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Frédéric Chyzak
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Centre international de rencontres mathématiques
U.M.S. 822 C.N.R.S./S.M.F.
Luminy (Marseille) FRANCE
Creative Telescoping for Parametrised Integration and Summation

Frédéric Chyzak

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CHAPTER 1

Introduction

This presentation is concerned with the algorithmic symbolic treatment of integrals and sums that appear in various fields like the theory of special functions, combinatorics, and mathematical physics, and more generally with exact algebraic manipulations of systems of linear functional equations, whether differential or of recurrence, and of their solutions. Our approach here is almost always algorithmic, whether with the goal of enlarging the class of systems and functions to which the approach applies, or with the goal of making the algorithms more efficient, as much as possible with a provably better arithmetic complexity. At the same time, we endeavour to propose a fair account on the context of the research in this domain, both ours and others’, so as to provide a global and coherent view on it.

The choice here is to focus on a body of research that centers around the method of Creative Telescoping. This can be viewed as a common formalism for several possibly surprisingly related operations on functions, series, and formal series. I shall present creative telescoping first as a method to perform integration and summation of special functions, combinatorial sequences, orthogonal polynomials, but its introduction in combinatorics was largely motivated by other operations like constant-coefficients extractions and the extraction of diagonals of generating functions in combinatorics. It also found an application to the evaluation of certain scalar products in the theory of the symmetric functions of combinatorics. This will be reviewed in the following text.

1. The Name “Creative Telescoping”

The phrase creative telescoping appears in an explanation by van der Poorten (1979, p. 211) of Apéry’s irrationality proof of $\zeta(3)$. One of van der Poorten’s steps is to establish that the sum

$$b_n = \sum_{k=0}^{n} b_{n,k}, \quad \text{where} \quad b_{n,k} = \binom{n}{k}^2 \binom{n+k}{k}^2,$$

satisfies the same second-order linear recurrence equation as another binomial sum. He mentions that, to get the recurrence explicitly, Cohen and Zagier “cleverly construct

$$B_{n,k} = 4(2n+1)(k(2k+1) - (2n+1)^2)b_{n,k},$$

with the motive that

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

so that summing over $k$ from 0 to $n+1$ results in the wanted recurrence,

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

Here, the series whose general term is the right-hand side of (1.2) reduces to the sum over $k$ of the term $B_{n,k} - B_{n,k-1}$, which telescopes, giving the name to the method. Works by Zeilberger to design algorithms for obtaining analogues of the key relation (1.2) for general summands popularised the approach (Zeilberger, 1982, 1990a, 1991).

The method has a differential analogue, which Almkvist and Zeilberger name the method of differentiating under the integral sign (1990), but this highlights only one aspect of the computation. For concreteness and to motivate my statement, I reproduce an example by Zeilberger (1982), which he borrowed from a classical textbook on integration: to evaluate the parametrised integral

$$f(b) = \int_{-\infty}^{+\infty} e^{-x^2} \cos 2bx \, dx,$$
first perform differentiation w.r.t. $b$ under the integral sign, followed by integration by parts w.r.t. $x$, to get the relation
\[ f'(b) = \int_{-x}^{+x} -2xe^{-x^2} \sin 2bx \, dx = \left[ e^{-x^2} \sin 2bx \right]_{-x}^{+x} + \int_{-x}^{+x} -2be^{-x^2} \cos 2bx \, dx = -2b f(b). \]

Solving the induced ODE requires to know an initial condition, $f(0)$, which amounts to getting an explicit form for the integral at $b = 0$. In the end, this results in the explicit form $f(b) = \sqrt{\pi} e^{-b^2}$. This calculation with integrals can be reconsidered on the level of integrands: after introducing an operator will be denoted as an inverse:
\[ D f = \frac{1}{2 \pi \pi} \int_{-\infty}^{\infty} b e^{-b^2} \cos b \, db. \]

It follows from the Leibniz rule and just the effect of substitution that
\[ \frac{df}{db}(b, x) - \frac{d}{dx} \left( e^{-x^2} \sin 2bx \right) - 2b f(b, x) - \frac{d}{dx} \left( -\frac{1}{2x} \frac{df}{db}(b, x) \right) = -2b f(b, x). \]

Reorganising terms delivers the following analogue of (1.1)–(1.2), with self-explanatory notation:
\begin{equation}
(1.4) \quad \frac{dF}{dx}(b, x) = \frac{df}{db}(b, x) + 2b f(b, x) \quad \text{for} \quad F(b, x) = -\frac{1}{2x} \frac{df}{db}(b, x).
\end{equation}

In view of the strong formal analogy between the recurrence case (1.2) and the differential case (1.4), and because “differentiating under the integral sign” is only one aspect of the approach, Salvy and I have started to use the same phrase “creative telescoping” in (Chyzak and Salvy, 1998) to denote these two similar situations, and specifically for the task of obtaining (1.2) or (1.4) in an algorithmic way.

As I will describe in the historical context below, creative telescoping is related to an elimination theory applied to a (non-commutative) polynomial representation of linear differential/difference operators. The absence of algorithms for linear operators in the early 1980s—or at least their relative immaturity—explains the difficult start of the creative-telescoping theory developed by Zeilberger.

2. **Linear Operators**

It has proved very fruitful in the works that will be developed in this text to represent the linear differential equations and linear recurrences under consideration as linear differential/difference “operators.” The following notation and conventions will be used throughout the whole text.

I shall constantly consider functions of (continuous) variables $x$, $y$, etc., and sequences of (discrete) variables $n$, $k$, etc., and more often than not variations like sequences of functions, parametrised families of functions, etc. All such objects will collectively be called “functions,” unless disambiguation is needed, and will be subject to respective derivation operators denoted $D_x$, $D_y$, etc., and (forward) shift operators denoted $S_n$, $S_k$, etc. When needed, a backward shift operator will be denoted as an inverse: $S_n^{-1}$, $S_k^{-1}$, etc. Composition will be denoted just by products and powers, so that, for example, $D_y S_n^{-1} S_k$ acts on a “function” $f$ by the rule:
\[ (D_y S_n^{-1} S_k f)(n, k, x) = \frac{\partial^3 f}{\partial x^3}(n + 1, k + 3, x). \]

These operators combine with operators of multiplication by a variable to generate more general operators. Operators of multiplication will be denoted by the variable itself, so as to enforce rules like:
\[ (xf)(n, x) = xf(n, x), \quad (nf)(n, x) = n f(n, x). \]

It follows from the Leibniz rule and just the effect of substitution that
\[ D_x xf = (D_x x)f - (D_x (xf)) = xD_x f + f - (xD_x + 1)f, \]
\[ S_n nf = (S_n n)f - (S_n (nf)) = (n + 1)S_n f, \]

where the operator 1 denotes an identity operator. These formal rules lead us to expect the following algebraic relations between non-commutative polynomials:
\[ D_x x = xD_x + 1, \quad S_n n = (n + 1)S_n. \]

A theory to make sense of such commutations has been developed in algebra, starting with Ore’s work in the 1930s. Since “operators” are considered in the present document for their algebraic properties, and not for any topological or analytic one, I will at times more properly speak of skew
polynomials for the objects originally studied by Ore. In the literature, they are also known as Ore polynomials, Ore operators, pseudo-linear transformations, and pseudo-linear operators.

The theory of skew polynomials started with Ore’s work on polynomials in a single derivation or shift operator: mainly with (1933), in which Ore developed a theory of one-sided gcd for skew polynomials, but also with (1931), in which he considered matrices of skew polynomials. Skew polynomials were later considered by (Jacobson, 1937) under the name pseudo-linear transformations, and algorithms for gcd and factorisation for general skew polynomials were discussed in (Bronstein and Petkovšek, 1994, 1996).

Ore’s construction produces rings of operators, a.k.a. skew polynomial rings. We thus have, for example: the ring \( \mathbb{Q}(x)\langle D_x \rangle \) of linear differential operators with coefficients in the rational-function field \( \mathbb{Q}(x) \); the ring \( \mathbb{Q}(n)\langle S_n \rangle \) of linear recurrence operators with coefficients in the rational-function field \( \mathbb{Q}(n) \); analogues \( \mathbb{Q}[x]\langle D_x \rangle \) and \( \mathbb{Q}[n]\langle S_n \rangle \) when we are interested in operators with polynomial coefficients only; an analogue \( \mathbb{Q}(n)\langle S_{n-1}^{-1} \rangle \) when considering backward shifts instead of forward shifts.

When several derivation/shift operators are needed in the same algebraic setting, Ore’s construction could be iterated abstractly, which introduces the possibility of derivations and shifts that do not commute with one another. We viewed this as a drawback in the work coauthored with Salvy (1998), as we would have lost good finiteness and algorithmic properties. In that article, we therefore developed a theory of so-called Ore algebras, in which derivations and shifts commute, while they need not commute with the coefficients. Coming back to the example of \( D_{x^2}S_{n-1}^{-1}S_k^3 \), this lives for example in the algebra \( \mathbb{Q}(n,k,x)\langle S_n, S_{n-1}^{-1}, S_k, S_{x^2}, D_x \rangle \), where \( S_n \), \( S_{n-1}^{-1} \), \( S_k \), and \( D_x \) commute pairwise, while none of them commutes with all elements from \( \mathbb{Q}(n,k,x) \).

In the present document, I chose to present neither Ore’s theory nor our theory of Ore algebras and to refrain from using the corresponding more heavy notation, \( \mathbb{Q}(x)\langle \overline{\sigma}; \overline{\sigma}, \delta \rangle \).

3. Important Classes of Functions and Sequences

A few specific classes of functions and sequences appear constantly in the present text, namely hypergeometric sequences, hyperexponential functions, D-finite functions, and \( \delta \)-finite functions, which are all solutions of linear functional operators. The distinction between those classes is based on the type of operators considered and the order of the equations that the functions solve.

Sequences of the index \( n \) (over \( \mathbb{N} \) or \( \mathbb{Z} \)) that solve a first-order linear recurrence equation with coefficients that are polynomial functions of \( n \) are called hypergeometric. Equivalently, a sequence \( u \equiv (u_n) \) is hypergeometric if there exists a rational function \( R(n) \) such that the ratio \( u_{n+1}/u_n \) is equal to \( R(n) \), except maybe for finitely many values of \( n \). In this case, I shall consider that \( S_n \equiv R(n) \) annihilates \( u \), disregarding the finite exceptions. This generalises to sequences \( u \equiv (u_{n_1}, \ldots, u_{n_r}) \) of several indices by requiring that there exist for each index \( R_{n_1}(1), \ldots, R_{n_r}(1) \) such that \( u \) is annihilated by each first-order operator \( S_{n_1} \cdots S_{n_r} \). Examples of hypergeometric sequences are given by the terms \( 2^n \), \( n! \), \( (n_1 + n_2)! \), \( 1/(n_1 - n_0)! \), \( 1/(n_1 + n_2) \), and \( \binom{n}{3} \). Rational functions of the indices are hypergeometric, as well as products of hypergeometric sequences.

The situation in analogous in the differential case, where a hyperexponential function is defined as a function \( f \) of continuous variables \( x_1, \ldots, x_r \), whose \( r \) logarithmic derivatives are rational functions of the \( r \) variables. Hyperexponential functions solve systems of first-order linear differential equations with coefficients that are polynomial functions of the \( x \)'s. Examples include rational functions, exponentials of rational functions, powers of rational functions to rational and transcendental constants. In addition, products of hyperexponential functions are hyperexponential.

