Automated & Certified Proofs of Summation Formulae

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Computer calculations and mathematical proofs

Using computer calculations is the only way we know to prove:

- The Four Color Theorem (Appel-Haken, 1976)
- The Kepler conjecture (Hales, 1998)
- ...
- The ternary Goldbach conjecture (Helfgott, 2013)
- ...

Summation/Integral identities

$$\sum_{k\in\mathbb{Z}} \frac{(3k)!}{k!(k+1)!(k+2)!27^k} = \frac{(81n^2+261n+200)(3n+2)!}{40(n+2)!(n+1)!n!27^n} - \frac{9}{2}$$

$$\sum_{k\in\mathbb{Z}} (-1)^k \binom{a+b}{a+k}\binom{a+c}{c+k}\binom{b+c}{b+k} = \frac{(a+b+c)!}{a!b!c!}$$

$$\int_0^{+\infty} \frac{e^{-px}T_n(x)}{\sqrt{1-x^2}}dx = (-1)^n \pi I_n(p)$$

Mathematical riddles

Some simple ones:

$$\sum_{k=0}^{n} \binom{n}{k} = 2^n \qquad \sum_{k=0}^{n} \binom{n}{k} (-1)^k = 0$$

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that can be obtained easily by specialization of the binomial formula:

$$(x+y)^n = \sum_{k=0}^{n} \binom{n}{k} x^k y^{n-k}$$

considering $(1+1)^n = 2^n$ and $((-1)+1)^n = 0$ respectively.

Answers as closed forms

By similar tricks:

$$\sum_{k=0}^{n} \binom{n}{k}^2 = \binom{2n}{n} \qquad \sum_{k=0}^{n} \binom{n}{k}^2 (-1)^k = 0$$

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but there is no hope to obtain any such *closed* form for higher powers of the binomial coefficients like $\sum_{k=0}^{n} \binom{n}{k}^3$, ...

Properties of sequences like $u_n := \sum_{k=0}^{n} \binom{n}{k}^3$ should be deduced from other informations than a closed form.

Answers as recurrences

A very informative data is a recurrence relation canceling the sequence:

- Optimized evaluation of the terms
- Asymptotic
- ...

Answers as recurrences: examples

- Our previous $u_n := \sum_{k=0}^{n} \binom{n}{k}^3$ is solution of:

$$(n+1)^2 a_{n+1} - (7n^2+7n+2)a_n - 8n^2 a_{n-1} = 0 \quad \text{(Franel, 1894)}$$

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- The sequence $u_n := \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2$ is solution of:

  $n^3 a_n - (34n^3 - 51n^2 + 27n - 5)a_{n-1} + (n-1)^3 a_{n-2} = 0$ (Apéry, 1978)

  which is a crucial point in its proof that $\zeta(3) := \sum_{k>0} \frac{1}{k^3}$ is irrational.

Checking a conjecture: easy cases

In these problems, checking a conjecture can be much easier than finding it. Example:

Let us prove the Cassini (1680) identity:

$$\forall n \in \mathbb{N}, F_{n+2}F_n - F_{n+1}^2 = (-1)^n$$

where F_n is the n-th Fibonacci number:

$$\forall n \in \mathbb{N}, F_{n+2} = F_{n+1} + F_n, \quad F(0) = 1, \quad F(1) = 1$$

Checking a conjecture: less easy cases

But checking a conjecture can also be extremely difficult:

Checking Apéry's claim that $u_n := \sum_k \binom{n}{k}^2 \binom{n+k}{k}^2$ verifies

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

took several months of effort to experts in number theory before being proved correct by Cohen and Zagier (1979).

Checking a conjecture: telescopes

In order to prove that $u_n := \sum_k v_{n,k}$ with $v_{n,k} := \binom{n}{k}^2 \binom{n+k}{k}^2$ verifies

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Cohen and Zagier construct $w_{n,k}$ such that:

$$n^3 v_{n,k} - (34n^3 - 51n^2 + 27n - 5)v_{n-1,k} + (n-1)^3 v_{n-2,k} = w_{n,k+1} - w_{n,k}$$

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$$= 0$$

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More than recipes

The collection of proofs we have seen so far is not a bag of tricks. There is:

- An algebraic framework and effective results
- Advances in algorithmics
- Efficient implementations in computer algebra systems

that systematize these lines of reasoning.

They provide automated ways of guessing and checking these identities/recurrences and their differential analogues.

Linear recurrences with polynomial coefficients

A sequence $u := (u_n)_{n\in\mathbb{N}} \in \mathbb{K}^{\mathbb{N}}$ is holonomic (or P-recursive) if it is a solution of a linear recurrence with coefficients in $\mathbb{K}[n]$.

