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A new proof of the irrationality of $\zeta(2)$ and $\zeta(3)$ using Padé approximants

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Dedicated to the memory of R. Apéry

Abstract

Using Padé approximants to the asymptotic expansion of the error term for the series $\sum_{k=1}^{\infty} 1/k^2$, $\sum_{k=1}^{\infty} 1/k^3$, and $\sum_{k=1}^{\infty}(-1)^{k+1}/k^2$, we recover Apéry's sequences which allow one to prove the irrationality of $\zeta(2)$ and of $\zeta(3)$. The same method applied to the partial sums of $\ln(1-t)$ also proves the irrationality of certain values of the logarithm.

Keywords: Diophantine approximation; Padé approximant

1. Introduction

In June 1978 at the "Journées Arithmétiques de Marseille Luminy", Apéry [3] astonished his audience by sketching a proof of the irrationality of $\zeta(3)$. To that end Apéry produced the recurrence relation

$$n^3 u_n + (n-1)^3 u_{n-2} = (34n^3 - 51n^2 + 27n - 5)\, u_{n-1}, \quad n \geqslant 2, \tag{1}$$

and two independent solutions thereof, namely the sequence (b_n) of integers determined by the initial conditions $b_0 = 1$ and $b_1 = 5$; and the sequences (a_n) of rationals defined by the initial conditions $a_0 = 0$ and $a_1 = 6$.

Set $d_n = [1, 2, \ldots, n]$, where the brackets denote the lowest common multiple. Then it is not too difficult to check that the $2d_n^3 a_n$ and the b_n are integers for all $n \in \mathbb{N}$. Since, moreover, $\lim_{n\to\infty} a_n/b_n = \zeta(3)$, one may then confirm that the convergence is so fast that it entails the irrationality of $\zeta(3)$. Indeed, it follows that for every infinite sequence of rational numbers p/q there

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is an $\varepsilon > 0$ such that

$$|\zeta(3) - p/q| > q^{-\theta-\varepsilon}, \quad \theta = 13.41782 \ldots .$$

Specifically, the numbers a_n and b_n can be expressed as sums:

$$b_n = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2, \quad a_n = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2 c_{n,k}, \tag{2}$$

where

$$c_{n,k} = \sum_{m=1}^{n} \frac{1}{m^3} + \sum_{m=1}^{k} \frac{(-1)^{m-1}}{2m^3 \binom{n}{m} \binom{n+m}{m}}.$$

Apéry also pointed out that the irrationality of $\zeta(2)$ similarly follows from consideration of the recurrence relation

$$n^2 u'_n - (n-1)^2 u'_{n-2} = (11n^2 - 11n + 3) u'_{n-1}, \quad n \geqslant 2, \tag{3}$$

and two of its solutions, namely the sequence (b'_n) determined by $b'_0 = 1$ and $b'_1 = 3$, and the sequence (a'_n) determined by $a'_0 = 0$ and $a'_1 = 5$. Then the b'_n and $d_n^2 a'_n$ all are integers and $\lim_{n\to\infty} a'_n / b'_n = \zeta(2)$. The convergence is sufficiently fast to entail the irrationality of $\zeta(2)$. In this case one has

$$a'_n = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k} c'_{n,k}, \quad b'_n = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}, \tag{4}$$

where

$$c'_{n,k} = 2 \sum_{m=1}^{n} \frac{(-1)^{m-1}}{m^2} + \sum_{m=1}^{k} \frac{(-1)^{n+m-1}}{m^2 \binom{n}{m} \binom{n+m}{m}}.$$

For details of the argument, see [10] or [17]. See also [4] for a generalization of the recurrence relations (1) and (3).

A little later, a particularly straightforward and elegant proof of the irrationality of $\zeta(2)$ and $\zeta(3)$ was given by Beukers [5]. Beukers considers the integral

$$I = -\frac{1}{2} \int_0^1 \int_0^1 \frac{P_n^*(x) P_n^*(y) \ln(xy)}{1 - xy} \, \mathrm{d}x \, \mathrm{d}y,$$

where

$$P_n^*(z) = \frac{1}{n!} \frac{\mathrm{d}^n}{\mathrm{d}z^n} (z^n (1-z)^n)$$

is the shifted Legendre polynomial on $[0, 1]$, and shows that $I = b_n \zeta(3) - a_n$ where the a_n and b_n are Apéry's numbers for $\zeta(3)$ mentioned above. Much the same method proves the irrationality of $\zeta(2)$, namely

$$\int_0^1 \int_0^1 \frac{(1-y)^n}{1-xy} P_n(x) \, \mathrm{d}x \, \mathrm{d}y = b'_n \zeta(2) - a'_n,$$

where the a'_n and b'_n are Apéry's numbers for $\zeta(2)$.

In this paper, we find Padé approximations to the asymptotic expansion of the partial sums of $\zeta(2)$ and of $\zeta(3)$, and show that the numbers a_n, a'_n, b_n, and b'_n arise in a very natural manner.