The generalisation to D-finite and \( \delta \)-finite functions is best explained after introducing the notion of annihilating ideals: indeed, the skew polynomials (with rational-function coefficients) from some skew-polynomial algebra \( A \equiv \mathbb{Q}(x,y, \ldots, m, n, \ldots)\langle D_x, D_y, \ldots, S_m, S_n, \ldots \rangle \) that cancel a given function \( f \) constitute a left ideal, denoted \( \text{ann}_A \ f \), or more simply \( \text{ann} \ f \) when no ambiguity can arise. When acting on \( f \), skew polynomials can be viewed modulo \( \text{ann} \ f \), as the function \( Pf \) obtained for \( P \in A \) is equal to any \( (P + Z) f \) for \( Z \in \text{ann} \ f \). So the \( Pf \) are actually described by classes \( P + \text{ann} \ f \) from the quotient module \( A/\text{ann} \ f \), and there is in fact an isomorphism from \( A/\text{ann} \ f \) to \( Af \) defined by mapping the class \( P + \text{ann} \ f \) to \( Pf \).
This leads to new definitions of hypergeometric and hyperexponential functions as functions $f$ whose corresponding quotient modules $A_f/\text{ann } f$ are vector spaces of dimension 1 over the rational-function field $\mathbb{Q}(x, y, \ldots, m, n, \ldots)$. The generalised notion of $\delta$-finite functions corresponds to finite-dimensional quotient modules of dimension possibly more than 1. In the purely differential situation, such a function is simply called differentiably finite, in short, $D$-finite. The special case of $D$-finite series was introduced and studied by Stanley (1980) in the univariate case and by Lipshitz (1989) in the multivariate case; see also Chapter 6 in the textbook (Stanley, 1999). I introduced the more general case of $\delta$-finite functions in my work (1998) with Salvy, as $\delta$ is the symbol we used in that work to denote derivation operators like $D_x$ and shift operators like $S_n$ in a unified way. Each class of functions is closed under additions and products, and algorithms exist to produce a defining system for $f + g$ and $fg$ from defining systems for $f$ and $g$; see the same references.

Now, a property of $D$-finite is that all its (infinitely-many) cross derivatives $f_x, D_x f, D_y f, \ldots, D_x^2 f, D_x D_y f, D_y^2 f, \ldots$, are so much linearly related that they span a finite-dimensional vector space over $\mathbb{Q}(x, y, \ldots)$. The similar property for $\delta$-finite functions is that all shifts of cross derivatives span a finite-dimensional vector space over $\mathbb{Q}(x, y, \ldots, m, n, \ldots)$. As a consequence, they also satisfy a (higher-order) purely differential equation for each derivation operator, and a (higher-order) purely difference equation for each shift operator.

4. $q$-Analogues

Just as many enumeration problems involve factorials and binomial terms, and thus lead to recurrences that relate values at $n$ with values at $n + 1$, $n + 2$, etc., using “additive shifts,” so do refined enumeration problems in combinatorics, in statistical physics, and in the theory of partitions involve recurrences that relate values at $x$ with values at $qx$, $q^2 x$, etc., using “multiplicative shifts” w.r.t. some fixed base $q$. A change of variables to replace $x$ with $q^n$ will bring multiplicative shifts back to additive ones, but if the recurrences under considerations had coefficients that were polynomials in $x$, the change of variables produces recurrences involving $q^n$ in the coefficients.

Many functions of the “classical” world, like counting numbers, special functions, and orthogonal polynomials, find a so-called $q$-analogue generalisation that recovers them at $q = 1$. In the tradition, the base $q$ is either a complex number with $|q| < 1$ or an indeterminate, whence the name of $q$-series for objects of the theory.

The simplest examples of terms that admit a $q$-analogue are the classical Pochhammer symbol, factorials, and binomial coefficients, which are related as follows: the Pochhammer symbol $(x)_n$ is defined for $x \in \mathbb{C}$ and $n \in \mathbb{Z}$ by

$$ (x)_n = \begin{cases} x(x+1) \cdots (x+n-1) & \text{if } n > 0, \\ 1 & \text{if } n = 0, \\ 1/((x-1) \cdots (x+n)) & \text{if } n < 0, \end{cases} $$

provided the quotient is well defined; the factorial sequence is then obtained by evaluation as

$$ n! - (1)_n; $$

finally, binomial coefficients are obtained by the well known formula

$$ \binom{n}{k} = \frac{n!}{k!(n-k)!}. $$

Note that the Pochhammer symbol satisfies the two recurrences

$$ (x + 1)_n = \frac{x + n}{x} (x)_n \quad \text{and} \quad (x)_{n+1} = (x + n)(x)_n, $$

from which recurrences can be derived for factorials and binomial coefficients. The $q$-Pochhammer symbol $(x; q)_n$ is defined for $x \in \mathbb{C}$ and $n \in \mathbb{Z}$ by

$$ (x; q)_n = \begin{cases} (1-x)(1-q x) \cdots (1-q^{n-1}x) & \text{if } n > 0, \\ 1 & \text{if } n = 0, \\ ((1 - \frac{x}{q}) \cdots (1 - \frac{x}{q^n}))^{-1} & \text{if } n < 0; \end{cases} $$

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it satisfies the two recurrences
\[
(qx; q)_n = \frac{1 - q^n x}{1 - x} (x; q)_n \quad \text{and} \quad (x; q)_{n+1} = (1 - q^n) (x; q)_n. 
\]
This is not a \(q\)-analogue of \((x)_n\), in the sense that setting \(q \to 1\) does not produce the classical Pochhammer symbol, but the \(q\)-factorial defined as \((q; q)_n\) is a \(q\)-analogue:
\[
\frac{(q; q)_n}{(1 - q)_n^+} = 1 \cdot (1 + q) \cdots \cdot (1 + q + \cdots + q^{n-1})
\]
goesto \(n!\) when \(q\) tends to \(1\). By way of consequence, the \(q\)-binomial coefficient defined as
\[
\left[ \begin{array}{c} n \\ k \end{array} \right]_q = \frac{(q; q)_n}{(q; q)_k (q; q)_{n-k}}
\]
becomes \(\binom{n}{k}\) when \(q\) goes to \(1\).

A nice introduction on \(q\)-analogue functions in identities that lift classical identities.

5. List of Examples

The primary goal of creative telescoping is the evaluation of integrals and sums involving combinatorial numbers and special functions, especially of hypergeometric/hyperexponential or D-finite type, and the proof of identities involving such sums and integrals. This contains and extends to:

- Binomial sums, as the equality
  \[
  \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2 - \sum_{k=0}^{n} \binom{n}{k} \binom{n+k}{k} \sum_{j=0}^{k} \binom{k}{j}^3,
  \]
  between sums, which appears in connection to Apéry’s proof of the irrationality of \(\zeta(3)\) and has been proved by creative telescoping by Strehl (1994), or the evaluation proposed by Blodgett (1990)
  \[
  \sum_{i=0}^{n} \sum_{j=0}^{n} \binom{i+j}{i}^2 \binom{4n-2i-2j}{2n-2i} = (2n+1) \binom{2n}{n}^2;
  \]

- Integrals of the theory of special functions, like the example of an integral
  \[
  \int_{0}^{\infty} x J_1(ax) I_1(ax) Y_0(x) K_0(x) \, dx = -\frac{\ln(1 - a^2)}{2\pi a^2}
  \]
  involving the four types of Bessel functions and first considered by Glasser and Montaldi (1994), or the double integral
  \[
  \int_{0}^{\infty} \int_{0}^{\infty} J_1(x) J_1(y) J_2(c\sqrt{xy}) \, dx \, dy \quad \text{for} \quad c > 0
  \]
  which, if it cannot be put to explicit form, can be proved by creative telescoping to satisfy a second-order linear ODE;

- Extractions of coefficients, for instance by the Cauchy formula, like with the formula
  \[
  \frac{1}{2\pi i} \oint \frac{(1 + 2xy + 4y^2) \exp \left( \frac{4x^2y^2}{1+4y^2} \right)}{y^{n+1}(1 + 4y^2)^{\frac{3}{2}}} \, dy = \frac{H_n(x)}{[n/2]!},
  \]
due to Doetsch (1930) and related to the Hermite orthogonal polynomials;

- Verifying identities in \(q\)-sums, that appear in the combinatorial theory of partitions, like
  \[
  \sum_{k=0}^{n} \frac{q^{k^2}}{(q; q)_k} - \sum_{k=-n}^{n} \frac{(-1)^k q^{(5k^2-k)/2}}{(q; q)_n (q; q)_{k+k}},
  \]
  \[
  \sum_{j=0}^{n-j} \frac{q^{(j+1)^2+j^2}}{(q; q)_{n-j} (q; q)_j} - \sum_{k=-n}^{n} \frac{(-1)^k q^{2k^2+1/2k}}{(q; q)_{n+k} (q; q)_{n-k}}.
  \]
which are finite forms of the Rogers–Ramanujan identities and of a generalisation and were respectively obtained by Andrews in 1974 and Paule in 1985;

- Computing explicit forms for scalar products with respect to various exponential/algebraic weights and in relation to families of orthogonal polynomials or of other parametrised families of functions, like the identities
  \[ \int_{-1}^{+\infty} e^{-px} T_n(x) \frac{dx}{\sqrt{1-x^2}} = (-1)^n n I_n(p), \]
  \[ \int_{0}^{+\infty} xe^{-px} J_n(bx) J_n(cx) \frac{dx}{2p} = \frac{1}{2p} \exp \left( \frac{e^2 - b^2}{4p} \right) J_n \left( \frac{bc}{2p} \right), \]
  which respectively involve Chebyshev orthogonal polynomials and Bessel functions;

- Scalar products that appear in the theory of symmetric functions, like
  \[ \left\langle \exp \left( \frac{p_1^2 - p_2^2}{2} - p_2^2/4 \right) \right| \exp \left( \frac{1}{2} t (t+2) \right) \right\rangle = e^{-\frac{1}{4} t (t+2)} \frac{1}{\sqrt{1-t}}, \]
  where \( p_1 \) and \( p_2 \) respectively denote the infinite symmetric power sums \( x_1 + x_2 + \cdots \) and \( x_1^2 + x_2^2 + \cdots \).

In all previous examples, the sequences and functions under consideration possess as many independent linear, whether differential, difference, or more general functional, equations as their number of variables. That is to say, they can be described as \( \varphi \)-finite functions, by a set of linear functional equations and finitely-many initial conditions. A recent extension of the approach, and still promising further developments, allows to deal as well with functions that possess fewer independent equations than variables; the general solutions of the linear functional systems that describe them therefore demand an arbitrary function of at least one variable in its description in explicit form. Examples include:

- Combinatorial identities involving: the graph-counting sequence \( k^{k-1} \), like
  \[ \sum_{k=0}^{n} \binom{n}{k} i (k+i)^{k-1} (n-k+j)^{n-k} - (n+i+j)^n, \]
  which is attributed to Abel; or Stirling numbers of the second kind and Eulerian numbers, like
  \[ \sum_{k=0}^{n} (-1)^{m-k} k! \binom{n+k}{m-k} \binom{n+1}{k+1} = \binom{n}{m}, \]
  attributed to Frobenius; or Bernoulli numbers, like
  \[ \sum_{k=0}^{m} \binom{m}{k} B_{n+k} = (-1)^{m+n} \sum_{k=0}^{n} \binom{n}{k} B_{m+k} \]
  to be found in (Gessel, 2003);

- Identities in more special functions, like Hurwitz’s zeta function, the beta function, polylogarithms, and the (upper) incomplete Gamma function, which appear in the following evaluations:
  \[ \int_{0}^{\infty} x^{k-1} \zeta(n, \alpha + \beta x) \frac{dx}{\zeta(n-k, \alpha)}, \]
  \[ \int_{0}^{\infty} x^{\alpha-1} \zeta(n, -xy) \frac{dx}{\zeta(n, \alpha)} = \frac{\pi (-\alpha)^n y^{-\alpha}}{\sin(\pi \alpha)}, \]
  \[ \int_{0}^{\infty} x^{\alpha-1} \exp(xy) \frac{dx}{\sin((a+s) \pi)} = \frac{\Gamma(s)}{\Gamma(1-a)}. \]

6. Notation

When discussing bounds, I shall most often consider asymptotic upper bounds, which I shall denote using the big-\( O \) notation: for example, \( u_n \in \mathcal{O}(n^3) \) means that the sequence \( u - (u_n) \) does not grow faster than a constant times the cubic function when \( n \) goes to infinity. On the other hand, I shall at times use the big-\( \Theta \) notation to denote that a sequence grows in proportion to another: for example, \( v_n \in \Theta(n^4) \) means that \( v_n \) is asymptotically equivalent to \( \kappa n^4 \) for some fixed
non-zero $\kappa$, as $n$ goes to infinity. This stronger notion is crucial in two cases: to express that an upper bound is tight and to express that, asymptotically, a sequence becomes strictly more than another.

