The Holonomic Systems Approach

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Abstract

The Holonomic Systems Approach was proposed in the early 1990s by Doron Zeilberger and has turned out to be extremely useful when dealing with special functions in computer algebra. Moreover, his celebrated algorithm for definite hypergeometric summation originates from this approach. We want to give an introduction to the underlying ideas—creative telescoping, Gröbner bases, Ore algebras—in an intuitive and therefore non-rigorous way. We also show various examples where these concepts can be successfully applied.

1 Telescoping

The basic principle of how summation (and integration) problems are attacked in the holonomic systems approach is *telescoping*. For indefinite summation this is quite natural: Computing the sum

$$\sum_{k=a}^{b} f(k)$$

for arbitrary $a, b \in \mathbb{Z}, b \geq a$ requires to find an antidifference $g(k)$ such that $f(k) = g(k+1) - g(k)$. By telescoping, the sum then equals $g(b+1) - g(a)$.

Depending on how the expression $g(k)$ looks like, this can be considered as a *closed form* (of course, one could just define $g(k) := \sum_{j=-\infty}^{k-1} f(j)$, but this would not provide a closed form).

Example 1. The antidifference of $k \cdot k!$ is $k!$ since $(k+1)! - k! = k \cdot k!$, hence

$$\sum_{k=a}^{b} k \cdot k! = (b+1)! - a!, \quad 0 \leq a \leq b.$$

2 Indefinite hypergeometric summation

We turn to a specific class of functions, namely the hypergeometric ones. A discrete function $f(k)$ is called *hypergeometric* if

$$\frac{f(k+1)}{f(k)} = r(k) \in \mathbb{K}(k)$$

where $\mathbb{K}$ is a field of characteristic 0. Usually we work with $\mathbb{K} = \mathbb{Q}$ or $\mathbb{K} = \mathbb{Q}(a_1, a_2, \dots)$ for some additional parameters a_i. In other words, hypergeometric functions satisfy a linear first-order recurrence. We want to study the question whether a given hypergeometric function $f(k)$ is indefinitely summable, or, more concretely, whether there exists an antidifference $g(k)$ that is hypergeometric, too.

Writing the telescoping equation as

$$g(k) \cdot \underbrace{\left(\frac{g(k+1)}{g(k)} - 1 \right)}_{\in \mathbb{K}(k)} = f(k)$$

reveals that a hypergeometric antidifference $g(k)$, if it exists at all, must be a rational function multiple of the summand $f(k)$. Therefore $g(k) = q(k)f(k)$ for some yet unknown $q \in \mathbb{K}(k)$. We plug this ansatz into the telescoping equation and obtain

$$q(k+1)f(k+1) - q(k)f(k) = f(k).$$

Dividing by $f(k)$ yields the equation

$$r(k)q(k+1) - q(k) = 1$$

that has to be solved for the unknown rational function $q(k)$ (we omit the details how this can be achieved; this is part of Gosper's algorithm [5]).

Example 2. For $f(k) = k \cdot k!$ we have to solve the equation

$$\frac{(k+1)^2}{k} q(k+1) - q(k) = 1.$$

The only rational function solution is $\frac{1}{k}$, and hence $g(k) = \frac{1}{k} f(k) = k!$.

Example 3. Let now $f(k) = \binom{n}{k}$, which is hypergeometric with respect to k as a simple computation shows:

$$\frac{\binom{n}{k+1}}{\binom{n}{k}} = \frac{n!(n-k)!k!}{(n-k-1)!(k+1)!n!} = \frac{n-k}{k+1} \in \mathbb{K}(k) \quad \text{with } \mathbb{K} = \mathbb{Q}(n).$$

According to the above results, we have to solve the equation

$$(n-k)q(k+1) - (k+1)q(k) = k+1$$

which turns out to have no solution $q(k) \in \mathbb{Q}(n)(k)$. Hence the binomial coefficients are not *indefinitely summable*.

