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Linear Differential Equations as a Data Structure

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Abstract
A lot of information concerning solutions of linear differential equations can be computed directly from the equation. It is therefore natural to consider these equations as a data structure, from which mathematical properties can be computed. A variety of algorithms has thus been designed in recent years that do not aim at "solving," but at computing with this representation. Many of these results are surveyed here.

Keywords Computer algebra · Linear differential equations · Algorithms · Complexity

Mathematics Subject Classification 68W30 · 33F10

1 Introduction

Computer algebra is a subfield of "foundations of computational mathematics" devoted to exact mathematical objects: their effectivity (what can be computed or decided?) and their complexity (how fast?). The first conference I am aware of that was devoted purely to symbolic and algebraic computation was held in Washington in 1966. Since then, for more than 50 years, numerous algorithms have been developed, many of which are available in today's popular computer algebra systems. This article presents a small fraction of the recent work in this area dedicated to linear differential equations and biased toward my own interests. It is mostly based on an invited talk at FoCM'17. The choice of presentation is to outline the underlying ideas through simple examples or algorithms and not put too much stress on proofs or general or formal statements, for which pointers to references are given.

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There are several motivations for exact computations with linear differential equations, depending on the origin of these equations.

Special Functions Many classical elementary or special functions are solutions of linear differential equations. This includes exponential, logarithm, rational functions, hypergeometric functions or generalized hypergeometric functions in their many variants (Bessel functions, Airy functions, Struve functions, etc.), orthogonal polynomials, etc. In this case, the differential equations have small order and the questions are to derive automatically formulas that practitioners currently look up in dedicated encyclopedias [4,106,115].

Generating Functions Another source of linear differential equations is provided by generating functions in combinatorics. There, the equations annihilate a power series whose nth coefficient counts the number of objects of interest of size n. The mere knowledge that this power series satisfies a linear differential equation gives information on the possible asymptotic behavior of those coefficients. From the actual differential equation, one can often derive precise asymptotics. In this area, the linear differential equations are often of high order. Their computation itself is difficult and requires efficient dedicated algorithms. A spectacular recent example was the study of so-called *Gessel walks* by Alin Bostan and Manuel Kauers [28]. These are walks confined to $\mathbb{N}^2$, starting from the origin and with steps restricted to $\{(-1, 0), (-1, -1), (1, 1), (1, 0)\}$. The coefficient of t^n in the generating function is a polynomial in two extra variables x and y, where the coefficient of $x^i y^j$ is the number of such walks of length n ending at the point with coordinates (i, j). In an intermediate step of their proof that this generating function is algebraic, they construct a linear differential equation of order 11 with coefficients that are polynomials of degree up to 96 in t and 78 in x and integer coefficients of up to 61 decimal digits. This is only for the value at $y = 0$ of the generating function! Such a computation would be impossible with straightforward algorithms.

Periods Linear differential equations of potentially high order also arise in more geometric contexts. The integral of a rational function in $n + 1$ variables over a cycle in $\mathbb{C}^n$ satisfies a linear differential equation in the remaining variable called a *Picard–Fuchs equation*. Algebraic integrands can also be allowed without changing the class of integrals, since algebraic functions can be expressed as residues of rational functions [61]. An early example of a linear differential equation arising in this way is Euler's computation of the perimeter of an ellipse as a function of its eccentricity. More recently, the computation of differential equations of this type has given rise to efficient algorithms for the computation of multiple binomial sums (see Sect. 15) and volumes of semi-algebraic sets [93].

The following two simple definitions make many statements more compact and set the notation for the sequel. There, as in the rest of this article, $\mathbb{K}$ denotes an arbitrary field of characteristic 0, even though some of the statements hold more generally.

Definition 1 A power series $S(z) \in \mathbb{K}[[z]]$ is called *differentially finite*, or in short, D-finite, when there exist polynomials $p_0(z), \dots, p_m(z)$ in $\mathbb{K}[z]$ with $p_m \neq 0$ such that

$$p_m(z)S^{(r)}(z) + \dots + p_0(z)S(z) = 0. \tag{1}$$

Definition 2 A sequence (u_n) of elements of $\mathbb{K}$ is called *polynomially recursive*, or in short, P-recursive, when there exist polynomials $a_0(n), \dots, a_r(n)$ in $\mathbb{K}[n]$ with $a_r \neq 0$ such that

$$a_r(n)u_{n+r} + \dots + a_0(n)u_n = 0, \qquad \text{for all } n \in \mathbb{N}. \tag{2}$$

A classical important observation relates these two families.

Proposition 1 *The power series $S(z) = \sum_{n\geq 0} u_n z^n \in \mathbb{K}[[z]]$ is differentially finite if and only if the sequence (u_n) is polynomially recursive.*

The computation of the recurrence from the differential equation or conversely is straightforward. (An efficient algorithm is known for large orders and degrees [19,23].) Even such a simple proposition has nontrivial computational consequences.

Example 1 In order to compute the coefficient of X^N in a high power like $P = (1 + X)^N(1 + X + X^2)^N$, an efficient method starts from the first-order linear differential equation satisfied by this polynomial:

$$\frac{P'}{P} = \frac{N}{1+X} + \frac{N(2X+1)}{1+X+X^2}.$$

From there, the proposition asserts the existence of a linear recurrence (of order 3 with coefficients of degree 1) for the coefficients of P. Using this recurrence makes it possible to obtain the Nth coefficient efficiently, without computing the previous ones, by the methods of Sect. 2.

The same reasoning extends to high-order coefficients of high-order powers of arbitrary polynomials, since the polynomial P^k satisfies the linear differential equation $Py' - kP'y = 0$, which is of order 1 with coefficients of degree at most deg P, leading to a linear recurrence of order deg P with coefficients of degree 1.

The plan of this article consists in visiting Fig. 1 from right to left. The central point is that linear differential equations with polynomial coefficients provide a useful representation for their solutions, even when the order or the degree of the coefficients of the equation is large. From the equation and its initial conditions, a lot of information concerning the solution can be computed exactly and often efficiently as well. This is covered in Part I. An important part of computer algebra that is not discussed here is the computation of closed-form solutions of these equations using differential Galois theory [116]. An advantage of having solutions in closed form is that these formulas provide analytic continuation “for free.” However, even when closed forms are available, which is rare, they are often not so appropriate for computations. Our approach will be to convert them into a linear differential equation, to which the algorithms described here apply. Once it is clear that many operations can be performed efficiently on linear differential equations, a natural objective is to design algorithms

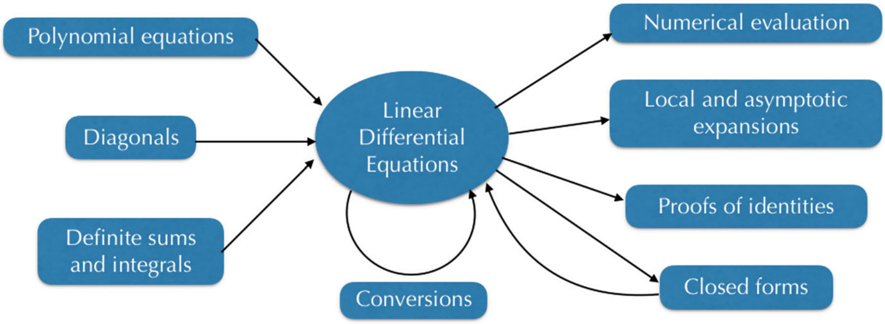

Fig. 1 Plan of the article

that compute such equations to solve other problems. This is the topic of Part III where differential equations are computed for algebraic functions, for multiple integrals and for generating functions of sums.

PART I. USING LINEAR DIFFERENTIAL EQUATIONS EXACTLY

2 Numerical Values from Linear Recurrences

Numerical values can be considered as exact mathematical objects when a bound on the approximation error is known and can be made arbitrarily small. It turns out that this can be achieved for all solutions of linear differential equations, with a very good complexity with respect to the desired precision, by exploiting linear recurrences and using only elementary ideas.

2.1 Fast Multiplication

In terms of complexity, the starting point is the fast Fourier transform (FFT). The theoretical complexity for multiplying two n-digit integers is $O(n \log n \log\log n)$ bit operations, with recent improvements [70,80] decreasing this bound slightly. We use the notation $\tilde{O}(n)$ for such complexities, meaning that they are in $O(n \log^k n)$ for some k. More generally, $\tilde{O}(f(n))$ for a function f tending to $+\infty$ means $O(f(n) \log^k f(n))$ for some $k > 0$. We say that an algorithm is *quasi-optimal* when its complexity is $\tilde{O}(n)$, for n the sum of the sizes of its input and output.

In practice, two integers of a million decimal digits can be multiplied in much less than one second on current laptops. Using Newton iteration, that same complexity of $\tilde{O}(n)$ and similar timings are reached for the computation of n digits of reciprocals, square roots and many other operations [34].

2.2 Efficient Computation of $n!$

Fast multiplication alone is not sufficient to compute $n!$ fast if one uses it naively. By Stirling's formula, the bit size of $k!$ grows roughly like $k \log k$, so that computing $n!$

as $((1 \times 2) \times 3) \cdots$ would lead to a complexity in $\tilde{O}(n^2)$, even if FFT is used. What happens is that all $k!$ for $k = 1, \ldots, n$ are obtained during intermediate computations and since the total bit size of those is $\tilde{O}(n^2)$, a lower bound in n^2 is unavoidable.

However, $n!$ can be computed more efficiently by a divide-and-conquer approach, using the equation

$$n! = \underbrace{n \times \cdots \times \lceil n/2 \rceil}_{\text{size } O(n \log n)} \times \underbrace{(\lceil n/2 \rceil - 1) \times \cdots \times 1}_{\text{size } O(n \log n)}.$$

By Stirling's formula, each half product has size growing asymptotically like $\frac{1}{2} n \log n$, so that their product can be computed in $\tilde{O}(n)$ bit operations. Applying the same divide-and-conquer approach recursively leads to a so-called "product tree," whose complete computation is performed in $\tilde{O}(n)$ bit operations [16]. For the special case of $n!$, it is even possible to save some of the logarithms hidden in the $\tilde{O}$ notation by looking at prime factors of n [18], but this idea does not generalize as much as the product tree technique.

2.3 Binary Splitting

The computation of $n!$ above does not make use of commutativity and thus extends to the efficient computation of products of matrices of integers. Rewriting a linear recurrence of order k over scalars into a first-order linear recurrence over vectors of dimension k therefore extends this method to arbitrary linear recurrences.

Example 2 The sequence

$$e_n = \sum_{k=0}^{n} \frac{1}{k!}, \tag{3}$$

is easily seen to satisfy the second-order linear recurrence $e_n = \frac{1}{n}((n+1)e_{n-1} - e_{n-2})$, $n \geq 2$, or equivalently

$$\begin{pmatrix} e_n \\ e_{n-1} \end{pmatrix} = \frac{1}{n} \underbrace{\begin{pmatrix} n+1 & -1 \\ n & 0 \end{pmatrix}}_{A(n)} \begin{pmatrix} e_{n-1} \\ e_{n-2} \end{pmatrix}.$$

Using the initial conditions leads to

$$\begin{pmatrix} e_n \\ e_{n-1} \end{pmatrix} = \frac{1}{n!} A!(n) \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

where $A!(n)$ denotes the *matrix factorial* $A(n)A(n-1)\cdots A(1)$. This product is computed as above by a divide-and-conquer method, which gives the nth element e_n in $\tilde{O}(n)$ bit operations, i.e., in a quasi-optimal way [33].

This reasoning leads to the following useful result.

Theorem 1 [48, Thm. 6.1] *If the sequence (u_n) is given by a linear recurrence with polynomial coefficients in $\mathbb{Q}[n]$ and initial conditions in $\mathbb{Q}$, all numerators and denominators of the rational numbers occurring in the initial conditions and in the coefficients* *of the recurrence being bounded by a fixed K, then as $N \to \infty$, the Nth element u_N is a rational number whose numerator and denominator have bit size bounded by $O(N \log N)$ and can be computed in $O(N \log^3 N \log\log N)$ bit operations. The result also holds for initial conditions as large as $O(N \log N)$ bits.*

Note that in the worst case, this computation is much faster than simply writing down all of $u_0, \dots, u_N$ (not to mention their computation), which would require a number of bits of order $N^2 \log N$.