As is usual in combinatorics, for a non-negative integer $\ell$, the falling factorial $n^\underline{\ell}$ denotes the polynomial $n(n-1)\cdots(n-\ell+1)$. 
CHAPTER 2

Early History of Creative Telescoping

Before the technical results in the next chapters, I provide a brief history of the research on creative telescoping. My goal here is to highlight the flow of ideas, while providing context and motivation to my past research orientations.

1. FROM ZEILBERGER’S EARLY ATTEMPT TO HIS “HOLONOMIC-SYSTEMS APPROACH”

Zeilberger (1982) made the first attempt in the literature at giving generality to Cohen and Zagier’s derivation (1.1)–(1.3), by exploiting a technique of Fasenmyer (1945, 1949). Although this work of Zeilberger’s makes good observations that have been used in later literature, it is flawed in several ways that make its main claims wrong. On the positive side, Zeilberger’s observation is that, given a hypergeometric summand \( h_{n,k} \), his variant of Fasenmyer’s technique provides, if it succeeds, a relation of the form

\[
\sum_{i=0}^{r} \sum_{j=0}^{s} c_{i,j}(n) h_{n+i,k+j} = 0
\]

from which an equation playing the role of (1.2) can be derived. In fact, Fasenmyer elaborated her original technique for hypergeometric series described in the form

\[
h_n(x) = \sum_k h_{n,k} x^k
\]

She used an analogue of (1.1) that involves shifts in \( n \) only, together with powers of \( x \):

\[
\sum_{i=0}^{r} \sum_{j=0}^{s} c_{i,j}(n) x^j h_{n+i}(x) = 0.
\]

Fasenmyer’s technique was later described by Rainville (1960), who also slightly generalised it to sums of the form \( h_n(x) = \sum_k h_{n,k} T_k(x) \), involving the \( k \)th Chebyshev polynomial \( T_k(x) \). It was also used by Verbaeten, a name that will appear again in what follows, for the quadrature of an integral problem parametrised by a Chebyshev series (Piessens and Verbaeten, 1973). In his paper, Zeilberger additionally observes that the approach generalises to sums of \( q \)-analogues and integrals of functions satisfying systems of first-order equations, and to all possible cases mixing these forms of operators.

It took Zeilberger a few more years before his seminal paper “A holonomic systems approach to special functions identities” (1990b), in which he introduced the proper definitions to prevent degenerate cases from occurring and ensure the existence of non-trivial (that is, non-zero) equations (1.2) and (1.1). This important paper bases on results of the theory of holonomic D-modules that had been developed in the 1970s (Bernšteín, 1971, 1972; Kashiwara, 1978). What is at stake here is the consideration of all linear differential/difference equations that a given summand or integrand satisfies. Viewing these equations as linear differential/difference operators results in (non-commutative) polynomials that constitute a (left) ideal in a non-commutative polynomial ring \( A_p = \mathbb{Q}[x,y,\ldots,m,n,\ldots] \langle D_x, D_y,\ldots,S_m, S_n,\ldots \rangle \) (in finitely many generators). This representation is now amenable to a theory of polynomial elimination, which was studied in depth in D-module theory.

Conceptually, however, a subtle distinction has to be done between the ideal of operators with rational-function coefficients in \( A_r = \mathbb{Q}(x,y,\ldots,m,n,\ldots) \langle D_x, D_y,\ldots,S_m, S_n,\ldots \rangle \) and the ideal of operators with polynomial coefficients in \( A_p \); the polynomial-elimination theory takes place in \( A_p \), not in \( A_r \). However, while the ideal of all operators in \( A_r \) that annihilate a given function is usually easily presented by finitely many explicit generators in applications involving special functions, the related ideal in \( A_p \) is not so easily described explicitly; in particular, generators in \( A_r \) cannot be used directly in \( A_p \), even after renormalisation to remove denominators. A simple illustration of the problem is given by the polynomial \( f = x^3 \) in the ordinary differential case. It is
annihilated by $x D_2 - 3$, and any annihilator in $A_r$ is a left multiple of the form $L(x D_2 - 3)$, with $L$ from $A_r$. But just restricting the cofactor $L$ to $A_p$ does not generate all annihilators from $A_p$; for example, $D_2^4$ cancels $f$, but $D_2^3$ factors as $(x^{-1} D_2^3)(x D_2 - 3)$, requiring a denominator $x$ in the cofactor. This phenomenon is part of the cause for the problems in (Zeilberger, 1982), and was not completely clarified even in (Zeilberger, 1990b). In the differential case, first algorithms for obtaining generators of the ideal with polynomial coefficients from generators of the ideal with rational coefficients were given by Tsai in the ordinary differential case (2000), then in the partial differential case (2002). This process was named Weyl closure. On the other hand, no “Ore closure” algorithm is known yet for other types of operators in the multivariate case.

2. OTHER EARLY ELIMINATION APPROACHES: CONSTANT TERMS AND DIAGONALS

It is worth noting that the polynomial notation for operators had already been used for combinatorial matters and in connexion to a polynomial elimination problem. Let me mention two works.

First, Zeilberger was studying already in (1980) means to derive difference equations satisfied by the constant term of products with symbolic exponents of multivariate Laurent polynomials. An example (simple, but of pedagogical nature) is the constant term with respect to $x_1$, $x_2$, and $x_3$ and viewed as a function of $a$, $b$, and $c$, of

$$F(a, b, c, x_1, x_2, x_3) = \left( \left( 1 - \frac{x_1}{x_2} \right) \left( 1 - \frac{x_2}{x_1} \right) \right)^a \left( \left( 1 - \frac{x_1}{x_3} \right) \left( 1 - \frac{x_3}{x_1} \right) \right)^b \left( \left( 1 - \frac{x_2}{x_3} \right) \left( 1 - \frac{x_3}{x_2} \right) \right)^c,$$

which turns out to be

$$(2a)! (2b)! (2c)! (a + b + c)! \frac{1}{a! b! c! (a + b)! (a + c)! (b + c)!}.$$  

(2.1)

Zeilberger’s approach was to consider the two-terms first-order difference equation

$$F(a + 1, b, c, x_1, x_2, x_3) = \left( 1 - \frac{x_1}{x_2} \right) \left( 1 - \frac{x_2}{x_1} \right) F(a, b, c, x_1, x_2, x_3),$$

or rather its normalised polynomial representation $x_1 x_2 S_a + (x_1 - x_2)^2$, together with its siblings obtained by shifting $b$ or $c$ instead of $a$. Then, eliminating $x_1$, $x_2$, and $x_3$ by successive runs of the fraction-free Euclidean algorithm in $\mathbb{Q}[S_a, S_b, S_c][x_1, x_2, x_3]$ yields the annihilator

$$S_a S_b S_c + S_a^2 + S_b^2 + S_c^2 - 2(S_a S_b + S_a S_c + S_b S_c)$$

of the constant term, from which checking that (2.1) is the constant term is easy. It is of interest that Zeilberger observed that the classical elimination theory for commutative polynomials can be applied to the case of partial difference operators with coefficients independent of the variables ($a$, $b$, and $c$ above), but dependent of extra parameters ($x_1$, $x_2$, and $x_3$ above). In contrast, algorithms by creative telescoping would represent the constant term by the Cauchy integral

$$\frac{1}{(2\pi i)^2} \oint \oint \oint F(a, b, c, x_1, x_2, x_3) \, dx_1 \, dx_2 \, dx_3,$$

then consider as well equations that are differential in $x_1$, $x_2$, and $x_3$, and perform an algorithmic elimination of $x_1$, $x_2$, and $x_3$ in $\mathbb{Q}(a, b, c)[x_1, x_2, x_3] < S_a, S_b, S_c, D_1, D_2, D_3 >$ (where $D_i$ denotes derivation w.r.t. $x_i$).

A second work is the proof by Lipshitz that the diagonal of a D-finite power series is D-finite (1988). These notions require definitions: Given a multivariate formal power series

$$f = \sum_{n_1, \ldots, n_r \in \mathbb{N}} c_{n_1, \ldots, n_r} x_1^{n_1} \cdots x_r^{n_r} \in \mathbb{Q}(x_1, \ldots, x_r),$$

its diagonal is defined as the univariate series

$$\Delta f = \sum_{n \in \mathbb{N}} c_n x^n.$$
The case studied by Lipshitz is that of a \textit{differentiably finite} series, in short \textit{D-finite} series, that is, of a series \( f \) whose derivatives \( D_1^{n_1} \cdots D_r^{n_r} f \) at all order \( (n_1, \ldots, n_r \geq 0) \) generate a finite-dimensional vector space over \( \mathbb{Q}(x_1, \ldots, x_r) \). (The power-series ring \( \mathbb{Q}[[x_1, \ldots, x_r]] \) can be included into a \( \mathbb{Q}(x_1, \ldots, x_r) \)-vector space.) An equivalent definition is that such an \( f \) possesses for each \( i \) between 1 and \( r \) an ordinary non-zero annihilator \( L_i \) from \( \mathbb{Q}(x_1, \ldots, x_r) \). Lipshitz’s approach does not appeal to any tool of D-modules theory, and remains on a very elementary level, but it bases on a counting argument that is at the heart of Bernstein’s dimension theory for D-modules. (It is difficult for me to imagine that Lipshitz was not inspired by the D-module theory, but this is pure speculation.) The derivation is as follows, after specialising to \( r = 2 \) for the sake of simplicity.

The first idea is to express the diagonal as a residue of a suitable transform of \( f \), namely by

\[
\Delta f = \text{res}_s g \quad \text{where} \quad g = \frac{1}{s} f \left( s, \frac{x}{s} \right).
\]

(Here, the \textit{residue} \( \text{res}_s \phi \) of a function \( \phi \) of the variables \( s \) and \( x \) that can be expressed as the sum \( \sum_{(p, q) \in \mathbb{Z}^2, p + q \geq m} \phi_{p, q} s^p x^q \) for some \( m \in \mathbb{Z} \) is just the univariate series \( \sum_{q = m+1}^{\infty} \phi_{-1, q} x^q \).) Note that the diagonal could be expressed as a constant term or a Cauchy integral, as well. Then, Lipshitz introduces the ordinary annihilators \( L_i \) mentioned above associated with \( g \) and proves that \( s \) can be eliminated from the family of the \( L_i \)’s. To this end, he considers the expressions

\[(2.2) \quad x^m D_i^o D_j^s g \quad \text{subject to} \quad m + n + o \leq N.\]

Then, he determines suitable integers \( a, b, \) and \( h \geq 1 \), and a suitable polynomial \( p \) to show that the expressions \( (2.2) \) all rewrite as linear combinations of terms of the form \( (q/p^N) D_i^a D_j^b g \), where \( 0 \leq i < a, 0 \leq j < b \), and \( q(s, x) \) is a polynomial of total degree bounded by \( Nh \). Now, the number of initial expressions is a multinomial number, growing in proportion to \( N^3 \), while the simplified expressions \( (2.2) \) live in a vector space of dimension \( O(N^2) \) over \( \mathbb{Q} \). Therefore, for large enough \( N \) there must be a \( \mathbb{Q} \)-linear combination \( Z(x, D_x, D_s) \) of the \( (2.2) \)’s that rewrites to 0 (as the rewriting is a linear map). He finally extracts the coefficient \( Z'(x, D_s) \) of \( Z \) of lowest exponent w.r.t. \( D_s \) and proves that \( Z' \) cancels the diagonal.
CHAPTER 3

Creative-Telescoping Algorithms for Equations of the First Order

1. Zeilberger’s Fast Algorithm for Hypergeometric Sums and its Variants

Zeilberger made explicit with (1990b) what was implied by the earlier works: designing algorithms based on the creative-telescoping approach for operations on integrals and series requires algorithmic means for non-commutative polynomial elimination in operator algebras. In (1980), Zeilberger had appealed to successive gcd computations by a sort of fraction-free Euclidean algorithm, which is likely to introduce spurious factors in the coefficients. The output (1.1) from Zeilberger’s modification of Fasenmyer’s technique in (1982) is essentially an operator from $\mathbb{Q}[n,S_n,S_k]$, and could be obtained by an elimination of $k$ from annihilators of $h_{n,k}$, provided the Ore closure problem was solved algorithmically. A searching algorithm by linear algebra is implied by the proof in (Lipshitz, 1988). In (1990b), Zeilberger based on a calculation he names “Sylvester’s dialytic elimination,” a classical process to compute Sylvester’s resultant (1840). This method is originally for univariate polynomials, but, despite non-commutativity, Zeilberger generalises it to an elimination method for operators viewed as bivariate polynomials in $n$ and $k$ with coefficients in $\mathbb{Q}[S_n,S_k]$. However, he dodges the question of Ore closure, which, in practice, becomes a large weakness of the method: one does not know if it will terminate if one starts with indiscriminate annihilators.

