

# A Computer-Algebra-Based Formal Proof of the Irrationality of $\zeta(3)$

**Frédéric Chyzak**

Joint work with A. Mahboubi, T. Sibut-Pinote, and E. Tassi

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# Apéry's Theorem (1978/1979): The Number $\zeta(3) = \sum_{m=1}^{\infty} \frac{1}{m^3}$ is Irrational

Sketch of proof, as in (van der Poorten, 1979)

- Define:

$$c_{n,k} = \binom{n}{k}^2 \binom{n+k}{k}^2, \quad z_n = \sum_{m=1}^n \frac{1}{m^3}, \quad u_{n,k} = z_n + \sum_{m=1}^k \frac{(-1)^{m+1}}{2m^3 \binom{n}{m} \binom{n+m}{m}},$$
$$v_{n,k} = c_{n,k} u_{n,k}, \quad a_n = \sum_{k=0}^n c_{n,k}, \quad b_n = \sum_{k=0}^n v_{n,k}.$$

- Prove:  $(a_n)$  and  $(b_n)$  satisfy the same 2nd-order recurrence, so that

$$0 < \zeta(3) - b_n/a_n = \mathcal{O}(a_n^{-2}), \quad a_n = \Theta(n^{-3/2}(\sqrt{2}+1)^{4n}).$$

- Define  $\ell_n = \text{lcm}(1, \dots, n)$  and prove  $2\ell_n^3 a_n \in \mathbb{N}$ ,  $2\ell_n^3 b_n \in \mathbb{Z}$ .
- Notice  $\ell_n = \mathcal{O}(e^n)$  and  $e^3(\sqrt{2}+1)^{-4} \simeq 0.59$  to conclude:

$$0 < 2\ell_n^3 (a_n \zeta(3) - b_n) = \mathcal{O}(n^{3/2} e^{3n} (\sqrt{2}+1)^{-4n}) \implies \zeta(3) \notin \mathbb{Q}.$$

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## Summary of ingredients of the proof

- Genius to invent the sequences  $(a_n)$  and  $(b_n)$
- Elementary number theory
- Deriving same second-order recurrence for  $(a_n)$  and  $(b_n)$
- Asymptotic estimates

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## Focus of the talk on proving the recurrence:

- this part is amenable to computer-algebra methods
- typical use of “creative telescoping” for summation

(Beukers, 1979)

Observe

$$I_n = \ell_n^3 \int_0^1 \int_0^1 \int_0^1 \frac{L_n(x) L_n(y)}{1-u(1-xy)} dx dy du \in \mathbb{Z} + \mathbb{Z} \zeta(3),$$

where

$$L_n(x) = \frac{1}{n!} \frac{d^n}{dx^n} x^n (1-x)^n \quad (\text{Legendre orthogonal polynomials}).$$

Integrations by parts and easy bounding yield

$$0 < I_n \leq 2\zeta(3) 3^{3n} (\sqrt{2} + 1)^{-4n}.$$

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Mathematically more elegant, but would not illustrate CA/FP interaction.

# Apéry's Recurrence for $(a_n)$ and $(b_n)$

Second-order recurrence (Apéry, 1978/1979)

$$(n+1)^3 s_{n+1} - (34n^3 + 51n^2 + 27n + 5) s_n + n^3 s_{n-1} = 0$$

Cohen and Zagier's "Creative Telescoping" (van der Poorten, 1979)

"[They] cleverly construct

$$q_{n,k} = 4(2n+1)(k(2k+1) - (2n+1)^2) c_{n,k}$$

with the motive that

$$(n+1)^3 c_{n+1,k} - (34n^3 + 51n^2 + 27n + 5) c_{n,k} + n^3 c_{n-1,k} = [q_{n,j}]_{j=k-1}^{j=k}."$$

After summation over  $k$  from 0 to  $n+1$ :

$$(n+1)^3 a_{n+1} - (34n^3 + 51n^2 + 27n + 5) a_n + n^3 a_{n-1} = \underbrace{[q_{n,j}]_{j=-1}^{j=n+1}}_{0-0=0}.$$

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with the motive that

$$\left( (n+1)^3 S_n - (34n^3 + 51n^2 + 27n + 5) + n^3 S_n^{-1} \right) \cdot c = (1 - S_k^{-1})(Q \cdot c)."$$

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$$P = (n+1)^3 S_n - (34n^3 + 51n^2 + 27n + 5) + n^3 S_n^{-1}$$

and

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$$P \cdot c = (1 - S_k^{-1})(Q \cdot c)."$$

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Skew-polynomial algebras:

$$S_n n = (n+1)S_n, \quad S_k k = (k+1)S_k \quad \text{in} \quad \mathbb{Q}(n, k) \langle S_n, S_k \rangle$$

## My Motivations to Reconsider CA from a FP Viewpoint

I do: study computer-algebra algorithms on special functions.

