Linear recurrences, linear differential equations, and fast computation

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[summary by Philippe Dumas]

Linear recurrences and linear differential equations with polynomial coefficients provide a finite representation of special functions or special sequences. Many algorithms are at our disposal; some give a way to automate the computation of recurrences or differential equations; some provide solutions to recurrences or differential equations; and some give the asymptotic behaviour of these solutions, directly from the recurrence or differential equation. All of this provides a method to efficiently compute special functions and special sequences.

1. Classical algorithms concerning formal power series

In the sequel, we use the ring $\mathbb{A}[[x]]$ of formal power series

$$F(x) = \sum_{n=0}^{+\infty} f_n x^n$$

with coefficients f_n in a commutative ring $\mathbb{A}$; this ring is assumed to contain the field $\mathbb{Q}$ of rational numbers, even though it is possible to consider a more general situation. Practically, one deals with truncated series

$$F(x) = \sum_{n=0}^{N} f_n x^n + O(x^{N+1}),$$

that is to say essentially polynomials. It must be noted that there exist lazy algorithms to deal with truncated series of arbitrary order, but their cost is generally excessive. We indicate how to deal with basic operations [7, Chap. 4].

Product of polynomials. The naive method to obtain the product of two polynomials of degree N has complexity $O(N^2)$ arithmetic operations. A better way is Karatsuba's algorithm, which has complexity $O(N^{\log_2 3}) = O(N^{1.59})$. The idea behind the algorithm resides in writing

$$P(x) = P_0(x) + x^k P_1(x), \qquad Q(x) = Q_0(x) + x^k Q_1(x),$$

$$P(x)Q(x) = P_0(x)Q_0(x) + R(x)x^k + P_1(x)Q_1(x)x^{2k},$$

$$R(x) = (P_0(x) + P_1(x))(Q_0(x) + Q_1(x)) - (P_0(x)Q_0(x) + P_1(x)Q_1(x)),$$

with $k \simeq N/2$; this formula needs only three multiplications of polynomials of degree less than k instead of four multiplications, and this leads to an efficient recursive computation.

From a practical standpoint, Karatsuba's method becomes efficient in Maple for an N greater than about a hundred. The fast Fourier transform algorithm needs a much larger value of N to be useful.

Composition. Here the goal is the computation of the first N coefficients of the series $F(G(x))$, where $g_0 = 0$. The naive method leads to a computation with $O(N)$ series multiplications. Brent and Kung's algorithm [2] has a better behaviour. It consists of three steps; first write $F(x)$ as

$$F(x) = F_0(x) + F_1(x)x^k + F_2(x)x^{2k} \cdots + F_{k-1}(x)x^{k(k-1)},$$

where $F_0(x)$, $F_1(x)$, ..., $F_{k-1}(x)$ are the series obtained by factoring out the powers of x^k, where $k = \lceil (N+1)^{1/2} \rceil$; next compute the powers $G^i(x)$ for i from 2 to $k-1$, and the series $F_i(G(x))$; finally, compute $T(x) = G^k(x)$ and $F(G(x))$ using a Horner scheme.

The algorithm uses $3k$ series multiplications and $O(N)$ coefficient multiplications, hence it has cost $O(N^{1/2})$ if the unit cost is series multiplication. Via Karatsuba's algorithm, this gives a cost of $O(N^{2.09})$ expressed in terms of coefficient multiplications, while the naive method has cost $O(N^3)$.

Powering and simple functions. Powering and simple functions are a particular case of composition, but in this case it is possible to be more efficient. We show the idea for the case of powering. If $H(x) = F^\alpha(x)$, then $H(x)$ satisfies the equation

$$H'(x)F(x) = \alpha F'(x)H(x),$$

therefore the coefficients of $H(x)$ are provided by the following recurrence

$$\sum_{k=0}^{n} k h_k f_{n-k} = \alpha \sum_{k=0}^{n} (n-k) h_k f_{n-k}.$$

This makes it possible to compute the first N coefficients at a cost of $O(N^2)$ coefficient multiplications, instead of $O(N^{2.09})$.