This theorem gives the complexity of computing the value u_N as an unreduced rational number. If it is necessary to reduce the result to lowest terms, the final gcd between numerator and denominator and subsequent divisions also fit within this complexity bound using a fast algorithm for the gcd. If what is needed is not a rational number but a numerical estimate, then by classical techniques based on Newton iteration, one can also obtain as many as $O(N \log^2 N/\log\log N)$ digits of the decimal expansion within the same complexity bound.

A more precise estimate of the size and complexity in this theorem, taking into account the degree of the polynomial coefficients of the recurrence, the bound K on the integers and the order of the recurrence can be obtained without any extra difficulty [23, chap. 15]. This method is very powerful, and much more complicated sums than the truncation (3) of exp(1) can be computed efficiently that way.

Example 3 In particular, all recent record computations of π use the following formula discovered in 1989 by the Chudnovsky's [49]:

$$\frac{1}{\pi} = \frac{12}{C^{3/2}} \sum_{n=0}^{\infty} \frac{(-1)^n (6n)!(A + nB)}{(3n)!n!^3 C^{3n}},$$

with $A = 13591409$, $B = 545140134$ and $C = 640320$. This series gives roughly 14 digits per term. That observation alone is not sufficient to yield a fast algorithm, which is obtained by observing that the summands satisfy a linear recurrence of order 1 which can be subjected to binary splitting. (The final division and square root are handled by Newton iteration.) In theory, the techniques based on the arithmetic-geometric mean give an algorithm that is faster by a factor of $\log N$ for the computation of N decimal digits, but that method is more delicate to implement and thus binary splitting is preferred, even for record computations [11,17,78].

3 Numerical Values from Linear Differential Equations

As the example above suggests, this efficient method for computing the Nth element of polynomially recursive sequences extends to give a fast algorithm for the numerical evaluation of differentially finite functions. If f is differentially finite, (f_m) are the coefficients of its Taylor expansion at the origin and x is a rational number inside the disk of convergence of f, then the value of $f(x)$ is the limit of the sequence

$$F_n(x) = \sum_{m=0}^{n} f_m x^m, \qquad n \to \infty.$$

From a linear recurrence of order k for (f_m), one deduces a linear recurrence of order $k+1$ for $F_n(x)$, whose nth element can be computed efficiently using a product tree for the matrix factorial as above [10,48]. Example 2 illustrates this idea on the differential equation $y' - y = 0$ with $y(0) = 1$ that, in our context, defines the exponential.

Rough estimates show that in all cases, the tail of the power series $\sum_{m>n} f_m x^m$ decreases sufficiently fast for $O(n)$ terms to be sufficient for the computation of n digits of $f(x)$. In order to deduce from this method an algorithm for numerical evaluation, it is thus sufficient to provide effective bounds on that tail. This can be achieved by using the linear recurrence on the coefficients (f_m) to produce a majorant series whose speed of convergence is under control [82,104].

3.1 Analytic Continuation

The same approach that gives arbitrarily precise estimates for the value of a differentially finite power series at a rational point inside its disk of convergence also applies to the case of a complex point with rational real and imaginary parts. It also applies to the first derivatives of the power series at such a point. Thus, one can compute arbitrarily precise initial conditions for the same differential equation translated at such a point. From there, applying the same process again makes it possible to compute numerical approximations at any point given by a polygonal path starting from the origin, using only points with (preferably small) rational coordinates as vertices and avoiding the (finitely many) singularities of the equation. This method produces numerical evaluation at precision N in quasi-optimal complexity $\tilde{O}(N)$. Again, the whole computation only involves rational numbers and no round-off errors occur.

Low complexity relies on a precise control over the integers occurring in intermediate computations. When the differential equation is translated at a point with large rational real or imaginary part, then the linear recurrence that results inherits large rational coefficients that weigh on its evaluation. If the point where the evaluation is required itself has small rational real and imaginary parts, then it is always possible to find intermediate points of the same kind in the analytic continuation path and the complexity remains moderate.

Example 4 Figure 2 displays the domains of convergence of the series obtained at the intermediate points taken by M. Mezzarobba's `ore_algebra_analytic` package [103] to evaluate $\arctan(2+i)$ starting from the origin, using this strategy with further refinements regarding the choice of intermediate points so that their bit size remains small.

3.2 Bit Burst

When the targeted evaluation point is not a rational number but is known only via an approximation (e.g., π) then one can use analytic continuation again. Even if the point is inside the disk of convergence, this makes it possible to trade integer size for number of terms in the power series by a technique called *bit burst* [48]. For instance, in order

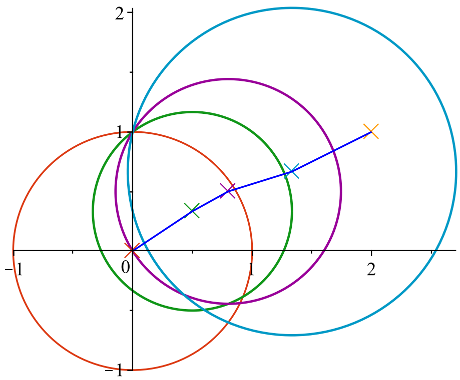

Fig. 2 Analytic continuation of arctan from 0 to $2+i$, using automatically selected intermediate points with small bit size inside the disk of convergence centered at the previous point. The circles of convergence of the successive power series are given, with the same color as their center

to evaluate at π a function given by its differential equation and initial conditions using this method, one would use as intermediate points the first rational numbers in the sequence $\left(\lfloor 2^{2^i}\pi\rfloor 2^{-2^i}\right)_{i\geq 0}$. While the size of the numerators and denominators of these rational numbers grows with i, the number of terms of the power series needed to obtain the desired accuracy decreases. These results are summarized in the following theorem.

Theorem 2 [48, Thm. 5.2] *If the power series $y(z)$ is given by a linear differential equation with polynomial coefficients in $\mathbb{Q}[z]$ and initial conditions, all numerators and denominators of the rational numbers occurring in the coefficients of the equation being bounded by 10^K, and all initial conditions being given at precision 10^{-K}, then given a point ζ inside the disk of convergence of $y(z)$ at precision 10^{-K}, the value of $y(\zeta)$ at precision 10^{-K} can be evaluated in $\tilde{O}(K)$ bit operations.*

More precise estimates can be derived in terms of all the parameters, with refinements for special cases and generalizations to singular points [23,48,50,83,84,102].

4 Local and Asymptotic Expansions

By the Picard–Lindelöf theorem (that we call Cauchy–Lipschitz in France), the linear differential equation (1) admits a basis of *analytic* solutions in the neighborhood of any point that is not a zero of its leading coefficient $p_m(z)$. For those solutions, Taylor expansions can be computed to arbitrary order efficiently using the linear recurrence that the coefficients satisfy.

4.1 Singular Behavior

In a neighborhood of a zero a of the leading coefficient, the Picard–Lindelöf theorem does not hold and the equation may present singular solutions. A classification of the possible behaviors of solutions is known. An important part is played by the *indicial polynomial* of the equation at a. This polynomial in $\mathbb{K}(a)[s]$ is obtained as the leading coefficient of the power series obtained by evaluating the linear differential equation at $(x-a)^s$ for a formal s and multiplying by $(x-a)^{-s}$. It is equal, up to an integer shift of s, to the leading coefficient of the recurrence satisfied by power series solutions of the differential equation at a. In the case of an *ordinary point*, i.e., when $p_m(a) \neq 0$, the indicial polynomial is simply $s(s-1)\cdots(s-m+1)$. More generally, when the degree of the indicial polynomial at a is equal to the order of the differential equation, the point a is called a *regular singular point* or a *Fuchsian* singularity. It is called an *irregular singular point* otherwise.

Theorem 3 [65] *If a is a regular singular point, then Eq.* (1) *admits a basis of formal solutions of the form*

$$(z-a)^\alpha \left(\phi_0(z) + \phi_1(z)\log(z-a) + \cdots + \phi_k(z)\log^k(z-a)\right) \tag{4}$$

where α (called an exponent *at the singularity a) is a root of the indicial polynomial and the coefficients ϕ_i are power series in $\mathbb{K}(\alpha)[[z-a]]$. When a is an irregular singular point, then Eq.* (1) *admits a basis of formal solutions of the form*

$$e^{P\left(1/(z-a)^{1/q}\right)}(z-a)^\alpha \left(\phi_0(z) + \phi_1(z)\log(z-a) + \cdots + \phi_k(z)\log^k(z-a)\right),$$

where P is a polynomial, q a nonnegative integer and the rest as in the regular singular case, except that the power series are now in powers of $(z-a)^{1/q}$.

(The behavior in the neighborhood of the point ∞ is obtained from the above by changing the variable z into $1/z$ in the equation and considering $a = 0$.)

The meaning of *formal* in this theorem is that these expressions satisfy the equation formally, but no convergence to an actual analytic solution is claimed. The formal aspects of this classical theory [57,86,113,126] have been transformed into computer algebra algorithms and code in the 1980s [60,122] and are now easily accessible. The analytic aspects are more delicate. In the regular singular case, Frobenius showed that the power series converge in a neighborhood of a. In the irregular singular case, they are generally divergent. Numerical sense can still be made of these expansions by resummation procedures [9,59,96,105].

A combination of these formal tools and those of the previous sections forms the basis of our *Dynamic Dictionary of Mathematical Functions* (DDMF) [13], an online encyclopedia[1] in the same spirit as the NIST DLMF[2] with two major differences: only solutions of linear differential equations are handled in the DDMF, and all the human expertise has been replaced by algorithms that provide an interactive access to the information, together with computer-generated proofs.

4.2 Proofs of Non-D-finiteness

The classification of the formal behavior of solutions of linear differential equations also provides an easy-to-use criterion to prove that a power series is *not* a solution of a

[1] Available at http://ddmf.msr-inria.inria.fr.

[2] https://dlmf.nist.gov.

linear differential equation with polynomial coefficients, or, by passing to generating functions, that a sequence is not the solution of a linear recurrence with polynomial coefficients. For instance, $\tan(z)$ cannot be a solution of such an equation, since it has infinitely many poles, while the singularities of solutions of linear differential equations can only lie at the roots of the leading coefficient. In an analogous way, the classical Bernoulli numbers that are present in Stirling's formula or in the Euler–Maclaurin formula have generating function $z/(\exp(z)-1)$ which has poles at all $2k\pi i$, $k \in \mathbb{Z} \setminus \{0\}$ and thus cannot satisfy a linear recurrence with polynomial coefficients. Exploiting not only the number of singularities but the classification of the local behavior given above is a natural way to prove that no linear recurrence with polynomial coefficients can be satisfied by sequences [66,67] like

$$\log n, \quad \sqrt{n}, \quad p_n \text{ (the } n\text{th prime number)}, \quad e^{\sqrt{n}}, \quad e^{1/n}, \quad \Gamma(n\sqrt{2}), \dots$$

4.3 Arithmetic Properties

Many generating functions $f \in \mathbb{Q}[[x]]$ arising in combinatorics possess the property of being *globally bounded*: f has positive radius of convergence and there exist a and b in $\mathbb{N} \setminus \{0\}$ such that $af(bx) \in \mathbb{Z}[[x]]$.

Theorem 4 [6,47,88] *If $F \in \mathbb{Q}[[x]]$ is differentially finite and globally bounded, then it satisfies a Fuchsian equation (all the singular points, including ∞, are regular) and all the exponents are rational numbers.*

This result also can be used to dismiss the possibility that a given sequence satisfies a linear recurrence.

Example 5 Many sequences arising in the enumeration of walks in the quarter plane can be proved not to satisfy a linear recurrence with polynomial coefficients [31]. A typical example is the number of walks on $\mathbb{N} \times \mathbb{N}$ using n steps, all taken in the set $\{(-1, 0), (0, 1), (1, 0), (1, -1), (0, -1)\}$, as pictured in Fig. 3. Using recent results connecting the asymptotic growth of this sequence to the first eigenvalue of the Laplacian on a spherical triangle, we obtained that this asymptotic growth is of the form $C\rho^n n^\alpha$ with $\alpha = -1 + \pi/\arccos(u)$, u a zero of $8u^3 - 8u^2 + 6u - 1$ so that $\alpha \notin \mathbb{Q}$, leading to a contradiction.