2. Padé approximants

Set $f = \sum_{i=0}^{\infty} c_i t^i$. Then the Padé approximant $[m/n]$ to f is defined to be a rational fraction $\tilde{Q}_m/\tilde{P}_n$ whose denominator $\tilde{P}_n$ has degree n and whose numerator $\tilde{Q}_n$ has degree m, so that the expansion of $\tilde{Q}_m/\tilde{P}_n$ in ascending powers of t coincides with the expansion of f up to the degree $m+n$; that is,

$$\tilde{P}_n(t)f(t) - \tilde{Q}_m(t) = 0(t^{m+n+1}), \quad t \to 0. \tag{5}$$

The theory of Padé approximation is linked with the theory of orthogonal polynomials. Suppose we define a linear functional c acting on $\mathscr{P}$, the space of polynomials,

$$\begin{aligned} c\colon\ & \mathscr{P} \to \mathbb{R} \text{ (or } \mathbb{C}), \\ & x^i \to \langle c, x^i \rangle = c_i, \quad i = 0,1,2,\ldots, \end{aligned}$$

and

$$\begin{aligned} \text{if } p \in \mathbb{Z} \quad c^{(p)}\colon\ & \mathscr{P} \to \mathbb{R} \text{ (or } \mathbb{C}), \\ & x^i \to \langle c^{(p)}, x^i \rangle := \langle c, x^{i+p} \rangle = c_{i+p}, \quad i = 0,1,2,\ldots. \end{aligned}$$

Then the denominators of the Padé approximants $[m/n]$ satisfy the orthogonality property

$$\langle c^{(m-n+1)}, x^i P_n(x) \rangle = 0, \quad i = 0,1,2,\ldots,n-1,$$

where $P_n(x) = x^n \tilde{P}_n(x^{-1})$.

We now define the associated polynomials:

$$R_{n-1}(t) := \left\langle c^{(m-n+1)}, \frac{P_n(x) - P_n(t)}{x - t} \right\rangle, \quad R_{n-1} \in \mathscr{P}_{n-1}, \tag{6}$$

where $c^{(m-n+1)}$ acts on the variable x. Then

$$\tilde{Q}_m(t) = \left(\sum_{i=0}^{n-m} c_i t^i \right) \tilde{P}_n(t) + t^{m-n+1} \tilde{R}_{n-1}(t), \tag{7}$$

where $\tilde{R}_{n-1}(t) = t^{n-1} R_{n-1}(t^{-1})$ and $c_j = 0$ for $j < 0$.

If c admits an integral representation with a nondecreasing function α of bounded variation

$$c_i = \int_{\mathbb{R}} x^i \, \mathrm{d}\alpha(x), \tag{8}$$

then the theory of Gaussian quadrature shows that the polynomials P_n, orthogonal with respect to c, have all their roots in the support of the function α. Moreover

$$\underline{\text{error}}\colon\ f(t) - [m/n]_f(t) = \frac{t^{m+n+1}}{\tilde{P}_n^2(t)} c^{(m-n+1)} \left(\frac{P_n^2(x)}{1 - xt} \right). \tag{9}$$

The above expression for the error is understood as a formal one if c is only a formal linear functional (see [7, Ch. 3]); but if c admits the integral representation (8) then the error becomes

$$f(t) - [m/n]_f(t) = f(t) - \frac{\tilde{Q}_m(t)}{\tilde{P}_n(t)} = \frac{t^{m+n+1}}{\tilde{P}_n^2(t)} \int_{\mathbb{R}} x^{m-n+1} \frac{P_n^2(x)}{1-xt}\,\mathrm{d}\alpha(x). \tag{10}$$

In the particular case $m = n - 1$,

$$f(t) - [n-1/n]_f(t) = \frac{t^{2n}}{\tilde{P}_n^2(t)} \int_{\mathbb{R}} \frac{P_n^2(x)}{1-xt}\,\mathrm{d}\alpha(x). \tag{11}$$

Note that if $c_0 = 0$ then

$$[n/n]_f(t) = t[n-1/n]_{f/t}(t)$$

and if $c_0 = 0$ and $c_1 = 0$

$$[n/n]_f(t) = t^2[n-2/n]_{f/t^2}(t).$$

Remark. If α is a nondecreasing function on $\mathbb{R}$, then

$$f(t) \neq [m/n]_f(t) \quad \forall t^{-1} \in \mathbb{C} - \operatorname{supp}(\alpha).$$

3. Irrationality of $\zeta(2)$ and $\zeta(3)$

The Riemann-zeta function is defined as

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}, \tag{12}$$

where the Dirichlet series on the right-hand side of (12) is convergent for $\mathrm{Re}(s) > 1$ and uniformly convergent in any finite region where $\mathrm{Re}(s) \geqslant 1 + \delta$ with $\delta > 0$. It defines an analytic function for $\mathrm{Re}(s) > 1$. The importance of the ζ-function to number theory is exhibited by the Euler product

$$\zeta(s) = \prod_p (1 - p^{-s})^{-1},$$

where p runs through the primes. Riemann's formula

$$\zeta(s) = \frac{1}{\Gamma(s)} \int_0^{\infty} \frac{x^{s-1}}{\mathrm{e}^x - 1}\,\mathrm{d}x, \quad \mathrm{Re}(s) > 1, \tag{13}$$

where

$$\Gamma(s) = \int_0^{\infty} y^{s-1}\mathrm{e}^{-y}\,\mathrm{d}y \tag{14}$$

is the gamma function, and

$$\zeta(s) = \frac{e^{-i\pi s}\Gamma(1-s)}{2i\pi}\int_C \frac{z^{s-1}}{e^z - 1}\,dz, \tag{15}$$

where C is some path in $\mathbb{C}$, provides the analytic continuation of $\zeta(s)$ over the whole s-plane.

