Computer Algebra Methods for Holonomic Functions

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The RISC Combinatorics Group

RISC: Research Institute for Symbolic Computation

- leader of the combinatorics group: Prof. Dr. Peter Paule
- computer algebra
- symbolic summation / integration
- computer proofs
- cooperation with colleagues from numerics (SFB F013)

Introductory Examples (1)

Task: Find a closed form for the sum

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

$\longrightarrow$ Use `fastZeil` (by P. Paule and M. Schorn)!

Solution:

$$s(n) = \begin{cases} \frac{(n-1)!!}{n!!} & n \text{ even} \\ 0 & n \text{ odd} \end{cases}$$

Introductory Examples (2)

Task: Find a closed form for the double sum

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

$\longrightarrow$ Use `MultiSum` (by K. Wegschaider)!

Solution:

$$s(m,n) = \delta_{m,n}$$

Introductory Examples (3)

Task: Prove

$$\sum_{j=-\infty}^{\infty}(-1)^j q^{4j^2-3j}\begin{bmatrix}2n+1\\ n+j\end{bmatrix}_2=(q^{2n+2};q^2)_{n+1}\sum_{j=0}^{\infty}\frac{q^{2j^2+2j}}{(-q;q^2)_{j+1}}\begin{bmatrix}n\\ j\end{bmatrix}_2.$$

$\longrightarrow$ Use `qZeil` (by A. Riese), `qGeneratingFunctions` (by C.K.)!

Solution strategy:

- Find recurrences for both sides of the identity
- Compute a recurrence for the sum of both
- Check initial values

Introductory Examples (4)

Task: Find a closed form for the sum

$$s(n) = \sum_{k=0}^{n} \frac{(-1)^k \binom{n}{k} H_k}{(1+k)^2}$$

$\longrightarrow$ Use `Sigma` (by C. Schneider)!

Solution:

$$s(n) = \frac{-2H_n - (n+1)H_n^2 + (n+1)H_n^{(2)}}{2(n+1)^2}$$

Main Topic

Generalization to

- multivariate (holonomic) functions
- both discrete and continuous variables
- mixed difference-differential equations
- handling of “standard” and q-problems in the same framework

The main ingredients to achieve this are

- translation to pure algebra, i.e., to operator algebras (Ore algebras)
- noncommutative Gröbner bases

$\longrightarrow$ D. Zeilberger's “Holonomic Systems Approach” (1991), with extensions and refinements by F. Chyzak (1998)

Notation

Notation:

- $\mathbb{K}$: field of characteristic 0
- $\mathcal{F}$: a $\mathbb{K}$-algebra (of "functions")
- A_n: Weyl algebra
- annihilating operator of $f \in \mathcal{F}$: an operator $P \in A_n$ s.t. $Pf = 0$
- $\operatorname{Ann}_{A_n} f$: the ideal of annihilating operators of f in A_n

Definition: Ore Algebra (1)

Given $\sigma, \delta \in \mathrm{End}_{\mathbb{K}} \mathcal{F}$ with

$$\delta(fg) = \sigma(f)\delta(g) + \delta(f)g \quad \text{for all } f, g \in \mathcal{F} \quad \text{(skew Leibniz law)}$$

The endomorphism δ is called a *σ-derivation*.

Let $\mathbb{A}$ be a $\mathbb{K}$-subalgebra of $\mathcal{F}$ (e.g., $\mathbb{A} = \mathbb{K}[x]$ or $\mathbb{A} = \mathbb{K}(x)$) and assume that σ, δ restrict to a σ-derivation on $\mathbb{A}$.
Define the skew polynomial ring $\mathbb{O} = \mathbb{A}[\partial; \sigma, \delta]$:

- polynomials in ∂
- coefficients in $\mathbb{A}$
- usual addition
- product that makes use of the commutation rule

$$\partial a = \sigma(a)\partial + \delta(a) \text{ for all } a \in \mathbb{A}$$

Definition: Ore Algebra (2)

We turn $\mathcal{F}$ into an $\mathbb{O}$-module by defining a "multiplication" (action) between an element in $\mathbb{O}$ and $f \in \mathcal{F}$:

$$\begin{aligned} a \bullet f &= a \cdot f, \\ \partial \bullet f &= \delta(f). \end{aligned}$$

Remark: In special cases we define the action $\partial \bullet f = \sigma(f)$.

Of course, this process can be iterated.

Ore Algebra: Examples

Example 1: $\mathbb{A} = \mathbb{K}[x]$, $\sigma = 1$, $\delta = \frac{\mathrm{d}}{\mathrm{d}x}$.

Then $\mathbb{K}[x][D_x; 1, \frac{\mathrm{d}}{\mathrm{d}x}] = \mathbb{K}[x][D_x; 1, D_x]$ is the Weyl algebra A_1.

Example 2: $\mathbb{A} = \mathbb{K}[n]$, $\sigma(n) = n + 1$, $\sigma(c) = c$ for $c \in \mathbb{K}$, $\delta = 0$.

Then $\mathbb{K}[n][S_n; S_n, 0]$ is a shift algebra.