Can an algorithmically-generated encyclopedia be authoritative?

E.g., Dynamic Dictionary of Mathematical Functions (DDMF).

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- some key papers are too informal to assess their correctness / I've lost proofs written too tersely in my own papers
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- hypergeometric sequence vs hypergeometric term? / holonomic vs rationally holonomic vs D-finite vs  $\partial$ -finite vs P-recursive?

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I want: banish underqualified phrasings and prevent shifts in meaning.

I don't want: reproduce informal interaction with the computer.

Example: Densities of short uniform random walks (Borwein, Straub, Wan, Zudilin, 2012).

Turning our attention to negative integers, we have for  $k \geq 0$  an integer:

$$(78) \quad W_3(-2k-1) = \frac{4}{\pi^3} \left( \frac{2^k k!}{(2k)!} \right)^2 \int_0^\infty t^{2k} K_0(t)^3 dt,$$

because the two sides satisfy the same recursion ([BBBG08, (8)]), and agree when  $k = 0, 1$  ([BBBG08, (47) and (48)]).

From (78), we experimentally determined a single hypergeometric for  $W_3(s)$  at negative odd integers:

**Lemma 2.** For  $k \geq 0$  an integer,

$$W_3(-2k-1) = \frac{\sqrt{3} \binom{2k}{k}^2}{2^{4k+1} 3^{2k}} {}_3F_2 \left( \begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ k+1, k+1 \end{matrix} \middle| \frac{1}{4} \right).$$

*Proof.* It is easy to check that both sides agree at  $k = 0, 1$ . Therefore we need only to show that they satisfy the same recursion. The recursion for the left-hand side implies a contiguous relation for the right-hand side, which can be verified by extracting the summand and applying Gosper's algorithm ([PWZ06]).  $\square$

## Example: Bounding error in high-precision computation of Euler's constant (Brent, Johansson, 2013).

The “lower” sum  $L$  is precisely  $\sum_{k=0}^{m/2-1} b_k x^{-2k}$ . Replacing  $k$  by  $2k$  in (21) (as the odd terms vanish by symmetry), we have to prove

$$\sum_{j=0}^{2k} \frac{(-1)^j [(2j)!]^2 [(4k-2j)!]^2}{(j!)^3 [(2k-j)!]^3 32^{2k}} = \frac{[(2k)!]^3}{(k!)^4 8^{2k}}. \quad (23)$$

This can be done algorithmically using the creative telescoping approach of Wilf and Zeilberger. For example, the implementation in the Mathematica package `HolonomicFunctions` by Koutschan [6] can be used. The command

```
a = ((2j)!)^2 / ((j!)^3 32^j);
CreativeTelescoping[(-1)^j a (a /. j -> 2k-j),
  {S[j]-1}, S[k]]
```

outputs the recurrence equation

$$(8 + 8k)b_{k+1} - (1 + 6k + 12k^2 + 8k^3)b_k = 0$$

matching the right-hand side of (23), together with a telescoping certificate. Since the summand in (23) vanishes for  $j < 0$  and  $j > 2k$ , no boundary conditions enter into the telescoping relation, and checking the initial value ( $k = 0$ ) suffices to prove the identity.<sup>1</sup>

<sup>1</sup>Curiously, the built-in `Sum` function in Mathematica 9.0.1 computes a closed form for the sum (23), but returns an answer that is wrong by a factor 2 if the factor  $[(4k-2j)!]^2$  in the summand is input as  $[(2(2k-j))!]^2$ .

Algorithmic theory for Special Functions and Combinatorial Sequences initiated by Zeilberger (1982, 1990, 1991)

- Replace named sequences by linear systems of recurrences (+ initial conditions to identify the right solutions)
- Develop algorithms on the level of systems for  $+$ ,  $\times$ ,  $\Sigma$

Implementations exist for Maple, Mathematica, Maxima, etc.