3 Definite hypergeometric summation

But we all know that the definite sum $\sum_{k=0}^{n} \binom{n}{k}$ has a nice evaluation. Now Zeilberger enters the game with his celebrated algorithm for definite hypergeometric summation [10]. It is based on the principle of *creative telescoping*: for this to work, the summand has to depend on at least one additional parameter n, and typically, the summation bounds involve this parameter, too. In this situation, $f(n,k)$ must be hypergeometric with respect to both n and k, i.e.,

$$\frac{f(n,k+1)}{f(n,k)} = r_1(n,k) \text{ and } \frac{f(n+1,k)}{f(n,k)} = r_2(n,k), \quad r_1, r_2 \in \mathbb{K}(n,k). \tag{1}$$

Instead of searching for a hypergeometric antidifference of the summand itself, we try the same for a $\mathbb{K}(n)$-linear combination of $f(n,k)$ and some of its n-shifts, i.e., $f(n+1,k), \dots, f(n+d,k)$. In other words, we try to find $g(n,k) = q(n,k)f(n,k), q \in \mathbb{K}(n,k)$ such that

$$p_0(n)f(n,k) + p_1(n)f(n+1,k) + \dots + p_d(n)f(n+d,k) = g(n,k+1) - g(n,k) \tag{2}$$

for some rational functions $p_i \in \mathbb{K}(n)$. A similar reasoning as before leads to the problem of solving the parameterized equation

$$p_0(n)+p_1(n)r_2(n,k)+\cdots+p_d(n)\prod_{i=0}^{d-1} r_2(n+i,k) = r_1(n,k)q(n,k+1)-q(n,k)$$

for rational solutions $q \in \mathbb{K}(n,k)$ and the parameters $p_0,\ldots,p_d \in \mathbb{K}(n)$. Under certain conditions (e.g., if the summand is *proper hypergeometric*), theory predicts that there must exist an integer d such that the above equation becomes solvable. Therefore Zeilberger's algorithm loops over $d = 0,1,2,\ldots$ until it finds a solution. We now sum over (2):

$$p_0(n)\sum_{k=a(n)}^{b(n)} f(n,k) + \cdots + p_d(n)\sum_{k=a(n)}^{b(n)} f(n+d,k) =$$
$$\sum_{k=a(n)}^{b(n)} \big(g(n,k+1)-g(n,k)\big) = g(n,b+1)-g(n,a).$$

Upon adjusting the summation ranges on the left-hand side and adding or subtracting correction terms, we have found a recurrence for the sum that has the form

$$p_0(n)F(n) + \cdots + p_d(n)F(n+d) = h(n), \quad \text{for } F(n) = \sum_{k=a(n)}^{b(n)} f(n,k).$$

In many cases this yields a closed-form solution, but in any case enables us to prove a given identity (by computing recurrences for both sides and comparing initial values).

Example 4. We continue with the binomial sum and perform the second loop of Zeilberger's algorithm (that corresponds to $d = 1$). We end up with the equation

$$p_0(n) + \frac{n+1}{n+1-k}p_1(n) = \frac{n-k}{k+1}q(n,k+1) - q(n,k)$$

which admits the solution

$$q(n,k) = \frac{c\,k}{k-n-1}, \quad p_0(n) = -2c, \quad p_1(n) = c, \quad \text{for some constant } c.$$

Summing both sides over $k = 0, \ldots, n+1$ delivers the recurrence

$$-2\sum_{k=0}^{n}\binom{n}{k} + \sum_{k=0}^{n+1}\binom{n+1}{k} = 0$$

which, together with the initial value $\sum_{k=0}^{0}\binom{n}{k} = 1$, yields the solution 2^n.

A nice and comprehensive introduction into hypergeometric summation is given in [8].

4 Hyperexponential integration

We want to stress that all the above can be translated to a continuous setting, then addressing integrals of *hyperexponential* functions, i.e., functions $f(x)$ with the property that the quotient $\frac{f'(x)}{f(x)}$ is a rational function in x. In other words, hyperexponential functions satisfy a linear first-order differential equation. Instead of antidifferences we then look for antiderivatives, and telescoping corresponds to invoke the Fundamental Theorem of Calculus. This method is sometimes referred to as *differentiating under the integral sign*, see for example [1, 9].

5 Holonomic systems

The main purpose of this talk is to introduce various generalizations of the above scenarios that allow to treat special function identities, summation and integration problems as well. The ideas go back to Zeilberger's seminal paper [11] and laid the foundations for his hypergeometric summation algorithm. These generalizations concern

- a unifying framework for dealing with shifts (summation) and derivatives (integration) at the same time,
- functions that are described by sufficiently many (possibly higher-order) recurrences or differential equations (*holonomic functions*)
- multivariate functions and multiple sums and integrals.