In addition, all these methods are merely existence proof turned into algorithms and tend to be very slow in practice. Although no sufficient study of lower bounds for their complexity is available yet, an explanation is that elimination constrains the output to be a polynomial in high degrees, and in a form like (1.1) that is more restrictive than what is required for the creative telescoping to work. Indeed, by way of comparison, representing (1.2) as an operator results in an operator that involves $k$:

$$(n + 1)^3S_n - (34n^3 + 51n^2 + 27n + 5) + n^3S_n^{-1} - (1 - S_n^{-1})4(2n + 1)(k(2k+1) - (2n + 1)^2).$$

A further consequence is that the order of the outputs from these methods cannot be expected to be minimal: when searching a fixed set of annihilators for elements of the form $P(n,S_n) + (S_k - 1)Q(n,k,S_n,S_k)$, the less constrained $Q$ is, the more pairs $(P,Q)$ will exist, and the lower the minimal order of a possible output $P$ is.

In view of this, Zeilberger called his algorithm in (1990b) his “slow algorithm,” and turned his attention back to the more restricted class of inputs he had studied in (1982): the special class of hypergeometric sequences, that is sequences $(h_{n,k})$ for which the two ratios

$$\frac{h_{n+1,k}}{h_{n,k}} \quad \text{and} \quad \frac{h_{n,k+1}}{h_{n,k}}$$

are given by two fixed rational functions in $n$ and $k$. For them, he designed a “fast algorithm” (1990a; 1991), which finally popularised the method of creative telescoping as an algorithm. Zeilberger based his fast approach for definite summation on Gosper’s decision algorithm for the indefinite summation of hypergeometric sequences (1978). Given a (univariate) hypergeometric sequence $(u_k)$, Gosper observed that any hypergeometric indefinite sum $(U_k)$, that is, any sequence satisfying $U_{k+1} - U_k = u_k$, must be a multiple of the summand by a fixed rational function $R$ of $k$:

$$(1.1) \quad U_k = R(k)u_k.$$
a non-trivial extension. Zeilberger realised that if the output from creative telescoping is known beforehand, like (1.3) in the example about \( \zeta(3) \), then the telescoping term (1.1) can be obtained just by calling Gosper’s algorithm on the right-hand side of (1.2). To make this into an algorithm, it was sufficient for Zeilberger to describe how to search at the same time for the coefficients of the output and for the rational function implied by Gosper’s algorithm: this amounts to a parametrised variant of Gosper’s calculation. Therefore, Zeilberger’s algorithm proceeds by increasing a tentative order \( r \) of maximal shifts w.r.t. \( n \) for the right-hand side of (1.2), trying to solve for \( B \) at each order. If there exists a non-zero family \( \{ \eta(n) \}_{n=1}^{\infty} \) of univariate rational functions and a bivariate rational function \( R(n,k) \) such that

\[
\eta_r(n) h_{n+r,k} + \cdots + \eta_0(n) h_{n,k} - R(k+1) h_{n,k+1} - R(k) h_{n,k},
\]

then the algorithm will terminate while producing such an identity with least possible order \( r \).

At about the same time, Almkvist and Zeilberger (1990) gave a differential analogue of Zeilberger’s fast algorithm, which applies to so-called hyperexponential function, that is, functions \( h \) of two variables \( x \) and \( y \) for which the two ratios

\[
\frac{\partial h(x,y)}{\partial x} \quad \text{and} \quad \frac{\partial h(x,y)}{\partial y}
\]

are two fixed rational functions in \( x \) and \( y \). To this end, they produced a differential analogue of Gosper’s algorithm and replaced (1.2) with an ansatz of the form

\[
\eta_r(x) D_x^r h(x,y) + \cdots + \eta_0(x) h(x,y) = (D_y R(x,y)) h(x,y) + R(x,y) (D_y h(x,y)).
\]

By the mid-1990s, Zeilberger had done a great job in popularising his theory, his fast algorithm, and his Maple implementation of it. A great deal of application papers were published, by he, admirers, and more often than not his computer whom he had named Shalosh B. Ekhad. The goal was to demonstrate that hypergeometric summation had become routine. To list a few of such papers: (Zeilberger, 1994; Ekhad and Zeilberger, 1994b,a, 1996; Prodinger, 1996). Still, there was some confusion around Zeilberger’s articles, caused by some allusiveness in the presentation and in algorithmic descriptions, especially in view of the many generalisations that were announced but not formalised rigorously.

This motivated Koornwinder to work on a new Maple implementation of Zeilberger’s fast algorithm as well as on a \( q \)-analogue; he wrote (1993) with the purpose to describe them in a very rigorous way, to ensure that the outputs produced could be trusted. In the same vein, Paule and Schorn (1995) provided a Mathematica implementation (for the classical case), with special emphasis on speed; in particular, they based on a notion of greatest falling factorial (GFF) from (Paule, 1995) to keep intermediate calculations in factored (therefore compact, efficient) form. The similar work for the \( q \)-analogue algorithm was done by Paule and Riese (1997), with a \( q \)-analogue of Gosper’s algorithm explained by a theory of \( q \)-GFFs; it was continued into a work on indefinite bibasic hypergeometric summation (Riese, 1996), that is, for identities involving an operator \( B \) such that

\[
(B f)(x,y) = f(qx,py).
\]

For a Maple counterpart, (Böing and Koepf, 1999) describes an analogue implementation of Zeilberger’s \( q \)-analogue fast algorithm and of Riese’s bibasic Gosper algorithm.

RISC: Lisoněk et al. ? + (Riese, 2001): fine-tuning (substitution heuristics, based on symmetries, which the user can tentatively apply to avoid memory explosion)

2. WILF AND ZEILBERGER’S APPROACH TO MULTIPLE SUMS AND INTEGRALS

After single hypergeometric/hyperexponential sums/integrals, there remained to understand on what inputs the method would terminate with certainty and if it could be extended to multiple sums and integrals. This was addressed to some extent by Wilf and Zeilberger (1992a); see also the result announcement in (Wilf and Zeilberger, 1992b)). There, they introduced the notion of a proper hypergeometric term, a special kind of hypergeometric term given as

\[
h_{n,k} = P(n,k) \zeta^n \xi^k \prod_{\ell=1}^{L} \Gamma(a\ell + bk + c\ell)\xi^\ell,
\]
where:
(1) the $a_i$’s and $b_i$’s are specific integers, and the $\epsilon_i$’s are $\pm 1$;
(2) the $c_i$, $\zeta$, and $\xi$ are constants independent from $n$ and $k$;
(3) $P$ is a polynomial in $n$ and $k$.

(The original definition separates the factors with $\epsilon = +1$ from those with $\epsilon = -1$ and insists on the $c_i$’s being integers, but I prefer this more formal view for what follows. Also, the term $\zeta^n$ was really introduced by Wegschaider (1997) only, but it alters what follows in no essential way.)

As a general hypergeometric term could be represented formally in the same way, but with a rational function in place of the polynomial $P$, the wording proper emphasises that the factor $P$ is polynomial. As we shall see, the crucial consequence of the definition (2.1) is the behaviour of $r$ and $s$ in (1.1) to ensure existence:

\begin{equation}
(2.2) \quad r - B \quad \text{and} \quad s - (A - 1)B + \deg_{kn}(P) + 1,
\end{equation}

where I have set

\begin{equation}
A = \sum_{\ell=1}^{L} |a_{\ell}| \quad \text{and} \quad B = \sum_{\ell=1}^{L} |b_{\ell}|.
\end{equation}

The proof can be sketched as follows: Each $h_{n+i,k+j}$ in (1.1) involves terms of the form $\Gamma(an + bk + c + \epsilon + u)$ for a shift $u$ bounded in absolute value by $|a| + |b|s$, that is, in a linear way. Now, observe that both

\begin{equation}
(2.3) \quad \frac{\Gamma(an + bk + c + \epsilon + u)}{\Gamma(an + bk + c + \epsilon - \sigma)} \quad \text{and} \quad \frac{\Gamma(an + bk + c + \epsilon + \sigma)}{\Gamma(an + bk + c + \epsilon + u)}
\end{equation}

are polynomials in $k$ of degree at most $\sigma$; the former will be used if $\epsilon = +1$, the latter if $\epsilon = -1$. Therefore, multiplying the hypergeometric relation (1.1) by the term

\begin{equation}
(2.4) \quad H_{n,k} = \zeta^{-n} \xi^{\ell} \left( \prod_{\ell=1, \epsilon=+1}^{L} \Gamma(an + bk + c + \epsilon - \sigma) \right)^{-1} \left( \prod_{\ell=1, \epsilon=-1}^{L} \Gamma(an + bk + c + \epsilon + \sigma) \right)
\end{equation}

results in an equivalent polynomial relation

\begin{equation}
(2.5) \quad \sum_{i=0}^{r} \sum_{j=0}^{s} c_{i,j}(n) \left( H_{n,k} h_{n+i,k+j} \right) = 0,
\end{equation}

where each product $H_{n,k} h_{n+i,k+j}$ is a polynomial of degree in $k$ not more than a linear function of $r$ and $s$. The full analysis gives the degree bound

\begin{equation}
(2.6) \quad \deg_{kn}(P) + \sum_{\ell=1}^{L} \sigma_{\ell} - \deg_{kn}(P) + Ar + Bs.
\end{equation}

Therefore, the left-hand side of (2.5) is a polynomial in $k$ of degree $O(r + s)$ while it is the combination of $O((r + s)^2)$ non-zero polynomials. For $r$ and $s$ large enough, there must be a non-trivial relation (2.5). More specifically, it is sufficient to ensure

\begin{equation}
(2.7) \quad (r + 1)(s + 1) > \deg_{kn}(P) + Ar + Bs + 1,
\end{equation}

and choosing $r - B$ immediately results in (2.2).

Of course, the formula should not be used blindly in an implementation. For instance, applying it to the simple binomial term $\binom{n + k}{k}^2$ results in $A - 4, B - 8, r - 8, s - 25$, and one has to expand products of 50 terms of the form $(n \pm k + u)^2$, leading to $6^{50}$ integer coefficients . . . over $8 \cdot 10^{38}$.

The second main contribution from (Wilf and Zeilberger, 1992a) is to show that the whole work extends to multiple sums and integrals, providing an algorithm to compute an analogue of (1.1)
when several \( k \)'s are involved. To this end, the notion of proper hypergeometric term extends to terms depending on several \( k \)'s in a natural way:

\[
h_{n,k_1,...,k_m} = P(n, k_1, \ldots, k_m) \zeta^n \xi_{k_1}^{k_1} \cdots \xi_{k_m}^{k_m} \prod_{\ell=1}^L \Gamma(a_{\ell n} + b_{\ell 1} k_1 + \cdots + b_{\ell m} k_m + c_{\ell})^\epsilon, \]

with the obvious generalisation of the constraints on (2.1). In case of an \( m \)-fold sum, (1.1) takes the form

\[
\sum_{i=0}^r \sum_{j_1=0}^{s_1} \cdots \sum_{j_m=0}^{s_m} c_{i,j_1,...,j_m}(n) h_{n+i+k_1+\cdots+k_m+j_m} = 0. \tag{2.8}
\]

The quantity \( A \) is defined as above while a sum \( B_i \) is associated with each \( k_i \). Inequality (2.7) is transformed by considering total degrees w.r.t. \( k_1, \ldots, k_m \), so as to compare the number of \( c \)'s in the \((m+1)\)-dimensional sum (2.8) with the \( m \)-dimensional combinatorics of monomials in \( k_1, \ldots, k_m \) of bounded total degree:

\[
(r+1)(s_1+1)\cdots(s_m+1) > \left( \deg_h(P) + Ar + B_1s_1 + \cdots + B_sm + m \right) + 1.
\]

Doing for instance \( r - s_1 - \cdots - s_m \) and comparing exponents shows the existence of a solution; Wilf and Zeilberger (1992a) (resp. Riese (2003)) gave a formula, but it is much less explicit than in the case \( m=1 \).