Great success:

- fast evaluation formulae:  $\pi$ , the Catalan constant,  $\zeta$ -values,  $\beta$ -values
- enumerative combinatorics: heap-ordered trees,  $q$ -analogue of totally symmetric plane partitions; positive 3D rook walks; small-step walks
- partition theory: Rogers-Ramanujan and Göllnitz-type identities
- knot theory: colored Jones functions
- mathematical physics: computation of Feynman diagrams



## Computer-algebra algorithms apply to Apéry's sums!

- Zeilberger's calculation ( $\leq 1992$ ) for  $(a_n)$
- Zudilin's alternate proof (1992) by two calls to Zeilberger's algorithm
- Apéry's original calculations using Zeilberger's and Chyzak's algorithms: Salvy's Maple worksheet (2003),  
<http://algo.inria.fr/libraries/autocomb/Apery2-html/apery.html>
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Our formalization follows the Apéry/van der Poorten/Salvy path.

# A Convolved Proof of Cassini's Identity $F_n F_{n+2} = F_{n+1}^2 + (-1)^n$

- Fibonacci numbers:  $F_{n+2} = F_{n+1} + F_n$ ,  $F_0 = F_1 = 1$ .
- Define  $(\sigma_n)$  by:  $\sigma_{n+1} = -\sigma_n$ ,  $\sigma_0 = 1$ .

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- Define  $(\sigma_n)$  by:  $\sigma_{n+1} = -\sigma_n$ ,  $\sigma_0 = 1$ .
- Introduce  $u_n := F_{n+1}^2 + \sigma_n$  and compute the **normal forms**:

$$\begin{aligned}u_n &= F_{n+1}^2 + \sigma_n, \\u_{n+1} &= F_n^2 + 2F_n F_{n+1} + F_{n+1}^2 - \sigma_n, \\u_{n+2} &= F_n^2 + 4F_n F_{n+1} + 4F_{n+1}^2 + \sigma_n, \\u_{n+3} &= 4F_n^2 + 12F_n F_{n+1} + 9F_{n+1}^2 - \sigma_n.\end{aligned}$$

- **Solving a linear system** yields:  $u_{n+3} - 2u_{n+2} - 2u_{n+1} + u_n = 0$ .

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- **Solving a linear system** yields:  $u_{n+3} - 2u_{n+2} - 2u_{n+1} + u_n = 0$ .
- Same process for  $v_n := F_n F_{n+2}$  delivers the same recurrence.
- Now, **checking initial conditions** and an induction ends the proof:

$$u_0 = v_0 = 2, \quad u_1 = v_1 = 3, \quad u_2 = v_2 = 10.$$

$(t_{n,k})$  is  $\partial$ -finite



the shifts  $(t_{n+i,k+j})$  span a **finite-dimensional**  $\mathbb{Q}(n,k)$ -vector space

$\Rightarrow$  linear functional equations with rational-function coefficients.

## A Generalization: $\partial$ -Finite Sequences (Chyzak, Salvy, 1998)

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Examples: Fibonacci numbers; binomial coefficients

$$\binom{n+1}{k} = \frac{n+1}{n+1-k} \binom{n}{k}, \quad \binom{n}{k+1} = \frac{n-k}{k+1} \binom{n}{k};$$

orthogonal polynomials, Bessel functions.

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Closures under  $+$ ,  $\times$ , shifts

- Annihilating ideal  $\rightarrow$  skew Gröbner basis  $\rightarrow$  normal forms in finite dim.
- Iterative algorithm to search for linear dependencies

$\rightsquigarrow$  simplification and zero test of  $\partial$ -finite polynomial expressions.



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Examples: Fibonacci numbers; binomial coefficients

$$\text{ann} \binom{n}{k} = \left\{ L_1 \left( S_n - \frac{n+1}{n+1-k} \right) + L_2 \left( S_k - \frac{n-k}{k+1} \right) : L_1, L_2 \in \mathbb{Q}(n,k) \langle S_n, S_k \rangle \right\};$$

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# A Convoluted Proof of $\sum_{k=0}^n \binom{n}{k} = 2^n$

- Define  $F_n := \sum_{k=0}^n \binom{n}{k}$ .