If we write (12) as

$$\zeta(s) = \sum_{k=1}^{n}\frac{1}{k^s} + \sum_{k=1}^{\infty}\frac{1}{(n+k)^s} \tag{16}$$

and set

$$\Psi_s(x) := \Gamma(s)\sum_{k=1}^{\infty}\left(\frac{x}{1+kx}\right)^s,$$

then

$$\zeta(s) = \sum_{k=1}^{n}\frac{1}{k^s} + \frac{1}{\Gamma(s)}\Psi_s(1/n). \tag{17}$$

The function

$$\sum_{k=1}^{\infty}\left(\frac{x}{1+kx}\right)^s$$

is known as the generalized ζ-function $\zeta(s, 1 + 1/x)$ [18, Ch. XIII]. So we get another expression for $\Psi_s(x)$,

$$\Psi_s(x) = \int_0^{\infty} u^{s-1}\frac{e^{-u/x}}{e^u - 1}\,du, \tag{18}$$

whose asymptotic expansion is

$$\Psi_s(x) = \sum_{k=0}^{\infty}\frac{B_k}{k!}\Gamma(k+s-1)\,x^{k+s-1}; \tag{19}$$

here the B_k are the Bernoulli numbers.

Outline of our method: In (17), we replace the unknown value $\Psi_s(1/n)$ by some Padé approximant to $\Psi_s(x)$, and get the approximation

$$\zeta(s) \approx \sum_{k=1}^{n}\frac{1}{k^s} + \frac{1}{\Gamma(s)}[p/q]_{\Psi_s}(x = 1/n). \tag{20}$$

We deal only with the particular case $p = q$.

3.1. Case $s = 2$

If $s = 2$ then (17) becomes

$$\zeta(2) = \sum_{k=1}^{n} \frac{1}{k^2} + \Psi_2(1/n) \tag{21}$$

and its approximation (20) becomes

$$\zeta(2) \approx \sum_{k=1}^{n} \frac{1}{k^2} + [p/q]_{\Psi_s}(x = 1/n), \tag{22}$$

where

$$\Psi_2(x) = \sum_{k=0}^{\infty} B_k x^{k+1} = B_0 x + B_1 x^2 + B_2 x^3 + \cdots \text{ (asymptotic expansion).} \tag{23}$$

The asymptotic expansion (23) is Borel-summable and its sum is

$$\Psi_2(x) = \int_0^{\infty} u \frac{e^{-u/x}}{e^u - 1} \, du. \tag{24}$$

Computation of $[p/q]_{\Psi_2}(x)$

The Padé approximants $[p/q]_{\Psi_2}$ are linked to the orthogonal polynomial with respect to the sequence $B_0, B_1, B_2 \ldots$. As in Section 2, we define the linear functional B acting on the space of polynomials by

$$B: \ \mathscr{P} \to \mathbb{R},$$
$$x^i \to \langle B, x^i \rangle = B_i, \ i = 0, 1 2, \ldots .$$

The orthogonal polynomials Ω_p satisfy

$$\langle B, x^i \Omega_p(x) \rangle = 0, \quad i = 0, 1, \ldots, p-1. \tag{25}$$

These polynomials were studied by Touchard [16, 6, 14, 15] and generalized by Carlitz [8, 9]. Wymann and Moser [20] found the expression

$$\Omega_p(x) = \sum_{2r \leqslant p} \binom{2x + p - 2r}{p - 2r} \binom{x}{r}^2 \tag{26}$$

for Ω_p, written by Carlitz as

$$\Omega_p(x) = (-1)^p \sum_{k=0}^{p} (-1)^k \binom{p}{k} \binom{p+k}{k} \binom{z+k}{k} = (-1)^p_3 F_2\left(\begin{matrix} -p, p+1, x+1 \\ 1, 1 \end{matrix}; 1 \right),$$

where ${}_pF_q$ is the hypergeometric function defined by

$${}_pF_q\left(\begin{matrix} a_1, \ldots, a_p \\ b_1, \ldots, b_q \end{matrix}; z \right) := \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_p)_k}{(b_1)_k \cdots (b_q)_k} \frac{z^k}{k!};$$

here $(a)_k := a(a+1) \cdots (a+k-1)$, with $(a)_0 := 1$, is Pochhammer's symbol.

From the identity

$$(-1)^p {}_3F_2\left(\begin{matrix}-p, p+1, z+1\\ 1,1\end{matrix}; 1\right) = {}_3F_2\left(\begin{matrix}-p, p+1, -z\\ 1,1\end{matrix}; 1\right), \tag{27}$$

we can give another expression for Ω_p:

$$\Omega_p(x) = {}_3F_2\left(\begin{matrix}-p, p+1, -x\\ 1,1\end{matrix}; 1\right) = \sum_{k=0}^{p} \binom{p}{k}\binom{p+k}{k}\binom{x}{k}. \tag{28}$$

Note that the Ω_p's are orthogonal polynomials and thus satisfy a three-term recurrence relation.

The associated polynomials Λ_p of degree $p-1$ are defined as

$$\Lambda_p(t) = \left\langle B, \frac{\Omega_p(x) - \Omega_p(t)}{x-t} \right\rangle, \tag{29}$$

where B acts on x.