5 Singularity Analysis

The asymptotic growth of a sequence (a_n) can often be analyzed by considering its generating function

$$A(z) := \sum_{n \geq 0} a_n z^n$$

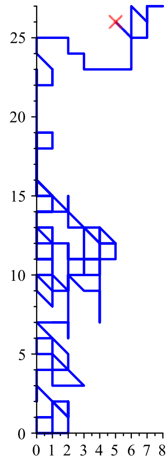

Fig. 3 A walk starting from (0,0), remaining in $\mathbb{N}^2$ and using 200 steps taken from $\{(-1,0),(0,1),(1,0),(1,-1),(0,-1)\}$. The number of such walks with n steps can be proved *not* to satisfy a linear recurrence with polynomial coefficients

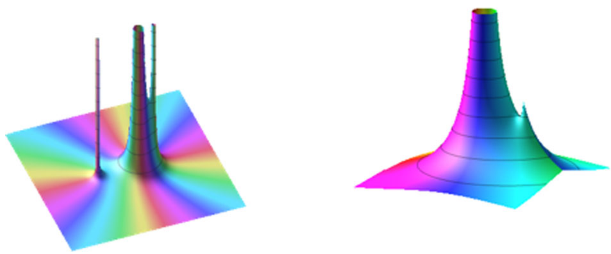

Fig. 4 A view of the first Fibonacci number (left) and Catalan number (right) in the complex plane. (The colors indicate the argument of the integrand) (Color figure online)

in the complex plane. When the radius of convergence is positive, the starting point is Cauchy's formula

$$a_n = \frac{1}{2\pi i}\oint \frac{A(z)}{z^{n+1}}\,\mathrm{d}z,$$

where the contour encloses the origin but no singularity of $A(z)$.

Example 6 Figure 4 displays the absolute value of the integrand for the cases when $n = 1$ and $A(z) = 1/(1 - z - z^2)$ (left) or $(1 - \sqrt{1-4z})/(2z)$ (right).

The value at 0 is infinite due to the division by z^{n+1}, which is shown by a sort of "chimney" in the middle of the pictures where the graph is truncated. As n increases, the "chimney" grows and the value of the integral concentrates in a neighborhood of the singularity of smallest modulus. This leads to a three-step method called *singularity analysis* [68,69]: (i) locate the singularities of minimal modulus; (ii) compute the local behavior of the generating function there; and (iii) translate into the asymptotic behavior of the sequence. In view of the previous two theorems, the following is the most useful result for polynomially recursive sequences from combinatorics.

Theorem 5 [87] *Let $A(z) = \sum_{n\geq 0} a_n z^n$ be a differentially finite power series with positive radius of convergence ρ. Assume that the only singularity of $A(z)$ of modulus ρ is at $z = \rho$ and that*

$$A(z) \sim c \left(1 - \frac{z}{\rho}\right)^{\alpha} \log^m \frac{1}{1 - \frac{z}{\rho}}, \quad z \to \rho-$$

with $\alpha \notin \mathbb{N}$, then

$$a_n \sim c\rho^{-n} \frac{n^{-\alpha-1}}{\Gamma(-\alpha)} \log^m n, \quad n \to \infty.$$

Full asymptotic expansions are available as well, and the case of several singularities on the circle of convergence can be dealt with too [69].

In the case of a polynomially recursive sequence, the linear differential equation gives the value of ρ as a root of minimal modulus of its leading coefficient. The computation of α and m can be obtained from the differential equation as mentioned before. The last point is the computation of the constant factor c: the initial conditions for the differential equation are known at the origin as the first elements of the sequence (a_n), and we need to express this solution as a linear combination of a basis of possible behaviors at ρ. In most cases, these constants can then be obtained numerically by analytic continuation (proving that one of the coefficients in this linear combination is 0 is a problem for which we only have a semi-decision algorithm).

Example 7 Pólya's random walk in $\mathbb{Z}^d$ starts at the origin and repeatedly moves one step along one of the axes with uniform probability. The question is to compute the probability p_d that the walk returns to the origin. It is a famous result of Pólya's that $p_2 = 1$. For higher dimension, the probability is smaller than 1. Here is how it can be computed numerically with arbitrary precision. The steps are given for dimension 3, and that approach has been used up to dimension 15 (where 100 digits are obtained in 1 min.):

1. the probability u_n that the walk returns to the origin in $2n$ steps satisfies

$$\begin{aligned}&(2n+3)(2n+1)(n+1)u_n - 2(2n+3)(10n^2+30n+23)u_{n+1}\\ &\quad +36(n+2)^3 u_{n+2} = 0\end{aligned}$$

   (this step is not trivial);
2. from there one could compute $a_n := \sum_{k=0}^{n} u_k$ which converges to $c := 1/(1 - p_3)$, but the convergence is slow, due to a singularity of the generating function at 1;
3. instead, given a_0, a_1, a_2, Mezzarobba's code mentioned above takes .4 sec. to produce 100 digits of c, c_2, c_3 such that

$$A(z) \approx c\left(\frac{1}{1-z} + \cdots\right) + c_2\left(\frac{1}{\sqrt{1-z}} + \cdots\right) + c_3(1 + \cdots),$$

   from there, the theorem above with $\alpha = -1, m = 0$ gives c and then p_3 follows.

In dimension 3, it turns out that a nice expression is available [74,127]:

$$c = \frac{\sqrt{6}}{32\pi^3}\Gamma\left(\frac{1}{24}\right)\Gamma\left(\frac{5}{24}\right)\Gamma\left(\frac{7}{24}\right)\Gamma\left(\frac{11}{24}\right),$$

which can be used to check our computations. In higher dimension, only the numerical values seem available currently [81].

6 Proofs of Identities

6.1 Confinement and Closure Properties

One way to prove that two power series are equal is to show that they are both solutions of a common linear differential equation, with the same initial conditions. Thus, the computation is reduced to finitely many operations.

Example 8 Here is how one can prove that

$$\sin^2(x) + \cos^2(x) = 1$$

with very little computation.

First, sin and cos are defined by a second-order linear differential equation $y'' + y = 0$. Next, the square of a solution to this equation is also solution of a linear differential equation. Indeed, using the differential equation to rewrite y'' as $-y$ shows that the $\mathbb{Q}$-vector space generated by $\{y^2, yy', y'^2\}$ is closed under differentiation. Thus, if $h = y^2$, then (h, h', h'', h''') are four vectors in a vector space of dimension at most 3, which implies that they must be linearly dependent. A linear dependency between them is precisely a linear differential equation satisfied by y^2. If needed, it is computed as the left kernel of the matrix

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ -2 & 0 & 2 \\ 0 & -8 & 0 \end{pmatrix}$$

that gives the coordinates of (h, h', h'', h''') on (y^2, yy', y'^2). This shows that $h''' + 4h' = 0$. However, at this stage, it is sufficient to know that this equation exists. Since this reasoning does not make use of the initial conditions, that same third-order differential equation is satisfied by $\sin^2$ and $\cos^2$ and, by linearity, by their sum.

The constant -1 is solution of a trivial first-order linear differential equation $y' = 0$, so that for any h as above, $(h - 1, h', h'', h''', h^{(4)})$ are five vectors in a vector space of dimension at most 4 generated by $(-1, h, h', h'')$, implying the existence of a linear differential equation of order at most 4, with constant coefficients, satisfied by $w := \sin^2 + \cos^2 - 1$.

Now, using the initial conditions for sin and cos to compute

$$\sin^2(x) + \cos^2(x) - 1 = O(x^4)$$

concludes the proof by the Picard–Lindelöf theorem: the initial conditions defining w are (0,0,0,0).

In summary, confining a power series and all its derivatives inside a finite-dimensional vector space makes it possible to use simple linear algebra for the proof of nonlinear identities involving products of power series. A similar reasoning applies to solutions of linear recurrences.

Example 9 It is a simple exercise to prove Cassini's identity

$$F_{n+1}F_{n-1} - F_n^2 = (-1)^n,$$

where F_n denotes the nth Fibonacci number along exactly the same lines, with the recurrence $F_{n+2} = F_{n+1} + F_n$ playing the role of $y'' + y = 0$.

With the same arguments, one can prove the following classical result.

Theorem 6 [119, Thm. 6.4.9] *The set of power series solutions of linear differential equations with coefficients in* $\mathbb{K}[x]$ *is a* $\mathbb{K}$*-algebra. So is the set of sequences solutions of linear recurrences with polynomial coefficients in* $\mathbb{K}[n]$.

More advanced example: Mehler's identity on the Hermite polynomials

$$\sum_{n=0}^{\infty} H_n(x)H_n(y)\frac{u^n}{n!} = \frac{\exp\left(\frac{4u(xy-u(x^2+y^2))}{1-4u^2}\right)}{\sqrt{1-4u^2}}. \tag{5}$$

The starting point of the automatic proof of this identity is to "define" the Hermite polynomials. It will be sufficient here to use the fact that they satisfy a linear recurrence of order 2. Next, the existence of this recurrence implies that all the sequences $H_{n+k}(x)H_{n+k}(y)/(n+k)!$ for integer $k \in \mathbb{N}$ are generated over $\mathbb{Q}(x, y, n)$ by

$$\frac{H_n(x)H_n(y)}{n!}, \quad \frac{H_{n+1}(x)H_n(y)}{n!}, \quad \frac{H_n(x)H_{n+1}(y)}{n!}, \quad \frac{H_{n+1}(x)H_{n+1}(y)}{n!},$$

so that the summand in the left-hand side of Eq. (5) satisfies a linear recurrence of order at most 4. That recurrence can then be translated directly into a linear differential equation satisfied by the generating function.

In that case, knowing only the order of the recurrence equation is not sufficient anymore. Fortunately, the linear-algebra-based algorithms that compute recurrences or differential equations for sums and products of solutions of recurrences or differential equations have been implemented in several packages [89,97,118]. Here, we use Maple's `gfun`. In this computation, the nth Hermite polynomial in the variable x is denoted $H_x(n)$ instead of the usual $H_n(x)$. We first define the Hermite polynomials:

```
> R[1] := {H[x](0) = 1, H[x](1) = 2*x,
H[x](n+2) = (-2*n-2)*H[x](n)+2*H[x](n+1)*x};
```

$$R_1 := \{H_x(0) = 1, H_x(1) = 2x, H_x(n+2) = (-2n-2)H_x(n) + 2H_x(n+1)x\}$$

```
> R[2] := subs(x = y, R[1]);
```

$$R_2 := \{H_y(0) = 1, H_y(1) = 2y, H_y(n+2) = (-2n-2)H_y(n) + 2H_y(n+1)y\}$$

The final term of the product, $1/n!$, is defined by the recurrence $(n+1)v_{n+1} = v_n$. Next, we compute the recurrence satisfied by the product $H_n(x)H_n(y)/n!$:

```
> R[3] := gfun:-poltorec(H[x](n)*H[y](n)*v(n),
[R[1], R[2], {v(n+1)*(n+1) = v(n), v(1) = 1}],
[H[x](n), H[y](n), v(n)], c(n));
```

$$\begin{aligned} R_3 := \Big\{&(16n+16)c(n) - 16xyc(n+1) + (8x^2 + 8y^2 - 8n - 20)c(n+2) \\ &- 4xyc(n+3) + (n+4)c(n+4), \\ &c(0) = 1, c(1) = 4xy, c(2) = 8x^2y^2 - 4x^2 - 4y^2 + 2, \\ &c(3) = \frac{32}{3}x^3y^3 - 16x^3y - 16xy^3 + 24xy, \\ &c(4) = \frac{32}{3}x^4y^4 - 32x^4y^2 - 32x^2y^4 + 8x^4 + 96x^2y^2 + 8y^4 - 24x^2 - 24y^2 + 6\Big\} \end{aligned}$$

The first element of that set is the recurrence, without the "$= 0$" part. The other ones give the corresponding initial conditions. This recurrence is then translated into a linear differential equation for the right-hand side of Eq. (5):

```
> gfun:-rectodiffeq(R[3], c(n), f(u));
```

$$\Big\{(-16u^2xy + 16u^3 + 8ux^2 + 8uy^2 - 4xy - 4u)f(u) + (16u^4 - 8u^2 + 1)f'(u), f(0) = 1\Big\}$$

Again, the "$= 0$" part is omitted from the first equation. At this stage, it is straightforward to solve this first-order equation and retrieve the desired result:

```
> dsolve(%,f(u)) assuming 0<u,u<1/2;
```

$$f(u) = \frac{e^{-\frac{4xyu - x^2 - y^2}{(2u-1)(2u+1)}}}{e^{-x^2-y^2}} \sqrt{\frac{1}{(2u+1)(-2u+1)}}$$

6.2 Application to Continued Fractions

Recently, we applied the same approach to the computation of explicit formulas for continued fractions by a guess-and-prove approach [99]. A typical example is provided by the continued fraction for $\tan z$. Starting from its definition by the Riccati equation

$y' = 1+y^2$ with initial condition $y(0) = 0$, it is easy to compute the first 15 coefficients of its Taylor expansion at 0. From there, repeatedly subtracting the first term, factoring out the next one and inverting the rest leads to the continued fraction

$$\tan z = \cfrac{z}{1 - \cfrac{z^2/3}{1 - \cfrac{z^2/15}{1 - \cfrac{z^2/63}{1 - \cfrac{z^2/99}{1 - \cfrac{z^2/143}{1 - \cdots}}}}}}.$$

From there, rational interpolation guesses automatically that the partial numerators are given by the formula

$$a_1(z) = z, \qquad a_n(z) = -\frac{z^2}{(2n-3)(2n-1)} \quad (n \geq 2). \tag{6}$$

This formula was the basis for Lambert's proof that π is irrational in 1761.