- Prove

$$\binom{n+1}{k} - 2\binom{n}{k} = \left[ \frac{-j\binom{n}{j}}{n+1-j} \right]_{j=k}^{j=k+1}$$

as a consequence of

$$\binom{n+1}{k} = \frac{n+1}{n+1-k} \binom{n}{k}, \quad \binom{n}{k+1} = \frac{n-k}{k+1} \binom{n}{k}.$$

- Sum from  $k = -1$  to  $k = n + 1$  to get  $F_{n+1} - 2F_n = 0$ .
- Now, observing  $F_0 = 1$  yields the result.

Zeilberger’s algorithm (1991)

INPUT: a hypergeometric term  $f_{n,k}$ , that is, first-order recurrences.

OUTPUT: rational functions  $p_0(n), \dots, p_r(n), Q(n, k)$  with minimal  $r$ , such that  $p_r(n) f_{n+r,k} + \dots + p_0(n) f_{n,k} = Q(n, k+1) f_{n,k+1} - Q(n, k) f_{n,k}$ .

# Algorithms for Summing “Holonomic” $\partial$ -Finite Sequences

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Chyzak’s algorithm (2000)

INPUT:  $\begin{cases} \text{a } \partial\text{-finite term } u \text{ w.r.t. } A = \mathbb{Q}(n, k)\langle S_n, S_k \rangle, \\ \text{a Gröbner basis } G \text{ of } \text{ann } u. \end{cases}$

OUTPUT:  $\begin{cases} P \in \mathbb{Q}(n)\langle S_n \rangle \text{ of } \text{minimal possible order,} \\ Q \in A \text{ reduced mod. } G \text{ and such that } P \cdot u = (S_k - 1)Q \cdot u. \end{cases}$

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Example: we can get the same 2nd-order operator  $P$  for both sides of

$$\underbrace{\sum_{r=0}^{\infty}}_{\text{by C}} \underbrace{\sum_{s=0}^{\infty}}_{\text{by Z}} (-1)^{n+r+s} \binom{n}{r} \binom{n}{s} \binom{n+r}{r} \binom{n+s}{s} \binom{2n-(r+s)}{n} = \underbrace{\sum_{k=0}^{\infty}}_{\text{by Z}} \binom{n}{k}^4.$$

## "Proving" an algorithm

- would prove all its results satisfy the specifications
- but it **is too much work** in our context

Instead, **use an external computer-algebra tool as an oracle**

- be as skeptical of the computer algebra as of the human
- approach of choice **when checking is simpler than discovering**

Inspired by (Harrison, Théry, 1997)

# A Program to Derive Recurrences for Apéry's Sums

Concrete sequences ...

step	explicit form	operation	input(s)
1	$c_{n,k} = \binom{n}{k}^2 \binom{n+k}{k}^2$	simplification	
2	$a_n = \sum_{k=1}^n c_{n,k}$	creative telescoping	$c_{n,k}$
3	$d_{n,m} = \frac{(-1)^{m+1}}{2m^3 \binom{n}{m} \binom{n+m}{m}}$	simplification	
4	$s_{n,k} = \sum_{m=1}^k d_{n,m}$	creative telescoping	$d_{n,m}$
5	$z_n = \sum_{m=1}^n \frac{1}{m^3}$	simplification	
6	$u_{n,k} = z_n + s_{n,k}$	addition	$z_n$ and $s_{n,k}$
7	$v_{n,k} = c_{n,k} u_{n,k}$	product	$c_{n,k}$ and $u_{n,k}$
8	$b_n = \sum_{k=1}^n v_{n,k}$	creative telescoping	$v_{n,k}$

# A Program to Derive Recurrences for Apéry's Sums

... replaced with abstract analogues: *any solution of a given GB*

step	explicit form	operation	input GB(s)	output GB
1	$c_{n,k} = \binom{n}{k}^2 \binom{n+k}{k}^2$	simplification		<i>C</i>
2	$a_n = \sum_{k=1}^n c_{n,k}$	creative telescoping	<i>C</i>	<i>A</i>
3	$d_{n,m} = \frac{(-1)^{m+1}}{2m^3 \binom{n}{m} \binom{n+m}{m}}$	simplification		<i>D</i>
4	$s_{n,k} = \sum_{m=1}^k d_{n,m}$	creative telescoping	<i>D</i>	<i>S</i>
5	$z_n = \sum_{m=1}^n \frac{1}{m^3}$	simplification		<i>Z</i>
6	$u_{n,k} = z_n + s_{n,k}$	addition	<i>Z</i> and <i>S</i>	<i>U</i>
7	$v_{n,k} = c_{n,k} u_{n,k}$	product	<i>C</i> and <i>U</i>	<i>V</i>
8	$b_n = \sum_{k=1}^n v_{n,k}$	creative telescoping	<i>V</i>	<i>B</i>



