Apéry Limits: Experiments and Proofs

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Abstract

An important component of Apéry's proof that $\zeta(3)$ is irrational involves representing $\zeta(3)$ as the limit of the quotient of two rational solutions to a three-term recurrence. We present various approaches to such Apéry limits and highlight connections to continued fractions as well as the famous theorems of Poincaré and Perron on difference equations. In the spirit of Jon Borwein, we advertise an experimental-mathematics approach by first exploring in detail a simple but instructive motivating example. We conclude with various open problems.

1 Introduction

A fundamental ingredient of Apéry's groundbreaking proof [Apé79] of the irrationality of $\zeta(3)$ is the binomial sum

$$A(n) = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2 \tag{1}$$

and the fact that it satisfies the three-term recurrence

$$(n+1)^3 u_{n+1} = (2n+1)(17n^2 + 17n + 5)u_n - n^3 u_{n-1} \tag{2}$$

with initial conditions $A(0) = 1$, $A(1) = 5$ — or, equivalently but more naturally, $A(-1) = 0$, $A(0) = 1$. Now let $B(n)$ be the solution to (2) with $B(0) = 0$ and $B(1) = 1$. Apéry showed that

$$\lim_{n\to\infty} \frac{B(n)}{A(n)} = \frac{\zeta(3)}{6} \tag{3}$$

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and that the rational approximations resulting from the left-hand side converge too rapidly to $\zeta(3)$ for $\zeta(3)$ itself to be rational. For details, we recommend the engaging account [Poo79] of Apéry's proof. In the sequel, we will not pursue questions of irrationality further. Instead, our focus will be on limits, like (3), of quotients of solutions to linear recurrences. Such limits are often called *Apéry limits* [AvSZ08], [Yan08].

Jon Borwein was a tireless advocate and champion of experimental mathematics and applied it with fantastic success. Jon was also a pioneer of teaching experimental mathematics, whether through numerous books, such as [BB08], or in the classroom (the second author is grateful for the opportunity to benefit from both). Before collecting known results on Apéry limits and general principles, we therefore find it fitting to explore in detail, in Section 2, a simple but instructive example using an experimental approach. We demonstrate how to discover the desired Apéry limit; and we show, even more importantly, how the exploratory process naturally leads us to discover additional structure that is helpful in understanding this and other such limits. We hope that the detailed discussion in Section 2 may be particularly useful to those seeking to integrate experimental mathematics into their own teaching.

After suggesting further examples in Section 3, we explain the observations made in Section 2 by giving in Section 4 some background on difference equations, introducing the Casoratian and the theorems of Poincaré and Perron. In Section 5, we connect with continued fractions and observe that, accordingly translated, many of the simpler examples are instances of classical results in the theory of continued fractions. We then outline in Section 6 several methods used in the literature to establish Apéry limits. To illustrate the limitations of these approaches, we conclude with several open problems in Sections 7 and 8.

Creative telescoping — including, for instance, Zeilberger's algorithm and the Wilf–Zeilberger (WZ) method — refers to a powerful set of tools that, among other applications, allow us to algorithmically derive the recurrence equations, like (2), that are satisfied by a given sum, like (1). In fact, as described in [Poo79], Zagier's proof of Apéry's claim that the sums (1) and (17) both satisfy the recurrence (2) may be viewed as giving birth to the modern method of creative telescoping. For an excellent introduction we refer to [PWZ96]. In the sequel, all claims that certain sums satisfy a recurrence can be established using creative telescoping.

2 A motivating example

At the end of van der Poorten's account [Poo79] of Apéry's proof, the reader is tasked with the exercise to consider the sequence

$$A(n) = \sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k} \tag{4}$$

and to apply to it Apéry's ideas to conclude the irrationality of $\ln(2)$. In this section, we will explore this exercise with an experimental mindset but without using the general tools and connections described later in the paper. In particular, we hope that the outline below could be handed out in an undergraduate experimental-math class and that the students could (with some help, depending on their familiarity with computer algebra systems) reproduce the steps, feel intrigued by the observations along the way, and then apply by themselves a similar approach to explore variations or extensions of this exercise. Readers familiar with the topic may want to skip ahead.

