The Algebra of Holonomic Equations

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Abstract. In this article algorithmic methods are presented that have essentially been introduced into computer algebra systems like Maple or Mathematica within the last decade. The main ideas are due to Stanley and Zeilberger. Some of them had already been discovered in the last century by Beke, but because of their complexity the underlying algorithms have fallen into oblivion. We give a survey of these techniques, show how they can be used to identify transcendental functions, and present implementations of these algorithms in computer algebra systems.

1 Algebraic Representation of Transcendental Functions

How can transcendental function be represented by algebraic means? To give this question another flavor: What is the main difference between the exponential function $f(x) = e^x$ and the function $g(x) = e^x + |x|/10^{1000}$, that makes f an elementary function, but not g, although f and g are numerically quite close on a part of the real axis?

Or let's consider an example of discrete mathematics: Why is the factorial function $a_n = n!$ considered to be the most important discrete function, and not $b_n = n! + n/10^{1000}$ or any other discrete function?

Although these examples refer to the most important continuous and discrete *transcendental* functions, oddly enough the answers to the above questions are *purely algebraic*: The exponential function f is characterized by any of the following algebraic properties:

1. f is continuous, $f(1) = e$, and for all x, y we have $f(x + y) = f(x) \cdot f(y)$;

2. f is differentiable, $f'(x) = f(x)$ and $f(0) = 1$;

3. $f \in C^\infty$, $f(x) = \sum\limits_{n=0}^{\infty} a_n \, x^n$ with $a_0 = 1$, and for all $n \geq 0$ we have $(n + 1) \, a_{n+1} = a_n$;

and the factorial function a_n is represented by any of the following algebraic properties:

4. $a_0 = 1$, and for all $n \geq 0$ we have $a_{n+1} = (n + 1) \, a_n$;

5. the generating function $f(x) = \sum\limits_{n=0}^{\infty} a_n x^n$ satisfies the differential equation $x^2 f'(x) + (x - 1)f(x) + 1 = 0$ with the initial condition $f(0) = 1$.

(Note here that one could argue that property (1.) is not algebraic since the symbol e is needed in the representation.) I do not know any method to represent transcendental functions using functional equations, such as property (1.), but I will show, why and how the other properties can be suitable for this purpose, being mainly concerned with properties (2.) and (4.). In § 4 we consider, how these representations can be viewed as purely polynomial cases.

Observe that the "generating function" of the factorial function is convergent only at the origin, and therefore must be considered as a formal series. In particular, a "closed representation" (whatever that should mean) of the generating function cannot be given. But this is not the main issue here. Rather than working with the generating function itself, it is much better to work with its differential equation which is purely algebraic (in fact, it is purely polynomial). The same argument applies to the exponential and factorial functions themselves. Rather than working with these transcendental objects, one should represent them by their corresponding differential and recurrence equations.

The given properties are *structural statements* about the corresponding functions. Any small modification (even changing the value at a single point) destroys this structure. For example, the function $g(x) = e^x + |x|/10^{1000}$ *cannot* be characterized by a rule analogous to one of the properties (2.)–(3.). On the other hand, the function $h(x) = e^x + x/10^{1000}$ can be represented by the differential equation $(x-1)\,h''(x) - x\,h'(x) + h(x) = 0$ with the initial values $h(0) = 1$ and $h'(0) = 1 + 10^{-1000}$.

Therefore, the special (and common) fact about the exponential and factorial functions is that they both satisfy a differential or recurrence equation, respectively, that is homogeneous, linear, of order one, and has polynomial coefficients.

We can generalize this observation [42]: A continuous function of one variable $f(x)$ is *holonomic*, if it satisfies a homogeneous linear differential equation with polynomial coefficients; we call such a differential equation also holonomic.

By linear algebra arguments, Stanley [36] showed that sums and products of holonomic functions and the composition with algebraic functions also form holonomic functions. This can be seen as follows: Assume f and g satisfy holonomic differential equations of order n and m, respectively. We consider the linear space L_f of functions with rational coefficients generated by $f, f', f'', \ldots, f^{(k)}, \ldots$. Since $f, f', \ldots, f^{(n)}$ are linearly dependent by the given holonomic differential equation and since by differentiation the same conclusion follows for $f', f'', \ldots, f^{(n+1)}$, and so on inductively, the dimension of L_f is $\leq n$. Similarly L_g has dimension $\leq m$. We now build the sum $L_f + L_g$ which is of dimension $\leq n + m$. As $f+g, (f+g)', \ldots, (f+g)^{(k)}, \ldots$ are elements of $L_f + L_g$, arbitrary $n + m + 1$ many of them are linearly dependent. In particular, $f + g$ satisfies a holonomic differential equation of order $\leq n + m$.

Similarly the product and composition cases can be handled. Note that the above proof provides a construction of the resulting holonomic equation by linear algebra techniques. It is remarkable that 100 years ago, Beke [4]–[5]

already described these algorithms to generate holonomic differential equations for the sum and product of f and g from the holonomic differential equations of f and g. Hence, he had discovered algorithmic versions of Stanley's results!

Analogously, a discrete function (sequence) of one variable is called holonomic, if it satisfies a homogeneous linear recurrence equation with polynomial coefficients. Such a recurrence equation is also called holonomic. Sums and products of discrete holonomic functions are again holonomic, and there are similar algorithms to calculate representing holonomic recurrence equations (s. [34], [25]).

A function

$$f(x) = \sum_{n=0}^{\infty} a_n \, x^n$$

represented by a power series is holonomic if and only if the corresponding power series coefficient a_n is a holonomic sequence. The holonomic equations for $f(x)$ and a_n can be converted equating coefficients.

Note that these algorithms were implemented by Salvy and Zimmermann in the `gfun` package of Maple's share library [34]. I wrote a Mathematica implementation, `SpecialFunctions`, to be obtained by World Wide Web from the address `ftp://ftp.zib-berlin.de/pub/UserHome/Koepf/SpecialFunctions`. Examples of this implementation will be given later.