Newton iteration. An ever better way to compute elementary functions is Newton's method. If we search for a series $y(x)$ such that $\Phi(x, y(x)) = 0$, we use the recurrence

$$y_{k+1}(x) = y_k(x) - \frac{\Phi(x, y_k(x))}{\partial\Phi/\partial y(x, y_k(x))} \mod x^{2k+2}.$$

We start from $y_0(x) = 0$ and the formula is iterated until $2k + 2 > N$. The number of correct coefficients is doubled at each step. For example, the reciprocal $y(x) = 1/F(x)$ satisfies the equation $\Phi(x, y) = 1/y - F(x) = 0$ and the recursion is $y_{k+1} = 2y_k - F(x)y_k^2$. In the same way one can compute the logarithm $\ln(F(x))$, the exponential $\exp(F(x))$, and solutions of simple differential equations. In all these cases the complexity of the computation is the complexity of the multiplication, that is $O(N^{1.59})$.

For the reversion of series the same method can be used. Given $F(x)$ with $f_0 = 0$, $f_1 \neq 0$, one looks for a series $y(x)$ such that $F(y(x)) = x$. This is carried out by Newton's method applied to the equation $F(y) - x = 0$; hence the recurrence is

$$y_{k+1}(x) = y_k(x) - \frac{F(y_k(x)) - x}{F'(y_k(x))} \mod x^{2k+2}.$$

The cost is of the same order as the composition cost, because of the terms $F(y_k(x))$ and $F'(y_k(x))$.

Linear differential equations. Assume that the power series $F(x)$ satisfies a linear differential equation

$$a_0(x)y^{(k)} + a_1(x)y^{(k-1)} + \cdots + a_k(x)y = 0,$$

whose coefficients are polynomials. If 0 is an ordinary point, this differential equation translates into a linear recurrence for the coefficients of $F(x)$. This leads to an algorithm whose cost is $O(N)$, while the preceding ones use at best $O(N^{1.59})$ basic operations.

Obviously, the complexity $O(N)$ is optimal, therefore for large N there is great interest in finding a linear differential equation with $F(x)$ as a solution, if possible. In the sequel, we will focus our attention on such power series.

2. Univariate holonomic series

A power series is said to be holonomic if it is a solution of a linear differential equation with polynomial coefficients. In the same manner, a sequence is said to be holonomic if it is a solution of a linear recurrence with polynomial coefficients.

It is easy to see that rational series, $\exp(x)$, $\sin x$, $\cos x$, $\log(1+x)$, and the Bessel functions $J_\nu(x)$ are all holonomic. Rational, factorial, Fibonacci, and hypergeometric sequences are all holonomic sequences. Recall that a sequence is hypergeometric if the sequence of quotients of consecutive terms is a rational sequence.

Both definitions are related by the following property: a sequence is holonomic if and only if its generating series is holonomic. The proof is easy and uses the simple but basic correspondences which may be summarized as follows,

$$\begin{aligned} F(x) &\quad\longleftrightarrow\quad f_n, \\ x^k F(x) &\quad\longleftrightarrow\quad f_{n-k}, \\ xF'(x) &\quad\longleftrightarrow\quad nf_n. \end{aligned}$$

Closure properties. The set of holonomic series is closed with respect to sum, Cauchy product, Hadamard product, Borel transform, and Laplace transform [10]. We give a sketch of the proof for the Cauchy product. If $F(x)$ satisfies a differential equation of order s and $G(x)$ satisfies a differential equation of order t, we formally compute the derivatives of $H(x) = F(x)G(x)$ and, using the equations satisfied by $F(x)$ and $G(x)$, we express them as linear combinations of the products $F^{(i)}(x)G^{(j)}(x)$ where the indices i and j vary from 0 to $s-1$ and from 0 to $t-1$ respectively. The space of such combinations has a finite dimension, hence the derivatives of $H(x)$ satisfy a dependance relation, that is a linear differential equation.

There is a similar result for holonomic sequences: the sum, product, and convolution of two holonomic sequences are holonomic; the indefinite summation of a holonomic sequence is holonomic. Both types of closure properties are interrelated, and the proofs use whichever is easier.