From the expression (28) for Ω_p, we get the following formula for $\Lambda_p(t)$:

$$\Lambda_p(t) = \sum_{k=0}^{p} \binom{p}{k}\binom{p+k}{k} \left\langle B, \frac{\binom{x}{k} - \binom{t}{k}}{x-t} \right\rangle. \tag{30}$$

The recurrence relation for the Bernoulli numbers B_i, implies that

$$\left\langle B, \binom{x}{k} \right\rangle = \frac{(-1)^k}{k+1}. \tag{31}$$

Using the expression

$$\frac{\binom{x}{k} - \binom{t}{k}}{x-t} = \binom{t}{k} \sum_{i=1}^{k} \frac{\binom{x}{i-1}}{i\binom{t}{i}}, \tag{32}$$

on the Newton basis on $0, 1, \ldots, k-1$, we can write a compact formula for Λ_p:

$$\Lambda_p(t) = \sum_{k=1}^{p} \binom{p}{k}\binom{p+k}{k}\binom{t}{k} \sum_{i=1}^{k} \frac{(-1)^{i-1}}{i^2\binom{t}{i}} \in \mathscr{P}_{p-1}. \tag{33}$$

The approximation (22) for $\zeta(2)$ becomes

$$\zeta(2) \approx \sum_{k=1}^{n} \frac{1}{k^2} + t\left.\frac{\tilde{\Lambda}_p(t)}{\tilde{\Omega}_p(t)}\right|_{t=1/n} = \sum_{k=1}^{n} \frac{1}{k^2} + \frac{\Lambda_p(n)}{\Omega_p(n)}. \tag{34}$$

Lemma 3.1.

$$\frac{d_n}{i\binom{n}{i}} \in \mathbb{N}, \quad \forall i \in \{1, 2, \ldots, n\}.$$

Proof. We have the partial fraction decomposition

$$\frac{1}{i\binom{n}{i}} = \frac{(i-1)!}{n(n-1)\cdots(n-i+1)} = \sum_{j=0}^{i-1} \frac{A_j}{n-j}$$

with $A_j = \binom{i-1}{j}(-1)^{i-j-1}$. Since the A_j are integers and $n-j \in \{1,2,\dots,n\}$, we deduce that $[1,2,\dots,n]\, i\binom{n}{i}$ is an integer for all $i \in \{1,\dots,n\}$. □

A consequence of the above lemma is

$$d_n^2 \Lambda_p(n) \in \mathbb{N}, \quad \forall p \in \mathbb{N},$$

and

$$d_n^2 \Omega_p(n)\zeta(2) - d_n^2(S_n \Omega_p(n) + \Lambda_p(n)) \tag{35}$$

is a diophantine approximation of $\zeta(2)$, for all integers p, where S_n denotes the partial sums:

$$S_n = \sum_{k=1}^{n} \frac{1}{k^2}.$$

It remains to estimate the error for the Padé approximation:

$$\Psi_2(t) - [p/p]_{\Psi_2}(t) = \Psi_2(t) - [p-1/p]_{\Psi_2/t}(t).$$

Touchard found the integral representation for the linear functional B:

$$\langle B, x^k \rangle := B_k = -\mathrm{i}\frac{\pi}{2}\int_{\alpha-\mathrm{i}\infty}^{\alpha+\mathrm{i}\infty} x^k \frac{\mathrm{d}x}{\sin^2(\pi x)}, \quad -1 < \alpha < 0. \tag{36}$$

Thus the formula (11) becomes

$$t^{-1}\Psi_2(t) - [p-1/p]_{\Psi_2/t}(t) = -\mathrm{i}\frac{\pi}{2}\frac{t^{2p}}{\tilde{\Omega}_p^2(t)}\int_{\alpha-\mathrm{i}\infty}^{\alpha+\mathrm{i}\infty} \frac{\Omega_p^2(x)}{1-xt}\frac{\mathrm{d}x}{\sin^2(\pi x)} \tag{37}$$

and we obtain the error for the Padé approximant to Ψ_2:

$$\Psi_2(t) - [p/p]_{\Psi_2}(t) = -\mathrm{i}\frac{\pi}{2}\frac{t}{\Omega_p^2(t^{-1})}\int_{\alpha-\mathrm{i}\infty}^{\alpha+\mathrm{i}\infty} \frac{\Omega_p^2(x)}{1-xt}\frac{\mathrm{d}x}{\sin^2(\pi x)}, \tag{38}$$

whilst the error for the formula in (35) is

$$d_n^2 \Omega_p(n)\zeta(2) - d_n^2(S_n\Omega_p(n) + \Lambda_p(n)) = -d_n^2\,\mathrm{i}\frac{\pi}{2n}\frac{1}{\Omega_p(n)}\int_{\alpha-\mathrm{i}\infty}^{\alpha+\mathrm{i}\infty} \frac{\Omega_p^2(x)}{1-x/n}\frac{\mathrm{d}x}{\sin^2(\pi x)}. \tag{39}$$

If $p = n$, we get Apéry's numbers:

$$\Omega_n(n) = b_n' = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k} \tag{40}$$

and

$$S_n\Omega_n(n) + \Lambda_n(n) = \left(\sum_{k=1}^{n} \frac{1}{k^2}\right) b'_n + \sum_{k=1}^{n} \binom{n}{k}^2 \binom{n+k}{k} \sum_{i=1}^{k} \frac{(-1)^{i-1}}{i^2 \binom{n}{i}} = a'_n. \tag{41}$$

So the error in formula (39) is

$$d_n^2 b'_n \zeta(2) - d_n^2 a'_n = -d_n^2 \,\mathrm{i} \frac{\pi}{2n} \frac{1}{b'_n} \int_{\alpha - \mathrm{i}\infty}^{\alpha + \mathrm{i}\infty} \frac{\Omega_n^2(x)}{1 - x/n} \frac{\mathrm{d}x}{\sin^2(\pi x)}. \tag{42}$$

In order to prove the irrationality of $\zeta(2)$ we have to show that the right-hand side of (42) tends to 0 as n tends to infinity.