2 Identification of Transcendental Functions

Note that the notion of holonomy provides a *normal form* for a suitably large number of transcendental functions, which can then be utilized for *identification* purposes. The holonomic equation *of lowest order* corresponding to a holonomic function constitutes such a normal form. Once we have calculated the normal form of a holonomic function, the latter is identified: Two holonomic functions are identical if and only if they have the same normal form, and satisfy the same initial conditions.

But also without having access to the *lowest order* holonomic equations, one can check whether two holonomic functions agree, since (by linear algebra, e.g.,) it is easy to see whether two holonomic equations are compatible with each other.

Therefore, we may ignore that $e^x, \sin x, \cos x, \arctan x, \arcsin x$ and others form transcendental functions, and take only their holonomic differential equations $f' = f$, $f'' = -f$, $f'' = -f$, $(1 + x^2)f'' + 2xf' = 0$, $(x^2 - 1)f'' + xf' = 0$ etc. into account. From these differential equations, corresponding differential equations for sums and products can be generated by the above mentioned technique, using only polynomial arithmetic and linear algebra. For example, the function $f(x) = \arcsin^2 x$ yields $(x^2 - 1)f''' + 3xf'' + f' = 0$. Note, however, that in the given case one can get even more: The resulting holonomic

differential equation is directly equivalent to the holonomic recurrence equation $n(1 + n)(2 + n)a_{n+2} = n^3 a_n$ for the coefficients a_n of the Taylor series of $\arcsin^2 x = \sum_{n=0}^{\infty} a_n x^n$, and since this holonomic recurrence equation fortunately contains only the two terms a_{n+2} and a_n, it can be solved explicitly, and leads to the representation

$$\arcsin^2 x = \sum_{n=0}^{\infty} \frac{4^n \, n!^2}{(1 + n)\,(1 + 2n)!} x^{2n+2}$$

(compare [18], [41], [20]–[21]).

Note that not only a function like the Airy function $\mathrm{Ai}\,(x)$ (s. e. [1], (10.4)) falls under the category of holonomic functions, since it satisfies the simple holonomic differential equation $f'' - xf = 0$, moreover the classical families of orthogonal polynomials[1] and many other special functions form holonomic functions [1]. These depend on several variables, and we will discuss this situation in § 4.

On the other hand, there are functions that are not holonomic, like the tangent function $\tan x$ (s. [36], [25]). The identification problem for expressions involving nonholonomic functions can only be treated after preprocessing the input. If, for example, we want to verify the addition formula for the tangent function

$$\tan (x + y) = \frac{\tan x + \tan y}{1 - \tan x \, \tan y}$$

by the given method, then we have to replace all occurrences of the tangent function by sines and cosines (which are holonomic) using the rewrite rule $\tan x = \sin x / \cos x$. We can then generate a polynomial equation by multiplying both sides by the common denominator. This procedure results in the equivalent representation

$$(\cos x \cos y - \sin x \sin y) \sin (x + y) = (\cos y \sin x + \cos x \sin y) \cos (x + y) \quad (1)$$

which is easily proved since the algorithms generate the common holonomic differential equation $f''(x) + 4f'(x) = 0$ with respect to x (or the common holonomic differential equation $f''(y) + 4f'(y) = 0$ with respect to y) for both sides of (1) where the common initial values are $f(0) = \cos y \sin y$, and $f'(0) = \cos y^2 - \sin y^2$. Assume that for the initial value functions we had obtained different representations (e.g. $\cos y \sin y$ and $\sin (2y)/2$). These could be verified by the same technique.

In the Mathematica package `SpecialFunctions` (s. also [22]), the procedure `HolonomicDE[f,x]` calculates the holonomic differential equation of f with respect to the variable x using the known holonomic differential equations of the primitive functions, and the sum and product algorithms by recursive decent

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[1]As families of orthogonal polynomials they are *not* polynomials!

through the expression tree. Here we call a function *primitive* if it is rational, or whenever we use a separate symbol for it and a holonomic differential equation is known. Therefore the above mentioned functions (besides the tangent function) are primitive.

The examples given are governed by the following Mathematica session:

```
In[1]:= <<SpecialFunctions`

In[2]:= HolonomicDE[ArcSin[x]^2,x]

                                                   (3)
Out[2]= F'[x] + 3 x F''[x] + (-1 + x) (1 + x) F    [x] == 0

In[3]:= DEtoRE[%,F,x,a,n]

          3
Out[3]= n  a[n] - n (1 + n) (2 + n) a[2 + n] == 0

In[4]:= Series[ArcSin[x]^2,{x,0}]

             k  2 + 2 k   2
            4 x         k!
Out[4]= Sum[------------------, {k, 0, Infinity}]
           (1 + k) (1 + 2 k)!

In[5]:= HolonomicDE[AiryAi[x],x]

Out[5]= -(x F[x]) + F''[x] == 0

In[6]:= HolonomicDE[AiryAi[x]^2,x]

                               (3)
Out[6]= 2 F[x] + 4 x F'[x] - F    [x] == 0

In[7]:= HolonomicDE[Sin[x+y]*(Sin[x]Sin[y]-Cos[x]Cos[y]),x]

                 (3)
Out[7]= 4 F'[x] + F    [x] == 0

In[8]:= HolonomicDE[Cos[x+y]*(Sin[x]Cos[y]+Cos[x]Sin[y]),x]

                 (3)
Out[8]= 4 F'[x] + F    [x] == 0

In[9]:= HolonomicDE[Cos[y]*Sin[y],y]

                 (3)
Out[9]= 4 F'[y] + F    [y] == 0
```