The numbers (4) are known as the central Delannoy numbers and count lattice paths from $(0,0)$ to (n,n) using the steps $(0,1)$, $(1,0)$ and $(1,1)$. They satisfy the recurrence

$$(n+1)u_{n+1} = 3(2n+1)u_n - nu_{n-1} \tag{5}$$

with initial conditions $A(-1) = 0$, $A(0) = 1$. Now let $B(n)$ be the sequence satisfying the same recurrence with initial conditions $B(0) = 0$, $B(1) = 1$. Numerically, we observe that the quotients $Q(n) = B(n)/A(n)$,

$$(Q(n))_{n \geq 0} = \left(0, \frac{1}{3}, \frac{9}{26}, \frac{131}{378}, \frac{445}{1284}, \frac{34997}{100980}, \frac{62307}{179780}, \frac{2359979}{6809460}, \ldots\right),$$

appear to converge rather quickly to a limit

$$L := \lim_{n \to \infty} Q(n) = 0.34657359\ldots$$

When we try to estimate the speed of convergence by computing the difference $Q(n) - Q(n-1)$ of consecutive terms, we find

$$(Q(n) - Q(n-1))_{n \geq 1} = \left(\frac{1}{3}, \frac{1}{78}, \frac{1}{2457}, \frac{1}{80892}, \frac{1}{2701215}, \frac{1}{90770922}, \ldots\right).$$

This suggests the probably-unexpected fact that these are all reciprocals of integers. Something interesting must be going on here! However, a cursory look-up of the denominators in the *On-Line Encyclopedia of Integer Sequences* (OEIS) [OEIS] does not result in a match. (Were we to investigate the factorizations of these integers, we might at this point discover the case $x = 1$ of (8). But we hold off on exploring that observation and continue to focus on the speed of convergence.) By, say, plotting the logarithm of $Q(n) - Q(n-1)$ versus n, we are led to realize that the number of digits to which $Q(n-1)$ and $Q(n)$ agree appears to increase (almost perfectly) linearly. This means that $Q(n)$ converges to L exponentially.

Exercise. For a computational challenge, quantify the exponential convergence by conjecturing an exact value for the limit of $(Q(n+1) - Q(n))/(Q(n) - Q(n-1))$ as $n \to \infty$. Then connect that value to the recurrence (5).

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At this point, we are confident that, say,

$$Q(50) = 0.34657359027997265470861606072908828403775006718\ldots \qquad (6)$$

agrees with the limit L to more than 75 digits. The ability to recognize constants from numerical data is a powerful asset in an experimental mathematician's toolbox. Several approaches to constant recognition are lucidly described in [BB08, Section 6.3]. The crucial ingredients are integer relation algorithms such as PSLQ or those based on lattice reduction algorithms like LLL. Readers new to constant recognition may find the *Inverse Symbolic Calculator* of particular value. This web service, created by Jon Borwein, Peter Borwein and Simon Plouffe, automates the constant-recognition process: it asks for a numerical approximation as input and determines, if successful, a suggested exact value. For instance, given (6), it suggests that

$$L = \frac{1}{2}\ln(2),$$

which one can then easily confirm further to any desired precision. Of course, while this provides overwhelming evidence, it does not constitute a proof. Given the success of our exploration, a natural next step would be to repeat this inquiry for the sequence of polynomials

$$A_x(n) = \sum_{k=0}^{n} \binom{n}{k}\binom{n+k}{k} x^k, \qquad (7)$$

which satisfies the recurrence (5) with the term $3(2n+1)$ replaced by $(2x+1)(2n+1)$. An important principle to keep in mind here is that introducing an additional parameter, like the x in (7), can make the underlying structure more apparent; and this may be crucial both for guessing patterns and for proving our assertions. Now define the secondary solution $B_x(n)$ satisfying the recurrence with $B_x(0) = 0$, $B_x(1) = 1$. Then, if we compute the difference of quotients $Q_x(n) = B_x(n)/A_x(n)$ as before, we find that

$$(Q_x(n) - Q_x(n-1))_{n \geq 1} = \left(\frac{1}{1+2x}, \frac{1}{2(1+2x)(1+6x+6x^2)}, \cdots \right).$$

Extending our earlier observation, these now appear to be the reciprocals of polynomials with integer coefficients. Moreover, in factored form, we are immediately led to conjecture that

$$Q_x(n) - Q_x(n-1) = \frac{1}{nA_x(n)A_x(n-1)}. \qquad (8)$$

Note that, since $Q_x(0) = 0$, this implies

$$Q_x(N) = \sum_{n=1}^{N}(Q_x(n) - Q_x(n-1)) = \sum_{n=1}^{N} \frac{1}{nA_x(n)A_x(n-1)} \qquad (9)$$

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and hence provides another way to compute the limit $L_x = \lim_{n\to\infty} Q_x(n)$ as

$$L_x = \sum_{n=1}^{\infty} \frac{1}{nA_x(n)A_x(n-1)},$$

which avoids reference to the secondary solution $B_x(n)$.