We have

$$\left| \int_{-1/2 - \mathrm{i}\infty}^{-1/2 + \mathrm{i}\infty} \frac{\Omega_n^2(x)}{1 - x/n} \frac{\mathrm{d}x}{\sin^2 \pi x} \right| \leqslant \left| \int_{-\infty}^{+\infty} \frac{\Omega_n^2(-\frac{1}{2} + \mathrm{i}u)}{1 + 1/2n} \frac{\mathrm{d}u}{\mathrm{ch}^2 \pi u} \right| \leqslant \frac{1}{1 + 1/2n} \langle B, \Omega_n^2(x) \rangle \tag{43}$$

since $\mathrm{ch}^2 \pi u$ is positive for $u \in \mathbb{R}$ and $\Omega_n^2(-\frac{1}{2} + \mathrm{i}u)$ real positive for u real (Ω_n has all its roots on the line $-\frac{1}{2} + \mathrm{i}\mathbb{R}$).

The quantity $\langle B, \Omega_n^2(x) \rangle$ can be computed from the three-term recurrence relation between the Ω_n's [16], namely

$$\langle B, \Omega_n^2(x) \rangle = \frac{(-1)^n}{2n+1}. \tag{44}$$

The diophantine approximation (42) satisfies

$$|d_n^2 b'_n \zeta(2) - d_n^2 a'_n| \leqslant d_n^2 \frac{\pi}{(2n+1)^2} \times \frac{1}{b'_n}. \tag{45}$$

In [13], Apéry proved that

$$b'_n = \mathrm{O}\left(\left(\frac{1+\sqrt{5}}{2}\right)^{5n}\right) \quad \text{when } n \to \infty, \tag{46}$$

and from a result concerning $d_n = [1, 2, \ldots, n]$, namely that $d_n \sim \mathrm{e}^n$ as $n \to \infty$, we get

$$\lim_{n \to \infty} |d_n^2 b'_n \zeta(2) - d_n^2 a'_n| = 0, \tag{47}$$

where the $d_n^2 b'_n$ and $d_n^2 a'_n$ are integers.

The relation (47) shows that $\zeta(2)$ is not rational and (46) gives a measure of irrationality for $\zeta(2)$: $\forall p \in \mathbb{N}$, $q \in \mathbb{N}$ sufficiently large relative to $\varepsilon > 0$

$$|\zeta(2) - p/q| > \frac{1}{q^{\theta + \varepsilon}} \quad \text{with } \theta' = 11.85, \ldots.$$

Remark. From relation (31), $\langle B, \binom{x}{k} \rangle = (-1)^k/(k+1)$, we can prove by induction that

$$\langle B, \gamma_k(x)\gamma_m(x) \rangle = (-1)^{k+m}/(k+m+1)!,$$

where $\gamma_i(x) = \binom{x}{i}(1/i!)$, and so another expression of Ω_n is

$$\Omega_n(x) = D_n \times \begin{vmatrix} \frac{1}{1!} & \frac{-1}{2!} & \cdots & \frac{(-1)^n}{n!} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{(-1)^{n-1}}{(n-1)!} & \frac{(-1)^n}{n!} & \cdots & \frac{(-1)^{2n-2}}{(2n-2)!} \\ \gamma_0(x) & \gamma_1(x) & \cdots & \gamma_n(x) \end{vmatrix},$$

D_n being a normalization factor. So, with the expression of the Padé approximant to the exponential function, the formula (28) may be recovered.

3.2. Case $s = 3$

If $s = 3$ then (17) becomes

$$\zeta(3) = \sum_{k=1}^{n} \frac{1}{k^3} + \frac{1}{2}\Psi_3(1/n), \tag{48}$$

and

$$\Psi_3(x) = \int_0^\infty u^2 \frac{e^{-u/x}}{e^u - 1}\, du, \tag{49}$$

with asymptotic expansion

$$\Psi_3(x) = \sum_{k=0}^{\infty} B_k(k+1)x^{k+2}. \tag{50}$$

Computation of $[p/p]_{\Psi_3}(x)$

We define the derivative of B by

$$\langle -B', x^k \rangle := \langle B, kx^{k-1} \rangle = kB_{k-1}, \quad k \geq 1,$$

$$\langle -B', 1 \rangle := 0,$$

so the functional B' admits an integral representation

$$\langle B', x^k \rangle = i\pi^2 \int_{\alpha - i\infty}^{\alpha + i\infty} x^k \frac{\cos(\pi x)}{\sin^3(\pi x)}\, dx, \quad -1 < \alpha < 0. \tag{51}$$

Let $(\Pi_n)_n$ be the sequence of orthogonal polynomial with respect to the sequence

$$-B'_0 := 0, \quad -B'_1 = B_0, \quad -B'_2 = 2B_1, \quad -B'_3 = 3B_2, \ldots .$$

The linear form B' is not definite and so the polynomials Π_n are not of exact degree n. More precisely, Π_{2n} has degree $2n$ and $\Pi_{2n+1} = \Pi_{2n}$. For the general theory of orthogonal polynomials with respect to a nondefinite functional, the reader is referred to [11]. If we take $\alpha = -\frac{1}{2}$, the weight $(\cos \pi x / \sin^3(\pi x))\,\mathrm{d}x$ on the line $-\frac{1}{2} + \mathrm{i}\mathbb{R}$ becomes $(\operatorname{sh}\pi t/\operatorname{ch}^3 \pi t)\,\mathrm{d}t$ on $\mathbb{R}$, which is symmetrical around 0. So $\Pi_{2n}(\mathrm{i}t - \frac{1}{2})$ only contains even powers of t and we can write

$$\Pi_{2n}(\mathrm{i}t - \tfrac{1}{2}) = W_n(t^2),$$

with W_n of exact degree n. Thus W_n satisfies

$$\int_{\mathbb{R}} W_n(t^2) W_m(t^2) \frac{t \operatorname{sh}\pi t}{\operatorname{ch}^3 \pi t}\,\mathrm{d}t = 0, \quad n \neq m. \tag{52}$$