5

```
In[10]:= HolonomicDE[Sin[2y]/2,y]

Out[10]= 4 F[y] + F''[y] == 0
```

One difficulty that may arise with the method described is that in some instances the sum and product algorithms will not generate the holonomic differential equation of lowest order, as in the above example for $\cos y \sin y$. In this case, the normal form property is lost. In fact, the sum algorithm calculates a holonomic equation that is valid for *any linear combination $af + bg$* rather than the particular given sum $f + g$. As a simple example, we consider the sum $\sqrt{1 + x} + \frac{1}{\sqrt{1+x}}$ satisfying the first order differential equation

$$2 \, (2 + x) \, (1 + x) \, F'(x) - xF(x) = 0 \; .$$

This differential equation can be found using a method given in [20]–[21], whereas the sum algorithm generates the second order differential equation

$$4 \, (1 + x)^2 \, F''(x) + 4 \, (1 + x) \, F'(x) - F(x) = 0 \; .$$

The reason for the existence of a differential equation of lower order is due to the fact that the ratio of the two summands $\sqrt{1 + x}$ and $\frac{1}{\sqrt{1+x}}$ forms a rational function.

Similarly, the sum of two consecutive Legendre polynomials $P_n(x) + P_{n+1}(x)$ satisfies the second order differential equation

$$(x - 1) \, (x + 1) \, F''(x) + (x + 1) \, F'(x) - (n + 1)^2 \, F(x) = 0 \; ,$$

whereas the sum algorithm generates the differential equation

$$\begin{aligned}
0 \;\; = \;\; & (x - 1)^2 \, (1 + x)^2 \, F''''(x) + 8 \, (x - 1) \, x \, (1 + x) \, F'''(x) \\
& + 2 \, \left(-2 + 2 \, n + n^2 + 6 \, x^2 - 2 \, n \, x^2 - n^2 \, x^2\right) \, F''(x) \\
& - 4 \, n \, (2 + n) \, x \, F'(x) + n \, (1 + n)^2 \, (2 + n) \, F(x)
\end{aligned}$$

of fourth order, which is also valid for the difference $P_n(x) - P_{n+1}(x)$ and for any other linear combination.

For the *verification of identities*, this is not an important issue, since the *compatibility* of two holonomic equations can be easily checked. This situation is similar to proving a rational identity by pure polynomial arithmetic without gcd computations (after having multiplied through by all denominators), and is actually equivalent to a noncommutative polynomial division, see § 4.

In the case that the normal form is needed for a particular problem, a *factorization algorithm* can be used, s. § 6.

For the discrete functions, the situation is quite similar. We call a function primitive whenever we use a separate symbol for it and a holonomic recurrence

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equation is known. To these primitive functions, we add the rational functions and the functions

$$(mn + b)! \, , \quad \frac{1}{(mn + b)!} \quad (m \in \mathbb{Q}) \, , \quad \text{and} \quad a^n \tag{2}$$

whose holonomic recurrence equations are known, as primitive functions with respect to the variable n. We consider the factorial function to be equivalent to the Γ function $\Gamma(a + 1) = a!$, and declare binomial coefficients etc. also via factorials. From the holonomic representations of the primitive functions the holonomic equations for all sums and products can be established. E. g. the two equations

$$(n - k + 1)^2 F(n + 1, k) - (1 + n)^2 F(n, k) = 0 \tag{3}$$

and

$$(k + 1)^2 F(n, k + 1) - (n - k)^2 F(n, k) = 0 \tag{4}$$

for $F(n, k) = \binom{n}{k}^2$. Whereas these are simple consequences of the representation of $F(n, k)$ by factorials, the given procedure can be applied, for example, to the more complicated function $F(n, k) = \frac{n! + k!^2}{k}$ to generate the two holonomic equations

$$nF(n + 2, k) - (1 + 3n + n^2)F(n + 1, k) + (1 + n)^2 F(n, k) = 0$$

and

$$k(2+k)^2 F(n, k+2) - (1+k)(1+3k+k^2)(3+3k+k^2)F(n, k+1) + k(1+k)^3 F(n, k) = 0 \, .$$

Note that the given approach also covers all kinds of orthogonal polynomials and special functions with respect to their discrete variables, see § 4.

In our Mathematica implementation `SpecialFunctions`, the procedure `HolonomicRE[a,n]` calculates the holonomic recurrence equation of a_n with respect to the variable n taking the known holonomic recurrence equations of the primitive functions into account, and using the sum and product algorithms by recursive decent through the expression tree. The above examples are governed by the following Mathematica session:

```
In[11]:= HolonomicRE[Binomial[n,k]^2,n]

                 2                   2
Out[11]= (1 + n)  a[n] - (1 - k + n)  a[1 + n] == 0

In[12]:= HolonomicRE[Binomial[n,k]^2,k]

                 2                   2
Out[12]= (-k + n)  a[k] - (1 + k)  a[1 + k] == 0
```

```
In[13]:= HolonomicRE[(n!+k!^2)/k,n]

                 2                      2
Out[13]= (1 + n)  a[n] + (-1 - 3 n - n ) a[1 + n] + n a[2 + n] == 0

In[14]:= HolonomicRE[(n!+k!^2)/k,k]

               3
Out[14]= k (1 + k)  (3 + k) a[k] -

                     2          2
>    (1 + k) (1 + 3 k + k ) (3 + 3 k + k ) a[1 + k] +

             2
>    k (2 + k)  a[2 + k] == 0
```

3   Hypergeometric Sums

Rather than having functions given as finite sums and products of primitive expressions, an important class of functions, particularly in analysis and combinatorics, is given by infinite sums of products of terms of the form (2)

$$s(n) = \sum_{k \in \mathbb{Z}} F(n, k) \ . \tag{5}$$

Then $F(n, k)$ is an (m, l)-fold *hypergeometric term*. That is, both $F(n + m, k)/F(n, k)$ and $F(n, k + l)/F(n, k)$ are rational functions with respect to n and k for a certain pair $(m, l) \in \mathbb{N}^2$. For example, by (3)–(4) this is valid for $F(n, k) = \binom{n}{k}^2$ with $m = l = 1$. We assume moreover that the sums (5) have finite support, i.e., they are finite sums for each particular $n \in \mathbb{N}$.