Can we experimentally identify the limit L_x? One approach could be to select special values for x and then proceed as we did for $x = 1$. For instance, we might numerically compute and then identify the following values:

	$x = 1$	$x = 2$	$x = 3$
L_x	$\frac{1}{2}\ln(2)$	$\frac{1}{2}\ln\left(\frac{3}{2}\right)$	$\frac{1}{2}\ln\left(\frac{4}{3}\right)$

We are lucky and the emerging pattern is transparent, suggesting that

$$L_x = \frac{1}{2}\ln\left(1 + \frac{1}{x}\right). \tag{10}$$

A possibly more robust approach to identifying L_x empirically is to fix some values of n and then expand the $Q_x(n)$, which are rational functions in x, into power series. If the initial terms of these power series appear to converge as $n \to \infty$ to identifiable values, then it is reasonable to expect that these values are the initial terms of the power series for the limit L_x. However, expanding around $x = 0$, we quickly realize that the power series

$$Q_x(n) = \sum_{k=0}^{\infty} q_k^{(n)} x^k$$

do not stabilize as $n \to \infty$, but that the coefficients increase in size: for instance, we find empirically that

$$q_1^{(n)} = -n(n+1), \quad q_2^{(n)} = \frac{1}{8}n(n+1)(5n^2 + 5n + 6),$$

and it appears that, for $k \geq 1$, $q_k^{(n)}$ is a polynomial in n of degree $2k$. Expanding the $Q_x(n)$ instead around some nonzero value of x — say, $x = 1$ — is more promising. Writing

$$Q_x(n) = \sum_{k=0}^{\infty} r_k^{(n)}(x-1)^k,$$

we observe empirically that

$$\left(\lim_{n\to\infty} r_k^{(n)}\right)_{k\geq 1} = \left(-\frac{1}{4}, \frac{3}{16}, -\frac{7}{48}, \frac{15}{128}, \ldots\right).$$

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Once we realize that the denominators are multiples of k, it is not difficult to conjecture that

$$\lim_{n \to \infty} r_k^{(n)} = (-1)^k \frac{2^k - 1}{k \cdot 2^{k+1}} \tag{11}$$

for $k \geq 1$. From our initial exploration, we already know that $\lim_{n \to \infty} r_0^{(n)} = \frac{1}{2} \ln(2)$ but we could also have (re)guessed this value as the formal limit of the right-hand side of (11) as $k \to 0$ (forgetting that k is really an integer). Anyway, (11) suggests that

$$L_x = L_1 + \sum_{k=1}^{\infty} (-1)^k \frac{2^k - 1}{k \cdot 2^{k+1}} (x - 1)^k = \frac{1}{2} \ln(2) + \frac{1}{2} \ln \left(\frac{x+1}{2x} \right),$$

leading again to (10). Finally, our life is easiest if we look at the power series of $Q_x(n)$ expanded around $x = \infty$. In that case, we find that the power series of $Q_x(n)$ and $Q_x(n+1)$ actually agree through order x^{-2n}. In hindsight — and to expand our experimental reach, it is always a good idea to reflect on the new data in front of us — this is a consequence of (8) and the fact that $A_x(n)$ has degree n in x (so that $A_x(n)A_x(n-1)$ has degree $2n-1$). Therefore, from just the case $n = 3$ we are confident that

$$L_x = Q_x(3) + O(x^{-7}) = \frac{1}{2x} - \frac{1}{4x^2} + \frac{1}{6x^3} - \frac{1}{8x^4} + \frac{1}{10x^5} - \frac{1}{12x^6} + O(x^{-7}).$$

At this point the pattern is evident, and we arrive, once more, at the conjectured formula (10) for L_x.

3 Searching for Apéry limits

Inspired by the approach laid out in the previous section, one can search for other Apéry limits as follows:

(a) Pick a binomial sum $A(n)$ and, using creative telescoping, compute a recurrence satisfied by $A(n)$.

(b) Compute the initial terms of a secondary solution $B(n)$ to the recurrence.

(c) Try to identify $\lim_{n \to \infty} B(n)/A(n)$ (either numerically or as a power series in an additional parameter).

It is important to realize, as will be indicated in Section 5, that if the binomial sum $A(n)$ satisfies a three-term recurrence, then the Apéry limit can be expressed as a continued fraction and compared to the (rather staggering) body of known results [Wal48], [JT80], [CPV+08], [BvSZ14].

Of course, the final step is to prove and/or generalize those discovered results that are sufficiently appealing. One benefit of an experimental approach is that we can discover

results, connections and generalizations, as well as discard less-fruitful avenues, before (or while!) working out a complete proof. Ideally, the processes of discovery and proof inform each other at every stage. For instance, experimentally finding a generalization may well lead to a simplified proof, while understanding a small piece of a puzzle can help set the direction of follow-up experiments. Jon Borwein's extensive legacy is filled with such delightful examples.