The weight $t \operatorname{sh}\pi t/\operatorname{ch}^3 \pi t$ equals $(1/4\pi^3)\,(|\Gamma\,\frac{1}{2} + \mathrm{i}t)|^8 / |\Gamma(2\mathrm{i}t)|^2)$ and has been studied by Wilson [19, 2]. Indeed,

$$W_n(t^2) = {}_4F_3\left(\begin{matrix} -n, n+1, \frac{1}{2} + \mathrm{i}t, \frac{1}{2} - \mathrm{i}t \\ 1, 1, 1 \end{matrix}; 1\right)$$

and thus for $n \geqslant 0$,

$$\Pi_{2n}(y) = {}_4F_3\left(\begin{matrix} -n, n+1, y+1, -y \\ 1, 1, 1 \end{matrix}; 1\right) \tag{53}$$

$$= \sum_{k=0}^{n} \binom{n}{k}\binom{y+k}{k}\binom{y}{k}\binom{n+k}{k}. \tag{54}$$

Set Θ_{2n} the polynomial associated to Π_{2n}, thus

$$\Theta_{2n}(t) = \left\langle -B', \frac{\Pi_{2n}(x) - \Pi_{2n}(t)}{x - t} \right\rangle; \quad B' \text{ acts on } x.$$

For the computation of Θ_{2n}, we need to expand the polynomial:

$$\left\{\binom{x+k}{k}\binom{x}{k} - \binom{t+k}{k}\binom{t}{k}\right\}\Big/(x-t)$$

on the Newton basis with abscissæ $\{0, 1, -1, \ldots, n, -n\}$:

$$\left\{\binom{x+k}{k}\binom{x}{k} - \binom{t+k}{k}\binom{t}{k}\right\}\Big/(x-t) = \sum_{i=1}^{2k} \frac{N_{2k}(t)}{N_i(t)} \frac{N_{i-1}(x)}{[(i+1)/2]}, \tag{55}$$

where

$$N_0(x) = 1, \quad N_1(x) = \binom{x}{1}, \quad N_2(x) = \binom{x}{1}\binom{x+1}{1}, \ldots,$$

$$N_{2i}(x) = \binom{x}{i}\binom{x+i}{i}, \quad N_{2i+1}(x) = \binom{x}{i+1}\binom{x+i}{i}.$$

By induction, the values $\langle -B', N_i(x)\rangle$, with $i \in \mathbb{N}$, can be found from

$$\langle -B', N_{2i}(x)\rangle = 0; \quad \langle -B', N_{2i+1}(x)\rangle = \frac{(-1)^i}{(i+1)^2}.$$

Now using the linearity of B', we get the expression for Θ_{2n},

$$\Theta_{2n}(t) = \sum_{k=0}^{n} \binom{n}{k}\binom{n+k}{k} \sum_{i=1}^{k} \frac{(-1)^{i+1}}{i^3} \frac{\binom{t+k}{k-i}\binom{t-i}{k-i}}{\binom{k}{i}^2} \in \mathscr{P}_{2n-2}. \tag{56}$$

But Lemma 1 implies that

$$d_n^3\, \Theta_{2n}(t) \in \mathbb{N}, \quad \forall t \in \mathbb{N}.$$

The link between Π_{2n}, Θ_{2n} and the Apéry numbers a_n, b_n is given by taking $y = n$ in (54) and $t = n$ in (56). Thus

$$\Pi_{2n}(n) = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2 = b_n, \tag{57}$$

and

$$\left(\sum_{k=1}^{n} \frac{1}{k^3}\right) \Pi_{2n}(n) + \tfrac{1}{2}\Theta_{2n}(n) = a_n. \tag{58}$$

Of course, since Apéry's numbers are recovered by the method of Padé approximants, we could conclude with the end of the proof given in [3] or [10]. However, it seems more coherent to end the proof of the irrationality of $\zeta(3)$ with the error term for the Padé approximation.

To that end we recall (48),

$$\zeta(3) = \sum_{k=1}^{n} \frac{1}{k^3} + \frac{1}{2}\Psi_3\left(\frac{1}{n}\right),$$

in which we replace the unknown term $\Psi_3(1/n)$ by its Padé approximant $[2n/2n]_{\Psi_3}$ $(x = 1/n)$. That leads to the following approximation for $\zeta(3)$,

$$\zeta(3) \approx \sum_{k=1}^{n} \frac{1}{k^3} + \frac{1}{2}\frac{\Theta_{2n}(n)}{\Pi_{2n}(n)}, \tag{59}$$

and to the diophantine approximation,

$$2d_n^3 \Pi_{2n}(n)\zeta(3) - \left[\left(\sum_{k=1}^{n} \frac{1}{k^3}\right)2\Pi_{2n}(n) + \Theta_{2n}(n)\right]d_n^3, \tag{60}$$

since $\Pi_{2n}(n)$ and $d_n^3 \Theta_{2n}(n)$ are integers.