## How Can a Candidate Recurrence be Checked?

Because

$$\binom{n+1}{k} = \frac{n+1}{n+1-k} \binom{n}{k}, \quad \binom{n}{k+1} = \frac{n-k}{k+1} \binom{n}{k},$$

it follows:

$$\begin{aligned} \binom{n+1}{k} - 2\binom{n}{k} + \left[ \frac{j\binom{n}{j}}{n+1-j} \right]_{j=k}^{j=k+1} &= \\ \binom{n+1}{k} - 2\binom{n}{k} + \frac{(k+1)\binom{n}{k+1}}{n-k} - \frac{k\binom{n}{k}}{n+1-k} &= \\ \underbrace{\left( \frac{n+1}{n+1-k} - 2 + \frac{k+1}{n-k} \frac{n-k}{k+1} - \frac{k}{n+1-k} \right)}_{=0} \binom{n}{k} &= 0. \end{aligned}$$

## How Can a Candidate Recurrence be Checked?

Because the annihilating (left) ideal  $I$  of  $\binom{n}{k}$  is generated by the GB

$$g_1 := S_n - \frac{n+1}{n+1-k}, \quad g_2 := S_k - \frac{n-k}{k+1},$$

it follows:

$$\begin{aligned} S_n - 2 + (S_k - 1) \frac{k}{n+1-k} &= \\ S_n - 2 + \frac{k+1}{n-k} S_k - \frac{k}{n+1-k} &= \\ g_1 + \frac{k+1}{n-k} g_2 + \underbrace{\left( \frac{n+1}{n+1-k} - 2 + \frac{k+1}{n-k} \frac{n-k}{k+1} - \frac{k}{n+1-k} \right)}_{=0} &\in I. \end{aligned}$$

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## How Can a Candidate Recurrence be Checked?

Because

$$k \neq n+1 \implies \binom{n+1}{k} = \frac{n+1}{n+1-k} \binom{n}{k}, \quad k \neq -1 \implies \binom{n}{k+1} = \frac{n-k}{k+1} \binom{n}{k},$$

it follows:

$$\begin{aligned} \binom{n+1}{k} - 2\binom{n}{k} + \left[ \frac{j\binom{n}{j}}{n+1-j} \right]_{j=k}^{j=k+1} &= \\ \binom{n+1}{k} - 2\binom{n}{k} + \frac{(k+1)\binom{n}{k+1}}{n-k} - \frac{k\binom{n}{k}}{n+1-k} &= \\ \underbrace{\left( \frac{n+1}{n+1-k} - 2 + \frac{k+1}{n-k} \frac{n-k}{k+1} - \frac{k}{n+1-k} \right)}_{=0} \binom{n}{k} &= 0 \end{aligned}$$

if  $k \neq n+1$ ,  $k \neq n$ , and  $k \neq -1$ .

Explanation:

- Recurrences are valid **out of an algebraic set  $\Delta$** .
- Closures under  $+$ ,  $\times$ ,  $S_i$  are sound, but out of an unknown  $\Delta$ .
- Meaning of summation is dubious if summation range intersects  $\Delta$ .

Hope:

- Easy: Discover the recurrences by a Maple session by algorithms.
- Uneasy: Guard each of them by a proviso, but how to get it?

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- Recurrences are valid **out of an algebraic set  $\Delta$** .
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Hope:

- Easy: Discover the recurrences by a Maple session by algorithms.
- Uneasy: Guard each of them by a proviso, but how to get it?

Remark:

- To the best of my knowledge, **correctness** of summation algorithms is addressed **only for very limited situations** (Abramov, Petkovšek, 2007).