A modification [23] of the (fast) *Zeilberger algorithm* ([43], see also [27], and [31]) returns a holonomic recurrence equation valid for $s(n)$. Zeilberger's algorithm is based on a decision procedure for indefinite summation due to Gosper [17]. In our example case, Zeilberger's algorithm finds the holonomic recurrence equation $(1 + n) s(n + 1) = 2(1 + 2n) s(n)$ for $s(n) = \sum_{k \in \mathbb{Z}} \binom{n}{k}^2 = \sum_{k=0}^{n} \binom{n}{k}^2$ which fortunately has only two terms. Therefore, we are led to the representation

$$s(n) = \sum_{k=0}^{n} \binom{n}{k}^2 = \frac{(2n)!}{n!^2} \ .$$

Even though, in general, the resulting recurrence equation has more than two terms, this holonomic equation contains very important structural information

about $s(n)$. This may be used to show that a certain family of polynomials is orthogonal or not [44], and can be an interesting property for numerical purposes (compare [11]–[12]).

In particular, as described in the last section, the generated structural information can be used for the identification of a transcendental function that is given as sum (5). Note that sums of type (5) in general form transcendental functions with respect to the discrete variable n.

For example, to check the identity (compare [37])

$$\sum_{k=0}^{n} \binom{n}{k}^3 = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{2k}{n} \tag{6}$$

which is nontrivial since for $n = 1$ it reads $1 + 1 = 0 + 2$, we need only to show that both sums $s(n)$ satisfy the common recurrence equation

$$(n+2)^2 s(n+2) - (16 + 21n + 7n^2)s(n+1) - (n+1)^2 s(n) = 0 \tag{7}$$

which is the result given by Zeilberger's algorithm. We also have the same initial values $s(0) = 1$ and $s(1) = 2$, so we are done.

In Mathematica these computations are done by

```
In[15]:= HolonomicRE[Sum[Binomial[n,k]^2,{k,0,n}],n]

Out[15]= -2 (1 + 2 n) a[n] + (1 + n) a[1 + n] == 0

In[16]:= HolonomicRE[Sum[Binomial[n,k]^3,{k,0,n}],n]

                 2                          2
Out[16]= -8 (1 + n)  a[n] + (-16 - 21 n - 7 n ) a[1 + n] +

              2
>        (2 + n)  a[2 + n] == 0

In[17]:= HolonomicRE[Sum[Binomial[n,k]^2*Binomial[2k,n],{k,0,n}],n]

                 2                          2
Out[17]= -8 (1 + n)  a[n] + (-16 - 21 n - 7 n ) a[1 + n] +

              2
>        (2 + n)  a[2 + n] == 0
```

Note that the example shows that transcendental functions can come in quite different disguises. Might the left or the right hand side of (6) be a preferable representation? This question cannot be answered satisfyingly. A holonomic recurrence equation like (7), defining the same transcendental function $s(n)$, is probably the simplest way to describe a function of a discrete variable, since

it postulates how the values of the function can be calculated iteratively. Not only is this a quite efficient way to calculate the values of $s(n)$, but moreover it is preferable to either of the two representations given in (6), since it gives a unique representation scheme. This is what a normal form is about.

As a further example, we consider the function ($\alpha, \beta, \gamma \in \mathbb{N}_0$, $z, M, d \in \mathbb{R}^+$)

$$
V(\alpha, \beta, \gamma) = (-1)^{\alpha+\beta+\gamma} \cdot \frac{\Gamma(\alpha+\beta+\gamma-d)\Gamma(d/2-\gamma)\Gamma(\alpha+\gamma-d/2)\Gamma(\beta+\gamma-d/2)}{\Gamma(\alpha)\Gamma(\beta)\Gamma(d/2)\Gamma(\alpha+\beta+2\gamma-d)M^{\alpha+\beta+\gamma-d}}
$$
$$
\cdot {}_2F_1\left(\begin{array}{cc} \alpha+\beta+\gamma-d, & \alpha+\gamma-d/2 \\ \alpha+\beta+2\gamma-d \end{array} \middle| z\right)
$$

(${}_2F_1$ here represents Gauß's hypergeometric function, see [1], Chapter 15), which plays a role for the computation of Feynman-diagrams [15][2], for which Zeilberger's algorithm generates the holonomic recurrence equation

$$
\begin{aligned}
0 = & (\alpha+\beta-d+\gamma)(2\alpha-d+2\gamma)V(\alpha, \beta, \gamma) \\
& + \alpha M(2\alpha+2\beta-2d+4\gamma-2z-4\alpha z-2\beta z+3dz-4\gamma z)V(\alpha+1, \beta, \gamma) \\
& + 2\alpha(1+\alpha)M^2(z-1)zV(\alpha+2, \beta, \gamma)
\end{aligned}
$$

and analogous recurrence equations with respect to the variables β and γ (see [24]). These, in particular, can be used for numerical purposes.