We now estimate the error in (59). The method is the same as for $\zeta(2)$ in (36)–(45). Firstly,

$$\Psi_3(t) - [2n/2n]_{\Psi_3}(t) = \Psi_3(t) - t^2[2n-2/2n]_{\Psi_3/t^2}(t) = \Psi_3(t) - \frac{\Theta_{2n}(t^{-1})}{\Pi_{2n}(t^{-1})}.$$

The integral representation for B' gives

$$\Psi_3(t) - [2n/2n]_{\Psi_3}(t) = -\frac{t\pi^2 \mathrm{i}}{\Pi_{2n}^2(t^{-1})} \int_{\alpha - \mathrm{i}\infty}^{\alpha + \mathrm{i}\infty} \frac{\Pi_{2n}^2(x)}{1 - xt} \frac{\cos \pi x}{\sin^3 \pi x}\, \mathrm{d}x, \tag{61}$$

which implies that

$$|\Psi_3(t) - [2n/2n]_{\Psi_3}(t)| \leqslant \frac{\pi^2 t}{\Pi_{2n}^2(t^{-1})} \frac{1}{1 + t/2} \int_{\mathbb{R}} W_n^2(u^2) \frac{u\, \mathrm{sh}\pi u}{\mathrm{ch}^3 \pi u}\, \mathrm{d}u, \quad t \in \mathbb{R}^+.$$

From the expression for the integral (see [19]) we get

$$|\Psi_3(1/n) - [2n/2n]_{\Psi_3}(1/n)| \leqslant \frac{4\pi^2}{(2n+1)^2 \Pi_{2n}^2(n)}. \tag{62}$$

The error term in the Padé approximation satisfies

$$\left| 2\zeta(3) - 2\sum_{k=1}^{n} \frac{1}{k^3} - [2n/2n]_{\Psi_3}(1/n) \right| \leqslant \frac{4\pi^2}{(2n+1)^2 \Pi_{2n}^2(n)} \tag{63}$$

so the error term in the diophantine approximation (60) is

$$\left| 2d_n^3 \Pi_{2n}(n)\zeta(3) - \left[2\left(\sum_{k=1}^{n} \frac{1}{k^3}\right)\Pi_{2n}(n) + \Theta_{2n}(n)\right]d_n^3 \right| \leqslant \frac{8\pi^2}{(2n+1)^2} \frac{d_n^3}{\Pi_{2n}(n)}. \tag{64}$$

Now $\Pi_{2n}(n) = b_n$ (see (57)) implies that

$$\Pi_{2n}(n) = 0((1+\sqrt{2})^{4n}) \quad \text{(see [10])}, \tag{65}$$

and so we get, recalling that $d_n \sim \mathrm{e}^n$ as $n \to \infty$,

$$|2d_n^3 b_n \zeta(3) - 2d_n^3 a_n| \to 0, \quad n \to \infty. \tag{66}$$

the point being that the $2d_n^3 b_n$ and $2d_n^3 a_n$ are integers.

The relation (66) shows that $\zeta(3)$ is irrational, and (65) gives a measure of irrationality of $\zeta(3)$ which is of course the same one as was found by Apéry.

4. Irrationality of $\ln(1+\lambda)$

In this section we use the same method as in the previous arguments. Thus we note

$$\ln(1+\lambda) = \sum_{k=1}^{n} (-1)^{k+1}\frac{\lambda^k}{k} + \sum_{k=1}^{\infty}\frac{(-1)^{k+n+1}}{k+n}\lambda^{k+n}. \tag{67}$$

From the formula

$$\frac{1}{k+n} = \int_0^\infty e^{-(k+n)v}\,dv,$$

we get an integral representation for the remainder term in (67):

$$\sum_{k=1}^{\infty}(-1)^{k+n+1}\frac{\lambda^{k+n}}{k+n} = (-1)^n\int_0^\infty \lambda^{n+1}\frac{e^{-nv}}{e^v+\lambda}\,dv. \tag{68}$$

If we expand the function

$$\frac{1+\lambda}{e^v+\lambda} = \sum_{k=0}^{\infty} R_k(-\lambda)\frac{v^k}{k!}, \tag{69}$$

where the $R_k(-\lambda)$'s are the Eulerian numbers [8], we get the asymptotic expansion

$$\sum_{k=1}^{\infty}(-1)^{k+n+1}\frac{\lambda^{k+n}}{k+n} = \frac{(-1)^n\lambda^{n+1}}{n(1+\lambda)}\left(\sum_{k=0}^{\infty} R_k(-\lambda)x^k\right)_{x=1/n}. \tag{70}$$

We now set

$$\Phi_1(x) = \sum_{k=0}^{\infty} R_k(-\lambda)x^k.$$

Carlitz has studied the orthogonal polynomials with respect to $R_0(-\lambda), R_1(-\lambda), \ldots$: If we define the linear function R by

$$\langle R, x^k\rangle := R_k(-\lambda),$$

then

$$\langle R, x^k P_n(x)\rangle = 0, \quad k = 0, 1, \ldots, n-1,$$

implies that

$$P_n(x) = \sum_{k=0}^{n}(1+\lambda)^k\binom{n}{k}\binom{x}{k} \quad [8].$$

The associated polynomials are

$$Q_n(t) = \sum_{k=0}^{n}(1+\lambda)^k\binom{n}{k}\left\langle R, \frac{\binom{x}{k}-\binom{t}{k}}{x-t}\right\rangle.$$

Carlitz showed that $\langle R, \binom{x}{k} \rangle = (-\lambda - 1)^{-k}$, and thus, using (32),

$$Q_n(t) = \sum_{k=0}^{n} (1+\lambda)^k \binom{n}{k} \binom{t}{k} \sum_{i=1}^{k} \frac{1}{i\binom{t}{i}} \left(\frac{-1}{\lambda+1} \right)^{i-1}. \tag{71}$$

If we set $\lambda = p/q$, with p and $q \in \mathbb{Z}$ and $t = n$, then $q^n d_n Q_n(n) \in \mathbb{Z}$.