Data of guarded recurrences for each abstracted composite sequence

- human-discovered and -written provisos for each of the recurrences
- Maple-generated coefficients of the recurrences, pretty-printed to Coq
- recurrences written in terms of the proviso name and coefficient names:
  - hypergeometric sequences  $(c_{n,k}, d_{n,m})$  and indefinite sum  $(z_n)$ : a GB directly obtained from the explicit form
  - composite under  $+$  or  $\times$   $(u_{n,k}$  and  $v_{n,k})$ : a GB directly obtained via algorithmic closure
  - composite under creative telescoping  $(a_n, s_{n,k}, b_n)$ : first, recurrences of the form  $P \cdot f = (S_k - 1)Q \cdot f$ ; then, conversion of the  $P$  into a GB

# Structure of Our Coq Files

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Proofs of recurrences for each abstracted sequence

- load guarded recurrences for arguments (assumed) and for the composite (being proved)
- assume arguments satisfying relevant recurrences; define the composite as a function of the arguments
- state and **prove** lemmas (recurrences) for the composite, e.g.:

Lemma:  $\forall c \in \mathbb{Q}^{\mathbb{Z}^2}, \forall u \in \mathbb{Q}^{\mathbb{Z}^2}, \forall v \in \mathbb{Q}^{\mathbb{Z}^2},$  if  $c$  solves  $C$  and  $u$  solves  $U$  and  $v = c \times u$ , then  $v$  solves  $V$ .



# Structure of Our Coq Files

Data of guarded recurrences for each abstracted composite sequence

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Proofs of recurrences for the concrete sequences

- ad-hoc means for initial sequences  $(c_{n,k}, d_{n,m}, z_n)$
- recurrences for other sequences follows immediately by instantiation
- finally, reduction of fourth-order recurrence for  $(b_n)$  to order 2

# A Lemma for Creative Telescoping?

$$\begin{aligned}
 p_0(n)u_{n,k} + p_1(n)u_{n+1,k} + \cdots + p_r(n)u_{n+r,k} &= Q(n, k+1)u_{n,k+1} - Q(n, k)u_{n,k} \\
 U_n &:= \sum_{k=\alpha}^{n+\beta} u_{n,k}
 \end{aligned}$$

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 \vdots &= \vdots \\
 p_0(n)u_{n,\alpha+1} + p_1(n)u_{n+1,\alpha+1} + \cdots + p_r(n)u_{n+r,\alpha+1} &= Q(n, \alpha+2)u_{n,\alpha+2} - Q(n, \alpha+1)u_{n,\alpha+1} \\
 p_0(n)u_{n,\alpha} + p_1(n)u_{n+1,\alpha} + \cdots + p_r(n)u_{n+r,\alpha} &= Q(n, \alpha+1)u_{n,\alpha+1} - Q(n, \alpha)u_{n,\alpha}
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$$p_0(n)U_n$$

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$$U_n := \sum_{k=\alpha}^{n+\beta} u_{n,k}$$

$$p_1(n)u_{n+1, n+\beta+1} = p_1(n)u_{n+1, n+\beta+1}$$

$$p_0(n)u_{n, n+\beta} + p_1(n)u_{n+1, n+\beta} + \cdots + p_r(n)u_{n+r, n+\beta} = Q(n, n+\beta+1)u_{n, n+\beta+1} - Q(n, n+\beta)u_{n, n+\beta}$$

$$\vdots = \vdots$$

$$p_0(n)u_{n, \alpha+1} + p_1(n)u_{n+1, \alpha+1} + \cdots + p_r(n)u_{n+r, \alpha+1} = Q(n, \alpha+2)u_{n, \alpha+2} - Q(n, \alpha+1)u_{n, \alpha+1}$$

$$p_0(n)u_{n, \alpha} + p_1(n)u_{n+1, \alpha} + \cdots + p_r(n)u_{n+r, \alpha} = Q(n, \alpha+1)u_{n, \alpha+1} - Q(n, \alpha)u_{n, \alpha}$$

$$p_0(n)U_n + p_1(n)U_{n+1}$$

# A Lemma for Creative Telescoping?

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$$p_0(n)U_n + p_1(n)U_{n+1} + \cdots + p_r(n)U_{n+r}$$

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$$+ \sum_{i=1}^r \sum_{j=1}^i p_i(n)u_{n+i,n+\beta+j}$$