Note that for the application of Zeilberger's algorithm our Mathematica program uses the Paule-Schorn implementation [31]. For the current example, the output is given by

```
In[18]:= HolonomicRE[(-1)^(alpha+beta+gamma)*Gamma[alpha+beta+gamma-d]*
            Gamma[d/2-gamma]*Gamma[alpha+gamma-d/2]*Gamma[beta+gamma-d/2]/
            (Gamma[alpha]*Gamma[beta]*Gamma[d/2]*
            Gamma[alpha+beta+2*gamma-d]*M^(alpha+beta+gamma-d))*
            Hypergeometric2F1[alpha+beta+gamma-d,alpha+gamma-d/2,
            alpha+beta+2*gamma-d,z],alpha,V]

Out[18]= (alpha + beta - d + gamma) (2 alpha - d + 2 gamma) V[alpha] +

>       alpha M (2 alpha + 2 beta - 2 d + 4 gamma - 2 z - 4 alpha z -

>          2 beta z + 3 d z - 4 gamma z) V[1 + alpha] +

                         2
>       2 alpha (1 + alpha) M  (-1 + z) z V[2 + alpha] == 0
```

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[2]I am indebted to Jochem Fleischer who informed me about a misprint in formula (31) of [15].

4 Holonomic Systems of Several Variables

In [42], Zeilberger considered the more general situation of functions F of several discrete and continuous variables. If we have d variables, and d (essentially independent) mixed homogeneous linear (partial) difference-differential equations with polynomial coefficients in all variables are given for F, then F is called a *holonomic system* (compare [6]–[8]). In most cases these holonomic equations together with suitably many initial values declare F uniquely.

In particular, we concentrate on the situation, when the given system of holonomic equations is separated, i.e. each of them is either an ordinary differential equation or a pure recurrence equation. These representing holonomic equations can be generated by the method described in § 2 whenever F is given in terms of sums and products of primitive functions.

For example, the Legendre polynomials $F(n, x) = P_n(x)$ ([1], Chapter 22) form a holonomic system by their holonomic differential equation

$$(x^2 - 1)F''(n, x) + 2xF'(n, x) - n(1 + n)F(n, x) = 0 \tag{8}$$

and their holonomic recurrence equation

$$(n + 2)F(n + 2, x) - (3 + 2n)xF(n + 1, x) + (n + 1)F(n, x) = 0 , \tag{9}$$

together with the initial values

$$F(0, 0) = 1 , \quad F(1, 0) = 0 , \quad F'(0, 0) = 0 , \quad F'(1, 0) = 1 . \tag{10}$$

Equations (8)–(10) therefore build a sufficient algebraic, even polynomial structure to represent the functions $P_n(x)$ as we shall see now.

If we interpret the (partial) differentiations and shifts that occur as operators, and the representing system of holonomic equations as operator equations, then these form a *polynomial equations system* in a noncommutative polynomial ring. For a continuous variable x with differential operator D given by $DF(n, x) = F'(n, x)$, the product rule implies $D(xf) - xDf = f$, and hence the commutator rule $Dx - xD = 1$ is valid. Similarly for a discrete variable n with the (forward) shift operator N given by $NF(n, x) = F(n + 1, x)$, we have $N(nF(n, x)) - nNF(n, x) = (n + 1)F(n + 1, x) - nF(n + 1, x) = F(n + 1, x) = NF(n, x)$, and therefore the commutator rule $Nn - nN = N$. Similar rules are valid for all variables involved, whereas all other commutators vanish.

The transformation of a holonomic system given by mixed holonomic difference-differential equations represents an elimination problem in the noncommutative polynomial ring considered, that can be solved by noncommutative Gröbner basis methods ([3], [16], [19], [42], [45], [38]–[40]), [23]).

Hence, we need the concept of a *Gröbner basis*. If one applies Gauß's algorithm to a linear system, the variables are eliminated iteratively, resulting in an equivalent system which is simpler in the sense that it contains some equations which are free of some variables involved. Note that connected with an application of Gauß's algorithm is a certain order of the variables.

The *Buchberger algorithm* is an elimination process, given a certain term order for the variables (a variable order is no longer sufficient), with which a polynomial system (rather than a linear one) is transformed, resulting in an equivalent system (i.e., constituting the same ideal) for which the terms that are largest with respect to the term order, are eliminated as far as possible. Note that—in contrast to the linear case—the resulting equivalent system may contain more polynomials than the original one. Such a rewritten system is called a Gröbner basis of the ideal generated by the polynomial system given. It turns out that Buchberger's algorithm can be extended to the noncommutative case that we consider here [19] as long as the rewrite process using the commutator does not increase the variable order.

As an example, we consider $F(n, k) = \binom{n}{k}$ in which case we have the Pascal triangle relation $F(n + 1, k + 1) = F(n, k) + F(n, k + 1)$, together with the pure recurrence equation $(n + 1 - k)F(n + 1, k) - (n + 1)F(n, k) = 0$ with respect to n, say. These equations read as $(KN - 1 - K)F(n, k) = 0$, and $((n + 1 - k)N - (n + 1))F(n, k) = 0$ in operator notation, K denoting the shift operator with respect to k. Therefore we have the polynomial system

$$KN - 1 - K \qquad \text{and} \qquad (n + 1 - k)N - (n + 1) . \qquad (11)$$

The Gröbner basis of the left ideal generated by (11) with respect to the lexicographical term order (k, n, K, N) is given by

$$\left\{ (k + 1)K + k - n, (n + 1 - k)N - (n + 1), KN - 1 - K \right\} ,$$

i.e., the elimination process has generated the pure recurrence equation

$$(k + 1)F(n, k + 1) + (k - n)F(n, k) = 0$$

with respect to k.

We used the REDUCE implementation [28] for the noncommutative Gröbner calculations of this article, but I would like to mention that there is also a Maple package `Mgfun` written by Chyzak [10] (to be obtained from `http://pauillac.inria.fr/algo/libraries/libraries.html#Mgfun`) which can be used for this purpose.