We want to exemplify this new class of holonomic functions with the Bessel function $J_\nu(z)$ which is defined to be one of the two solutions of Bessel's differential equation

$$z^2 J_\nu''(z) + z J_\nu'(z) + (z^2 - \nu^2) J_\nu(z) = 0.$$

A necessary condition for a function to be holonomic is that for each variable under consideration there exists a pure recurrence or differential equation. For the Bessel functions $J_\nu(z)$ there exists also a relation for the variable ν, namely the following recurrence:

$$z J_{\nu+2}(z) - 2(\nu+1) J_{\nu+1}(z) + z J_\nu(z) = 0.$$

These two relations (together with finitely many initial values) completely define the Bessel functions. Here is an incomplete list of functions that are holonomic:

- rational functions, algebraic functions, logarithms, exponentials,
- sine, cosine, all arc functions, hyperbolic sine and cosine, all inverse hyperbolic functions,
- factorials, binomial coefficients, Gamma function, hypergeometric ${}_pF_q$
- Fibonacci, harmonic, and Catalan numbers,
- Airy, Bessel, Appell, Struve, Hankel, Whittaker, Kelvin functions
- orthogonal polynomials: Legendre, Chebyshev, Hermite, Gegenbauer, Laguerre, Jacobi
- error function, elliptic functions, sine, cosine, and exponential integrals, Fresnel integrals

We give two examples of identities that can be proven by means of the holonomic systems approach in a completely algorithmic fashion (and hence by the computer):

$$\frac{(\nu+1)}{x} J_{\nu+1}(x) + \frac{\partial J_{\nu+1}(x)}{\partial x} = J_\nu(x), \tag{3}$$

$$\int_0^\infty J_m(ax)J_n(bx)\,\mathrm{d}x = \frac{a^{-n-1}b^n\Gamma\left(\frac{m+n+1}{2}\right)}{\Gamma(n+1)\Gamma\left(\frac{m-n+1}{2}\right)}\,{}_2F_1\!\left(\tfrac{m+n+1}{2}, \tfrac{n-m+1}{2}, n+1, \tfrac{b^2}{a^2}\right). \tag{4}$$

For convenience we introduce the following operator notation. Let S_n denote the forward shift operator with respect to n, i.e., $S_n(f(n)) = f(n+1)$. Similarly, we denote by D_x the differentiation operator with respect to x, i.e., $D_x(f(x)) = f'(x)$. Variables like n or x, interpreted as operators, are defined as the multiplication by this variable. As such, they do not commute with the corresponding shift or differential operator as the some simple computations show:

$$\begin{aligned}(S_n \cdot n)(f(n)) &= S_n(n(f(n))) = S_n(n \cdot f(n)) = (n+1) \cdot f(n+1)\\ (D_x \cdot x)(f(x)) &= D_x(x(f(x))) = (x \cdot f(x))' = x \cdot f'(x) + f(x)\end{aligned}$$

Hence we get the commutation rules $S_n n = nS_n + S_n$ and $D_x x = xD_x + 1$ which can be used to define a noncommutative polynomial ring

$$\begin{aligned}\mathbb{K}\langle n, x, S_n, D_x\rangle \,/\, \langle &S_n n - nS_n - S_n, D_x x - xD_x - 1,\\ &nx - xn, S_n D_x - D_x S_n, nD_x - D_x n, xS_n - S_n x\rangle.\end{aligned}$$

Informally speaking, this is the polynomial ring $\mathbb{K}[n, x, S_n, D_x]$ in four variables subject to the above commutation rules. We will prefer to allow division by the variables too, hence working in a structure that could—by abuse of notation—be denoted by $\mathbb{K}(n, x)[S_n, D_x]$. This is now a polynomial ring in the two indeterminates S_n and D_x, with coefficients being rational functions in n and x. Note that the noncommutativity is now hidden between the indeterminates of the polynomial ring and its coefficients. Such structures are called *Ore algebras*.