The next step is to obtain an automatic proof that the continued fraction defined by these elements $a_n(z)$ converges to the unique solution of the Riccati equation with $y(0) = 0$. Defining

$$H_n := Q_n^2 \left(\left(\frac{P_n}{Q_n} \right)' - 1 - \left(\frac{P_n}{Q_n} \right)^2 \right),$$

where P_n/Q_n is the nth convergent of the continued fraction gives a polynomial in P_n, Q_n, P_n', Q_n'. A fundamental result in the theory of continued fractions is that the *linear recurrence* $u_n = u_{n-1}+a_n u_{n-2}$ is satisfied by both P_n and Q_n, with different initial conditions. In view of our candidate a_n, we deduce that all H_{n+k} for $k \in \mathbb{N}$ can be rewritten as linear combinations of $P_{n+i}P_{n+j}$, $Q_{n+i}Q_{n+j}$, $P'_{n+i}Q_{n+j}$, $P_{n+i}Q'_{n+j}$, for i and j in $\{0, 1\}$. It follows that the sequence H_n satisfies a linear recurrence that can be computed. The computation produces a linear recurrence of order 4 obtained without taking into account the initial conditions for P_n and Q_n. Using the actual sequences makes it possible to guess the simpler

$$H_{n+1} = -\frac{z^2}{(2n+1)^2} H_n,$$

which is then proved by Euclidean division of the recurrence operators (see Sect. 10). Thus, $H_n = O(z^{2n})$ tends to 0 as a power series, which concludes the proof of the formula (6) without any human intervention.

This method has been applied to all explicit C-fractions in the recent compendium by Cuyt et al. [58], starting from one of

– a Riccati equation: $y' = A(z) + B(z)y + C(z)y^2$;
– a q-Riccati equation: $y(qz) = A(z) + B(z)y(z) + C(z)y(z)y(qz)$;
– a difference Riccati equation: $y(s+1) = A(s) + B(s)y(s) + C(s)y(s)y(s+1)$.

The surprising observation is that this method works in all cases, including Gauss's classical continued fraction for the quotient of contiguous hypergeometric series, its q-analogue due to Heine, Brouncker's continued fraction for the Gamma function. In all cases, the corresponding sequence H_n satisfies a linear recurrence of small order that is sufficient to prove the convergence. Work is in progress to explain why this method works so well and classify the formulas it yields [100].

Part II. Conversions

This short second part is devoted to the middle part of Fig. 1: conversions from linear differential equations to linear recurrences. It also serves as an introduction to the operator formalism used in the next part.

7 Ore Polynomials

The differentiation operator D_x and the operator x of multiplication by x act on power series in x and obey the commutation law $D_x x = x D_x + 1$, where 1 denotes the identity operator. This is an operator view of the usual relation $(xf)' = xf' + f$.

Similarly, the shift operator S_n and the operator n of multiplication by n act on sequences indexed by n, with commutation $S_n n = (n+1)S_n$ reflecting the relation $(nu_n)|_{n\mapsto n+1} = (n+1)u_{n+1}$.

The analogy between these operators and polynomials has been observed at least since the 1830s [32,95]. The modern point of view was introduced by Ore a century later [107,108].

Definition 3 Let $\mathbb{A}$ be a ring with no zero divisor, σ a ring endomorphism of $\mathbb{A}$ and δ a σ-derivation, which means that for all a, b in $\mathbb{A}$, $\delta(ab) = \sigma(a)\delta(b) + \delta(a)b$. Then the *skew polynomial ring* $\mathbb{A}\langle\partial; \sigma, \delta\rangle$ is the ring of polynomials in ∂ with coefficients in $\mathbb{A}$ with usual addition and a product defined by associativity from the commutation

$$\forall a \in \mathbb{A}, \quad \partial a = \sigma(a)\partial + \delta(a).$$

The elements of $\mathbb{A}\langle\partial; \sigma, \delta\rangle$ are called *Ore polynomials*.

Special cases are the classical polynomial ring $\mathbb{A}[x] = \mathbb{A}\langle x; \mathrm{Id}, 0\rangle$; the ring of linear differential operators $\mathbb{K}(x)\langle D_x\rangle := \mathbb{K}(x)\langle D_x; \mathrm{Id}, \mathrm{d}/\mathrm{d}x\rangle$; the ring of difference operators $\mathbb{K}(n)\langle\Delta_n\rangle := \mathbb{K}\langle\Delta_n; (a(n) \mapsto a(n+1)), (a(n) \mapsto a(n+1) - a(n)\rangle$; its close relative the ring of recurrence operators $\mathbb{K}(n)\langle S_n\rangle := \mathbb{K}(n)\langle S_n; (a(n) \mapsto a(n+1)), 0\rangle$. In cases like this last one, where $\delta = 0$ and σ is invertible, it is also natural to consider the ring of Laurent Ore polynomials in S_n, denoted $\mathbb{K}(n)\langle S_n, S_n^{-1}\rangle$, with the obvious commutations $S_n^{-1}a(n) = a(n-1)S_n^{-1}$ and $S_n S_n^{-1} = S_n^{-1}S_n = 1$ [131].

Ore polynomials have played an increasing role in the design of algorithms in computer algebra since their introduction in this area around 20 years ago [35].

8 Taylor Morphism

In this setting, the correspondence between linear differential equations and linear recurrence satisfied by the sequences of coefficients of their power series solutions becomes a ring morphism between $\mathbb{Q}[x, x^{-1}]\langle D_x\rangle$ and $\mathbb{Q}[n]\langle S_n, S_n^{-1}\rangle$, defined by

$$D_x \mapsto (n+1)S_n, \qquad x \mapsto S_n^{-1}. \tag{7}$$

(See, e.g., [36, p. 58] for a more general statement.)

Example 10 The Airy function $\mathrm{Ai}(x)$ is defined by the equation

$$y'' - xy = 0, \qquad y(0) = \frac{\sqrt[3]{3}}{3\Gamma(2/3)}, \quad y'(0) = -\frac{\sqrt[6]{3}\Gamma(2/3)}{2\pi}.$$

The Taylor morphism applied to differential operator $D_x^2 - x$ yields

$$D_x^2 - x \mapsto (n+1)S_n(n+1)S_n - S_n^{-1} = (n+1)(n+2)S_n^2 - S_n^{-1},$$

the last operator being obtained by the commutation $S_n(n+1) = (n+2)S_n$. This recovers the recurrence

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

from which one deduces the classical Taylor expansion

$$\mathrm{Ai}(x) = \frac{\sqrt[3]{3}}{3\Gamma(2/3)} \sum_{n\geq 0} \frac{x^{3n}}{\Gamma(n+2/3)9^n n!} - \frac{3^{2/3}}{9} \sum_{n\geq 0} \frac{x^{3n+1}}{\Gamma(n+4/3)9^n n!}.$$

9 Chebyshev Expansions

Taylor expansions converge well inside their disk of convergence, but when the aim is to approximate a function on a real interval, it is usually preferable to use Chebyshev expansions [43,98,123]. This is exemplified on the case of the function arctan on the interval $[-1, 1]$ in Fig. 5. On the left, the graphs of $S_n(x)$ and of $\arctan x - S_n(x)$ are displayed for $n = 0, \ldots, 4$, with

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

the truncation of the Taylor expansion. On the same scale, the graphs of $C_n(x)$ and $\arctan x - C_n(x)$ are displayed on the right, with

$$C_n(x) = 2(\sqrt{2}-1)T_1(x) + \cdots + \frac{(-1)^n(\sqrt{2}-1)^{2n+1}}{n+1/2} T_{2n+1}(x),$$

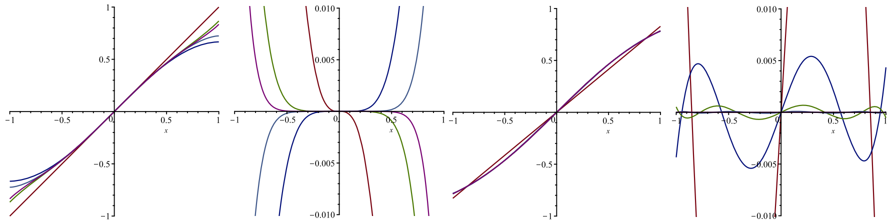

Fig. 5 Truncations of Taylor expansions (left) and Chebyshev expansions (right) to arctan, with the corresponding errors

where $T_i(x)$ denotes the ith Chebyshev polynomial of the first kind, defined for instance by $T_i(\cos x) = \cos(ix)$. Already for C_1, the difference with the next ones and with arctan cannot be seen on the graph. The graphs of differences show how the error is spread out more uniformly over the interval in the Chebyshev expansions.

Obviously, the situation would be even more contrasted on an interval $[-c, c]$ with $c > 1$, where the Taylor expansion does not converge anymore due to the logarithmic singularities at $\pm i$, while the Chebyshev expansion

$$\sum_{n\geq 0} \frac{(-1)^n \left(\frac{\sqrt{c^2+1}-1}{c}\right)^{2n+1}}{n+1/2} T_{2n+1}(x/c) \tag{8}$$

still converges very well.

Both expansions have the property that their coefficients satisfy a linear recurrence that can be computed automatically from the linear differential equation. While the case of Taylor expansions uses Ore polynomials, that of Chebyshev expansions can be computed using Ore fractions that we now discuss.

10 Ore Fractions

By design, the degree of the product of two Ore polynomials is the sum of their degrees. (In particular, there are no zero divisors.) Next, for two Ore polynomials A and B *with coefficients in a field*, a right Euclidean division $A = QB + R$ can be defined and computed as for commutative polynomials, except that all multiplications of B take place on the left. From there, Euclid's algorithm for the greatest common right divisor of A and B follows, as well as the extended version that computes the cofactors. Moreover, performing a final iteration of this extended Euclidean algorithm provides least common left multiples.

Theorem 7 [108] *Given two Ore polynomials A and B in a skew polynomial ring $\mathbb{K}\langle\partial; \sigma, \delta\rangle$ over a field $\mathbb{K}$, the Euclidean algorithm produces polynomials u, v, G, U, V in $\mathbb{K}\langle\partial; \sigma, \delta\rangle$ such that*

$$uA + vB = G, \quad UA + VB = 0,$$

G is a greatest common right divisor (gcrd) of A and B, while UA is a least common left multiple (lclm) of them.