- $F_{n+2} = F_{n+1} + F_n$
- $nu_{n+2} - (n^2 + 100)u_{n+1} - u_n = 0$

In the special case when the recurrence is of order 1 (and $u_0 \neq 0$) the sequence u is said to be hypergeometric.

- $(n+1)u_{n+1} = nu_n$

The definition extends obviously to sequences with several indexes and multivariate polynomial coefficients.

Linear recurrences with polynomial coefficients

- Elementary remark: Linear recurrences impose a structure of vector space to their set of solution.
- Hence in order to prove the equality of two holonomic sequences it is sufficient to:
  - Find a common linear recurrence relation
  - Check that the two sequences coincide on sufficiently many initial conditions.

Remember the Cassini identity $F_{n+2}F_n - F_{n+1}^2 = (-1)^n$.

Linear recurrences with polynomial coefficients

- Less obvious remark: The set of holonomic sequences on a field $\mathbb{K}$ is a $\mathbb{K}$-algebra.
- Hence if u and v are holonomic it is possible to:
  - Find a recurrence canceling $(u + v)$
  - Find a recurrence canceling $(u * v)$

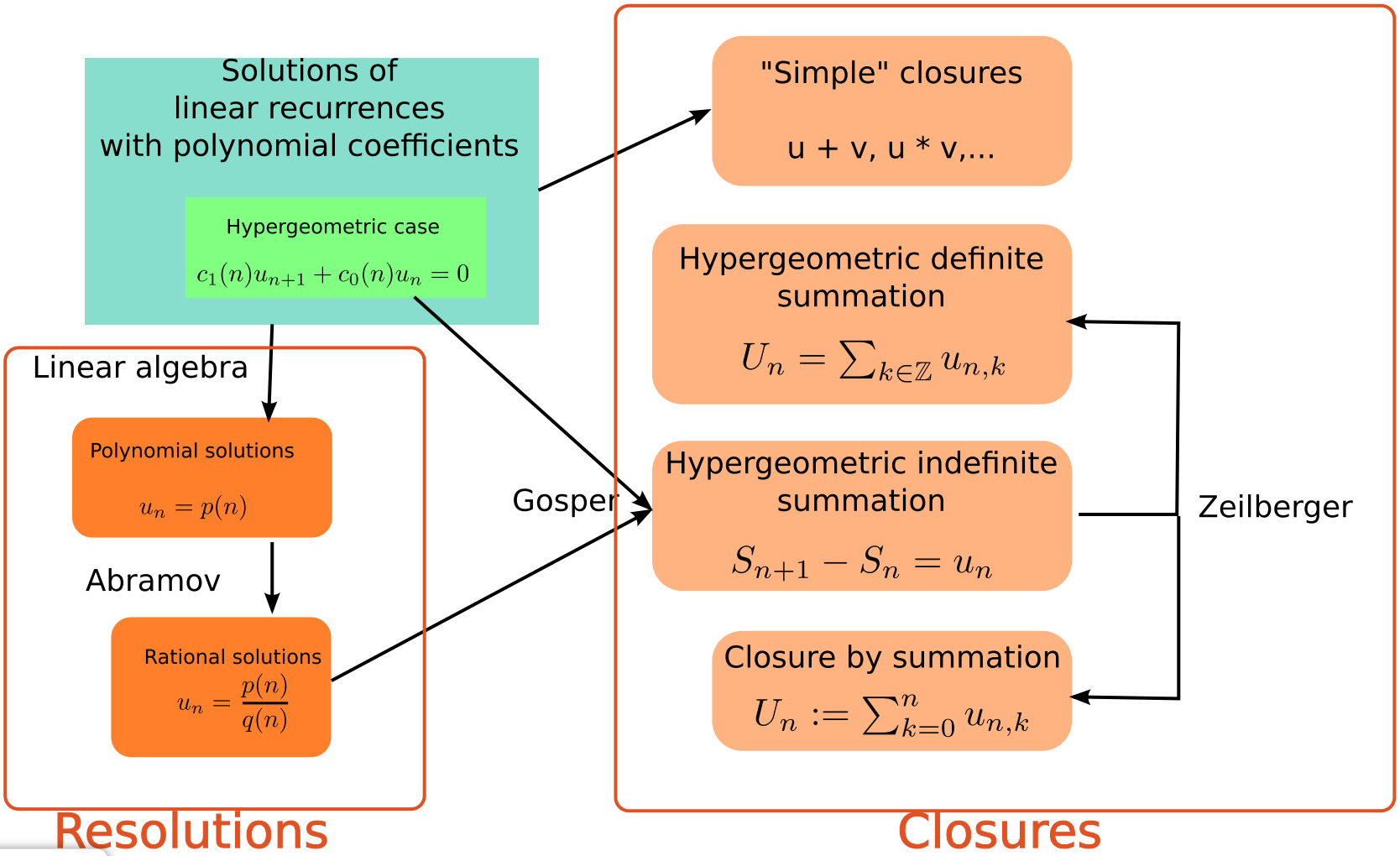
Find a recurrence canceling $\binom{n}{k} + k!F_n$.