Of course, one could just start with a recurrence; however, selecting a binomial sum increases the odds that the recurrence has desirable properties (it is a difficult open problem to "invert creative telescoping" in the sense of producing a binomial sum satisfying a given recurrence). Some simple suggestions for binomial sums, as well as the corresponding Apéry limits, are as follows (in each case, we choose the secondary solution with initial conditions $B(0) = 0$, $B(1) = 1$).

$\displaystyle\sum_{k=0}^{n}\binom{n}{2k}x^k$	$\dfrac{1}{\sqrt{x}}$ (around $x = 1$)
$\displaystyle\sum_{k=0}^{n}\binom{n-k}{k}x^k$	$\dfrac{2}{1+\sqrt{1+4x}}$ (around $x = 0$)
$\displaystyle\sum_{k=0}^{n}\binom{n}{k}\binom{n-k}{k}x^k$	$\dfrac{\arctan\left(\sqrt{4x-1}\right)}{\sqrt{4x-1}}$ (around $x = \frac{1}{4}$)

Example 1. Setting $x = 1/2$ in the last instance leads to the limit being $\arctan(1) = \pi/4$ and therefore to a way of computing π as

$$\pi = \lim_{n\to\infty} \frac{4B(n)}{A(n)},$$

where $A(n)$ and $B(n)$ both solve the recurrence $(n+1)u_{n+1} = (2n+1)u_n + nu_{n-1}$ with $A(-1) = 0$, $A(0) = 1$ and $B(0) = 0$, $B(1) = 1$. In an experimental-math class, this could be used to segue into the fascinating world of computing π, a topic to which Jon Borwein, sometimes admiringly referred to as Dr. Pi, has contributed so much — one example being the groundbreaking work in [BB87] with his brother Peter. Let us note that this is not a new result. Indeed, with the substitution $z = \sqrt{4x-1}$, it follows from the discussion in Section 5 that the Apéry limit in question is equivalent to the well-known continued fraction

$$\arctan(z) = \frac{z}{1+}\frac{1^2z^2}{3+}\frac{2^2z^2}{5+}\cdots\frac{n^2z^2}{(2n+1)+}\cdots$$

[Wal48, p. 343, eq. (90.3)]. The reader finds, for instance, in [BCP05, Theorem 2] that this continued fraction, as well as corresponding ones for the tails of $\arctan(z)$, is a special case of Gauss' famous continued fraction for quotients of hypergeometric functions $_2F_1$. We hope that some readers and students, in particular, enjoy the fact that they are able to rediscover such results themselves.

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Example 2. For more challenging explorations, the reader is invited to consider the binomial sums

$$A_x(n) = \sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k}^2 x^k, \quad \sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k}^3 x^k,$$

and to compare the findings with those by Zudilin [Zud07] who obtains simultaneous approximations to the logarithm, dilogarithm and trilogarithm.

Example 3. Increasing the level of difficulty further, one may consider, for instance, the binomial sum

$$A(n) = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{3k}{n},$$

which is an appealing instance, randomly selected from many others, for which Almkvist, van Straten and Zudilin [AvSZ08, Section 4, #219] have numerically identified an Apéry limit (in this case, depending on the initial conditions of the secondary solution, the Apéry limit can be empirically expressed as a rational multiple of π^2 or of the L-function evaluation $L_{-3}(2)$, or, in general, a linear combination of those). To our knowledge, proving the conjectured Apéry limits for most cases in [AvSZ08, Section 4], including the one above, remains open. While the techniques discussed in Section 6 can likely be used to prove some individual limits, it would be of particular interest to establish all these Apéry limits in a uniform fashion.

Choosing an appropriate binomial sum as a starting point, the present approach could be used to construct challenges for students in an experimental-math class, with varying levels of difficulty (or that students could explore themselves with minimal guidance). As illustrated by Example 1, simple cases can be connected with existing classical results, and opportunities abound to connect with other topics such as hypergeometric functions, computer algebra, orthogonal polynomials, or Padé approximation, which we couldn't properly discuss here. However, much about Apéry limits is not well understood and we believe that more serious investigations, possibly along the lines outlined here, can help improve our understanding. To highlight this point, we present in Sections 7 and 8 several specific open problems and challenges.

4 Difference equations

In our initial motivating example, we started with a solution $A(n)$ to the three-term recurrence (5) and considered a second, linearly independent solution $B(n)$ of that same recurrence. We then discovered in (9) that

$$B(n) = A(n) \sum_{k=1}^{n} \frac{1}{kA(k)A(k-1)}.$$

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That the secondary solution is expressible in terms of the primary solution is a consequence of a general principle in the theory of difference equations, which we outline in this section. For a gentle introduction to difference equations, we refer to [KP01].