Identity proving. An application of holonomy, widely exemplified by D. Zeilberger, is identity proving [12]. The idea is the following: to prove $F(x) = G(x)$, build the equation satisfied by $F(x) - G(x)$, and compute sufficiently many initial conditions to ensure $F(x) - G(x) = 0$.

Here is a simple example. Suppose we want to prove the identity

$$\sqrt{x}J_{1/2}(x) = \sqrt{\frac{2}{\pi}}\sin x,$$

where $J_{1/2}(x)$ is a Bessel function of index $1/2$. This function satisfies a second order differential equation, while the square root satisfies a first order equation; hence the product is a solution of an equation of order not greater than 2. On the other hand, sine satisfies a second order equation; therefore the difference of the two sides of the formula satisfies an equation of order not greater than 4. It suffices to verify that the power series of the difference is $O(x^4)$, using the differential equations and the initial conditions defining the components. The alert reader may think we were lucky, because $\sqrt{x}J_{1/2}(x)$ has a power series expansion at 0, while $J_{1/2}(x)$ has not. But, if this had not been the case, we would have used use another point than 0.

Algebraic functions. Algebraic functions are holonomic. Comtet [4] gave an algorithm to compute the differential equation satisfied by a function $F(x)$ solution of $P(x, y) = 0$, where P is an irreducible polynomial. The idea is to find a Bezout relation $UP + VP_y = 1$ by the extended Euclidean algorithm and use $P_x + P_yF' = 0$ to express the successive derivatives of $F(x)$ as polynomials in $F(x)$ of degree less than $d = \deg_y P$. The family of powers 1, $F(x)$, ..., $F^{d-1}(x)$ is a basis of the space generated by the derivatives of $F(x)$, and there is a dependance relation between $F(x)$, $F'(x)$, ..., $F^{(d)}(x)$.

Algebraic substitution. If $F(x)$ is holonomic and $G(x)$ is algebraic, then $F(G(x))$ is holonomic by the same kind of technique as above. An immediate application of this result is the following: if f_n is a holonomic sequence, then its Euler transform

$$h_n = \sum_{k=0}^{n} (-1)^k \binom{n}{k} f_k$$

is holonomic too. This is obvious because the two generating functions are connected by $H(x) = F(-x/(1-x))/(1-x)$.

3. Search for solutions

Recurrence relations and differential equations almost never have explicit solutions, but if an explicit solution exists it might be important to recognize it, and find the solution. Above all an explicit solution gives a global information about the equation.

Rational solutions to recurrences. Abramov [1] gives a method to obtain the rational solutions $u_n = P(n)/Q(n)$ of a recurrence

$$a_0(n)u_{n+k} + \cdots + a_k(n)u_n = b(n),$$

where a_0, ..., a_k, and b are polynomials. The principle which guides the algorithm is: the zeros of the coefficients must match the poles of u_n and its shifts $u_{n+\ell}$. As a consequence, Q must be a multiple of $\gcd(a_0(n-k), \ldots, a_k(n))$ if the roots of Q do not differ by an integer. The last condition is not necessarily fulfilled; to avoid this problem one considers a recurrence satisfied by the sequence $v_n = u_{nh}$, where h is the maximal difference between two roots of Q. It must be noted that the number h is not greater than the maximal difference between the roots of $a_k(n)$ and $a_0(n-k)$.

Indefinite hypergeometric summation. The indefinite sum [6] of f_k is equivalent to finding a closed formula for $F_n = \sum^n f_k$ where f_k is a given sequence. This relation means

$$F_n - F_{n-1} = f_n$$

for all n. If f_n is assumed to be hypergeometric, and we look for a hypergeometric F_n, the relation $1 - F_{n-1}/F_n = f_n/F_n$ shows that the sequence $u_n = F_n/f_n$ must be rational. Hence we are led to search for a rational solution of the equation

$$u_n - \frac{f_{n-1}}{f_n} u_{n-1} = 1.$$

Hypergeometric solutions to recurrences. Petkovšek's algorithm [8] provides the hypergeometric solutions of a linear recurrence