Wilf and Zeilberger’s method also has a \( q \)-analogue, for simple and multiple sums. They adapted their definition to call proper \( q \)-hypergeometric a term of the form:

\[
h_{n,k} = P(q^n, q^k) \zeta^n \xi^k q^{an^2 + \beta nk + \gamma n^2 + \delta/2} \prod_{\ell=1}^L ((q;c_{\ell})_{a \ell n + b \ell k})^{\epsilon_{\ell}}, \tag{2.9}
\]

where, in addition to the constraints of the classical case:

1. \((q; x)_N \) denotes the \( q \)-Pochhammer symbol, defined by \((q; x)_0 = 1 \) and, for \( N > 0 \):

\[
(q; x)_N = (1 - x)(1 - qx)\cdots(1 - q^{N-1}x) \quad \text{and} \quad (q; x)_{-N} = \left( 1 - \frac{x}{q} \right)^{-1} \left( 1 - \frac{x}{q^2} \right)^{-1} \cdots \left( 1 - \frac{x}{q^N} \right)^{-1};
\]

2. the constants \( c_{\ell} \)'s, \( \zeta \), and \( \xi \), as well as the coefficients of \( P \) may now be rational functions of \( q \);

3. \( \alpha, \beta, \gamma, \lambda, \) and \( \mu \) are all relative integers.

(Again, I have used here the generalised form by Riese (2003), with no essential change in what follows.) As for the classical case, Wilf and Zeilberger (1992a) (resp. Riese (2003)) showed that a non-trivial relation

\[
\sum_{i=0}^r \sum_{j=0}^s c_{i,j}(q^n)h_{n+i+k+j} = 0 \tag{2.10}
\]

always exist. Here, an additional difficulty over the classical case is that the analogues of the factors (2.3) are no longer polynomial, but in general Laurent polynomials in \( q^n \) and \( q^k \); this adds a lot of technicalities. This all generalises to the case of multiple \( q \)-sums. Furthermore, under the assumption \( m - P - \zeta - 1 \) (single \( q \)-sums), Wilf and Zeilberger gave the bound

\[
|\gamma| + \sum_{\ell=1}^L b_{\ell}^2 \tag{2.11}
\]

on \( r \) for a relation (2.10) to exist.

Another analogue of Wilf and Zeilberger’s approach was developed by Tefera (2000, 2002) for the case of multiple integrals of functions that are (essentially) proper-hypergeometric w.r.t. one discrete variable \( n \) and hyperexponential w.r.t. several continuous variables \( x_1, \ldots, x_n \). Written in the case of a single continuous variable, the corresponding “proper terms” are of the form

\[
h_{n}(x) = P(n, x)e^{G(x)}\zeta_1(x)^n \zeta_2(x)^d \prod_{\ell=1}^L \Gamma(a_{\ell n} + b_{\ell k} + c_{\ell})^{\epsilon_{\ell}},
\]

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where $P$ is again a polynomial, and the $\zeta$'s are now univariate rational functions, the $c$'s and $d$ are constant w.r.t. both $n$ and $x$, and the $a$'s, $b$'s and $\epsilon$'s are like before.

3. Verbaeten’s Completion and Non-$k$-Free Recurrences

Practical experimentation with the WZ-method soon revealed two shortcomings in formula (1.1), both causing the need for too high upper bounds $r$ and $s$ of the double sum, and too high running times in implementations.

Firstly, the support of the double sum being a rectangular box, as opposed to a more flexible set of pairs $(i, j)$, it is an artificial hindrance to the satisfiability of inequality (2.7). A solution was studied in the similar context of obtaining the so-called “pure recurrence relation” (1.2) by Verbaeten in his PhD thesis (1974; 1976). The idea consists in enlarging the support of the sum (1.1) insofar as this does not increase the degree in $k$ of (2.5), a process that is called Verbaeten’s completion. Incidentally, by considering special maximal sets of pairs, Verbaeten had already obtained an existence proof for a relation (1.1), for a special case of proper hypergeometric terms: so-called irreducible terms such that $P$ in (2.1) is 1 and no two factors $\Gamma(an + bk + c)$ with opposite $\epsilon$'s have the same $a$'s and $b$'s, and $c$'s that differ by an integer. Verbaeten’s proof was later greatly simplified by Hornegger (1992) and a sketch of it is available in (Wegschaider, 1997). It involves a very fine analysis of the degree of polynomials in an equivalent of (2.5) where the rectangular double sum is replaced with some convex polygon. The approach proceeds by counting the points on the integer-lattice that lie in a convex polygon defined by extremal directions related to the $a_\ell$'s and $b_\ell$'s. In addition, by thoroughly studying Verbaeten’s completion, Wegschaider was able in his master’s thesis (1997) to fill a gap in the proof in (Wilf and Zeilberger, 1992a) of the existence theorem of a recurrence in $n$ for the sum $\sum_k h_{n,k}$ in the case of a proper hypergeometric term that is not necessarily irreducible.

Secondly, the way (1.1) is used to get a recurrence on the sum over $k$ suggests that banning $k$ from the coefficients $c_{i,j}$ in an absolute way is not optimal, as is best explained by observing how the recurrence (1.1) on the term $h_{n,k}$ is transformed into a recurrence

$$
\sum_{i=0}^{r} a_i(n) h_{n+i} = 0 \quad \text{for} \quad h_n - \sum_{k=0}^{\beta} h_{n,k}. 
$$

This transformation proceeds by rewriting (1.1) by the relations

$$
h_{n+i,k+j} - h_{n+i,k} - (h_{n+i,k}^{(j)} - h_{n,i+k}^{(j)}) \quad \text{for} \quad h_{n+i,k}^{(j)} - h_{n+i,k} + \cdots + h_{n+i,k+j-1},
$$

which results in a term $g_{n,k}$ satisfying

$$
\sum_{i=0}^{r} c_i(n) h_{n+i,k} = g_{n,k+1} - g_{n,k} \quad \text{for} \quad c_i(n) = \sum_{j=0}^{s} c_{i,j}(n).
$$

Now, summation over $k$ yields

$$
\sum_{i=0}^{r} c_i(n) h_{n+i} = g_{n,\beta+1} - g_{n,\alpha}.
$$

In applications, either the right-hand side is zero by itself, or it can be canceled by applying a linear recurrence operator. In the former case, the output recurrence (3.1) is just (3.4), with $p = r$ and $a_i = c_i$ for each $i$. In the latter case, applying the proper operator to both sides of (3.4) results in a new recurrence (of order $p$ more than $r$), satisfied by $(h_n)$. In the derivation above, the term $g_{n,k}$ is of the form $L f_{n,k}$ for $L \in \mathbb{Q}[n] S_n, S_k$, but this limitation on $g$ is inessential for the derivation. In particular, allowing $L$ to be in the larger set $\mathbb{Q}[n, k] S_n, S_k$ should allow “more” $g$'s to be tested, and “more” relations (3.4) to be found, with the hope of lower orders for the final recurrences. Wilf and Zeilberger (1992a) attribute this observation to Gerdt Almkvist. Wegschaider (1997, Sec. 3.5.1) developed a heuristic to allow $L$ to involve $k$. To this end, he considers the equation

$$
\sum_{i=0}^{r} \sum_{j=0}^{s} \sum_{\ell=0}^{t} c_{i,j,\ell}(n) k^\ell h_{n+i,k+j} = 0
$$

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in place of equation (1.1) and the following analogue for the transformations (3.2):
\[ k^t h_{n+i+1,j} = (k-j)^t h_{n+i,k} - \left( h_{n+i,k}^{(j,t)} - h_{n+i,k+1}^{(j,t)} \right) \]
for \( h_{n+i,k}^{(j,t)} = (k-j)^t h_{n+i,k} + \cdots + (k-1)^t h_{n+i,k+j-1} \).

Using this in (3.5) before any calculations involving the actual value of \( h \) results in linear constraints on the \( c \)'s for the ansatz to lead to a recurrence of the form (3.4), best expressed as the \( r \times t \) linear constraints that each polynomial
\[ \sum_{j=0}^s \sum_{t=0}^t c_{j,t}(n) (k-j)^t \]
should actually not involve \( k \). As no study is available of what a suitable degree \( t \) should be, Wegschaider’s implementation lets the user heuristically input a value for it; his manuscript shows tremendous speed-ups by using this improvement.

The case of \( q \)-sums is amenable to the same two improvements, Verbaeten’s completion and the reintroduction of the summation variable in the ansatz. This has been worked out thoroughly by Riese (2003), both theoretically and in his implementation.

4. FROM ELIMINATION TO EQUATIONS ON SUMS AND INTEGRALS

In the recurrence case, creative telescoping crucially relies on transforming (1.1) to (3.3), and on an analogue transformation in the differential case. In operator notation, this transformation derives from an operator \( L \) free of the summation and integration variables an operator \( P \) that involves exclusively the parameters of the sum/integral and the corresponding shifts and derivatives. A cause of concern is that nothing guarantees a priori that (3.3) or its analogue is not a tautology of the form \( 0 = 0 \), that is, that the transformed operator is non-zero. As a matter of fact, the reader will only find handwaving in (Zeilberger, 1990b; Almkvist and Zeilberger, 1990), and no proof attempt at all in either of (Zeilberger, 1991; Wilf and Zeilberger, 1992a).

To the best of my knowledge, this problem was fixed first by Wegschaider (1997) in the case of recurrences. A similar idea works in the differential case. This late stage in the creative-teleconping method is the topic of the current section.

The differential case is a bit less technical, so let us start with it. Creative telescoping for the integration of a function \( f \) of variables \( x_1, \ldots, x_r \) w.r.t. \( x_2, \ldots, x_r \) first obtains a non-zero skew polynomial \( L \in \mathbb{C}[x_1]\langle D_1, \ldots, D_r \rangle \) that annihilates \( f \). Then, to obtain \( P \), it rewrites \( L \) by successive divisions by \( D_2, \ldots, D_r \) on the left as
\[ (4.1) \quad L = P(x_1, D_1) + D_2 Q_2(x_1, D_1, \ldots, D_r) + \cdots + D_r Q_r(x_1, D_1, \ldots, D_r). \]
(There, the family of \( Q \)'s is not uniquely defined). Upon application to \( f \) and integrating over \( (x_2, \ldots, x_r) \) in some domain \( \Omega \), and under the assumption that the boundary terms (induced by the integration of derivatives) vanish, we obtain the equation
\[ P(x_1, D_1)F(x_1) = 0 \quad \text{where} \quad F(x_1) = \int_{\Omega} f(x_1, \ldots, x_r) \, dx_2 \cdots dx_r. \]
This is a meaningful relation on the integral \( F \) provided the remainder \( P \) is not zero. In general, a transformation is needed to ensure that \( P \) be non-zero. To this end, consider a monomial \( D_1^{e_1} \cdots D_r^{e_r} \) that divides \( L \) on the left and that is maximal with this property (that is, increasing any of the \( v \)'s would result in a monomial that is no left factor of \( L \)). Then, \( L \) can be written as
\[ L = D_1^{e_1} \cdots D_r^{e_r} \left( \hat{P}(x_1, D_1) + D_2 Q_2(x_1, D_1, \ldots, D_r) + \cdots + D_r Q_r(x_1, D_1, \ldots, D_r) \right), \]
where, now, \( \hat{P} \) cannot be zero by maximality. By repeated use of the relation \( x_1 D_1^t = D_1^t x_1 - tD_1^{t-1} \) and using (*) to denote an expression that I do not want to write explicitly, we get:
\[ (4.2) \quad x_2^{e_2} \cdots x_r^{e_r} L = (-1)^{e_2 + \cdots + e_r} v_2 \cdots v_r! \hat{P}(x_1, D_1) + D_2 (*) + \cdots + D_r (*). \]
As this new operator also cancels \( f \), \( \hat{P} \) is a non-zero operator that cancels the integral \( F \) (provided the suitable boundary terms vanish). For future reference, note that the total degree of \( \hat{P} \), and for
that matter, of the \((\ast)\)'s as well, is not more than twice the degree of \(L\), while total and partial degree in the \(D_i\)'s are not increased.