Consider the general homogeneous linear difference equation

$$u(n + d) + p_{d-1}(n)u(n + d - 1) + \cdots + p_1(n)u(n + 1) + p_0(n)u(n) = 0 \qquad (12)$$

of order d, where we normalize the leading coefficient to 1. If $u_1(n), \ldots, u_d(n)$ are solutions to (12), then their *Casoratian* $w(n)$ is defined as

$$w(n) = \det \begin{bmatrix} u_1(n) & u_2(n) & \cdots & u_d(n) \\ u_1(n+1) & u_2(n+1) & \cdots & u_d(n+1) \\ \vdots & \vdots & \ddots & \vdots \\ u_1(n+d-1) & u_2(n+d-1) & \cdots & u_d(n+d-1) \end{bmatrix}.$$

This is the discrete analog of the Wronskian that is discussed in most introductory courses on differential equations. By applying the difference equation (12) to the last row in $w(n+1)$ and then subtracting off multiples of earlier rows, one finds that the Casoratian satisfies [KP01, Lemma 3.1]

$$w(n + 1) = (-1)^d p_0(n)w(n)$$

and hence

$$w(n) = (-1)^{dn} p_0(0)p_0(1) \cdots p_0(n - 1)w(0). \qquad (13)$$

In the case of second order difference equations ($d = 2$), we have

$$\frac{u_2(n+1)}{u_1(n+1)} - \frac{u_2(n)}{u_1(n)} = \frac{u_1(n)u_2(n+1) - u_1(n+1)u_2(n)}{u_1(n)u_1(n+1)} = \frac{w(n)}{u_1(n)u_1(n+1)},$$

which implies that we can construct a second solution from a given solution as follows.

Lemma 4. *Let $d = 2$ and suppose that $u_1(n)$ solves (12) and that $u_1(n) \neq 0$ for all $n \geq 0$. Then a second solution of (12) is given by*

$$u_2(n) = u_1(n) \sum_{k=0}^{n-1} \frac{w(k)}{u_1(k)u_1(k+1)}, \qquad (14)$$

where $w(k) = p_0(0)p_0(1) \cdots p_0(k - 1)$.

Here we have normalized the solution u_2 by choosing $w(0) = 1$: this entails $u_2(0) = 0$ and $u_2(1) = 1/u_1(0)$. Note also that if $p_0(0) \neq 0$, then $w(1) \neq 0$, which implies that the solution u_2 is linearly independent from u_1.

Example 5. For the Delannoy difference equation (5) and the solutions $A(n)$, $B(n)$ with initial conditions as before, we have $d = 2$ and $p_0(n) = (n + 1)/(n + 2)$, hence $w(n) = 1/(n + 1)$. In particular, equation (14) is equivalent to (9).

Now suppose that $p_k(n) \to c_k$ as $n \to \infty$, for each $k \in \{0, 1, \ldots, d-1\}$. Then the characteristic polynomial of the recurrence (12) is, by definition,

$$\lambda^d + c_{d-1}\lambda^{d-1} + \cdots + c_1\lambda + c_0 = \prod_{k=1}^{d}(\lambda - \lambda_k)$$

with characteristic roots $\lambda_1, \ldots, \lambda_d$. Poincare's famous theorem [KP01, Theorem 5.1] states, under a modest additional hypothesis, that each nontrivial solution to (12) has asymptotic growth according to one of the characteristic roots.

Theorem 6 (Poincaré). *Suppose further that the characteristic roots have distinct moduli. If $u(n)$ solves the recurrence (12), then either $u(n) = 0$ for all sufficiently large n, or*

$$\lim_{n\to\infty} \frac{u(n+1)}{u(n)} = \lambda_k \tag{15}$$

for some $k \in \{1, \ldots, d\}$.

If, in addition, $p_0(n) \neq 0$ for all $n \geq 0$ (so that, by (13), the Casoratian $w(n)$ is either zero for all n or nonzero for all n), then Perron's theorem guarantees that, for each k, there exists a solution such that (15) holds.

5 Continued Fractions

In this section, we briefly connect with (irregular) continued fractions

$$C = b_0 + \frac{a_1}{b_1+} \frac{a_2}{b_2+} \frac{a_3}{b_3+} \ldots := b_0 + \cfrac{a_1}{b_1 + \cfrac{a_2}{b_2 + \cfrac{a_3}{b_3 + \ldots}}},$$

as introduced, for instance, in [JT80], [Ber89, Entry 12.1] or [BvSZ14, Chapter 9]. The n-th convergent of C is

$$C_n = b_0 + \frac{a_1}{b_1+} \frac{a_2}{b_2+} \ldots \frac{a_n}{b_n}.$$

It is well known, and readily proved by induction, that $C_n = B(n)/A(n)$ where both $A(n)$ and $B(n)$ solve the second-order recurrence

$$u_n = b_n u_{n-1} + a_n u_{n-2} \tag{16}$$

with $A(-1) = 0$, $A(0) = 1$ and $B(-1) = 1$, $B(0) = b_0$. (Note that, if $b_0 = 0$, then the initial conditions for $B(n)$ are equivalent to $B(0) = 0$, $B(1) = a_1$.)