The two defining relations for the Bessel functions can now be written as elements of such an Ore algebra:

$$z^2D_z^2 + zD_z + (z^2 - \nu^2) \quad \text{and} \quad zS_\nu^2 - 2(\nu+1)S_\nu + z, \tag{5}$$

and are called *annihilating operators* for $J_\nu(z)$. These relations can be multiplied by ν or by z, they can be differentiated by z (corresponds to multiplication by D_z from the left), they can be shifted in n (which corresponds to multiplication by S_n from the left), and they still will be true. Hence every operator that lies in the left ideal generated by (5) will be an annihilating operator for $J_\nu(z)$. Or, the other way round, all annihilating operators of $J_\nu(z)$ form a left ideal in the corresponding Ore algebra.

Questions: How can we decide whether the operator $S_\nu D_z + \frac{\nu+1}{z} S_\nu - 1$, that corresponds to (3), lies in the left ideal generated by (5), and hence is a valid identity between Bessel functions? How can we check whether two given sets of operators generate the same annihilating ideal?

6 Gröbner bases

The above questions can be answered by means of *Gröbner bases*. This concept has been invented by Bruno Buchberger (the founder of RISC, see his PhD thesis [2]), and since then has been very successfully applied in various fields of mathematics. The original work deals with commutative polynomial rings only, and has been extended later to certain noncommutative polynomial rings as well.

We try to give an intuition why Gröbner bases are useful. For sake of simplicity we choose an example with commutative bivariate polynomials. We consider the ideal $I \trianglelefteq \mathbb{Q}[x, y]$ that is generated by $xy - 1$ and $x^2 + y + 1$. When working in multivariate polynomial rings it is essential to define a *monomial order*, i.e., a total order on the set of monomials that is compatible with multiplication. In this example we use a total degree order, breaking ties by the exponent of x. Informally speaking, a Gröbner basis is a unique representation of a polynomial ideal in terms of a generating set; it depends on the monomial order. In our example, the Gröbner basis of I with respect to total degree order is

$$G = \left\{y^2 + x + y,\, xy - 1,\, x^2 + y + 1\right\}.$$

Gröbner bases can be computed by Buchberger's algorithm.

Example 5. Compute the remainder of the division of $x^2 y$ by the ideal I. In other words, we are interested in the residue classes of $\mathbb{K}[x, y]$ modulo I. In some steps of the polynomial division procedure we can choose which generator we take for reduction. This might lead to different results as the following shows

$$x^2 y - x(xy - 1) = x \quad \text{or} \quad x^2 y - y(x^2 + y + 1) = -y^2 - y.$$

When using a Gröbner basis, the remainder of the polynomial division will be unique and independent of possible choices: taking the first element in G for performing another division step gives the remainder x also in the second case.

Note that by making the remainder unique, Gröbner bases solve the ideal membership problem: a polynomial is element of an ideal if and only if its remainder modulo a Gröbner basis of this ideal is zero.

Example 6. Consider the ideal $J \trianglelefteq \mathbb{Q}[x,y]$ that is generated by

$$\left\{x^3y^3 + y^3 - 2y^2 - 3x - 3y, y^4 + y^3 + y^2 + x + 2y, xy^2 + 2xy + y^2 + x - 2\right\}.$$

In which relation are I and J, e.g., $J \subset I$, $I = J$, or are they incomparable with respect to the subset relation? The Gröbner basis of J equals G revealing that indeed we have $I = J$.

Example 7. How can we compute the zero set of I, i.e., the set of common zeros in $\mathbb{C}^2$? Alternatively, we can ask: are there univariate polynomials contained in I? Also these questions can be answered by Gröbner bases. If $y \prec x$, the Gröbner basis of I with respect to *lexicographic order* is

$$\left\{y^3 + y^2 + 1,\ x + y^2 + y\right\}.$$

The first element depends only on y (in other words "x has been eliminated") and allows to compute the common zeros. Lexicographic order always gives a Gröbner basis in triangular form with respect to occurrence of the variables, and therefore is used for elimination problems. In fact, in the special case of linear polynomials, Buchberger's algorithm reduces to Gaussian elimination.