Now, as in the commutative case, fractions are equivalence classes of pairs of polynomials. For our purpose, they are written with the denominator on the left. Two fractions $B^{-1}A$ and $D^{-1}C$ are equal when $uA = vC$ where u and v are such that $uB = vD = \operatorname{lclm}(B, D)$. (Proceeding formally gives $B^{-1}A = B^{-1}u^{-1}uA = (uB)^{-1}uA = (vD)^{-1}vC = D^{-1}v^{-1}vC = D^{-1}C$, which explains where this formula comes from.) It is then a simple exercise to determine the algorithms for addition and multiplication:

$$B^{-1}A + D^{-1}C = \operatorname{lclm}(B, D)^{-1}(uA + vC) \qquad \text{where} \quad uB = vD = \operatorname{lclm}(B, D),$$
$$B^{-1}AD^{-1}C = (uB)^{-1}vC \qquad \text{where} \quad uA = vD = \operatorname{lclm}(A, D).$$

These operations turn the set of fractions into a (non-commutative) field [108].

11 Application to Chebyshev Expansions

The Taylor morphism (7) is a reflection of the action of d/dx and x on the basis (x^n): $(x^n)' = nx^{n-1}$ and $x(x^n) = x^{n+1}$. Basic trigonometric identities give the analogous relations

$$2xT_n(x) = T_{n+1}(x) + T_{n-1}(x), \quad 2(1 - x^2)T_n'(x) = -nT_{n+1}(x) + nT_{n-1}(x) \quad (9)$$

for the Chebyshev polynomials. The first one indicates that x should be mapped to $X := (S_n + S_n^{-1})/2$. The factor $(1 - x^2)$ in the second one prevents such a direct translation. Proceeding formally in terms of operators suggests that d/dx should be mapped to the Ore fraction $D := (1 - X^2)^{-1}n(S_n - S_n^{-1})/2$. Indeed, if $L(x, d/dx)$ cancels a sufficiently smooth function f, then any numerator of the Ore fraction $L(X, D)$ cancels the coefficients of its Chebyshev expansion [15]. This approach sheds new light on previous algorithms in this area [94,109,117].

Example 11 For $\arctan(cx)$, A. Benoit's package `GFS` (for Generalized Fourier Series) [12] produces:

```
> deq := (c^2*x^2+1)*(diff(y(x),x,x))+2*c^2*x*(diff(y(x),x));
> diffeqToGFSRec(deq,y(x),u(n),functions=ChebyshevT(n,x));
```

$$c^2nu(n) + 2(c^2 + 2)(n + 2)u(n + 2) + c^2(n + 4)u(n + 4)$$

Together with initial conditions, this leads to the formula for the Chebyshev expansion (8).

The numerical use of these recurrences is delicate: generally, as in this example, the characteristic polynomial of the leading coefficient in n, here $c^2 + 2(c^2 + 1)X + c^2X^2$, is reciprocal, which implies that its asymptotically dominant solutions tend to infinity, while the coefficients of Chebyshev expansions tend to 0. Thus, when unrolling the recurrence naively, any numerical round-off error is eventually amplified exponentially. Nonetheless, a recent work of Benoit, Joldes and Mezzarobba shows how these recurrences can be exploited, leading to an efficient algorithm in the context of validated numerical evaluation [14].

Part III. Computing Linear Differential Equations (Efficiently)

The previous parts have shown how information can be extracted from linear differential equations. This motivates the search of algorithms computing linear differential equations in different contexts.

12 Algebraic Series and Questions of Size

12.1 Algebraic Series Can Be Computed Fast

A power series $Y(X)$ with coefficients in $\mathbb{K}$ is called *algebraic* when it is a zero of a nonzero polynomial $P(X, Y) \in \mathbb{K}[X, Y]$.

Theorem 8 *Algebraic power series are differentially finite.*

This is an old result that appears in notes of Abel's [1, p. 287] and was rediscovered many times [56,79,121]. It implies for instance that the first N coefficients of the power series solutions of such polynomials can be computed in $O(N)$ arithmetic operations in $\mathbb{K}$ (by unrolling the recurrence).

The proof is a nontrivial but not exceedingly complicated algorithm. Without loss of generality, P can be assumed irreducible and we denote by D its degree. Differentiating the polynomial equation implies

$$P_X(X, Y(X)) + P_Y(X, Y(X))Y'(X) = 0,$$

where P_X and P_Y denote the partial derivatives of P with respect to X and Y. Being irreducible, P is relatively prime to its derivative P_Y. Using the (commutative) extended Euclidean algorithm produces two polynomials U and V in $\mathbb{K}(X)[Y]$ such that

$$UP_Y + VP = 1.$$

This is the standard way of computing the inverse U of P_Y modulo P. Denoting by $R^{[1]}$ the remainder of the Euclidean division of $-UP_X$ by P gives

$$Y'(X) = R^{[1]}(X, Y(X)),$$

with $R^{[1]}$ a *polynomial* in $\mathbb{K}(X)[Y]$ of degree in Y smaller than D. Differentiating again gives

$$Y'' = R_X^{[1]} + R_Y^{[1]}Y' = R_X^{[1]} + R_Y^{[1]}R^{[1]} = Q_2P + R^{[2]},$$

the last term being a Euclidean division. Evaluating at $Y(X)$ implies that $Y''(X) = R^{[2]}(X, Y(X))$, with $R^{[2]}$ a polynomial in $\mathbb{K}(X)[Y]$ of degree in Y smaller than D. Iterating this process shows that all the power series $Y^{(k)}(X)$ for $k \in \mathbb{N}$ belong to the finite-dimensional vector space over $\mathbb{K}(X)$ generated by $(1, Y, \dots, Y^{d-1})$. This proves that Y satisfies a linear differential equation of order at most D that can be obtained by linear algebra.

The same argument shows that for any F solution of a linear differential equation and any algebraic Y, $F(Y(X))$ is also solution of a linear differential equation.

12.2 Order–Degree Curve

The differential equation obtained by the algorithm described above has minimal order, but the degree of its coefficients may be large. If D is also the degree of P with respect to X, then the coefficients of the differential equation have degree $O(D^3)$ and that bound is tight in general. This implies that the linear recurrence that can be deduced for the coefficients of the power series has order $O(D^3)$. Conversely, the minimal order recurrence can be shown to have order only $O(D^2)$ with coefficients of degree also $O(D^2)$, thus again, the cost of looking for minimality is a size of $O(D^4)$ coefficients for the equation. If instead, one relaxes the constraint on the order of the differential equation, then there always exists a linear differential equation of order $O(D)$ and coefficients of degree only $O(D^2)$ [25], leading to a non-minimal recurrence of order only $O(D^2)$ with coefficients of degree $O(D)$, which brings efficiency improvements when it needs to be unrolled. These observations are summarized in Fig. 6.

The large degree of the coefficients of the minimal order linear differential equation is a general phenomenon that goes beyond the algebraic case. It is due to the presence of numerous *apparent singularities* that are zeros of the leading coefficient of the differential equation, but not singularities of any of its solutions (e.g., xe^x is a nonzero solution of a first-order linear differential equation, but with $y(0) = 0$, which means that the Picard–Lindelöf theorem cannot apply at 0). Left multiples of the differential operator let those apparent singularities disappear and a precise analysis of the "order–degree curve" is possible [39]. The apparent singularities can all be removed algorithmically [124], but the resulting equation can have arbitrarily large order (e.g., $xy' - 1000y = 0$ has for solution x^{1000} and the only way to get rid of 0 as an apparent singularity is to go to order 1000.) Instead, recent work has been considering ways to trade order for degree without necessarily looking for minimal degree [21,40].

13 Creative Telescoping

Creative telescoping is a method introduced by Zeilberger in the 1990s [5,132,133] that computes definite integrals or sums with a free parameter, in the sense that it produces linear differential or recurrence equations for them. From there, the algorithms of the previous parts can be used to compute information concerning the sum or the integral.

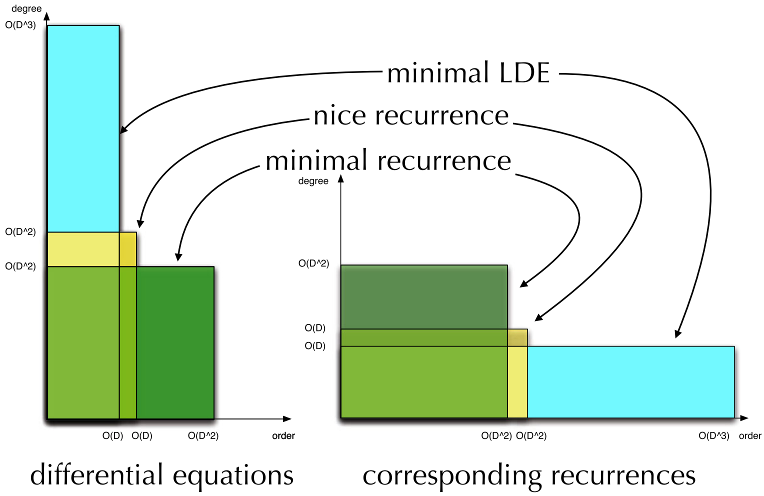

Fig. 6 Differential equations and recurrences for algebraic series

Example 12 Typical examples of formulas that can be computed or proved by this method are [7,62,73,75,115,120]:

$$\sum_{k=0}^{n}\binom{n}{k}^2\binom{n+k}{k}^2=\sum_{k=0}^{n}\binom{n}{k}\binom{n+k}{k}\sum_{j=0}^{k}\binom{k}{j}^3, \tag{10}$$

$$\sum_{j,k}(-1)^{j+k}\binom{j+k}{k+\ell}\binom{r}{j}\binom{n}{k}\binom{s+n-j-k}{m-j}=(-1)^{\ell}\binom{n+r}{n+\ell}\binom{s-r}{m-n-\ell}, \tag{11}$$

$$\int_0^{+\infty} x J_1(ax)I_1(ax)Y_0(x)K_0(x)\,\mathrm{d}x=\frac{1}{2\pi a^2}\ln\frac{1}{1-a^4}, \tag{12}$$

$$\int_{-1}^{1}\frac{e^{-px}T_n(x)}{\sqrt{1-x^2}}\,\mathrm{d}x=(-1)^n\pi I_n(p), \tag{13}$$

$$\frac{1}{2\pi i}\oint\frac{(1+2xy+4y^2)\exp\left(\frac{4x^2y^2}{1+4y^2}\right)}{y^{n+1}(1+4y^2)^{3/2}}\,\mathrm{d}y=\frac{H_n(x)}{\lfloor n/2\rfloor!}, \tag{14}$$

$$\sum_{k=0}^{n}\frac{q^{k^2}}{(q;q)_k(q;q)_{n-k}}=\sum_{k=-n}^{n}\frac{(-1)^k q^{(5k^2-k)/2}}{(q;q)_{n-k}(q;q)_{n+k}}. \tag{15}$$

They involve binomial coefficients, orthogonal polynomials, special functions and their q-analogues. The aim of these algorithms is to prove such identities automatically and, when the right-hand side does not itself involve a sum or an integral, compute it from the left-hand side. In all cases, at least one free variable remains: n in (10); ℓ, r, n, k, s in (11); a in (12); n and p in (13); n and x in (14); n and q in (15). This is important since the algorithms start by computing linear recurrences or differential equations or q-equations in these free variables.

This part of computer algebra has made a lot of progress in terms of generality and efficiency and is still very active. We describe here the general context and a few of the recent developments. More information can be found in recent surveys [53,91].

The name "creative telescoping" appears in van der Poorten's enjoyable account [114] of Apéry's proof of the irrationality of $\zeta(3)$. There, it was used to prove that the sum

$$A_n := \sum_{k=0}^{n} a_{n,k}, \qquad \text{with} \quad a_{n,k} = \binom{n}{k}^2 \binom{n+k}{k}^2, \tag{16}$$

satisfies the linear recurrence

$$(n+1)^3 A_{n+1} - (34n^3 + 51n^2 + 27n + 5)A_n + n^3 A_{n-1} = 0.$$

For this, an intermediate sequence

$$b_{n,k} = 4(2n+1)\left(k(2k+1) - (2n+1)^2\right) a_{n,k},$$

called *the certificate* of the identity was introduced. It is then sufficient to use simple properties of the binomial coefficients to observe that

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

and sum over k, letting the right-hand side telescope.