The case of recurrences is more technical, although it is essentially the same idea. To mimic the formula \(x_i^\ell D_i^\ell = -\ell! + D_i(\ast)\), Wegschaider (1997) introduced the falling factorial \((n - a)^\ell\) (for a constant \(a\)). Now, we have the identities

\[
(n - a)^\ell(S_n - 1) - S_n(n - a - 1)^\ell - (n - a)^\ell - (S_n - 1)(n - a - 1)^\ell - ((n - a)^\ell - (n - a - 1)^\ell) = \]

\[
(S_n - 1)(n - a - 1)^\ell - \ell(n - a - 1)^\ell - 1.
\]

An iterated use of this identity yields \(n^\ell - (-1)^\ell \ell! + (S_n - 1)(\ast)\). The proof in the recurrence case then proceeds in a way similar to the differential case, by using a left factor of the form \(n_2^\ell \cdots n_r^\ell\) instead of \(x_2^\ell \cdots x_r^\ell\). Again, the degree after transformation is not more than twice the degree of \(L\), and the transformation does not increase the expected order of the output recurrence.

This also has a \(q\)-analogue.

I end this section by a remark that can explain why the gap about the possible nullity of \(P\) had long been overlooked in different works: The terms \((\ast)\) in (4.2) denote skew polynomials from \(\mathbb{C}[x_1, \ldots, x_r] \langle D_1, \ldots, D_r \rangle\), so that the existence of an annihilator of the form (4.1) implies the existence of an annihilator of the form

\[
(4.3) \quad \tilde{L} = \tilde{P}(x_1, D_1) + D_2 \tilde{Q}_2(x_1, \ldots, x_r, D_1, \ldots, D_r) + \cdots + D_r \tilde{Q}_r(x_1, \ldots, x_r, D_1, \ldots, D_r),
\]

with non-zero \(\tilde{P}\). The point is that Zeilberger promoted his fast algorithm for the case \(r = 2\), which implicitly searches directly for a relation similar to the form (4.3). As was remarked above, the order bound for a non-zero telescoper is not higher than the order bound for a \(k\)-free recurrence, and so, calculations and just order considerations could not detect the problem in the proof.
CHAPTER 4

Termination Questions: Criteria and Bounds

Zeilberger’s fast algorithm and its variants and extensions all perform an exhaustive search of an analogue of (3.4) in some suitable space of equations, in relation to the annihilator of the input summand or integrand. Thus described, the approach is only a heuristic, as no argument justifies its termination, especially in the non-purely differential situations. This has motivated a number of works to prove termination properties, which I shall separate in two main bodies.

First, a series of works endeavor to determine a criteria that is able to decide, before any complicated calculation, whether Zeilberger’s approach will be successful. Such results give no hint as to the order of the outputs from the method.

Second, for certain classes of inputs, a bound on the output order has been developed, which is based on degrees and other arithmetic parameters of the input. The bounds (2.2) already mentioned for proper hypergeometric terms are of this type, as any order bound for Wilf and Zeilberger’s approach is a bound for Zeilberger’s fast algorithm. When they exist, bounds can hopefully be reused in estimating the complexity of some summation or integration algorithm.

1. CONSEQUENCE OF HOLOMONY

In this section, I recall the notions of holonomic functions and sequences, and the sufficient condition of holonomy for the existence of (3.4) or its differential variant. These notions are adapted from the notion of holonomic module, itself borrowed from D-module theory.

A series \( f \), possibly of Taylor kind or a formal power series, or more generally a function, of variables \( x_1, \ldots, x_r \) is called holonomic when the functions \( x_1^{a_1} \cdots x_r^{a_r} \partial_1^{b_1} \cdots \partial_r^{b_r} f \) obtained by multiplying monomials in the variables and higher-order derivatives of \( f \) subject to the constraint \( a_1 + \cdots + a_r + b_1 + \cdots + b_r \leq N \) span a vector space \( V_N(f) \) whose dimension over \( \mathbb{C} \) grows like \( O(N^r) \). For comparison sake, note that the number of generator for this vector space grows like \( \Theta(N^{2r}) \). Even the vector space of elements from \( \mathbb{C}[x_1]\langle D_1, \ldots, D_r \rangle \) with total degree not more than \( N \) grows “faster” than the \( V_N(f) \)’s, with a dimension \( \Theta(N^{r+1}) \). As a consequence, there must exist for large enough \( N \) a non-zero skew polynomial \( L \) that maps \( f \) to 0. The implied identity \( LF = 0 \) is a differential analogue to (1.1). This means that a differential analogue of Wilf and Zeilberger’s approach will always terminate. After all, this was Lipshitz’s argument in (1988).

Furthermore, \( L \) can be put in the form (4.1) and transformed into (4.3) for a non-zero \( \tilde{L}(x_1, D_1) \). This means that the differential analogue of Zeilberger’s fast algorithm (Almkvist and Zeilberger, 1990) will always terminate.

A sequence \( u = (u_{n_1, \ldots, n_r})_{n_1, \ldots, n_r \geq 0} \) is often called holonomic when its generating function

\[
U(x_1, \ldots, x_r) = \sum_{n_1, \ldots, n_r \geq 0} u_{n_1, \ldots, n_r} x_1^{n_1} \cdots x_r^{n_r}
\]

is holonomic in the original sense. I shall show the existence of an equation of the form (2.8) for \( h - u \), but, for the sake of presentation, I shall give the idea in the bivariate case, with \( x_1 \) and \( x_r \) respectively denoted \( x \) and \( y \). By the same type of reasoning as above, there exists a non-zero \( L \in \mathbb{C}[x, y]\langle D_x \rangle \) that annihilates \( U \). We proceed to make the relation \( LU = 0 \) explicit on the coefficient level. To this end, remark that \( L \) rewrites as a (Laurent) polynomial \( A(x, y, \theta_x) \in \mathbb{C}[x^{-1}, y]\langle \theta_x \rangle \), where \( \theta_x \) is the Euler derivative \( xD_x \). Next, for any sum \( V \) of the form

\[
V(x, y) = \sum_{n \geq 0, k \geq 0} v_{n,k} x^n y^k,
\]

we have the formulas

\[
\theta_x^n V = \sum_{n \geq 0, k \geq 0} n^b v_{n,k} x^n y^k \quad \text{and} \quad x^a y^b V = \sum_{n \geq 0, k \geq b} v_{n-a, k-b} x^n y^k,
\]
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for any $a \in \mathbb{Z}$ and $b \in \mathbb{N}$. Write $\Lambda$ more explicitly as a sum

$$\Lambda = \sum_{(a,b) \in S} x^a y^b \lambda_{a,b}(\theta_x),$$

where $S$ is a finite set of pairs $(a, b)$ satisfying $a \in \mathbb{Z}$ and $b \in \mathbb{N}$. Denote by $A$ and $B$ the partial degrees in $x$ and $y$, respectively. Applying $\Lambda$ to $U$ results in

$$\Lambda U = \sum_{(a,b) \in S} \sum_{n \geq a, k \geq b} \lambda_{a,b}(n-a) u_{n-a,k-b} x^a y^k.$$

Extracting the coefficient of $x^a y^k$ proves that the relation

$$\sum_{(a,b) \in S} \lambda_{a,b}(n-a) u_{n-a,k-b} = 0$$

holds for all $n \geq A$ and all $k \geq B$. This is a non-trivial $k$-free recurrence.

As in the differential case, this means that Wilf and Zeilberger’s approach and Zeilberger’s fast algorithm both terminate on holonomic inputs.

2. Termination of Zeilberger’s Fast Algorithm


rational case: (Abramov and Le, 2000; Le, 2001; Abramov and Le, 2002)

Wilf and Zeilberger’s conjecture: (Abramov and Petkovšek, 2002; Hou, 2004)

(voir aussi la thèse de Hou en 2001 (références dans (Abramov and Petkovšek, 2002), qui fait la conjecture dans le cas bivarié, en parallèle de AbPe (autres réfs))

rq: ici, holonome est défini comme P-récursif de Stanley ; il faudrait montrer/rappeler l’équivalence

2.1. Termination Criteria for Hypergeometric-Hyperexponential Terms. The criteria in (Chen, 2011) are also valid for non-proper terms. This will be the topic of (Chen, Chyzak, Feng, and Li, 2011).

3. Proving Identities by Numerical Evaluations

An application of creative telescoping is to decide—prove or disprove—a conjectured identity of the form

$$(3.1) \quad \sum_{k=a}^b u_{n,k} - U(n).$$

Performing creative telescoping, either in the form of Zeilberger’s fast algorithm or of Wilf and Zeilberger’s approach, produces a $k$-free recurrence from which a recurrence for the sum is derived. The identity is decided by:

- verifying that $U$ satisfies the computed recurrence;
- specialising (3.1) on sufficiently many values of $n$ and observing equality or mismatch.

Indeed, if the recurrence is of order $r$ and expressed as

$$a_0(n) w_n + \cdots + a_r(n) w_{n-r} = 0,$$

and if $n_0$ is defined as the maximal integer root of $a_0(n)$ if it has one, or 0 if it has none, the values of $w_n$ at $n_0, \ldots, n_0 - (r - 1)$ define uniquely the values at $n > n_0$.

This is the starting point of a strategy, initiated by Yen (1993, 1996, 1997), for deciding identities of the form (3.1) by numerical evaluations. Yen’s approach is to rewrite the relation (3.3) predicted by Wilf and Zeilberger’s theory as

$$a_0(n) u_{n,k} + \cdots + a_r(n) u_{n-r,k} - R(n,k) u_{n,k} - R(n,k-1) u_{n,k-1}$$

for a rational function $R$. The approach in section 2, and especially the bounds (2.2) and (2.6), allow to bound the degree $\beta$ in $k$ of the numerator $c_0(n) + \cdots + c_\beta(n) k^\beta$ of $R$, then to view the $a_i$’s and $c_i$’s as solutions of a linear system of size $(\delta+1) \times (r+\beta+2)$, where $\delta$ is the value of (2.6). Then, expressing the unknown $a$’s and $c$’s by Cramer’s rules and using Hadamard-type bounds allows to derive bounds on the degrees and heights of those polynomials that are polynomial functions in

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parameters of the input (degrees of \(P\), heights of \(P, A, B, L\), in (2.1)–(2.2)), then an exponential bound on the maximal integer root of \(a_0(n)\).

The exponential nature of the bound makes it absolutely impractical: the simplest possible example of the sum \(\sum \binom{n}{k} 2^k\) would be proved by checking the identity on a number of consecutive integers that is much more than \(10^{38000}\), according to the formula in (Yen, 1993)!

Yen’s evaluation was later refined dramatically by Zhang (2003) and (Guo, Hou, and Sun, 2008). There, no explicit lower bound is provided: rather, an algorithm to produce a lower bound is developed, which experimentally provides dramatically lower values: for the same simple sum of the binomial coefficients, the bound goes down to just 4 by the method in (Guo et al., 2008)!

I shall give details about the latter work only.

At the time of writing, I must confess that I cannot say if the possibility of the simultaneous cancellation of all the \(c_i\)'s in (3.3) has been integrated in either of the works mentioned above. However, Wegschaider’s transformation presented in section 4 does not increase degrees and heights by much, which should not drastically change the results.

4. Bounds related to First-Order Equations

A series of works has produced sharper and sharper bounds on the minimal order of a telescoper that can be obtained for a proper, respectively \(q\)-proper, hypergeometric term by Wilf and Zeilberger’s approach and by Zeilberger’s fast algorithm. However, bound improvements seemingly require a genericity assumption of some kind.