$$a_0(n)u_{n+k} + \cdots + a_k(n)u_n = 0,$$

where $a_0, \ldots, a_k$, and b are polynomials. Writing $u_{n+1}/u_n = P(n)/Q(n)$ and substituting leads to a non-linear equation, which is not tractable. There exists a decomposition

$$\frac{u_{n+1}}{u_n} = \frac{P(n)}{Q(n)} \frac{A(n+1)}{A(n)}$$

in which all pairs $(A(n), P(n))$, $(A(n), P(n))$, $(P(n), Q(n))$, $(P(n), Q(n+1))$, ..., $(P(n), Q(n+k))$ are relatively prime. With this decomposition a substitution gives

$$a_0(n)A(n+k)P(n+k)\cdots P(n) + a_1(n)A(n+k-1)P(n+k-1)\cdots P(n)Q(n+k) \\ + \cdots + a_k(n)A(n)Q(n+k)\cdots Q(n) = 0.$$

This equation is still non-linear, but it shows that $P(n)$ divides $a_k(n)$, and $Q(n+k)$ divides $a_0(n)$. Finally it suffices to test all pairs of factors of $a_0(n-k)$ and $a_k(n)$.

Note that this algorithm is a powerful tool; it is equivalent to finding factors of order 1 on the right of the recurrence.

Symbolic solutions to differential equations. Searching for generalized hypergeometric solutions is a first approach to a linear differential equation: the recurrence satisfied by the coefficients of the series is computed; the hypergeometric solutions to this recurrence are found; finally the result is translated from sequences to generating functions.

The more general class of Liouvillian functions may be used. Liouvillian functions are obtained from rational functions with rational coefficients by repeated use of the four elementary operations, taking exponentials and logarithms, integration, and algebraic extensions. Singer gives a purely theoretic algorithm to obtain Liouvillian solutions of linear differential equations of arbitrary order. Kovacic's algorithm for equations of order 2 is partially implemented in most computer algebra systems. The theory behind all these algorithms is differential Galois theory. It is difficult to use, because for each order it is necessary to classify the Galois groups which come into play [11].

4. Asymptotic analysis

Even when no explicit solution of a differential equation is known, it is possible to perform an asymptotic analysis. The theory of linear differential equations prescribes the asymptotic behaviour of a solution near a singularity and this asymptotic behaviour is strongly related to the asymptotic behaviour of the Taylor coefficients of the solution.

Singular points. The solutions of a linear differential equation

$$a_0(x)y^{(k)}(x) + \cdots + a_k(x)y(x) = 0$$

may only have singularities at the roots of the dominant coefficient $a_0(x)$, and possibly at infinity. In addition all formal solutions to the equation are known. A logarithmic sum is a formal series

$$\lambda(z) = z^\alpha \sum_{j=1}^{J} \sum_{i \geq 0} c_{ij} z^i \log^j z,$$

and a formal solution in the neighbourhood of the root a of $a_0(x)$ is a finite combination of logarithmic sums

$$y(x) = \sum_{k=0}^{K} \lambda_k(z) \exp(P_k(z)), \qquad z = \frac{1}{(1 - x/a)^{1/r}},$$

which formally satisfies the differential equation. All quantities involved in these formulae can be explicitly computed. In the case where the point a is a regular singular point, that is to say $a_\ell(x) = (x-a)^{k-\ell} A(x)$ for $\ell = 0, \ldots, k$, and $A_\ell(x)$ is analytic in the neighbourhood of a, the formal solutions are logarithmic sums and locally define actual solutions, with a possible ramification point at a. Conversely, in the case of an irregular singular point the formal solutions are generally divergent series, but provide asymptotic expansions for actual solutions in a sector with origin a.

The preceding classification demonstrates that the composition of two holonomic functions is not necessarily holonomic. For instance $1/\sin x$, which is the composition of the two holonomic functions $\sin x$ and $1/x$, is not holonomic because it has an infinite number of singularities. The sequence of Bell numbers is not holonomic because its exponential generating function $\exp(e^x - 1)$ does not have the right form, given by the formula above (after changing x into $1/x$).