Example 13 For the much simpler example of the sum

$$U_n := \sum_{k=0}^{n} \binom{n}{k} = (1+1)^n = 2^n,$$

the computation by this method produces

$$U_{n+1} = \sum_k \binom{n+1}{k} = \sum_k \Bigg(\underbrace{\binom{n+1}{k} - \boxed{\binom{n+1}{k+1}}}\, + \underbrace{\boxed{\binom{n}{k+1}} - \binom{n}{k}} + 2\boxed{\binom{n}{k}} \Bigg) = 2U_n.$$

The summands above the braces telescope and the boxed parts sum to 0 by Pascal's relation that the method has to synthesize somehow.

More generally, in order to compute equations satisfied by an integral or a sum, the method takes as input a system of equations satisfied by the summand or integrand and relies on two operations: integration (resp. summation) by parts and differentiation (resp. difference) under the integral (resp. sum) sign. The first part gives the certificate, i.e., the multivariate expression whose difference (or derivative) telescopes; the second part gives the desired operator, called the *telescoper*.

14 Telescoping Ideal

Since the skew polynomial ring $\mathbb{A}\langle\partial;\sigma,\delta\rangle$ does not have zero divisors when $\mathbb{A}$ does not, one can iterate the construction of Ore polynomials and obtain multivariate Ore polynomial rings $\mathbb{A}\langle\partial_1;\sigma_1,\delta_1\rangle\cdots\langle\partial_r;\sigma_r,\delta_r\rangle$. The case when moreover $\partial_i\partial_j=\partial_j\partial_i$ for all (i,j) is called an *Ore algebra* and denoted $\mathbb{A}\langle\partial_1,\ldots,\partial_r;\sigma_1,\ldots,\sigma_r,\delta_1,\ldots,\delta_r\rangle$ or even $\mathbb{A}\langle\partial_1,\ldots,\partial_r\rangle$ where the σ_is and δ_is are clear from the context. If $\mathbb{O}$ is such an algebra and f a function on which its elements act, then the *annihilator* of f with respect to $\mathbb{O}$,

$$\operatorname{Ann}(f):=\{P\in\mathbb{O}\mid P(f)=0\},$$

is a left ideal in $\mathbb{O}$. For example, the annihilator of $\sin x$ in $\mathbb{Q}(x)\langle D_x\rangle$ is generated by D_x^2+1. More generally, in the case of operators in one variable over the rational functions, the ideals are principal by Ore's theorem (Thm. 7 above), thus the annihilator of a function f is given by the greatest common right divisor of its elements, and rewriting on a basis of the quotient $\mathbb{O}/\operatorname{Ann}(f)$ is performed by Euclidean division. This is the univariate situation considered in the previous parts.

14.1 ∂-Finite Ideals

The notions of D-finiteness or P-recursiveness generalize as follows.

Definition 4 A left ideal $\mathcal{I}$ in a multivariate Ore algebra $\mathbb{O}=\mathbb{K}(\mathbf{x})\langle\boldsymbol{\partial}\rangle$ is called ∂-finite when the quotient $\mathbb{O}/\mathcal{I}$ is a finite-dimensional vector space over $\mathbb{K}(\mathbf{x})$. A function whose annihilator is ∂-finite is called ∂-finite too.

(We introduced this name with Frédéric Chyzak [55], but it was probably not such a good idea, since it is pronounced like D-finite, leading to some confusion.)

These ideals are a non-commutative analogue of zero-dimensional ideals in polynomial rings. Thus, like in the commutative case, Euclidean division and (right) gcd can be replaced by Gröbner bases [55] that provide an access to a basis of the finite-dimensional vector space $\mathbb{O}/\operatorname{Ann}(f)$ and to rewriting rules reducing any element of $\mathbb{O}/\operatorname{Ann}(f)$ to a linear combination of the elements of this basis. It is important to stress that the use of Gröbner bases does not raise any efficiency issue in these computations.

Instead of a formal definition of the Gröbner basis of an ideal $\operatorname{Ann}(f)$, we use Fig. 7 to illustrate their main features. Each point with integer coordinates corresponds to a monomial in $\partial_x,\partial_y,\partial_z$ with these coordinates as exponents. The red points, located "below" the stairs, correspond to a basis of the quotient $\mathbb{O}/\operatorname{Ann}(f)$. Since the stairs are bounded, there are finitely many red points, which shows that f is ∂-finite. The blue points indicate elements of the Gröbner basis: each corresponds to a rewriting rule expressing this monomial as a linear combination of the red ones. Any monomial that is neither red nor blue is a multiple of one of the blue ones and thus can also be reduced, possibly in several steps, to a linear combination of the red points.

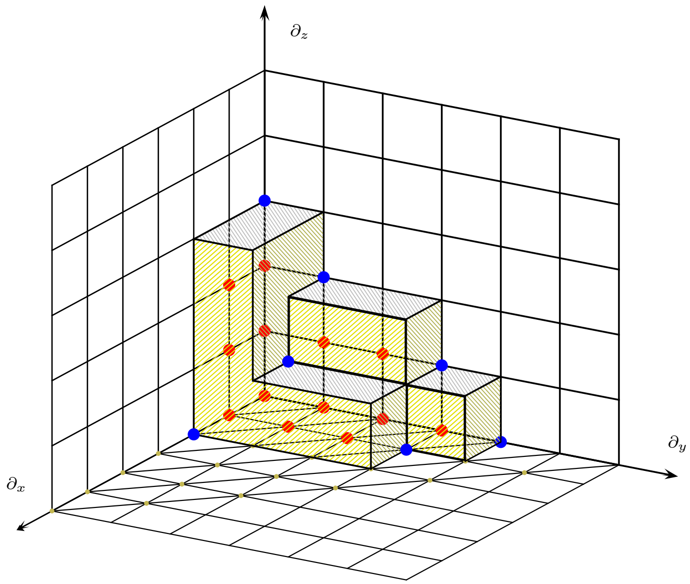

Fig. 7 Illustration of Gröbner bases and of Chyzak's algorithm

Example 14 The operators defining the Chebyshev polynomials of the first kind $T_n(x)$, namely

$$(1-x^2)D_x^2 - xD_x + n^2, \quad nS_n + (1-x^2)D_x + nx$$

make it possible to reduce any polynomial in $\mathbb{Q}(x,n)\langle D_x, S_n\rangle$ to a linear combination of 1 and D_x and constitute a Gröbner basis of the ideal $\operatorname{Ann}(T_n(x))$ is this Ore algebra. In other words, using this basis, any $T_{n+k}^{(i)}(x)$ (i, k nonnegative integers) rewrites as a linear combination of T_n and T_n', with coefficients in $\mathbb{Q}(x,n)$. (One could also have chosen the operators corresponding to Eq. (9). They also give a Gröbner basis in this algebra, for a different term order.)

Example 15 Using the basis of the previous example together with the operators defining e^{-px}, namely $(D_p + x, D_x + p)$ that form a Gröbner basis of $\operatorname{Ann}(e^{-px})$ in $\mathbb{Q}(p,x)\langle D_p, D_x\rangle$, simple manipulations like those used for the proofs of univariate identities (Sect. 6) reduce to linear algebra in finite-dimensional vector space and show that the integrand in Eq. (13) is annihilated by the operators

$$\begin{aligned} D_p + x, \quad nS_n - (x^2-1)D_x - (p(1-x^2) - (n+1)x), \\ (1-x^2)D_x^2 - (2px^2 + 3x - 2p)D_x - (p^2x^2 + 3px - n^2 - p^2 + 1), \end{aligned} \tag{17}$$

which constitute a Gröbner basis of the annihilator, showing that the quotient in this example has dimension 2, being generated by 1 and D_x. In other words, if $F_n(p,x)$ denotes the integrand of (13), all $\frac{\partial^{i+j}}{\partial x^i \partial p^j} F_{n+k}(p,x)$ for $(i,j,k) \in \mathbb{N}^3$ can be rewritten as linear combinations of F_n and $\partial F_n/\partial x$, with coefficients in $\mathbb{Q}(n,p,x)$.

14.2 Telescoping Ideal

In this framework, let the Ore algebra $\mathbb{O}$ be $\mathbb{K}(\mathbf{x}, t)\langle \boldsymbol{\partial}_{\mathbf{x}}, D_t\rangle$ with $\mathbf{x} = (x_1, \ldots, x_r)$ and $\boldsymbol{\partial}_{\mathbf{x}} = (\partial_1, \ldots, \partial_r)$ the corresponding Ore operators, while D_t is the differentiation with respect to t. If the aim is to compute an integral of f with respect to the variable t, its representation is given by the *telescoping ideal*

$$T_t(f) := \Big(\mathrm{Ann}(f) + \underbrace{D_t\mathbb{K}(\mathbf{x}, t)\langle \boldsymbol{\partial}_{\mathbf{x}}, D_t\rangle}_{\text{int. by parts}}\Big) \cap \underbrace{\mathbb{K}(\mathbf{x})\langle \boldsymbol{\partial}_{\mathbf{x}}\rangle}_{\text{diff. under } \int} .$$

Indeed, canceling the derivatives that are used during the successive integrations by parts amounts to computing modulo the *right* ideal $D_t\mathbb{K}(\mathbf{x}, t)\langle \boldsymbol{\partial}_{\mathbf{x}}, D_t\rangle$. The situation in the computation of sums is completely similar, with the differentiation operator D_t replaced by the difference operator $\Delta_k = S_k - 1$.

Example 16 The ideal generated by the operators in Eq. (17) contains

$$P = p^2D_p^2 + pD_p + nD_xS_n + (px^2 - nx - p)D_x + (2px - n^2 - p^2 - n),$$

as can be checked by reduction with the Gröbner basis. Rewriting this operator as

$$P = p^2D_p^2 + pD_p - (n^2 + p^2) + D_x(nS_n + (px^2 - nx - p))$$

shows that $p^2D_p^2 + pD_p - (n^2 + p^2)$ is an operator in $\mathbb{Q}(n, p)\langle S_n, D_p\rangle$ that belongs to the telescoping ideal of the integrand of (13) with respect to x.

A major source of difficulty is that while $T_t(f)$ is a left ideal, the sum of the left ideal $\mathrm{Ann}(f)$ and the right ideal $D_t\mathbb{O}$ or $\Delta_n\mathbb{O}$ is not an ideal in general, so that new algorithms are required to perform this computation or to find approximations (i.e., subideals) of the telescoping ideal.

Zeilberger's Slow Algorithm The first general approach was Zeilberger's slow algorithm [132], as he named it later. The idea is to restrict integration by parts by considering only the ideal $D_t\mathbb{K}(\mathbf{x})\langle \boldsymbol{\partial}_{\mathbf{x}}, D_t\rangle$. Now D_t commutes with all the elements of $\mathbb{K}(\mathbf{x})\langle \boldsymbol{\partial}_{\mathbf{x}}, D_t\rangle$, which makes the computation easier. However, by restricting to a subideal, one may be led to compute generators of much higher degree than necessary, or even fail to find any equation. This last problem disappears when a sufficient condition called "holonomy" in D-module theory holds. Holonomy was then a starting point for Zeilberger's approach [132].

14.3 Toward a Basis of the Telescoping Ideal

Generators of the telescoping ideal can be obtained by looking for Ore polynomials of the form

$$\underbrace{\sum_{\mathbf{m}} c_{\mathbf{m}}(\mathbf{x})\boldsymbol{\partial}^{\mathbf{m}}}_{\text{telescoper}} + \partial_t \underbrace{\sum_{(\mathbf{i},j)\in\mathcal{S}} a_{\mathbf{i},j}(\mathbf{x},t)\boldsymbol{\partial}^{\mathbf{i}}\partial_t^j}_{\text{certificate}} \in \operatorname{Ann}(f), \tag{18}$$

where, with the notations above, $\mathbf{m} = (m_1, \ldots, m_r)$, $\mathbf{i} = (i_1, \ldots, i_r)$ and the multi-exponent notation is $\boldsymbol{\partial}^{\mathbf{m}} = \partial_1^{m_1} \cdots \partial_r^{m_r}$. In this formula, the range of the first sum is *a priori* unknown and that of the second one depends on the function f under consideration.