Wilf and Zeilberger (1992a) formulated the linear bound (2.2), that is

\[ r \leq \sum_{\ell=1}^{L} |b_\ell|, \]

for a proper hypergeometric term, together with a quadratic bound (2.11) for \(q\)-analogues. This was refined by Yen (1993), who produced the bound

\[ r \leq \sum_{\ell=1}^{L} b_\ell^+ + \sum_{\ell=1, c=-1}^{L} (-b_\ell)^+ + \left( - \sum_{\ell=1, c=-1}^{L} e b_\ell \right)^+, \]

where the notation \(x^+\) denotes \(\max(0, x)\); this bound relies on distinguishing terms that are factorials and terms that are inverses of factorials. An even sharper bound can be obtained by further collecting the terms according to the signs of the \(b_\ell\)'s in (2.1), respectively in (2.9). Under presentation and genericity hypotheses, specifically that all \(a\)'s are non-negative and that the polynomial part \(P(n, k)\) has maximal degree, Mohammed and Zeilberger (2005) derived the better bound

\[ \max \left( \sum_{c=-1, b_\ell \geq 0} b_\ell - \sum_{c=-1, b_\ell \leq 0} b_\ell, - \sum_{c=+1, b_\ell \geq 0} b_\ell + \sum_{c=+1, b_\ell \leq 0} b_\ell \right). \]

Apagodu (after Mohammed changed his name to this) and Zeilberger (Apagodu, 2006; Apagodu and Zeilberger, 2006) obtained similar bounds for various classes of hyperexponential functions, for mixed hypergeometric-hyperexponential functions, for \(q\)-analogues, and for multiple summations and integrations. For example, for the class of non-rational hyperexponential functions of the form

\[ p(x, y) \exp \left( \frac{a(x, y)}{b(x, y)} \right) \prod_{s \in S} s(x, y)^{\alpha_s}, \]

where

- \(p, a,\) and \(b\) are polynomial such that \(a/b\) is a non-constant function of \(y,\)
- the \(s\)'s are polynomials with no non-trivial content w.r.t. \(y,\)
- the \(\alpha\)'s are transcendental constants,

the bound is given as

\[ \deg_y(b) + \max(\deg_y(a), \deg_y(b)) + \left( \sum_{s \in S} \deg_y(s) \right) - 1. \]

(The choice of hypotheses in (Apagodu and Zeilberger, 2006) for their proof to be valid is not cautious, so I chose here a combination that makes the paper work with no additional idea.)
Beside bounds on the output order, (Wilf and Zeilberger, 1992a; Yen, 1993) provide bounds on the degree of the output that are, informally speaking, quadratic in the quantities that appear in the order bound. In contrast, no degree bound can be found in (Mohammed and Zeilberger, 2005), but the polynomial bound in the differential analogue, to be found in the ongoing work (Bostan, Chyzak, and Lairez, 2011), makes me expect that degrees have the same polynomial behaviour. However, this discussion means nothing as to the degree of the telescoper of minimal order. It may well be that (Apagodu and Zeilberger, 2006) describes the generic case, with polynomial order and degree for the minimal-order telescoper, but that degenerate cases require non-polynomial degrees, as suggested by the encoding of these degrees as roots of a resultant in (Almkvist and Zeilberger, 1990).
CHAPTER 5

Creative Telescoping Algorithms for Equations of Arbitrary Order

The algorithms and considerations of Chapters 3 and 4 all discuss how to obtain a $k$-free relation like (1.1), a differential variant, or a non-$k$-free generalisation like (3.5). In each case, the calculation can be viewed as some sort of skew-polynomial elimination of the summation index or integration variable, possibly modulo derivatives like in (4.3) or modulo finite differences like in (3.4). In each case, too, the application of operators to a function $f$ can be expressed very explicitly, owing to the assumption on the hypergeometric-hyperexponential nature of $f$, as an explicit rational function times $f$.

Both aspects lose their simplicity in presence of higher-order equations, and a common solution lies in an algorithmic theory for skew-polynomial elimination, which was modeled after the classical commutative theory of Gröbner bases. This is why the present chapter begins with an account on a non-commutative analogue for the theory of Gröbner bases that is well adapted to the skew algebras under consideration. In relation to (non-commutative) ideal theory, many termination arguments or arguments that some calculation returns a non-trivial output more often than not rely on a non-commutative analogue of the dimension theory of algebraic geometry. Dimension is a quantity that, on an intuitive level, distinguishes between the infinite vector space dimensions over $\mathbb{Q}$ of $\mathbb{Q}[x]$, $\mathbb{Q}[x, y]$, $\mathbb{Q}[x, y, z]$, etc., and is able to capture such notions as $\partial$-finiteness and holonomy.

Algorithms in the later sections all rely on this Gröbner-basis theory in a way or another.

1. Skew Gröbner Bases and a Dimension Theory

As Galligo and Takayama noticed, respectively, in the differential case (1985) and in the differential-difference case (1989), and as was developed by Kandri-Rody and Weispfenning in the more general setting of polynomial rings of solvable type (1990), Buchberger’s algorithm for Gröbner bases can be adapted to our non-commutative context: whether $\mathbb{Q}(x, y, m, n, \ldots)$, $\mathbb{Q}[x, y, m, n, \ldots]$, $\mathbb{Q}[x, y, z, \ldots]$, etc., or polynomial coefficients, or any intermediate situation. This theory provides:

- a procedure for putting the presentation of an ideal in normal form: two ideals given by sets of generators can be compared for equality by testing equality of the normalised sets, and additionally, inclusion of ideals can be tested easily;
- a procedure for division of an element of $A$ by an ideal $I \subset A$ with unique remainder, or, equivalently, for normal forms in the quotient module $A/I$;
- a procedure for (skew-)polynomial elimination: for a sub-algebra $B$ of $A$ given by a subset of the generators of $A$ (the $D_x, D_y, \ldots, S_m, S_n, \ldots$, and possibly the $x, y, \ldots, m, n, \ldots$ in the variant with polynomial coefficients), a Gröbner-basis calculation results in a presentation of the intersection ideal $I \cap B$.

2. Elimination Based on Gröbner Bases

This section is just a summary, due to lack of time. I should discuss:

- algorithms by plain elimination of the summation/integration variable (Takayama, 1992; Chyzak, 1998b,a);
- Takayama’s algorithm by truncation of ideals and module Gröbner bases (1990b; 1990a), the variant of it I developed with Salvy in (Chyzak and Salvy, 1998), its extension to systems of non-homogeneous equations (Nakayama and Nishiyama, 2010);
• algorithms by homogenisation of the algebra (Sturmfels and Takayama, 1998; Saito, Sturmfels, and Takayama, 2000) or by Oaku’s homogenisation of the ideal (Oaku, 1997; Oaku and Takayama, 1998; Oaku, Takayama, and Walther, 2000; Oaku and Takayama, 2001; Saito et al., 2000; Oaku, 2011).

3. Summation and Integration of $\partial$-Finite Functions

Zeilberger’s fast algorithm for definite hypergeometric sums of the form

$$U_n = \sum_{k=a}^{b} u_{n,k}$$

and the differential analogue by Almkvist and Zeilberger for definite hyperexponential integrals of the form

$$U(n) = \int_{a}^{b} u(x,y) \, dy$$

are dedicated to hypergeometric/hyperexponential terms by their choice of an ansatz, $P(n,S_{n}) u - (S_{k} - 1)(R(n,k) u)$ for $P \in \mathbb{C}(n)\langle S_{n} \rangle$ and $R \in \mathbb{C}(n,k)$ in the discrete case and

$$(3.1) \quad P(x,D_{x}) u - D_{y}(R(x,y) u) \quad \text{for} \quad P \in \mathbb{C}(x)\langle D_{x} \rangle \quad \text{and} \quad R \in \mathbb{C}(x,y)$$

in the continuous case. In each case, the rationale to ask for a term of the form $P(x,D_{x})$ and of some $Q(x,y,D_{x},D_{y}) \in \mathbb{C}[x,y][D_{x},D_{y}]$, respectively $Q \in \mathbb{C}(x,y)[D_{x},D_{y}]$, is just a rational multiple of $u$ when $u$ is hypergeometric, respectively hyperexponential.

But more general classes of functions $u$ require more general terms to take the role of $R u$. With the motivation of section (4), which, in the (differential) holonomic case, guarantees the existence of a non-zero $P(x,D_{x})$ and of some $Q(x,y,D_{x},D_{y}) \in \mathbb{C}[x,y][D_{x},D_{y}]$ such that

$$(3.2) \quad P(x,D_{x}) u = D_{y} v \quad \text{for} \quad v = Q(x,y,D_{x},D_{y}) u,$$

it is just natural to replace $R u$ with an expression that can represent all the possible $Q u$’s. I realised in (Chyzak, 2000) that a nice solution is available for a D-finite $u$, which is the topic of the present section.

3.1. Chyzak’s algorithm in basic form. Indeed, given that there exists a finite basis $\{v_{i}\}$, indexed by $1 \leq i \leq d$, for the vector space $V$ over $\mathbb{C}(x,y)$ generated by all the derivatives $D_{x}^{a}D_{y}^{b}u$ at any orders, the ansatz (3.2) in the unknown operator $Q$ can be replaced with the ansatz

$$(3.3) \quad P(x,D_{x}) u = D_{y} v \quad \text{for} \quad v = \sum_{i=1}^{d} \phi_{i} v_{i}$$

in the unknown bivariate rational functions $\phi_{i}$’s from $\mathbb{C}(x,y)$. Now, expanding $D_{y} v$ results in an expression that is linear in the $\phi_{i}$ and $D_{y} v_{i}$, on the one hand, and linear in the $\phi_{i}$ and the $D_{y} \phi_{i}$, on the other hand. As the $D_{y} v_{i}$’s are also in $V$, the derivative $D_{y} v$ can be rewritten in the form

$$(3.4) \quad D_{y} v = \sum_{j=1}^{d} (D_{y} \phi_{j}) v_{j} + \sum_{i,j=1}^{d} \phi_{i} a_{i,j} v_{j}$$

for explicit rational functions $a_{i,j} \in \mathbb{C}(x,y)$. As in the case of (1.3) for hyperexponential functions (that is, when $d = 1$), an ansatz $P = \eta_{0}(x) D_{x}^{r} + \cdots + \eta_{r}(x)$ is made, and leads to writing $P u$ as a linear combination of the $v_{j}$ with coefficients that are linear in the $\eta$’s:

$$P u = \sum_{j=1}^{d} \sum_{i=0}^{r} \eta_{i} b_{i,j} v_{j}$$
for explicit rational functions $b_{i,j} \in \mathbb{C}(x,y)$. For each $i$ between 1 and $d$, extracting from (3.3) the coefficients w.r.t. the basis element $v_j$ results in a non-homogeneous linear differential relation between $D_y\phi_j$ and the $\phi_i$’s, with non-homogeneous part involving the $\eta_i$’s:

\begin{equation}
D_y\phi_j + \sum_{i=1}^{d} a_{i,j}\phi_i - \sum_{i=0}^{r} b_{i,j}\eta_i \quad (1 \leq j \leq d).
\end{equation}

This system is solved by eliminating all $\phi_i$’s but one (say, $\psi = \phi_d$), which results in a non-homogeneous higher-order linear differential equation in $\psi(x,y)$, with derivations w.r.t. $y$ only and a non-homogeneous part this is linear in the $\eta_i(x)$. This can be solved by a non-homogeneous variant of Abramov’s decision algorithm for rational solutions of a linear ODE in (1991). Then, if Abramov’s algorithm proves the absence of solutions, there is provably no solution to the ansatz (3.3) for the current value of $r$. Else, putting the solution $\psi$ back into the system (3.5) results in a similar system in fewer unknown $\phi$’s, which can in turn be examined for solutions.

The algorithm I formulated in (2000) applies to general operators in place of just the derivations $D_x$ and $D_y$, as long as the same kind of finiteness as with D-finite functions is preserved. This is why I presented my algorithm for $\delta$-finite functions. This includes sequences defined by recurrences or $q$-recurrences, functions defined by mixed differential-difference equations. What varies with the nature of operators is how $D_yv$ is changed in (3.3) and the exact form it takes in the analogue of (3.4). Still, the induced system that plays the role of (3.5) can each time be solved by resorting to a variant of Abramov’s algorithms for rational solutions in (1991; 1995).

In practice, one takes for the $v_i$’s a family of derivatives $\{D_x^i D_y^j u\}_{1 \leq i \leq d}$ with good properties with respect to derivation, and the matrix $(a_{i,j})$ is rather sparse. Such a family is obtained naturally when manipulating the $\delta$-finite function in an algorithmic way. A $\delta$-finite function $f$ is given by a family operators $P_1, \ldots, P_s$ that generate the annihilating ideal ann $f$ w.r.t. a skew-polynomial algebra $A = \mathbb{Q}(x,y,\ldots,m,n,\ldots)\langle D_x, D_y, \ldots, S_m, S_n, \ldots \rangle$. But most often, as the result of a preceding calculation, the $P_i$’s constitute moreover a Gröbner basis of ann $f$ w.r.t. some monomial order. So there is a natural family of derivatives that are reduced with respect to the $P_i$’s, that is, that are equal to their remainder after division by the $P_i$’s.