Linear recurrences with polynomial coefficients

- Non obvious at all: If $(u_{n,k})$ is holonomic, it is possible to:
  - Find a recurrence canceling $U_n := \sum_{k=0}^{+\infty} u_{n,k}$
  - Find a recurrence canceling $U_n := \sum_{k=0}^{n} u_{n,k}$

Remember Apéry's sequence $u_n := \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2$

From existence theorems to efficient algorithms



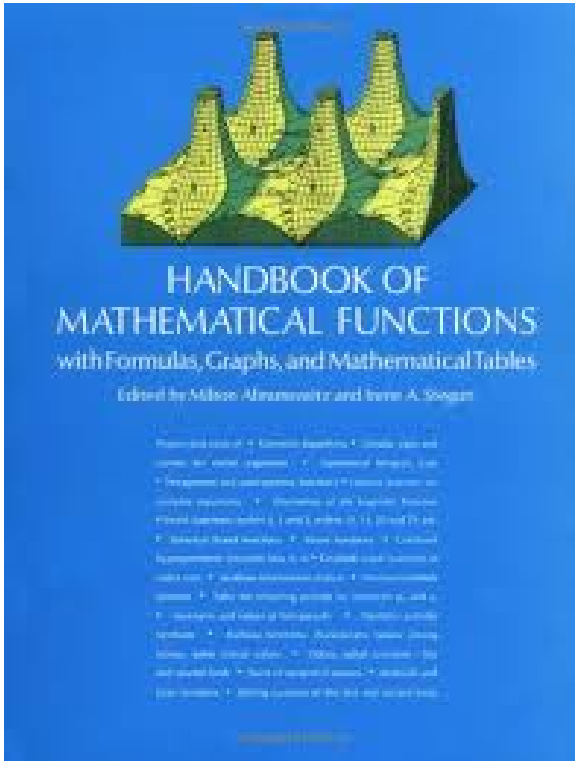
Linear differential operators with polynomial coefficients

The underlying theory (of D-modules and Ore/Weyl algebra) applies just as well to functions of a continuous variable:

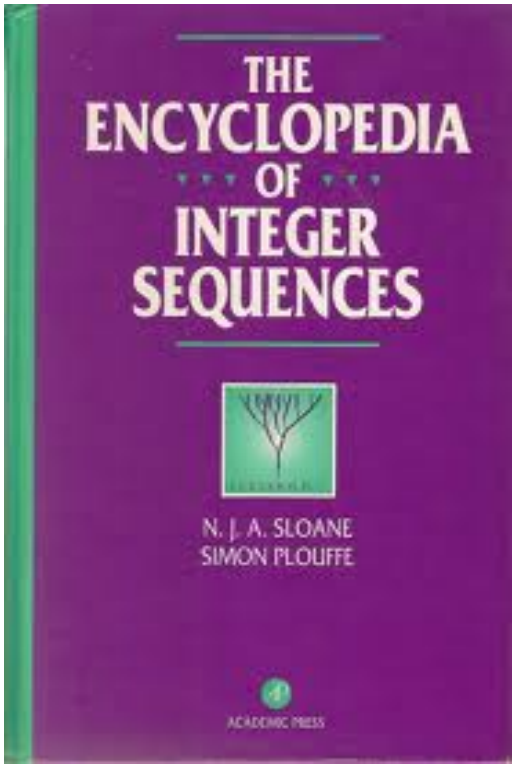
- A formal series $\sum_{n\geq 0} a_n X^n$ is holonomic (or D-finite) if it is solution of a differential equation with polynomial coefficients.
- Remark: A formal series is holonomic $\sum_{n\geq 0} a_n X^n$ if and only if the sequence (a_n) of its coefficients is holonomic.

And algorithms also transpose.

A large class of objects



Abramowitz and Stegun
$\sim 60\%$ of the entries are holonomic



Plouffe and Sloane
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Implementations and their applications

- Several packages are available in mainstream computer algebra systems (Maple, Mathematica).
- Computer-algebra aided proofs of several theorems (irrationality of $\zeta(3)$, q-TSPP conjecture,...)
- A Dynamic Dictionary of Mathematical Functions

  `http://ddmf.msr-inria.inria.fr/1.9.1/ddmf`

Confidence

- Static large tables of formulae are quite error-prone.
- Data-bases generated by generic computer-algebra algorithms are much more reliable.
- Generating these data-bases benchmarks the computer-algebra libraries and increase the confidence in computer algebra aided proofs.