Zeilberger's Fast Algorithm Historically, the first algorithm in this family was Zeilberger's algorithm [133] for the definite summation of hypergeometric sequences. These are bivariate sequences (i.e., $r = 1$) whose annihilator is generated by two recurrence operators of the form $S_n - r(n,k)$ and $S_k - t(n,k)$ with r and t rational functions. Typical examples are the binomial coefficients or Apéry's sequence $a_{n,k}$ from Eq. (16). Reducing any operator in $\mathbb{O} := \mathbb{Q}(n,k)\langle S_n, S_k\rangle$ with these two first-order ones leads to rational functions times the identity. In other words, the quotient $\mathbb{O}/\operatorname{Ann}(f)$ is a vector space over $\mathbb{Q}(n,k)$ of dimension 1. As a consequence, the set of indices in the second sum of Eq. (18) (with $\partial_t = \Delta_k = S_k - 1$) can be taken as $\mathcal{S} = \{(0,0)\}$ without any loss. Thus, the certificate is reduced to one rational function. Zeilberger's algorithm takes $m \in \{0, \ldots, r\}$ for increasing r as the set of indices for the first sum. For each such r, it looks for the existence of rational $c_0, \ldots, c_r$ and $a_{0,0}$ by a variant of Gosper's classical algorithm for *indefinite* summation. If a solution is found, the algorithm stops and returns the generator of the telescoping ideal $T_k(f)$, which is principal since this is a univariate situation. Otherwise, the failure to find a solution is actually a proof that none exists and the algorithm proceeds to the next value of r. Necessary and sufficient conditions for the algorithm to terminate are known [2,3,129]. Variants of this algorithm with quotients of dimension 1 have been developed by Almkvist and Zeilberger [5] for integrals of hyperexponential functions (given by two first-order differential equations) and for integrals of functions that satisfy both a first-order linear recurrence and a first-order linear differential equation.

Chyzak's Algorithm A vast generalization of Zeilberger's algorithm was designed by Chyzak [52] for the case when the quotient $\mathbb{O}/\operatorname{Ann}(f)$ is only required to have *finite dimension* over $\mathbb{K}(\mathbf{x}, t)$. A basis of the quotient gives the set of indices $\mathcal{S}$ to be used in Eq. (18). Then, as in Zeilberger's algorithm, Chyzak's algorithm uses increasingly large sets of monomials with unknown rational functions $c_{\mathbf{m}}$ and one unknown rational function $a_{\mathbf{i},j}$ per element of this set $\mathcal{S}$. Multiplying by ∂_t on the left and reducing the resulting expression on the basis of the quotient gives a set of linear differential equations if ∂_t is a differentiation operator (or recurrence equations if it is a difference operator) for these unknown functions. The generalization of Gosper's algorithm is replaced by algorithms for rational solutions for such systems.

Figure 7 suggests how the algorithm proceeds in a case with 3 variables where integration (or summation) is performed with respect to z. During the execution of Chyzak's algorithm, an unknown rational function $a_{\mathbf{i},j}$ is associated to each of the red points. The first sum in Eq. (18) runs over more and more of the (small yellow) monomials in the remaining variables ∂_x and ∂_y, by increasing order for the computation of a Gröbner basis of the telescoping ideal.

Example 17 For the integral in Eq. (13), the Gröbner basis (17) leads to considering operators of the form

$$\sum_{(k,m)} c_{k,m}(n,p) D_p^k S_n^m + D_x\Big(a_0(n,p,x) + a_1(n,p,x) D_x\Big)$$

and finding rational functions $c_{k,m}$, a_0 and a_1 so that they belong to $\mathrm{Ann}(F_n(p,x))$, or equivalently so that they reduce to 0 by the Gröbner basis.

The second part of the expression does not depend on the range of the first sum and reduces to

$$\frac{\partial a_0}{\partial x} + a_0 D_x + \frac{\partial a_1}{\partial x} D_x + \frac{a_1}{1-x^2}\Big((p^2x^2 + 3px - n^2 - p_1^2) + (2px^2 + 3x - 2p)D_x\Big).$$

Next, each monomial $D_p^k S_n^m$ reduces to a linear combination $u_{k,m}^{(0)} + u_{k,m}^{(1)} D_x$. Thus, by canceling the coordinates of 1 and D_x in the sum, the problem is reduced to looking for rational solutions of the inhomogeneous linear differential system

$$\begin{aligned}
\frac{\partial a_0}{\partial x} + \frac{a_1}{1-x^2}(p^2x^2 + 3px - n^2 - p_1^2) &= -\sum_{(k,m)} c_{k,m} u_{k,m}^{(0)},\\
\frac{\partial a_1}{\partial x} + a_0 + \frac{a_1}{1-x^2}(2px^2 + 3x - 2p) &= -\sum_{(k,m)} c_{k,m} u_{k,m}^{(1)}.
\end{aligned}$$

More precisely, the algorithm looks for values of rational $c_{k,m}$ such that the system admits a rational solution. Several algorithms are available for this. A solution is to: decouple the system; observe that the poles and their multiplicities in possible rational solutions a_0, a_1 are dictated by the homogeneous part; use undetermined coefficients on the numerator to reduce the problem to linear algebra over the coefficients of the numerator and the $c_{k,m}$.

The first two cases when solutions are found is when the indices run over the sets $\{(0,0),(0,1),(1,0)\}$ and $\{(0,0),(0,1),(0,2)\}$, giving

$$F_{n+1} + \frac{\partial F_n}{\partial p} - \frac{n}{p} F_n = \frac{\partial\, \mathrm{Cert}_1}{\partial x}, \quad p^2 \frac{\partial^2 F_n}{\partial p^2} + p\frac{\partial F_n}{\partial p} - (n^2 + p^2) F_n = \frac{\partial\, \mathrm{Cert}_2}{\partial x}, \quad (19)$$

for two explicit functions Cert_1 and Cert_2. These equations can be integrated from -1 to 1, and the left-hand sides provide a Gröbner basis of the annihilator of the integral. These can easily be checked to cancel the Bessel function $I_n(p)$ multiplied by $(-1)^n$, and initial conditions can be used to conclude the proof of Eq. (13).

Infinite Dimension That same method also extends to cases where the dimension of the quotient is not finite, by proceeding by increasing total degree. Again, termination of the algorithm is problematic, but this method allows the automatic derivation of identities for a much larger class of functions or sequences, including Stirling numbers, Bernoulli numbers, the Beta function and the Hurwitz zeta function [54].

Multiple Sums or Integrals Formally, the situation is very similar. The Ore algebra $\mathbb{O}$ is $\mathbb{K}(\mathbf{x}, \mathbf{t})\langle \boldsymbol{\partial}_{\mathbf{x}}, \boldsymbol{\partial}_{\mathbf{t}}\rangle$, with $\mathbf{x} = (x_1, \ldots, x_r)$, $\boldsymbol{\partial}_{\mathbf{x}} = (\partial_{x_1}, \ldots, \partial_{x_r})$, $\mathbf{t} = (t_1, \ldots, t_m)$, $\boldsymbol{\partial}_{\mathbf{t}} = (\partial_{t_1}, \ldots, \partial_{t_r})$. The aim is to compute an integral (or sum or other depending on the Ore operators) of f with respect to the variables $\mathbf{t}$. The telescoping ideal becomes

$$T_{\mathbf{t}}(f) := \Big(\mathrm{Ann}(f) + \partial_{t_1}\mathbb{K}(\mathbf{x}, \mathbf{t})\langle \boldsymbol{\partial}_{\mathbf{x}}, \boldsymbol{\partial}_{\mathbf{t}}\rangle + \cdots + \partial_{t_m}\mathbb{K}(\mathbf{x}, \mathbf{t})\langle \boldsymbol{\partial}_{\mathbf{x}}, \boldsymbol{\partial}_{\mathbf{t}}\rangle\Big) \cap \mathbb{K}(\mathbf{x})\langle \boldsymbol{\partial}_{\mathbf{x}}\rangle.$$

Under a sufficient condition based on holonomy, Wilf and Zeilberger have given a generalization of Zeilberger's slow algorithm and showed that it terminates [130]. This was improved by Wegschaider [128].

Without restricting the integration by parts, proceeding with unknown rational functions as above is also possible, but it leads to a system of linear partial differential equations for which algorithms are still missing in general. In the case of a quotient of dimension 1, Zeilberger's fast algorithm for hypergeometric summation has been generalized [8,72]. Another approach for multiple binomial sums is described below. In the general case, except for special families mentioned below, one resorts to proceeding variable by variable, with some optimizations [53].

15 Creative Telescoping: New Generation

The certificate computed by these algorithms is sometimes necessary: if the integration (or summation) domain is such that the integral (or sum) of a derivative (or a difference) is not zero, then one needs to evaluate the certificate at the boundary of the domain. In many cases however, it is useless. This is the case when integrating over a cycle in $\mathbb{C}^n$ or when summing over $\mathbb{Z}^n$ a product of binomial coefficients with finite support, provided it can be ensured that the certificate does not present singularities on the domain of integration (or summation) that were not present in the input. However, by their design, the algorithms described above cannot avoid the computation of that certificate.

15.1 Certificates are Big

Being formed of rational functions in more variables than the telescoper, certificates tend to be bigger, which impacts the complexity.

Example 18 The double sum

$$C_n := \sum_{r\geq 0}\sum_{s\geq 0}(-1)^{n+r+s}\binom{n}{r}\binom{n}{s}\binom{n+s}{s}\binom{n+r}{r}\binom{2n-r-s}{n} \tag{20}$$

satisfies the linear recurrence

$$(n+2)^3C_{n+2}-2(2n+3)(3n^2+9n+7)C_{n+1}-(4n+3)(4n+4)(4n+5)C_n = 0, \tag{21}$$

the corresponding certificate being 180kB large (approximately 2 pages of text).

Example 19 Similarly, the triple integral

$$I(z) = \oint \frac{(1+t_3)^2\,\mathrm{d}t_1\mathrm{d}t_2\mathrm{d}t_3}{t_1t_2t_3(1+t_3(1+t_1))(1+t_3(1+t_2)) + z(1+t_1)(1+t_2)(1+t_3)^4} \quad (22)$$

satisfies the linear differential equation

$$\begin{aligned} &z^2(1+4z)(1-16z)I'''(z) + 3z(1-18z-128z^2)I''(z) \\ &\quad - (11-40z-444z^2)I'(z) + 2(1+30z)I(z) = 0, \end{aligned}$$

with a certificate that fits in 12 pages.

Thus, for efficiency reasons, the design of a new generation of algorithms avoiding the computation of the certificate has been an active research area recently.

15.2 Hermite Reduction

The linear system of equations obtained by reducing Eq. (18) modulo the annihilator of f has a fixed homogeneous part in the unknown rational coefficients $a_{\mathbf{i},j}$ and a variable inhomogeneous part coming from the telescoper. The idea of algorithms based on Hermite reduction is to work modulo the image of the linear map constituted by the homogeneous part. When a finite basis of the quotient by this image is available, generalized Hermite reduction is the process of reducing (vectors of) rational functions to this basis. This generalizes the classical Hermite reduction, which reduces modulo the image of a derivation D_x.

This was first exploited in the case of dimension 1 for bivariate rational functions [21], for hyperexponential functions [22], for bivariate hypergeometric terms [38, 85], for mixed hypergeometric-hyperexponential functions [26]. Next, it was extended to algebraic functions [41,42], to Fuchsian functions [37], to solutions of differential systems [125] and finally to the integration of ∂-finite functions [24].

A further simplification is brought by the use of adjoint operators. If $L = c_r D_x^r + \cdots + c_0 \in \mathbb{K}(x)\langle D_x\rangle$, then its adjoint is defined as $L^* = c_0 + \cdots + (-D_x)^r c_r$. It is related to integration by parts via Lagrange's identity

$$uL(f) - L^*(u)f = D_x(P_L(f,u)),$$

satisfied for any u and f, with an explicit P_L. Thus, if f is a solution of L, any rational function R in $L^*(\mathbb{K}(x))$ is such that Rf is a derivative. Now, if, as in the case of Example 17, all the other operators in the algebra rewrite as linear combinations of powers of D_x (see Eq. (17)), then all operations boil down to Hermite reductions of rational functions. This specific form can always be achieved by the use of a so-called *cyclic vector* [51].