Conversely, see [BvSZ14, Theorem 9.4], two such solutions to a second-order difference equation with non-vanishing Casoratian correspond to a unique continued fraction. In particular, Apéry limits $\lim_{n\to\infty} B(n)/A(n)$ arising from second-order difference equations can be equivalently expressed as continued fractions.

Example 7. The Apéry limit (10) is equivalent to the continued fraction

$$\frac{1}{2}\ln\left(1+\frac{1}{x}\right) = \frac{1}{(2x+1)-}\frac{1^2}{3(2x+1)-}\frac{2^2}{5(2x+1)-}\cdots\frac{n^2}{(2n+1)(2x+1)-}\cdots$$

[Wal48, p. 343, eq. (90.4)]. To see this, it suffices to note that, if $A_x(n)$ and $B_x(n)$ are as in Section 2, then $n!A_x(n)$ and $n!B_x(n)$ solve the adjusted recurrence

$$u_{n+1} = (2x+1)(2n+1)u_n - n^2 u_{n-1}$$

of the form (16).

The interested reader can find a detailed discussion of the continued fractions corresponding to Apéry's limits for $\zeta(2)$ and $\zeta(3)$ in [BvSZ14, Section 9.5], which then proceeds to proving the respective irrationality results.

6 Proving Apéry limits

In the sequel, we briefly indicate several approaches towards proving Apéry limits. In case of the Apéry numbers (1), Apéry established the limit (3) by finding the explicit expression

$$B(n) = \frac{1}{6}\sum_{k=0}^{n}\binom{n}{k}^2\binom{n+k}{k}^2\left(\sum_{j=1}^{n}\frac{1}{j^3} + \sum_{m=1}^{k}\frac{(-1)^{m-1}}{2m^3\binom{n}{m}\binom{n+m}{m}}\right)\tag{17}$$

for the secondary solution $B(n)$. Observe how, indeed, the presence of the truncated sum for $\zeta(3)$ in (17) makes the limit (3) transparent. While, nowadays, it is routine [Sch07] to verify that the sum (17) satisfies the recurrence (2), it is much less clear how to discover sums like (17) that are suitable for proving a desired Apéry limit.

Shortly after, and inspired by, Apéry's proof, Beukers [Beu79] gave shorter and more elegant proofs of the irrationality of $\zeta(2)$ and $\zeta(3)$ by considering double and triple integrals that result in small linear forms in the zeta value and 1. For instance, for $\zeta(3)$, Beukers establishes that

$$(-1)^n\int_0^1\int_0^1\int_0^1\frac{x^n(1-x)^n y^n(1-y)^n z^n(1-z)^n}{(1-(1-xy)z)^{n+1}}\mathrm{d}x\mathrm{d}y\mathrm{d}z$$
$$= A(n)\zeta(3) - 6B(n),\tag{18}$$

where $A(n)$ and $B(n)$ are precisely the Apéry numbers (1) and the corresponding secondary solution (17). By bounding the integrand, it is straightforward to show that the triple integral approaches 0 as $n \to \infty$. From this we directly obtain the Apéry limit (3), namely, $\lim_{n\to\infty} B(n)/A(n) = \zeta(3)/6$.

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Example 8. In the same spirit, the Apéry limit (10) can be deduced from

$$\int_0^1 \frac{t^n(1-t)^n}{(x+t)^{n+1}}\mathrm{d}t = A_n(x)\ln\left(1+\frac{1}{x}\right) - 2B_n(x),$$

which holds for $x > 0$ with $A_n(x)$ and $B_n(x)$ as in Section 2. We note that this integral is a variation of the integral that Alladi and Robinson [AR80] have used to prove explicit irrationality measures for numbers of the form $\ln(1+\lambda)$ for certain algebraic λ.

As a powerful variation of this approach, the same kind of linear forms can be constructed through hypergeometric sums obtained from rational functions. For instance, Zudilin [Zud04] studies a general construction, a special case of which is the relation, originally due to Gutnik,

$$-\frac{1}{2}\sum_{t=1}^{\infty} R_n'(t) = A(n)\zeta(3) - 6B(n), \quad \text{where } R_n(t) = \left(\frac{(t-1)\cdots(t-n)}{t(t+1)\cdots(t+n)}\right)^2,$$

which once more equals (18). We refer to [Zud04], [Zud07] and [AvSZ08, Section 2.3] for further details and references. A detailed discussion of the case of $\zeta(2)$ is included in [BvSZ14, Sections 9.5 and 9.6].