As another example, we consider the Legendre polynomials. In operator notation the holonomic equations (8)–(9) constitute the polynomials

$$(x^2 - 1)D^2 + 2xD - n(1 + n) \quad \text{and} \quad (n + 2)N^2 - (3 + 2n)xN + (n + 1) . \ (12)$$

The Gröbner basis of the left ideal generated by (12) with respect to the lexicographical term order (D, N, n, x) is given by

$$\Big\{ (x^2 - 1)D^2 + 2xD - n(1 + n),$$

$$(1 + n)ND - (1 + n)xD - (1 + n)^2, \qquad (13)$$

$$(x^2 - 1)ND - (1+n)xN + (1+n), \tag{14}$$

$$(1+n)(x^2-1)D - (1+n)^2N + x(1+n)^2, \tag{15}$$

$$\left.(n+2)N^2 - (3+2n)xN + (n+1)\right\} .$$

After the calculation of the Gröbner basis, for better readability I positioned the operators D and N back to the right, so that the equations can be easily understood as operator equations, again. By the term order chosen, the Gröbner basis contains those equations for which the D-powers are eliminated as far as possible, and (13)–(15) correspond to the relations

$$P'_{n+1}(x) = x\,P'_n(x) + (1+n)\,P_n(x)\,,$$

$$(x^2-1)P'_{n+1}(x) = (1+n)\,(xP_{n+1}(x) - P_n(x))\,,$$

$$(x^2-1)P'_n(x) = (1+n)\,(P_{n+1}(x) - xP_n(x)) \tag{16}$$

between the Legendre polynomials and their derivatives.

If we are interested in a relation between the Legendre polynomials and their derivatives that is x-free (which is of importance for example for spectral approximation, see [9]), we choose the term order (x, D, N, n) to eliminate x in the first place, and obtain a different Gröbner basis containing the x-free polynomial

$$-(n+2)(n+1)D - (2n+3)(n+2)(n+1)N + (n+2)(n+1)N^2D$$

equivalent to the identity

$$(2n+1)P_n(x) = P'_{n+1}(x) - P'_{n-1}(x)$$

for the Legendre polynomials (see e.g. [9], formula (2.3.16)).

Here, we present the REDUCE output for the above examples:

```
1: load ncpoly;

2: nc_setup({D,NN,n,x},{NN*n-n*NN=NN,D*x-x*D=1},left);

3: p1:=(x^2-1)*D^2+2*x*D-n*(1+n)$ % differential equation

4: p2:=(n+2)*NN^2-(3+2*n)*x*NN+(n+1)$ % recurrence equation

5: nc_groebner({p1,p2});

  2 2    2             2
{d *x  - d  - 2*d*x - n  - n,


                  2
 d*nn*n - d*n*x - d*x - n  - n,
```

```
       2
 d*nn*x  - d*nn - nn*n*x - 2*nn*x + n + 1,

      2           2          2   2
 d*n*x  - d*n + d*x  - d - nn*n  + n *x - x,

   2
 nn *n - 2*nn*n*x - nn*x + n + 1}

6: nc_setup({x,D,NN,n},{NN*n-n*NN=NN,D*x-x*D=1},left);

7: result:=nc_groebner({p1,p2});

           2 2         2    2
result := {x *d  + 2*x*d - d  - n  - n,

                  2                 2
         x*d*nn - d*nn *n + d*n + d + 2*nn*n  + 2*nn*n + nn,

                          2
         x*d*n + x*d - d*nn*n + n  + 2*n + 1,

                       2
         2*x*nn*n + x*nn - nn *n - n - 1,

            2 2       2      2                3          2
         d*nn *n  - d*nn *n - d*n  - 3*d*n - 2*d - 2*nn*n  - 3*nn*n  - nn*n}

8: nc_setup({n,x,NN,D},{NN*n-n*NN=NN,D*x-x*D=1},left);

9: nc_compact(part(result,5));

                                                   2
 - (2*n + 3)*(n + 2)*(n + 1)*nn + (n + 2)*(n + 1)*nn *d - (n + 2)*(n + 1)*d
```

We see, therefore, that by the given procedure new relations (between the binomial coefficients, and between the derivatives of the Legendre polynomials) can be *discovered*. The generation of derivative rules like (16), and the algorithmic work with them is described in [23].

5   Holonomic Sums and Integrals

Analogously, with the method in the last section, holonomic recurrence equations for *holonomic sums* can be generated. Note that the idea to use recurrence equations for the summand to deduce a recurrence equation for the sum is origi-

nally due to Sister Celine Fasenmyer ([13]–[14], see [33], Chapter 14). Zeilberger [42] brought this into a more general setting.

Consider for example

$$s(n) = \sum_{k=0}^{n} F(n, k) = \sum_{k=0}^{n} \binom{n}{k} P_n(x) \ ,$$

then by the product algorithm, we find the holonomic recurrence equations

$$(n - k + 1)F(n + 1, k) - (1 + n)F(n, k) = 0$$

and

$$(2+k)^2 F(n, k+2) - (3+2k)(n-k-1)xF(n, k+1) + (n-k)(n-k-1)F(n, k) = 0$$

for the summand $F(n, k)$. The Gröbner basis of the left ideal generated by the corresponding polynomials

$$(n-k+1)N-(1+n) \quad \text{and} \quad (2+k)^2 K^2 - (3+2k)(n-k-1)xK + (n-k)(n-k-1)$$

with respect to the lexicographical term order (k, N, n, K) contains the k-free polynomial

$$(2+n)^2 K^2 N^2 - K(2+n)(3+2n)(K+x)N + (1+n)(2+n)(1+K^2+2Kx) \ , \quad (17)$$

which corresponds to a k-free recurrence equation for $F(n, k)$. We use the order (k, N, n, K) because then k-powers are eliminated as far as possible (since we like to find a k-free recurrence), and N-powers come next in the elimination process (since the recurrence equation obtained should be of lowest possible order).

Because all shifted sums

$$s(n) = \sum_{k \in \mathbb{Z}} F(n, k) = \sum_{k \in \mathbb{Z}} F(n, k + 1) = \sum_{k \in \mathbb{Z}} F(n, k + 2)$$

generate the same function $s(n)$, and since summing the k-free recurrence equation is equivalent to setting $K = 1$ in the corresponding operator equation (check!), the substitution $K = 1$ in (17) generates the valid holonomic recurrence equation

$$(2 + n)s(n + 2) - (3 + 2n)(1 + x)s(n + 1) + 2(1 + n)(1 + x)s(n) = 0$$

for $s(n)$.