7 Applications of holonomic systems

Back to the Bessel examples. Running the noncommutative version of Buchberger's algorithm delivers a Gröbner basis for the ideal generated by (5):

$$\{zS_\nu + zD_z - \nu,\ z^2D_z^2 + zD_z + (z^2 - \nu^2)\}.$$

In order to prove identity (3), we just have to reduce it with the Gröbner basis! In the first division step, we can only use the first element of the Gröbner basis:

$$\begin{array}{lcll}
S_\nu D_z + \frac{\nu+1}{z}S_\nu - 1 & - & \frac{1}{z}D_z(zS_\nu + zD_z - \nu) & = \\
S_\nu D_z + \frac{\nu+1}{z}S_\nu - 1 & - & \frac{1}{z}((zD_z+1)S_\nu + (zD_z+1)D_z - \nu D_z) & = \\
S_\nu D_z + \frac{\nu+1}{z}S_\nu - 1 & - & (S_\nu D_z + \frac{1}{z}S_\nu + D_z^2 + \frac{1-\nu}{z}D_z) & = \\
-D_z^2 + \frac{\nu}{z}S_\nu + \frac{\nu-1}{z}D_z - 1 & & &
\end{array}$$

In the second step, only the second element of the Gröbner basis is eligible for reduction:

$$-D_z^2 + \tfrac{\nu}{z}S_\nu + \tfrac{\nu-1}{z}D_z - 1 \quad + \quad \tfrac{1}{z^2}(z^2D_z^2 + zD_z + (z^2-\nu^2)) =$$
$$\tfrac{\nu}{z}S_\nu + \tfrac{\nu}{z}D_z - \tfrac{\nu^2}{z^2}$$

Now it is obvious that a third reduction step delivers 0, since the above is just a multiple of the first Gröbner basis element by $\frac{\nu}{z^2}$. This means that the relation (3) lies in the left ideal generated by (5) and therefore is true.

Identity (4) is more involved: First because an integral appears, and second because the integrand consists not only of one Bessel function, but of a combination of those. Fortunately there are algorithms for performing *closure properties* of holonomic functions. Important closure properties are sum, product, algebraic substitution of continuous variables, and rational-linear substitution of discrete variables. This means, given an annihilating ideal for $J_n(z)$, we can compute an annihilating ideal for $J_m(ax)$. The closure property "product" then delivers an annihilating ideal for $J_m(ax)J_n(bx)$:

$$\begin{aligned}
\{&bxS_m + axS_n + xD_x - m - n,\\
&bD_b - axS_n - xD_x + n,\\
&aD_a + axS_n - n,\\
&2ax^2S_nD_x + x^2D_x^2 + 2axS_n + (x-2nx)D_x - a^2x^2 + b^2x^2 - m^2 + n^2,\\
&axS_n^2 + (-2n-2)S_n + ax,\\
&x^3D_x^3 + 3x^2D_x^2 + (2a^3x^3 - 2ab^2x^3 + 2am^2x - 2an^2x)S_n\\
&\quad + (3a^2x^3 + b^2x^3 - m^2x - 3n^2x + x)D_x\\
&\quad - 2a^2nx^2 + 2a^2x^2 + 2b^2nx^2 + 2b^2x^2 - 2m^2n + 2n^3\}.
\end{aligned}$$

Some examples of functions that are not holonomic in both n and x: $1/J_n(z)$ (division is not among the closure properties), $J_n(\sin(x))$ (the substitution $z \to \sin(x)$ is not algebraic), and $J_{n^2}(z)$ or $J_{\pi n}(z)$ (the substitutions for the discrete variable n are not rational-linear). In general, it is highly nontrivial to prove non-holonomicity!

The algorithms for executing closure properties make essential use of Gröbner bases (in fact, any annihilating ideal that is encountered here, is presented by its Gröbner basis). They have first been described in [3].

Now that we have a holonomic description of the integrand, we can care about the integration. As in Zeilberger's algorithm this is done by creative telescoping. Frédéric Chyzak has extended Zeilberger's algorithm to general holonomic functions [4]. Recall that for a hypergeometric function $f(n, k)$, we were able to express any shifted version $f(n+i, k+j)$ as a rational function times $f(n,k)$ itself. For holonomic functions, this is not true in general. However, we can reduce any shifted or differentiated version of the function to a linear combination of a finite set of base cases. This basis can be read off from the Gröbner basis of the annihilating ideal: it corresponds exactly to the monomials that cannot be reduced by the Gröbner basis (the residue classes). In our example, let $f(a,b,m,n,x) = J_m(ax)J_n(bx)$. Then