An integral representation for $R_k(-\lambda)$,

$$R_k(-\lambda) = -\frac{1+\lambda}{2i\lambda} \int_{\alpha - i\infty}^{\alpha + i\infty} z^k \frac{\lambda^{-z}}{\sin \pi z} \, dz, \quad -1 < \alpha < 0, \tag{72}$$

is given by Carlitz, and thus

$$\Phi_1(x) = -\frac{1+\lambda}{2i\lambda} \int_{\alpha - i\infty}^{\alpha + i\infty} \frac{1}{1 - xz} \frac{\lambda^{-z}}{\sin \pi z} \, dz. \tag{73}$$

The orthogonal polynomial P_n satisfies

$$\int_{\alpha - i\infty}^{\alpha + i\infty} P_n^2(z) \frac{\lambda^{-z}}{\sin \pi z} \, dz = \frac{+2i}{i+\lambda} (-\lambda)^{n+1} \quad [8], \tag{74}$$

and since $\mathrm{Re}(\lambda^{-z}/\sin \pi z) > 0$ for $z \in -\frac{1}{2} + i\mathbb{R}$, we obtain an upper bound for the error in the Padé approximation to Φ_1,

$$x > 0, \quad |\Phi_1(x) - [n-1/n]_{\Phi_1}(x)| \leqslant \frac{\lambda^n}{|1 + x/2|}. \tag{75}$$

In particular, if $x = 1/n$, we get

$$\left| \Phi_1\left(\frac{1}{n}\right) - [n-1/n]_{\Phi_1}(1/n) \right| \leqslant \frac{|\lambda|^n}{1 + 1/2n}. \tag{76}$$

In (67) we now replace the remainder term by its Padé approximant

$$\ln(1+\lambda) \approx \sum_{k=1}^{n} (-1)^{k+1} \frac{\lambda^k}{k} + \frac{(-1)^n \lambda^{n+1}}{(1+\lambda)n} [n-1/n]_{\Phi_1}(1/n),$$

and obtain a diophantine approximation for $\ln(1 + p/q)$:

$$|\ln(1 + p/q) d_n q^{2n} P_n(n) - d_n q^{2n} T_n(n)| \leqslant \frac{\lambda^{2n} d_n q^{2n}}{(n+2) P_n(n)}, \tag{77}$$

where

$$T_n(n) = P_n(n) \sum_{k=1}^{n} (-1)^{k+1} \frac{p^k}{kq^k} + (-1)^{n+1} Q_n(n) q^n.$$

From the expression of $P_n(x)$ we can conclude that

$$P_n(n) = \sum_{k=0}^{n} (1+\lambda)^k \binom{n}{k}^2 = \text{Legendre}\left(n, \frac{2}{\lambda}+1\right)\lambda^n,$$

where Legendre(n, x) is the nth Legendre polynomial. Thus

$$\frac{T_n(n)}{P_n(n)} = [n/n]_{\ln(1+x)} \quad (x = 1). \tag{78}$$

So, the classical proof for the irrationality of $\ln(1 + p/q)$ based on Padé approximations to the function $\ln(1 + x)$, is recovered by the formula (77).

5. Proof of irrationality of $\zeta(2)$ with alternating series

Another expression for $\zeta(2)$ is

$$\zeta(2) = 2\sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^2}. \tag{79}$$

Suppose we write it as a sum

$$\zeta(2) = 2\sum_{k=1}^{n} \frac{(-1)^{k-1}}{k^2} + 2\sum_{k=1}^{\infty} \frac{(-1)^{k+n+1}}{(k+n)^2}. \tag{80}$$

We define Φ_2 by $\Phi_2(x) = \sum_{k=0}^{\infty} R_k(-1)(k+1)x^k$. So

$$\zeta(2) = 2\sum_{k=1}^{n} \frac{(-1)^{k-1}}{k^2} + \frac{(-1)^n}{n^2}\Phi_2(1/n). \tag{81}$$

With the same method as in Section 3.1, we can now show that the Padé approximant $[2n/2n]_{\Phi_2}(x)$ computed at $x = 1/n$ leads to Apéry' numbers a'_n and b'_n and so yields the irrationality of $\zeta(2)$ with the integral representation for the sequence $(kR_{k-1}(-1))_k$,

$$kR_{k-1}(-1) = -\frac{\pi(1+\lambda)}{2i\lambda}\int_{\alpha-i\infty}^{\alpha+i\infty} z^k \frac{\cos\pi z}{\sin^2\pi z}\,dz, \quad k \geqslant 1,$$

obtained from an integration by parts applied to (72).

6. Conclusion

The substitution of the asymptotic expansion of the remainder term of a series by its Padé approximant makes it possible to recover Apéry's numbers in a natural way, and also yields the standard proof for the irrationality of some logarithms. Unfortunately, the method does not generalize because the "weight function" underlying the functions Ψ_s, when $s \geqslant 4$, is no longer positive on its support. So, Padé approximation is not appropriate to constructing good approximations to $\zeta(s)$, $s \geqslant 4$. Nonetheless, the free choice of poles in the Padé-type approximation could lead to some interesting results.

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