus Variation". In: *Maple Transactions* 1.2 (Nov. 2021). DOI: 10.5206/mt.v1i2.14500 (cit. on pp. 16, 17).
- [6] Robert M. Corless and Leili Rafiee Sevyeri. "Stirling's Original Asymptotic Series from a Formula Like One of Binet's and its Evaluation by Sequence Acceleration". In: *Experimental Mathematics* (Apr. 2019), pp. 1–8. DOI: 10.1080/10586458.2019.1593898 (cit. on pp. 9, 16).
- [7] Annie Cuyt. *Padé approximants for operators: theory and applications.* Vol. 1065. Springer, 2006 (cit. on p. 9).
- [8] Annie Cuyt and Luc Wuytack. *Nonlinear methods in numerical analysis.* Elsevier, 1987 (cit. on p. 9).
- [9] Philip J. Davis. *Spirals: From Theodorus to Chaos*. Wellesley, Massachussetts: AK Peters, 1993 (cit. on p. 16).
- [10] Ronald L. Graham, Donald E. Knuth, and Oren Patashnik. *Concrete Mathematics: A Foundation for Computer Science*. Reading: Addison-Wesley, 1989 (cit. on p. 12).
- [11] Godfrey Harold Hardy. *Divergent Series*. Clarendon: Oxford University Press, 1949 (cit. on pp. 1, 2, 7, 8, 19).
- [12] Nicholas J Higham. Accuracy and stability of numerical algorithms. SIAM, 2002 (cit. on p. 20).
- [13] David Levin. "Development of non-linear transformations for improving convergence of sequences". In: *International Journal of Computer Mathematics* 3.1-4 (1972), pp. 371–388 (cit. on p. 16).
- [14] Henri Poincaré. *New methods of celestial mechanics*. Vol. II. Original date of publication in 1892–1899. Edited and Introduced by Daniel Goroff. American Institute of Physics, 1993 (cit. on p. 7).
- [15] George Pólya and Gabor Szegő. *Problems and Theorems in Analysis: Series, integral calculus, theory of functions.* Vol. I. Springer, 1972 (cit. on p. 20).
- [16] Lewis F Richardson. *Statistics of deadly quarrels*. Vol. 10. Boxwood Press, 1960. URL: libkey.io/www.icpsr.umich.edu/web/ICPSR/studies/5407 (cit. on p. 10).
- [17] David A. Smith and William F. Ford. "Numerical comparisons of nonlinear convergence accelerators". In: *Mathematics of Computation* 38.158 (1982), pp. 481–499. DOI: 10.1090/s0025-5718-1982-0645665-1. URL: https://doi.org/10.1090/s0025-5718-1982-0645665-1 (cit. on p. 16).
- [18] Yong-Kang Zhu and Wayne B Hayes. "Algorithm 908: Online exact summation of floating-point streams". In: *ACM Transactions on Mathematical Software (TOMS)* 37.3 (2010), pp. 1–13 (cit. on p. 20).
- [19] Yong-Kang Zhu and Wayne B Hayes. "Correct rounding and a hybrid approach to exact floating-point summation". In: *SIAM Journal on Scientific Computing* 31.4 (2009), pp. 2981–3001 (cit. on p. 20).