Example 20 The adjoint of the last operator in the basis (17) is

$$M := (x^2-1)D_x^2 + (x - 2p(x^2-1))D_x + (p^2(x^2-1) - px - n^2).$$

If one wants to reduce a polynomial with respect to M, the first step is to determine the intersection of $M(\mathbb{Q}(x))$ with $\mathbb{Q}[x]$. Considering $M(x^k)$ for $k \in \mathbb{N}$ shows that all polynomials of degree at least 2 belong to $M(\mathbb{Q}(x)) \cap \mathbb{Q}[x]$. To prove that no other polynomial belongs to this set, it is sufficient to consider the singularities at ± 1 and observe that M increases the orders of the poles there. Thus, 1 and x reduce to themselves with respect to M and the Hermite reduction of any polynomial is a linear combination of 1 and x with coefficients in $\mathbb{Q}(n, p)$. In particular, using $M(1)$ reduces x^2 to $x/p + 1 + n^2/p^2$.

This means first that F_n itself is not a derivative (or 1 would be reduced to 0) and that no linear combination of F_n and $\partial F_n/\partial p$ is a derivative (since 1 and x are linearly independent). Next, D_p reduces to x by the Gröbner basis, so D_p^2 reduces to x^2 and the Hermite reduction of x^2 implies that

$$p^2 \frac{\partial^2 F_n}{\partial p^2} + p \frac{\partial F_n}{\partial p} - (n^2 + p^2) F_n$$

is a derivative, which recovers the second part of Eq. (19). Finally, rewriting the equation for F_{n+1} in the Gröbner basis (17) by a Euclidean right division by D_x gives

$$n S_n - D_x (x^2 - 1) + (p x^2 + (n-1)x - p),$$

so that again, the Hermite reduction of x^2 helps conclude that

$$F_{n+1} + \frac{\partial F_n}{\partial p} - \frac{n}{p} F_n$$

is a derivative, which is the first part of Eq. (19), obtained without computing the certificates.

15.3 Periods

Integrals of rational functions over cycles provide an important class of *multiple* integrals where the computation of the certificate is unnecessary. What we call *period* here is an integral of a rational function in $\mathbb{Q}(\mathbf{t})$ with $\mathbf{t} = (t_1, \ldots, t_m)$ over a cycle in $\mathbb{C}^m$ that avoids the zero set of the denominator. These numbers form an important subclass of the countable class of periods considered by Kontsevich and Zagier [90], with fewer constraints on the domain of integration.

If instead one integrates in $\mathbb{C}^m$ a function F in $\mathbb{Q}(x, \mathbf{t})$ for an extra variable x and if the denominator does not vanish in a neighborhood of the cycle of integration, then the period is a function of x. Moreover, this function satisfies a linear differential equation, called a *Picard–Fuchs equation* after early work by Picard [111] in the bivariate case.

Without loss of generality, $F \in \mathbb{Q}(x, \mathbf{t})$ can be written P/Q^ℓ with Q a square-free polynomial. An algorithm finding the Picard–Fuchs equation is obtained by a process called Griffiths–Dwork reduction, which can be seen as a generalization of Hermite's reduction [45,63,76]. A first technicality is that in order to get a better control over the degrees, one homogenizes the integrand by introducing a new variable t_0. Next, a key step is to introduce the ideal generated by the partial derivatives $\partial_0 Q, \dots, \partial_m Q$. The reduction takes the remainder modulo (a Gröbner basis of) this ideal of the numerators that appear and use integration by parts: if $P = r + v_0\partial_0 Q + \cdots + v_m\partial_m Q$ and $\ell > 1$, then

$$\frac{P}{Q^\ell} = \frac{r}{Q^\ell} - \frac{1}{\ell-1}\left(\partial_0\frac{v_0}{Q^{\ell-1}} + \cdots + \partial_m\frac{v_m}{Q^{\ell-1}}\right) + \frac{1}{\ell-1}\frac{\partial_0 v_0 + \cdots + \partial_m v_m}{Q^{\ell-1}}.$$

Thus, modulo derivatives, P/Q^ℓ reduces to r/Q^ℓ and a rational function with denominator only $Q^{\ell-1}$ on which the process is repeated until $\ell = 1$ is reached. A result of Griffiths [76] shows that, under some regularity condition, F is reduced to 0 by this process if and only if the integral of F over cycles is 0. The computation of the Picard–Fuchs equation then consists in computing the reductions of the successive derivatives with respect to the free variable x and looking for a linear relation between the reductions, whose coefficients are those of the differential equation. When the regularity conditions are not met, they can be recovered by a perturbation method [63]. Counting dimensions carefully and using recent efficient algorithms for the reduction stage lead to the following [29,92].

Theorem 9 *Let $F = P/Q$ be a rational function in $\mathbb{Q}(x, \mathbf{t})$ with $\mathbf{t} = (t_1, \dots, t_m)$, let*

$$N = \max(\deg_{\mathbf{t}} P + m + 1, \deg_{\mathbf{t}} Q) \quad \text{and} \quad d_x = \max(\deg_x P, \deg_x Q).$$

Then F admits a telescoper whose certificate is singular only where $Q = 0$. This telescoper has order at most N^m and degree $O(N^{3m} d_x)$. It can be computed in $O(N^{8m} d_x)$ arithmetic operations in $\mathbb{Q}$.

The bound on the order is tight. It is important to note that generically, the certificate has a number of monomials growing like $N^{n^2/2}$ and thus cannot even be written within that complexity.

Recent work has exploited these differential equations for the computation of volumes of semi-algebraic sets [93] and of multiple binomial sums (see below).

16 Diagonals

Diagonals form an important class of such multiple integrals of rational functions. If $F(\mathbf{t}) = G(\mathbf{t})/H(\mathbf{t})$ with $\mathbf{t} = (t_1, \dots, t_m)$ is a multivariate rational function such that $H(0) \neq 0$, then it admits a Taylor expansion

$$F(\mathbf{t}) = \sum_{\mathbf{i} \in \mathbb{N}^m} c_{\mathbf{i}} \mathbf{t}^{\mathbf{i}}$$

and its *diagonal* is the power series

$$\Delta F(t) := \sum_{k \in \mathbb{N}} c_{k,k,\dots,k} t^k.$$

Example 21 The simplest example is the diagonal of Pascal's triangle: the binomial coefficients are the Taylor coefficients of $f = 1/(1-x-y)$ and the central binomial coefficients $\binom{2k}{k}$ have for generating function Δf. Less obvious are

$$\sum_{k=0}^{\infty} \frac{1}{k+1}\binom{2k}{k} t^k = \Delta \frac{1-2x}{(1-x-y)(1-x)},$$
$$\sum_{k=0}^{\infty} A_k t^k = \Delta \frac{1}{1-t(1+x)(1+y)(1+z)(1+y+z+yz+xyz)},$$

where the first one is the generating function of the Catalan numbers and the second one is that of the Apéry numbers from Eq. (16).

Since diagonals can be rewritten as multidimensional residues

$$\Delta F(t) = \left(\frac{1}{2\pi i}\right)^{m-1} \oint F\left(t_1, \dots, t_{m-1}, \frac{t}{t_1 \cdots t_{m-1}}\right) \frac{\mathrm{d}t_1 \cdots \mathrm{d}t_{m-1}}{t_1 \cdots t_{m-1}},$$

the results of the previous section apply and lead to the following.

Theorem 10 [44] *Diagonals of rational functions are differentially finite.*

Moreover, if F has degree d, then, by Theorem 9, the differential equation satisfied by the diagonal has order that grows like d^m and its coefficients have degree bounded by $d^{O(m)}$. It can be computed in good complexity.

Much more is known about diagonals. Algebraic series are the diagonals of bivariate rational functions [71,112] (the degree of the polynomial may be large [27]); diagonals are closed under sum, product and Hadamard product. They are globally bounded and therefore satisfy the hypothesis of Theorem 4; Christol conjectures that the converse holds: all globally bounded D-finite power series would be diagonals. More information on diagonals can be found in recent surveys [20,46].

Also, for the most regular of those rational functions, the constant involved in the asymptotic behavior of the coefficients of their diagonals, as discussed in Sect. 5, can sometimes be computed explicitly and moreover algorithmically [101,110].

17 Multiple Binomial Sums

These are sums like that of Eq. (20). A more formal definition is the following.

Definition 5 The class of *multiple binomial sums* over $\mathbb{K}$ is the class of sequences of elements of $\mathbb{K}$ obtained from: geometric sequences $n \mapsto C^n$ (for $C \in \mathbb{K} \setminus \{0\}$), binomial coefficients $(n, k) \mapsto \binom{n}{k}$, the Kronecker delta sequence $n \mapsto \delta_n$ (which is 1 at index n and 0 everywhere else) using the operations of: addition, multiplication, multiplication by a scalar, affine change of indices $u_{\mathbf{n}} \mapsto u_{\Lambda\mathbf{n}}$ with Λ an affine map from $\mathbb{Z}^d$ to $\mathbb{Z}^e$ and indefinite summation

$$(\mathbf{m}, n) \mapsto \sum_{k=0}^{n} u_{\mathbf{m},k}.$$

These sums are very closely related to diagonals, by the following not too difficult result, whose proof is effective.

Theorem 11 [30] *A sequence $u : \mathbb{N} \to \mathbb{K}$ is a multiple binomial sum if and only if the generating function $\sum_{n\geq 0} u_n t^n$ is the diagonal of a rational power series.*

In order to compute a linear recurrence for a multiple binomial sum, it is actually not necessary to rewrite it as a diagonal, and a residue expression is sufficient. This provides a fast algorithm for single or multiple summation [30] that makes effective a classical approach sometimes called the generating function method [64].

Example 22 Dixon's classical identity

$$\sum_{k=0}^{2n} (-1)^k \binom{2n}{k}^3 = (-1)^n \frac{(3n)!}{n!^3}$$

is computed automatically by first expressing the generating function of the sum as the integral of a rational function as follows. A starting point is to define $\binom{n}{k}$ as the coefficient of x^k in $(1+x)^n$, hence, by Cauchy's formula, as

$$\binom{n}{k} = \frac{1}{2\pi i} \oint \frac{(1+x)^n}{x^k} \frac{\mathrm{d}x}{x},$$

where the contour is a small circle (of radius smaller than 1) around the origin. Then the summand has for integral representation

$$(-1)^k \binom{2n}{k}^3 = \frac{1}{(2\pi i)^3} \oint \left(\prod_{i=1}^{3} (1+x_i)^2 \right)^n \left(\frac{-1}{x_1x_2x_3} \right)^k \frac{\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3}{x_1x_2x_3},$$

where the contour is the product of three of those small circles. Multiplying by t^n and summing the geometric series over k and n finally gives the generating function of the sum as

$$\frac{1}{(2\pi i)^3} \oint \frac{x_1x_2x_3 - t\prod_{i=1}^{3}(1+x_i)^2}{\left(x_1^2x_2^2x_3^2 - t\prod_{i=1}^{3}(1+x_i)^2\right)\left(1 - t\prod_{i=1}^{3}(1+x_i)^2\right)} \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3.$$

Next, the algorithm detects that the integral with respect to one of the variables, say x_3, can be obtained by residue computation, taking into account that as $t \to 0$, the first factor of the denominator has all its roots that remain small, while those of the second one do not contribute. The integral is thus simplified to

$$\frac{1}{(2\pi i)^2} \oint \frac{x_1x_2\,\mathrm{d}x_1\mathrm{d}x_2}{x_1^2x_2^2 - t(1+x_1)^2(1+x_2)^2(1-x_1x_2)^2}.$$

From there, the algorithms of Sect. 15.3 produce the following linear differential equation for the generating function:

$$t(1+27t)y'' + (1+54t)y' + 6y = 0,$$

which in turn gives the linear recurrence

$$3(3n+2)(3n+1)u_n + (n+1)^2 u_{n+1} = 0,$$

concluding the proof of Dixon's formula after checking one initial condition. Actually, the right-hand side is discovered automatically by this computation.

Example 23 From the double sum from Eq. (20), the rational function integrand of Eq. (22) is obtained automatically. From there, the Picard–Fuchs equation is deduced and then by direct translation into a recurrence, Eq. (21) follows.

And again, from the linear differential equation or linear recurrence, a lot of information can be obtained for the sum by the methods of the first part.

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