$$
\begin{aligned}
&\frac{\partial^{s+t+u}}{\partial a^s \partial b^t \partial x^u} f(a,b,m+i,n+j,x) = \\
&\quad r_1(a,b,m,n,x) f(a,b,m,n,x) + r_2(a,b,m,n,x) \frac{\partial}{\partial x} f(a,b,m,n,x) + \\
&\quad r_3(a,b,m,n,x) f(a,b,m,n+1,x) + r_4(a,b,m,n,x) \frac{\partial^2}{\partial x^2} f(a,b,m,n,x)
\end{aligned}
$$

for some rational functions $r_1, \ldots, r_4$. This corresponds to the monomials $\{1, D_x, S_n, D_x^2\}$ which cannot be reduced ("lie under the stairs") of the Gröbner basis (they can be found by investigating the *leading monomials* of the Gröbner basis elements, i.e., the maximal monomials w.r.t. the monomial order). For finding a recurrence in n for the integral, we therefore start with the ansatz

$$
\underbrace{p_0 + p_1 S_n + \cdots + p_d S_n^d}_{P} \quad - \quad D_x \cdot \underbrace{(q_1 + q_2 D_x + q_3 S_n + q_4 D_x^2)}_{Q} \tag{6}
$$

for unknowns $p_i \in \mathbb{K}(a,b,m,n)$ and $q_i \in \mathbb{K}(a,b,m,n,x)$. This ansatz encodes that we are looking for an antiderivative Q of P. We reduce this ansatz with the Gröbner basis obtaining some remainder (*normal form*):

$$
c_1 + c_2 D_x + c_3 S_n + c_4 D_x^2, \quad c_i \in \mathbb{K}(a,b,m,n,x)[p_0, \ldots, p_d].
$$

This step corresponds exactly to the rewriting in the hypergeometric case where we expressed for example $f(n+d,k)$ as a rational function multiple of $f(n,k)$. The condition that (6) is a valid relation for the integrand is equivalent to claiming that its remainder modulo the annihilating ideal is 0. Equating all coefficients c_i to zero yields a parameterized coupled system of linear differential equations of the form:

$$
\begin{aligned}
q_1' &= r_{1,1} q_1 + \cdots + r_{1,4} q_4 + r_1(a,b,m,n,x,p_0,\ldots,p_d) \\
&\vdots \\
q_4' &= r_{4,1} q_1 + \cdots + r_{4,4} q_4 + r_4(a,b,m,n,x,p_0,\ldots,p_d)
\end{aligned}
$$

where $r_{i,j} \in \mathbb{K}(a,b,m,n,x)$ and $r_i \in \mathbb{K}(a,b,m,n,x)[p_0,\dots,p_d]$. We just mention that there are algorithms for solving such systems, but don't go into detail here.

Finally, integrating (6) will deliver a recurrence of the form

$$p_0 F(a,b,m,n) + p_1 F(a,b,m,n+1) + \cdots + p_d F(a,b,m,n+d) = h(a,b,m,n)$$

where $F(a,b,m,n) = \int_0^\infty J_m(ax) J_n(bx)\,\mathrm{d}x$. Similarly, we can find a recurrence in m and differential equations in a and b, obtaining a holonomic system for the integral. It turns out that it equals exactly the holonomic system that closure properties deliver for the right-hand side (again by Gröbner basis reasoning).

8 Advanced applications of the HSA

This is the title of our PhD thesis [7]. Part of this work was to implement (in Mathematica) all the algorithms mentioned above, and related ones (noncommutative arithmetic with Ore polynomials and Buchberger's algorithm for these, closure properties for holonomic functions, Chyzak's algorithm, algorithms for finding rational solutions of linear difference or differential equations, uncoupling of systems of such equations, etc.). The package is named `HolonomicFunctions` and is freely available from the RISC combinatorics software page

http://www.risc.uni-linz.ac.at/research/combinat/software/

In the thesis, three "advanced applications" are presented:

- proof of a conjecture by Ira Gessel about the enumeration formula for certain lattice walks, see also [6],
- derivation of certain relations between basis functions that are used in finite element methods for numerical simulations (these basis functions are products of Legendre and Jacobi polynomials and hence holonomic),
- a computer proof of Stembridge's theorem about the counting formula of totally symmetric plane partitions.

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