Singularity analysis. The smallest singularity ρ of a function analytic in a neighbourhood of zero prescribes the behaviour of the Taylor coefficients of the function. This rough correspondence may be strongly refined [5]; indeed an asymptotic expansion in some sufficiently large neighborhood of the singularity a of smallest modulus

$$f(x) \underset{x \to a}{=} c_0 (1 - x/a)^{\alpha_0} \log^{\beta_0} \frac{1}{1 - x/a} + c_1 (1 - x/a)^{\alpha_1} \log^{\beta_1} \frac{1}{1 - x/a} + \cdots$$

translates into an asymptotic expansion for the coefficient of the Taylor expansion of $f(x)$ at 0

$$f_n \underset{n \to \infty}{=} \rho^{-n} \frac{n^{-\alpha_0 - 1}}{\Gamma(-\alpha_0)} \log^{\beta_0} n \left(c_0 + \frac{d_1}{\log n} + \cdots \right).$$

This result leads to the following idea: to study the asymptotic behaviour of a sequence which satisfies a linear recurrence it suffices to translate the recurrence into a differential equation for the generating function; next a singularity analysis of this function gives the asymptotic behaviour of the sequence. This simple method presents a difficulty. The function is determined as a solution of a differential equation and some initial conditions, which are specified at the point 0. The study of the differential equation provides a basis of formal solutions near the smallest singularity, but there is no direct way to express the generating function with respect to this basis. Obviously if a closed form of the function is available it is possible to realize the connection between the data at 0 and the behaviour at the smallest singularity; but in that case more direct procedures may be used. Generally, it is necessary to use analytic continuation and a resummation method [9]. Note that such a method needs to know about the singularities of the Borel transform of the function; and we have seen that it is possible to compute the differential equation satisfied by the Borel transform of a holonomic function.

5. Multivariate holonomy

The machinery of holonomic sequences or functions is so powerful that it is tempting to generalize holonomy for sequences or functions with more than one variable.

Weyl algebra. The Weyl algebra $A_N(\mathbb{K})$ is an algebra of linear operators which is defined over the space of polynomials $\mathbb{K}[\mathbf{x}] = \mathbb{K}[x_1, \dots, x_N]$. These operators are the partial derivatives ∂_j, the multiplications by the variable x_i's, and all their combinations. The generators $\partial_1, \dots, \partial_N, x_1, \dots, x_N$ satisfy the following commutation rules:

$$\partial_i \partial_j = \partial_j \partial_i, \qquad x_i x_j = x_j x_i$$

$$\partial_i x_j = x_j \partial_i \quad \text{for } i \neq j, \qquad \partial_i x_i = x_i \partial_i + 1.$$

Then, an element f of a module over the Weyl algebra is D-finite if the submodule spanned by f and all its derivatives $\boldsymbol{\partial}^\alpha f$ has a finite dimension over the field of rational functions $\mathbb{K}(\mathbf{x})$. An equivalent definition is obtained as follows: for f from an $A_N(\mathbb{K})$-module, consider the set of all equations $P(\mathbf{x}, \boldsymbol{\partial})f = 0$ satisfied by f; the polynomials $P(\mathbf{x}, \boldsymbol{\partial})$ are elements of the left ideal $\operatorname{Ann}(f)$ in the Weyl algebra; then f is D-finite if the quotient $A_N(\mathbb{K})/\operatorname{Ann}(f)$ of the Weyl algebra by the annihilator ideal $\operatorname{Ann}(f)$ has a finite dimension over $\mathbb{K}(\mathbf{x})$ as a vector space.