In the general case, we search for a k-free recurrence equation contained in a Gröbner basis of the corresponding left ideal with respect to a suitably chosen weighted [30] (or lexicographical (k, N, n, K)) term order. For example, the elimination problems described in [45] are automated by this procedure.

On the other hand, it turns out that in many cases the holonomic recurrence equation derived is not of the lowest order. In the next section, we will discuss how this problem can be resolved.

Note that by a similar technique, holonomic integrals can be treated [2]. To find a holonomic equation for

$$I(y) := \int_a^b F(y, x) \, dx$$

for holonomic $F(y, x)$ with respect to the discrete or continuous variable y, calculate the Gröbner basis of the left ideal constituted by the holonomic equations of $F(y, x)$ with respect to a suitably chosen weighted or the lexicographical term order (x, D_y, y, D_x). We search for an x-free holonomic equation $\mathcal{E}$ contained in such a Gröbner basis. In case, that $F(y, a) = F(y, b) \equiv 0$, and enough derivatives of $F(y, x)$ with respect to x vanish at $x = a$ and $x = b$, by partial integration it follows that the holonomic equation valid for $I(y)$ is given by the substitution $D_x = 0$ into $\mathcal{E}$ (see [2]).

As an example, we consider

$$I(n) := \int_{-\infty}^{\infty} e^{-x^2} H_n(x) \, dx \ ,$$

$H_n(x)$ denoting the Hermite polynomials. The method of § 2 yields the holonomic polynomials

$$2(1 + n) + N^2 - 2xN \qquad \text{and} \qquad D^2 + 2(1 + n) + 2xD$$

for the integrand. Note that since $H_n(x)$ is an odd function for odd n, it is immediately clear that $I(n) = 0$ in this case. However, what about even values of n?

The Gröbner basis of the corresponding left ideal contains the two x-free polynomials

$$N^2 + ND \qquad \text{and} \qquad Nn + nD + D$$

so that setting $D = 0$ we get for $I(n)$ the recurrence equation $I(n + 1) = 0$. Indeed, this proves that $I(n) = 0$ for $n \geq 1$.

As another example, we consider the Abramowitz functions ([1], 27.5))

$$A(n, y) := \int_0^{\infty} x^n e^{-x^2 - y/x} \, dx \ .$$

By the method in § 2 for the integrand $F(n, y, x) = x^n e^{-x^2 - y/x}$ we get the three holonomic polynomials

$$x - N \ , \qquad -nx + x^2 D_x + 2x^3 - y \qquad \text{and} \qquad 1 + x D_y \ .$$

Using the term order (x, D_y, y, D_x), the differential equation

$$y\, A'''(n, y) - (n - 1)\, A''(n, y) + 2A(n, y) = 0 \; ,$$

and using (x, N, n, D), the recurrence equation

$$2A(n + 3, y) - (n + 2)\, A(n + 1, y) - y\, A(n, y) = 0$$

is automatically generated by the given approach (compare [1], (27.5.1), (27.5.3)).

Finally, we mention that similarly an identity like ([1], (11.4.28))

$$\int\limits_0^\infty e^{-a^2\,x^2}\, x^{m-1}\, J_n(bx)\, dx = \frac{\Gamma\left(n/2 + m/2\right) b^n}{2^{n+1}\, a^{n+m}\, \Gamma\left(n + 1\right)}\, {}_1F_1\left(\begin{array}{c} n/2 + m/2 \\ n + 1 \end{array}\ \middle|\ -\frac{b^2}{4a^2}\right)$$

(18)

(${}_1F_1$ representing Kummer's confluent hypergeometric function) for the Bessel function is proved by the calculation of the common holonomic recurrence equation

$$\begin{aligned}
0 \;=\; & -(n + 3)\,(n + m)\,b^2 I(n) \\
& +2\,(n + 2)\left(4\,a^2 n^2 + 16\,a^2 n + 12\,a^2 - b^2 m + b^2\right) I(n + 2) \\
& +(n + 1)\,(n + 4 - m)\,b^2 I(n + 4)
\end{aligned}$$

for the left and right hand sides of (18). Note that Zeilberger's algorithm is not directly applicable to the right hand side, but the extended version of [23] gives the result.

6 Noncommutative Factorization and Holonomic Normal Form

Note that neither the sum and product algorithms of § 2, nor Zeilberger's algorithm or its extension [23], nor the algorithms for holonomic sums and integrals of § 5 can guarantee to present the holonomic equation $\mathcal{N}$ of lowest order, and therefore the normal form searched for.

In [29][3] a Gröbner basis based factorization algorithm was introduced for polynomials in noncommutative polynomial rings given by Lie bracket commutator rules. This method is implemented in [28]. Given an expression f, and a holonomic equation $\mathcal{P}$ of order m of f, one may find the normal form $\mathcal{N}$ of f using this factorization algorithm by generating the right factors of the noncommutative polynomial p corresponding to $\mathcal{P}$, and checking if any of them, $\mathcal{Q}$, say, (having order $l < m$, say) and $m - l$ derivatives (shifts) of $\mathcal{Q}$ are satisfied by f at a certain initial point. In the affirmative case, $\mathcal{Q}$ is compatible with f, and corresponds to a valid holonomic equation for f.

---

[3] Due to a severe bicycle accident of Herbert Melenk, this paper is still unfinished.