A lemma instead of a case-by-case analysis

Given  $(u_{n,k}) \in \mathbb{Q}^{\mathbb{Z}^2}$ , define  $U_n = \sum_{k=\alpha}^{n+\beta} u_{n,k}$ . Given a set  $\Delta$  such that

$$(n,k) \notin \Delta \Rightarrow (P \cdot u_{\bullet,k})_n = (Q \cdot u)_{n,k+1} - (Q \cdot u)_{n,k},$$

the following identity holds for any  $n$  such that  $\alpha \leq n + \beta$ :

$$\begin{aligned} (P \cdot U)_n &= \left( (Q \cdot u)_{n,n+\beta+1} - (Q \cdot u)_{n,\alpha} \right) + \sum_{i=1}^r \sum_{j=1}^i p_i(n) u_{n+i,n+\beta+j} \\ &+ \sum_{\alpha \leq k \leq n+\beta \wedge (n,k) \in \Delta} (P \cdot u_{\bullet,k})_n - (Q \cdot u)_{n,k+1} + (Q \cdot u)_{n,k}. \end{aligned}$$



# Sound Creative Telescoping

A lemma instead of a case-by-case analysis

Given  $(u_{n,k}) \in \mathbb{Q}^{\mathbb{Z}^2}$ , define  $U_n = \sum_{k=\alpha}^{n+\beta} u_{n,k}$ . Given a set  $\Delta$  such that

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In practice: Coq's  $u, U, P, Q$  are total maps, extending the mathematical objects.

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In practice: Coq's  $u, U, P, Q$  are total maps, extending the mathematical objects.

Use of the lemma: normalizing the right-hand side (to 0)

- **Ill-formed terms** should cancel (manual inspection)
- Normalize modulo GB (several copies of stairs:  $u_{n,\alpha}, u_{n,n+\beta}$ )
- Use rational-function normalization to get 0 (Coq's field)

## Elementary number theory

- definition of binomials over  $\mathbb{Z}^2$
- standard properties +  $1 \leq i \leq j \leq n \implies j \binom{i}{j} \mid \ell_n$

## Asymptotic estimates

- of  $a_n$ :
  - implicit use of Poincaré–Perron–Kreuser theorem(s) in Apéry’s proof
  - replaced with the more elementary  $33^n = \mathcal{O}(a^n)$
- of  $\ell_n$ :
  - original proof uses  $\ell_n = e^{n+o(1)}$ , implied by the Prime Number Theorem
  - replaced with  $\ell_n = \mathcal{O}(3^n)$

## Numbers: libraries used

- proof-dedicated integers and rationals of MathComp (Gonthier *et al.*)
- computation-dedicated integers and rationals of CoqEAL (Cohen, Mörtberg, Dénès)
- algebraic numbers (Cohen)
- Cauchy reals to encode  $\zeta(3)$  as  $(z_n)_{n \in \mathbb{N}}$  and a Cauchy-CV proof

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We have machine-checked (a stronger statement of):

Theorem:  $\ell_n = \mathcal{O}(3^n) \implies \zeta(3) \notin \mathbb{Q}$ .

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```
Coq < Print lcmn_asymptotic_bound.  
lcmn_asymptotic_bound =  
exists (K2 K3 : rat) (N : nat),  
  0 < K2 /\ 0 < K3 /\ K2 ^ 3 < 33%:~R /\  
  forall (n : nat),  
    (N <= n)%N -> (iter_lcmn n)%:~R < K3 * K2 ^ n  
  : Prop
```

```
Coq < About zeta_3_irrational.  
zeta_3_irrational :  
lcmn_asymptotic_bound ->  
  not (exists (r : rat), (z3 = (r%:CR))%CR)
```

An excessively difficult endeavour: a very shallow learning curve

- different methodologies over the years  $\rightsquigarrow$  documentation out of sync  $\rightsquigarrow$  oral transmission
- too difficult to read *through* notation + coercions + structure inference
- understanding libraries requires a knowledge of Coq's most advanced features

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Formalization: opposing goals?

- mimicking the mathematical informal interaction
- flushing doubts on proofs/interpretation of mathematical objects



- (Ongoing) Complete proof by formalizing bound on  $\text{lcm}(1, \dots, n)$
- Test robustness of approach by more examples of sums
- Understanding why it works, so as to automate our protocol
- (Ongoing) Differential analogue: similar approach to prove the second-order ODE for the square-lattice Green function

$$\int_0^1 \int_0^1 \frac{1}{(1 - xyz)\sqrt{1 - x^2}\sqrt{1 - y^2}} dx dy$$

- Dedicated data structure to keep (skew-)polynomials normalized