A more effective definition uses the idea of a rectangular system. A set of N polynomials $P_k(\mathbf{x}, \boldsymbol{\partial})$ from the Weyl algebra is a rectangular system if each polynomial involves only one partial derivative ∂_i, and each partial derivative appears in exactly one of these polynomials $P_k(\mathbf{x}, \boldsymbol{\partial})$. One proves that f is D-finite if and only if there exists a rectangular system contained in the annihilator ideal $\operatorname{Ann}(f)$. As a consequence a D-finite element f satisfies a special set of equations of the form

$$P_1(\mathbf{x}, \partial_1)f = 0, \qquad P_2(\mathbf{x}, \partial_2)f = 0, \qquad \dots, \qquad P_N(\mathbf{x}, \partial_N)f = 0.$$

In addition, Bernstein worked out the concept of multivariate holonomy. The Weyl algebra is naturally graded by the degree: the degree of the monomial $\mathbf{x}^\alpha \boldsymbol{\partial}^\beta$ is $|\alpha| + |\beta|$, and the component F_d of the natural filtration is composed of the polynomials of degree not greater than d. For f from a module over the Weyl algebra, this induces a filtration of the submodule $A_N(\mathbb{K})f$; the component Γ_d is merely $F_d f$. It turns out that the dimension of Γ_d over $\mathbb{K}$ is expressed as a polynomial in d for all sufficiently large d. The degree of this polynomial is the Bernstein dimension of the module $A_N(\mathbb{K})f$. Moreover it is shown that the Bernstein dimension of $A_N(\mathbb{K})f$ is greater or equal to N. Now, f is *holonomic* if the Bernstein dimension of $A_N(\mathbb{K})f$ is exactly N.

Kashiwara's theorem proves that D-finiteness and holonomy are the same concept. But each one has its own merits. The D-finiteness property makes it easy to show that sums and products of holonomic functions are holonomic too. On the other hand, definite integration with respect to one of the x_i's preserves holonomy, and this is more easily shown using the definition of holonomy.

The link between sequences and generating functions is not as nice in the multivariate case as in the univariate case. A sequence u_ν, where the index ν is an N-tuple $(n_1, \dots, n_N)$ is P-finite if the sequence u_ν and all its shifts $u_{\nu+\tau}$ span a finite dimensional space over $\mathbb{K}(\tau_1, \dots, \tau_N)$. An equivalent formulation of the P-finiteness can be written as follows: there exists a rectangular system

$$P_1(\nu, S_1)u = 0, \qquad P_2(\nu, S_2)u = 0, \qquad \dots, \qquad P_N(\nu, S_N)u = 0,$$

where S_i is the shift operator defined by $S_i u_\nu = u_{n_1, \dots, n_i+1, \dots, n_N}$. One proves that a sequence is P-finite if its multivariate generating function is D-finite. The reciprocal assertion is false.

The study of P-finite sequences shows it is interesting to consider a more general concept than Weyl algebras. This leads to Ore algebras, which are defined as polynomial algebras with some commutation rules for the variables [3]. For instance, the finite difference calculus in one variable is formalized by the algebra $\mathbb{K}\langle n, \Delta\rangle$ with $\Delta n = (n+1)\Delta + 1$.

Creative telescoping. We search for a recurrence relation for the definite sum $U_n = \sum_k u_{n,k}$, where the double sequence $u_{n,k}$ is P-finite. The idea is to find an equation $P(n, S_n, \Delta_k)u = 0$, where the variable k does not occur, S_n is the shift operator with respect to n, and Δ_k is the difference operator with respect to k; then, U satisfies $P(n, S_n, \Delta_k)U = 0$. Contrary to the case of holonomic functions such an equation does not exist a priori; but if it exists, it is possible to find it by a Gröbner basis technique. As an example we want to rederive the Franel relation on the sum

$$U_n = \sum_{k=0}^{n} \binom{n}{k}^3.$$

First we give a rectangular system for the double sequence $u_{n,k} = \binom{n}{k}^3$,

$$[(n-k+1)^3 S_n - (n+1)^3]u = 0, \qquad [(k+1)^3 S_k - (n-k)^3]u = 0.$$

Here the analogue to the Bernstein dimension is 2, hence elimination provides a relation $P(n, S_k, S_n)u = 0$. Next the summation with respect to k, and the substitution $S_k = 1$, or equivalently $\Delta_k = 0$, give the desired formula:

$$\begin{aligned}\big[(n+3)^3(3n+4)S_n^3 - (18n^3 + 114n^2 + 232n + 148)S_n^2 \\ -(3n+5)(15n^2 + 55n + 48)S_n - 8(n+1)^2(3n+7)\big]\, U = 0.\end{aligned}$$

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