### 3.2. Iterated integrals and sums

Multiple summation and integration can also be computed by the same approach, as I explained in the case of natural boundaries in (2000) and as we later extended to all kinds of boundaries in (Bostan, Chyzak, van Hoeij, and Pech, 2011). For presentation sake, I shall only present the case of double integration with respect to $y$ and $z$ of a hyperexponential function $u$ of variables $x$, $y$, and $z$.

The case of double integrals leads to generalising (3.1) into a form

\begin{equation}
P(x,D_x)u = D_y(R_1(x,y,z)u) + D_z(R_2(x,y,z)u) \quad \text{for } P \in \mathbb{C}(x)\langle D_x \rangle \text{ and } (R_1, R_2) \in \mathbb{C}(x,y,z)^2,
\end{equation}

but the solving for $R_1$ and $R_2$ does not generalise so smoothly: an attempt yields a linear partial differential equation relating $R_1$ and $R_2$ with $D_y R_1$ and $D_z R_2$. To the best of our knowledge, although this overdetermined linear partial differential equation has a very specific form, no algorithm is available to solve it for its rational solutions.

Therefore, instead of a direct approach, I developed in (2000) a cascading approach which I shall now summarise. Noting that the dependency of $P$ on a single derivation $D_x$ in (3.1) is inessential, the same approach is possible for the creative telescoping with respect to the (single) variable $z$ of a trivariate hyperexponential function $u$ from $\mathbb{Q}(x,y,z)$. Indeed, setting $P$ to the undetermined form

\begin{equation}
P = \sum_{0 \leq i+j \leq r} \eta_{i,j}(x,y) D_x^i D_y^j
\end{equation}

for some tentative total order $r$ and unknown rational functions $\eta_{i,j}$ from $\mathbb{Q}(x,y)$ and performing the same solving as previously, now relying on linear algebra over $\mathbb{Q}(x,y)$, leads to a basis of $P^{(\alpha)}$’s of total order at most $r$ for which there exists a rational function $\phi^{(\alpha)}(x,y,z)$ satisfying

\begin{equation}
P^{(\alpha)}u = D_z \left( \phi^{(\alpha)}(x,y,z) \right).
\end{equation}
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The theory (as developed, e.g., by Zeilberger (1990b)) guarantees that the set of $P^{(\alpha)}$'s obtained for sufficiently large $r$ describes a D-finite function $\hat{u}$ of $x$ and $y$, and can therefore be used to determine the finite set needed as an input to the algorithm in (Chyzak, 2000) and in (3.3).

Finally, a double integration algorithm is obtained by continuing the approach used for natural boundaries in (Chyzak, 2000) (Stages A and B below) by a suitable recombination of the outputs (Stage C below). The resulting treatment of multiple integrals over non-natural boundaries is an extension over (Chyzak, 2000), and the corresponding algorithm is as follows:

- **Stage A: First iteration of creative telescoping.** Using the univariate algorithm for trivariate hyperexponential functions in variables $(x, y, z)$ delivers identities

$$P^{(\alpha)}(x, y, D_x, D_y) u - D_z (\phi^{(\alpha)}(x, y, z) u). \tag{3.7}$$

- **Stage B: Second iteration of creative telescoping.** Considering a function $\hat{u}$ of $(x, y)$ that is annihilated by all $P^{(\alpha)}$ and using the univariate algorithm for D-finite functions in variables $(x, y)$ delivers identity

$$P(x, D_x) \hat{u} - D_y (Q(x, y, D_x, D_y) \hat{u}). \tag{3.8}$$

- **Stage C: Recombination.** By the theory of linear-differential-operators ideals, the calculations of the algorithm can be interpreted as a proof of existence of operators $L^{(\alpha)}(x, y, D_x, D_y)$ satisfying

$$P(x, D_x) - D_y Q(x, y, D_x, D_y) = \sum_\alpha L^{(\alpha)}(x, y, D_x, D_y) P^{(\alpha)}(x, y, D_x, D_y). \tag{3.9}$$

These $L^{(\alpha)}$ can effectively be obtained either by following the calculations step by step or (less efficiently) by a postprocessing (non-commutative multivariate division). Hence, defining

$$R_1 - u^{-1} (Q(x, y, D_x, D_y) u) \quad \text{and} \quad R_2 - u^{-1} \sum_\alpha L^{(\alpha)}(x, y, D_x, D_y) (\phi^{(\alpha)}(x, y, z) u)$$

leads to a solution $(P, R_1, R_2)$ of (3.6).

Note that this two-stage process inherently introduces a dissymmetry in the treatment of the variables $y$ and $z$: the output from the first iteration tends to be larger than its input; in turn, the output from the second is larger than the output from the first. As a consequence, the order we deal with the variables may have an impact on the running time.

3.3. Koutschan’s heuristics. Mainly two aspects of the algorithms for $\hat{c}$-finite functions make them slow in practice. Firstly, solving of (3.5) by uncoupling is sub-optimal. Algorithms for direct solving of a system exist in the ordinary differential/difference case, and should be used. Secondly, even if no algorithm is known to solve (3.6) as an overdetermined linear partial differential equation, patterns in the orders of poles emerge by experimentation. This all has motivated Koutschan (2010) to develop heuristics to guess the exponents in the denominators, which have allowed to solve difficult problems in sizes that can so far not be attacked by the algorithmic approaches.

4. Scalar Product of Symmetric Functions

Intriguingly enough, creative telescoping has been applied to functions—and equations—in infinitely many variables, for the calculation of a classical scalar product in the combinatorial theory of symmetric functions. Mishna, Salvy, and I described algorithms in (2005).

5. Beyond Holonomy

Another direction of extension concerns functions or sequences that cannot be defined by a $\hat{c}$-finite ideal. Majewicz (1996, 1997) has given an algorithm that is able to produce Abel’s summation identity

$$\sum_{k=0}^n \binom{n}{k} (k + i)^{k-1} (n - k + j)^{n-k} = (n + i + j)^n$$

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automatically and to find similar new identities. Kauers (2007) has suggested a summation algorithm applicable to sums involving Stirling numbers and similar sequences defined by triangular recurrence equations. This algorithm finds, for instance, the identity

$$\sum_{k=0}^{n} (-1)^{m-k} k! \binom{n-k}{m-k} S_2(n+1,k+1) - E_1(n,m),$$

where $S_2$ and $E_1$ refer to the Stirling numbers of second kind and the Eulerian numbers of first kind, respectively. A summation algorithm of Chen and Sun (2009) is able to discover certain summation identities involving Bernoulli numbers $B_n$ or similar quantities, for example

$$\sum_{k=0}^{m} \binom{m}{k} B_{m+k} - (-1)^{m+n} \sum_{k=0}^{n} \binom{n}{k} B_{m+k}.$$

None of the quantities covered by these algorithms admits a definition via a $\partial$-finite ideal, but all three algorithms are based on principles that resemble those employed for holonomic systems and $\partial$-finite ideals. In each case, it turns out that the differential/difference equations defining the integrand/summand are of a form that permits to prove the existence of at least one non-trivial differential/difference equation for the integral/sum by a counting argument.

In (Chyzak, Kauers, and Salvy, 2009), we have given algorithms dealing with functions described by ideals of linear functional operators that are not $\partial$-finite. They generalize the algorithms known for the $\partial$-finite case and cover the extensions to non-holonomic functions discussed so far. Holonomy being lost, it is not always the case that creative telescoping can succeed—whatever the algorithm. However, holonomy being only a sufficient condition, it is shown that by considering more generally the dimension of the ideals and another quantity that we have called polynomial growth, it is possible to predict termination of a generalisation of Chyzak’s generalisation of Zeilberger’s fast algorithm.

To state it in a nutshell, the lower the dimension of the annihilating ideal of a function, the more variables can be summed and integrated by creative telescoping. It is therefore natural to try and bound the dimension related to a multiple sum/integral in terms of the dimension of the summand/integrand. In doing this, the bound we could find is parametrised by the new notion of possible growth.

The notion of polynomial growth originates in observing how the “common denominator” $H_{n,k}$ could be chosen in Wilf and Zeilberger’s treatment of proper hypergeometric sums, in contrast to the behaviour of the approach confronted with the non-proper input $1/(n^2 + k^2)$. In the former case, the common denominator has a number of factors that is linear with respect to $r + s$; in the latter case, it has to be chosen as

$$\prod_{i=0}^{r} \prod_{j=0}^{s} ((n+i)^2 + (k+j)^2)$$

and thus has a quadratic number of factors. The same difference in behaviours—linear versus quadratic—occurs for the numerators. Intuitively speaking, the exponent in this polynomial growth of the degree is our notion of polynomial growth.

To make this formal, let us distinguish between variables $x_1, \ldots, x_\xi$ that are parameters of the integral/sum and variables $t_1, \ldots, t_\tau$ that are integration/summation variables. That is, we consider a multiple integral/sum of the form

$$F(x_1, \ldots, x_\xi) = \int f(x_1, \ldots, x_\xi, t_1, \ldots, t_\tau) \, dt_1 \cdots dt_\tau,$$

or

$$F(x_1, \ldots, x_\xi) = \sum_{(t_1, \ldots, t_\tau) \in I} f(x_1, \ldots, x_\xi, t_1, \ldots, t_\tau),$$

viewed as a sequence with indices $x_1, \ldots, x_\xi$, or some mixed case of integrations and summations. As creative telescoping has to do with the elimination of the $t$’s, we consider how reduction modulo (a fixed Gröbner basis for) the ideal ann $f$ lets the degrees in the $t$’s grow. In what follows, $\partial_{t_1}$ denotes either $D_{x_1}$ or $S_{x_1}$, according to the case, and similarly for $\partial_{t_\tau}$. For any given integer $s \geq 0$, there exists a polynomial $P_s(x_1, \ldots, x_\xi, t_1, \ldots, t_\tau)$ such that each of the
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$P_s(x_1,x_\xi,t_1,\ldots,t_\tau)\partial_{x_1}^{\alpha_1}\ldots\partial_{x_\xi}^{\alpha_\xi}\partial_{t_1}^{\beta_1}\ldots\partial_{t_\tau}^{\beta_\tau}$ has a remainder that is a linear combination of monomials in the $\partial$’s with coefficients in $\mathbb{Q}(x_1,x_\xi,t_1,\ldots,t_\tau)$: such a polynomial $P_s$ can be found as a common denominator, for instance. When, additionally, there is an integer $p \in \mathbb{N}$ such that the coefficients in $\mathbb{Q}(x_1,x_\xi,t_1,\ldots,t_\tau)$ have total degree in the $t$’s bounded by $O(s^p)$, then the annihilating ideal of $f$ is said to have polynomial growth $p$.

The main result of (Chyzak et al., 2009) is to bound the dimension of the ideal of annihilators that can be obtained by creative telescoping, respectively

\[
\left(\text{ann } f + \sum_{i=1}^{s} D_t, A_{x,t} \right) \cap A_x \quad \text{and} \quad \left(\text{ann } f + \sum_{i=1}^{s} (S_t - 1)A_{x,t} \right) \cap A_x
\]

in the integration and in the summation cases, where we have set $A_{x,y} = \mathbb{Q}(x)[[\partial_x,\partial_y]]$ and $A_x = \mathbb{Q}(x)[\partial_x]$. Under natural technical assumptions, this bound can be expressed in terms of the dimension and polynomial growth of ann $f$ (w.r.t. $A_{x,t}$): the dimension of the output (w.r.t. $A_x$) is bounded by

\[
d + (p - 1) \tau.
\]

Two nice cases correspond to polynomial growth $p = 1$: the case of functions considered only with respect to differential operators and the the case of proper-hypergeometric terms. In both cases, starting with a $\partial$-finite function results in a sum/integral that is $\partial$-finite as well.
Bibliography


INRIA (FRANCE) • frederic.chyzak@inria.fr • http://algo.inria.fr/chyzak/