Limits of computer algebra aided proofs

Beyond the possible but rather rare bugs that can affect these programs:

- Computer algebra systems manipulate symbolic expressions, not functions

$$\frac{0}{0} = \text{Error}, \qquad \frac{x-y}{x-y} = 1$$

- Equality almost everywhere is equality.
- Experts know the dark corners of the algorithms they design, but not necessarily the user.

Non-expert users can go wrong very quickly.

Limits of computer algebra aided proofs

Examples of dark corners:

- Singularities: $(n-4)u_{n+1} - (n-4)u_n = 0 \quad u_5 = ?$

  $\Rightarrow$ germs of sequences, not sequences.

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- Summation of rational fractions: $\sum_k (u_{n,k+1} - \frac{1}{k-4}u_{n,k})$
  $\Rightarrow$ Are we sure it never happens?

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Proof assistants

In a proof assistant, like the Coq system, the situation is much different:

- The user defines the mathematical objects inside the logic.
- The user specifies the mathematical objects inside the logic.
- For instance, the comparison relation between objects or the behavior of partial operations are made precise.
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But the efficiency of computations is poorer and certification is not an easy task.

Computer algebra aided formal proofs

We can benefit from both ways of doing mathematics with a computer:

- We guess recurrence operators using a computer algebra system (here Maple).
- We check formally their validity inside the proof assistant (here Coq).

We just pretty-print the output of a Maple session is some files, later included in the files describing the formal proof.

Formally proving Maple's recurrences

- We prove new recurrences from known ones.
- We normalize the conjectured recurrence using the known relations.
- The recurrence is reduced on independent shifts of the known sequences (Grobner basis).
- We normalize their (rational fraction) coefficients: they should be zero.

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But we should handle denominators with care, which makes the normalization less systematic.

Example: Apéry's proof that $\zeta(3) \notin \mathbb{Q}$

The crux of the proof is to verify that the two sequences:

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

satisfy the same linear recurrence of order two.

Example: Apéry's proof that $\zeta(3) \notin \mathbb{Q}$

For this we follow the syntactic tree of the expressions defining a_n and b_n:

- We (easily) know the recurrences canceling the leaves of the expressions of a_n and b_n: $\binom{n}{m}$, $\binom{n+m}{m}$, $\sum_{k=1}^{n} \frac{1}{k^3}$.

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- We prove formally and independently Maple's conjectures using the recurrences previously formally established.
- When proving a conjecture produced by Maple, we decorate it with the necessary side conditions.

Sketch of the proof

In order to prove that $\zeta(3) \notin \mathbb{Q}$ we show that otherwise we could exhibit a sequence S_n such that:

- $\forall n, \quad S_n$ is an integer
- $\forall n, \quad S_n > 0$
- $\lim_{n \to \infty} S_n = 0$

Sketch of the proof

In fact prove that:

$$a_n\zeta(3) - b_n \to 0 \quad \text{and} \quad \forall n, a_n \in \mathbb{Z}^* \quad b_n \in \mathbb{Q}^*$$

Now in fact if we pose $d_n := lcm(1, \ldots, n)$ we even have:

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In fact:

$S_n := 2d_n^3(a_n\zeta(3) - b_n)$ is the desired absurd sequence.

Steps in the proof

- $a_n\zeta(3) - b_n \to 0$

  considered elementary.
- $2d_n^3 b_n \in \mathbb{Z}$:

  considered as elementary arithmetic.
- $d_n \sim e^n$:

  considered as standard.
- $a_n\zeta(3) - b_n > 0$:

  asymptotic of a remainder since $a_n\zeta(3) - b_n \to 0$
- $2d_n^3(a_n\zeta(3) - b_n) \to 0$:

  asymptotic of the sequence $a_n\zeta(3) - b_n$

Current state of the formalization

Today we have checked in Coq that: $d_n = O(3^n) \Rightarrow \zeta(3) \notin \mathbb{Q}$.

- Proof of the common recurrence using a Maple session;
- Some elementary number theory (p-valuation, discrete log, binomials);
- A formal study of creative telescoping filling holes in the computer algebra literature;
- Improved formal proof-producing normalization procedures for ring/field expressions;
- Asymptotic reasoning using Cauchy reals and tactics for the bureaucracy of $\epsilon\delta$ reasoning.

Conclusion

- We now dispose of a systematic protocol to validate with a formal proof the recurrences for holonomic sequences guessed by th Algolib Maple library.
- We have used this protocol to formalize a large part of Apéry's proof that $\zeta(3) \in \mathbb{Q}$.
- Libraries from the Feit-Thompson proof have been instrumental in many places.
- But good data structures are still to be found (for proofs and for computations).
- Obtaining formal proofs in the differential case will be the next challenge, but a lot more formalized material is needed.