Beukers [Beu87] further realized that, in Apéry's cases, the differential equations associated to the recurrences have a description in terms of modular forms. Zagier [Zag09] has used such modular parametrizations to prove Apéry limits in several cases, including for the Franel numbers, the case $d = 3$ in (19). The limits occuring in his cases are rational multiples of

$$\zeta(2), \quad L_{-3}(2) = \sum_{n=1}^{\infty} \frac{\left(\frac{-3}{n}\right)}{n^2}, \quad L_{-4}(2) = \sum_{n=1}^{\infty} \frac{\left(\frac{-4}{n}\right)}{n^2} = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^2},$$

where $\left(\frac{a}{n}\right)$ is a Legendre symbol and $L_{-4}(2)$ is Catalan's constant (whose irrationality remains famously unproven). A general method for obtaining Apéry limits in cases of modular origin has been described by Yang [Yan08], who proves various Apéry limits in terms of special values of L-functions.

7 Sums of powers of binomials

Let us consider the family

$$A^{(d)}(n) = \sum_{k=0}^{n}\binom{n}{k}^d \tag{19}$$

of sums of powers of binomial coefficients. It is easy to see that $A^{(1)}(n) = 2^n$ and $A^{(2)}(n) = \binom{2n}{n}$. The numbers $A^{(3)}(n)$ are known as *Franel numbers* [OEIS, A000172]. Almost a

century before the availability of computer-algebra approaches like creative telescoping, Franel [Fra94] obtained explicit recurrences for $A^{(3)}(n)$ as well as, in a second paper, $A^{(4)}(n)$, and he conjectured that $A^{(d)}(n)$ satisfies a linear recurrence of order $\lfloor (d+1)/2 \rfloor$ with polynomial coefficients. This conjecture was proved by Stoll in [Sto97], to which we refer for details and references. It remains an open problem to show that, in general, no recurrence of lower order exists.

Van der Poorten [Poo79, p. 202] reports that the following Apéry limits in the cases $d = 3$ and $d = 4$ (in which case the binomial sums satisfy second-order recurrences like Apéry's sequences) have been numerically observed by Tom Cusick:

$$\lim_{n\to\infty} \frac{B^{(3)}(n)}{A^{(3)}(n)} = \frac{\pi^2}{24}, \quad \lim_{n\to\infty} \frac{B^{(4)}(n)}{A^{(4)}(n)} = \frac{\pi^2}{30}. \tag{20}$$

In each case, $B^{(d)}(n)$ is the (unique) secondary solution with initial conditions $B^{(d)}(0) = 0$, $B^{(d)}(1) = 1$. The case $d = 3$ was proved by Zagier [Zag09] using modular forms. Since the case $d = 4$ is similarly connected to modular forms [Coo12], we expect that it can be established using the methods in [Yan08], [Zag09] as well. Based on numerical evidence, following the approach in Section 3, we make the following general conjecture extending (20):

Conjecture 9. *For $d \geq 3$, the minimal-order recurrence satisfied by $A^{(d)}(n)$ has a unique solution $B^{(d)}(n)$ with $B^{(d)}(0) = 0$ and $B^{(d)}(1) = 1$ that also satisfies*

$$\lim_{n\to\infty} \frac{B^{(d)}(n)}{A^{(d)}(n)} = \frac{\zeta(2)}{d+1}. \tag{21}$$

Note that for $d \geq 5$, the recurrence is of order ≥ 3, and so the solution $B^{(d)}(n)$ is not uniquely determined by the two initial conditions $B^{(d)}(0) = 0$ and $B^{(d)}(1) = 1$. Conjecture 9 asserts that precisely one of these solutions satisfies (21).

Subsequent to making this conjecture, we realized that the case $d = 5$ was already conjectured in [AvSZ08, Section 4.1] as sequence #22. We are not aware of previous conjectures for the cases $d \geq 6$. We have numerically confirmed each of the cases $d \leq 10$ to more than 100 digits.