To present some examples, we consider Zeilberger's algorithm first. An example for which Zeilberger's algorithm does not generate the holonomic recurrence equation of lowest order is given by the sum (see e.g. [31])

$$s_n := \sum_{k=0}^{n}(-1)^k \binom{n}{k}\binom{3k}{n}$$

for which the holonomic equation

$$2\,(2\,n+3)\,s_{n+2} + 3\,(5\,n+7)\,s_{n+1} + 9\,(n+1)\,s_n = 0 \tag{19}$$

is generated. Note that there is an algorithm due to Petkovšek [32] to find all hypergeometric solutions of holonomic recurrence equations which could be used as next step. However, we may also proceed as follows: The corresponding noncommutative polynomial $2(2n+3)N^2 + 3(5n+7)N + 9(n+1)$ is factorized by implementation [28] as

$$2(2n+3)\,N^2 + 3(5n+7)\,N + 9(n+1) = ((4n+6)\,N + 3(n+1))\,(N+3)\,.$$

The right factor $N+3$ corresponds to the holonomic recurrence equation

$$S_{n+1} + 3S_n = 0\,, \tag{20}$$

which, together with the initial value $S_0 = s_0 = 1$ uniquely defines a sequence $(S_n)_{n\in\mathbb{N}_0}$. Since $S_1 = -3$ turns out to be compatible with the given sum

$$s_1 = \sum_{k=0}^{1}(-1)^k \binom{1}{k}\binom{3k}{1} = -3\,,$$

and since (20) implies (19) (right factor!), the sequence s_n, which is the unique solution of (19) with $s_0 = 1$ and $s_1 = -3$, must equal S_n. From (20), however, the closed form $s_n = (-3)^n$ follows.

Similarly, for any particular $d \in \mathbb{N}$, $d \geq 3$, the identity

$$\sum_{k=0}^{n}(-1)^k \binom{n}{k}\binom{dk}{n} = (-d)^n$$

can be established, for whose left hand side Zeilberger's algorithm generates a recurrence equation of order $d-1$ (see [31]).

Whereas Petkovšek's algorithm finds hypergeometric solutions of holonomic recurrence equations as in the example, and therefore not only verifies identities, but *generates* closed-form results, our approach is more general in the following sense. Factorizations with polynomial coefficients of ordinary holonomic differential equations (see [4], [35] for other methods) as well as of any mixed holonomic difference-differential equation can be calculated.

We give an example of that type for the sum algorithm: Consider the difference of successive Gegenbauer polynomials $h(x) = C_{n+1}^{(-1/2)}(x) - C_n^{(-1/2)}(x)$ that were used in [26]. Here the summand $f(x) := C_n^{(-1/2)}(x)$ satisfies the holonomic equation

$$(x^2 - 1)\,f''(x) + (n - n^2)\,f(x) = 0 \ ,$$

and the sum algorithm yields the fourth order equation

$$(x^2 - 1)^2\,h''''(x) + 4\,x\,(x^2 - 1)\,h'''(x) - 2\,(n^2 - 1)(x^2 - 1)\,h''(x) + n^2\,(n^2 - 1)\,h(x) = 0$$

for $h(x)$. The implementation [28] finds (besides others) the noncommutative factorization

$$\Big((x^2 - 1)\,D^2 + (1 + x)\,D - n^2\Big)\Big((x^2 - 1)\,D^2 - (1 + x)\,D + (1 - n^2)\Big)$$

of the corresponding noncommutative polynomial, whose right factor

$$(x^2 - 1)\,D^2 - (1 + x)\,D + (1 - n^2)$$

turns out to be compatible with the given function $h(x)$. That is, the corresponding differential equation and two derivatives thereof are satisfied by $h(x)$, at $x = 1$. Therefore the holonomic normal form of $h(x)$ is the corresponding differential equation

$$(1 - n^2)\,h(x) - (1 + x)\,h'(x) + (x^2 - 1)\,h''(x) = 0$$

that was a tool in [26]. This result can also be obtained by the method given in [20]–[21].

To evaluate the integrals

$$I_n := \int\limits_{-\infty}^{\infty} x^n\,e^{-x^2}\,H_n(x)\,dx \ ,$$

we may deduce the holonomic system

$$N^2 - 2x^2 N + 2(1 + n)x^2$$

and

$$x^2\,D^2 + 2x(x^2 - n)\,D + (n + n^2 + 2x^2)$$

of the integrand. The Gröbner basis of this system with respect to the weighted lexicographical order with weights $(3, 1, 0, 0)$ for (x, N, n, D) (i.e. the term x is considered larger than N^3, whereas x is smaller than N^4, and any power of n and D is smaller than x and N) contains an x-free polynomial, which when evaluated at $D = 0$ yields

$$
\begin{aligned}
P(n, N) \ = \ & (n + 5)(n + 4)(n + 3)N^3 - (3n + 7)(n + 5)(n + 4)(n + 3)N^2 \\
& + (3n + 5)(n + 5)(n + 4)(n + 3)(n + 2)N \quad\quad\quad\quad\quad (21) \\
& - (n + 5)(n + 4)(n + 3)(n + 2)(n + 1)^2
\end{aligned}
$$

corresponding to a recurrence equation of order three.

On the other hand, $P(n, N)$ obviously has the trivial (commutative) factorization

$$P(n,N) = (n+5)(n+4)(n+3)\Big(N^3 - (3n+7)N^2 + (3n+5)(n+2)N - (n+2)(n+1)^2\Big)$$

and the remaining right factor can be represented as

$$N^3 - (3n+7)N^2 + (3n+5)(n+2)N - (n+2)(n+1)^2 = (N-n-2)(N-n-1)(N-n-1)$$

(note that [28] finds four different right factors). This leads to the valid recurrence equation $I_{n+1} = (n+1)I_n$ that together with the initial value

$$I_0 = \int\limits_{-\infty}^{\infty} e^{-x^2}\, dx = \sqrt{\pi}$$

gives finally $I_n = \sqrt{\pi}\, n!$.

Acknowledgement

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