Example 10. For $d = 5$, the sum $A^{(5)}(n)$ satisfies a recurrence of order 3, spelled out in [Per87], of the form

$$(n+3)^4 p(n+1) u(n+3) + \ldots + 32(n+1)^4 p(n+2) u(n) = 0 \tag{22}$$

where $p(n) = 55n^2 + 33n + 6$. The solution $B^{(5)}(n)$ from Conjecture 9 is characterized by $B^{(5)}(0) = 0$ and $B^{(5)}(1) = 1$ and insisting that the recurrence (22) also holds for $n = -1$ (note that this does not require a value for $B^{(5)}(-1)$ because of the term $(n+1)^4$). Similarly, for $d = 6, 7, 8, 9$ the sequence $B^{(d)}(n)$ in Conjecture 9 can be characterized by enforcing

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the recurrence for small negative n and by setting $B^{(d)}(n) = 0$ for $n < 0$. By contrast, for $d = 10$, there is a two-dimensional space of sequences $u(n)$ solving (22) for all integers n with the constraint that $u(n) = 0$ for $n \leq 0$. Among these, $B^{(10)}(n)$ is characterized by $B^{(10)}(1) = 1$ and $B^{(10)}(2) = 381/4$.

Now return to the case $d = 5$ and let $C^{(5)}(n)$ be the third solution to the same recurrence with $C^{(5)}(0) = 0$, $C^{(5)}(1) = 1$, $C^{(5)}(2) = \frac{48}{7}$. Numerical evidence suggests that we have the Apéry limits

$$\lim_{n \to \infty} \frac{B^{(5)}(n)}{A^{(5)}(n)} = \frac{1}{6}\zeta(2), \quad \lim_{n \to \infty} \frac{C^{(5)}(n)}{A^{(5)}(n)} = \frac{3\pi^4}{1120} = \frac{27}{112}\zeta(4).$$

Extending this idea to $d = 5, 6, \ldots, 10$, we numerically find Apéry limits $C^{(d)}(n)/A^{(d)}(n) \to \lambda\zeta(4)$ with the following rational values for λ:

$$\frac{27}{112}, \frac{4}{21}, \frac{37}{240}, \frac{7}{55}, \frac{47}{440}, \frac{1}{11}.$$

These values suggest that λ can be expressed as a simple rational function of d:

Conjecture 11. *For $d \geq 5$, the minimal-order recurrence satisfied by $A^{(d)}(n)$ has a unique solution $C^{(d)}(n)$ with $C^{(d)}(0) = 0$ and $C^{(d)}(1) = 1$ that also satisfies*

$$\lim_{n \to \infty} \frac{C^{(d)}(n)}{A^{(d)}(n)} = \frac{3(5d + 2)}{(d + 1)(d + 2)(d + 3)}\zeta(4).$$

More generally, we expect that, for $d \geq 2m+1$, there exist such Apéry limits for rational multiples of $\zeta(2), \zeta(4), \ldots, \zeta(2m)$. It is part of the challenge presented here to explicitly describe all of these limits. As communicated to us by Zudilin, one could approach the challenge, uniformly in d, by considering the rational functions

$$R_n^{(d)}(t) = \left(\frac{(-1)^t n!}{t(t + 1) \cdots (t + n)} \right)^d$$

in the spirit of [Zud04], [Zud07] and [AvSZ08, Section 2.3], as indicated in Section 6.

8 Further challenges and open problems

Although many things are known about Apéry limits, much deserves to be better understood. The explicit conjectures we offer in the previous section can be supplemented with similar ones for other families of binomial sums. In addition, many conjectural Apéry limits that were discovered numerically are listed in [AvSZ08, Section 4] for sequences that arise from fourth- and fifth-order differential equations of Calabi–Yau type. As mentioned

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in Example 3, it would be of particular interest to establish all these Apéry limits in a uniform fashion.

It is natural to wonder whether a better understanding of Apéry limits can lead to new irrationality results. Despite considerable efforts and progress (we refer the reader to [Zud04] and [Bro16] as well as the references therein), it remains a wide-open challenge to prove the irrationality of, say, $\zeta(5)$ or Catalan's constant. As a recent promising construction in this direction, we mention Brown's cellular integrals [Bro16] which are linear forms in (multiple) zeta values that are constructed to have certain vanishing properties that make them amenable to irrationality proofs. In particular, Brown's general construction includes Apéry's results as (unique) special cases occuring as initial instances.

In another direction, it would be of interest to systematically study q-analogs and, in particular, to generalize from difference equations to q-difference equations. For instance, Amdeberhan and Zeilberger [AZ98] offer an Apéry-style proof of the irrationality of the q-analog of $\ln(2)$ based on a q-version of the Delannoy numbers (4).

Perron's theorem, which we have mentioned after Poincaré's Theorem 6, guarantees that, for each characteristic root λ of an appropriate difference equation, there exists a solution $u(n)$ such that $u(n+1)/u(n)$ approaches λ. We note that, for instance, Apéry's linear form (18) is precisely the unique (up to a constant multiple) solution corresponding to the λ of smallest modulus. General tools to explicitly construct such Perron solutions from the difference equation would be of great utility.

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