Example 3: $\mathbb{K}(n)[S_n; S_n, 0]$

Special functions (1)

A sequence $(P_n)_{n\in\mathbb{N}}$ of polynomials $P_n \in \mathbb{R}[x]$ is orthogonal if

$$\int_a^b \rho(x)P_m(x)P_n(x)\mathrm{d}x = 0 \quad \forall m,n\in\mathbb{N} \text{ s.t. } m \neq n$$

for a given interval $[a,b]$ and a weight function $\rho(x)$.

$\longrightarrow$ Start with the standard basis $\{x^n\}$ and do Gram-Schmidt.

Example: $a=-1$, $b=1$ and $\rho(x)=1$: Legendre polynomials.

$$\begin{aligned} P_0(x) &= 1 \\ P_1(x) &= x \\ P_2(x) &= \tfrac{1}{2}(3x^2-1) \\ P_3(x) &= \tfrac{1}{2}(5x^3-3x) \end{aligned}$$

Special functions (2)

Ore algebras are very well suited for representing special functions.

Example: Legendre polynomials $P_n(x)$.
Well-known formulae for Legendre polynomials:

$$(1-x^2)P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0,$$
$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x).$$

They translate to the following annihilating operators in the Ore algebra $\mathbb{K}[n,x][S_n;S_n,0][D_x;1,D_x]$:

$$(1-x^2)D_x^2 - 2xD_x + (n^2+n),$$
$$(n+2)S_n^2 - (2nx+3x)S_n + (n+1).$$

Definition: Holonomic function

Definition:
$f \in \mathcal{F}$ is said to be holonomic if $A_n / \operatorname{Ann}_{A_n} f$ is a holonomic module.

Properties of holonomic functions

Closure properties:

- sum
- product
- definite integration

Elimination property:
Given an ideal I in A_n s.t. A_n/I is holonomic; then for any choice of $n+1$ among the generators of A_n there exists a nonzero operator in I that depends only on these. In other words, we can eliminate $n-1$ variables.

Holonomy for sequences

Let $f(k_1, \ldots, k_r)$ be a sequence in $\mathbb{C}^{\mathbb{N}^r}$. The multivariate generating function of f is

$$F(x_1, \ldots, x_r) = \sum_{k_1=0}^{\infty} \cdots \sum_{k_r=0}^{\infty} f(k_1, \ldots, k_r) x_1^{k_1} \cdots x_r^{k_r}.$$

The sequence f is called holonomic if its generating function is a holonomic function.

$\longrightarrow$ The elimination property carries over!

Remark: Bernstein's inequality does not hold in the shift case.

Definite integration of holonomic functions (1)

Given: $\operatorname{Ann}_{\mathbb{O}} f$, the annihilator of a holonomic function $f(x,y)$ in the Ore algebra $\mathbb{O} = \mathbb{K}[x,y][D_x;1;D_x][D_y;1,D_y]$.
Find: The annihilator of $F(y) = \int_a^b f(x,y)\mathrm{d}x$
Since $\operatorname{Ann}_{\mathbb{O}} f$ is holonomic, there exists $P(y,D_x,D_y) \in \operatorname{Ann}_{\mathbb{O}} f$ that does not contain x.

$$P(y,D_x,D_y) = Q(y,D_y) + D_x R(y,D_x,D_y)$$

Performing the integration on $Pf = 0$ gives

$$Q(y,D_y)F(y) + [R(y,D_x,D_y)f(x,y)]_{x=a}^{x=b} = 0$$

Definite integration of holonomic functions (2)

Given: $\operatorname{Ann}_{\mathbb{O}} f$, the annihilator of a holonomic function $f(x, y)$ in the Ore algebra $\mathbb{O} = \mathbb{K}[x, y][D_x; 1; D_x][D_y; 1, D_y]$.

Find: The annihilator of $F(y) = \int_a^b f(x, y)\mathrm{d}x$

Find $P \in \operatorname{Ann}_{\mathbb{O}} f$ which can be written in the form

$$P(x, y, D_x, D_y) = Q(y, D_y) + D_x R(x, y, D_x, D_y)$$

$$\begin{aligned} 0 &= \int_a^b P(x, y, D_x, D_y) f(x, y)\mathrm{d}x \\ &= \int_a^b Q(y, D_y) f(x, y)\mathrm{d}x + \int_a^b D_x R(x, y, D_x, D_y) f(x, y)\mathrm{d}x \end{aligned}$$

Hence $Q(y, D_y)F(y) = 0$ (in the case of "natural boundaries")

The operator Q can be computed with Takayama's algorithm (noncommutative Gröbner bases over modules). The theory of holonomy guarantees that such an operator exists.

Definite summation of holonomic functions

Given: $\operatorname{Ann}_{\mathbb{O}} f$, the annihilator of a holonomic sequence $f(k,n)$ in the Ore algebra $\mathbb{O} = \mathbb{K}[k,n][S_k; S_k, 0][S_n; S_n, 0]$.
Find: The annihilator of $F(n) = \sum_k f(k,n)$
Find $P \in \operatorname{Ann} f$ which can be written in the form

$$P(k,n,S_k,S_n) = Q(n,S_n) + \Delta_k R(k,n,S_k,S_n)$$

$$\begin{aligned} 0 &= \sum_k P(k,n,S_k,S_n) f(k,n) \\ &= \sum_k Q(n,S_n) f(k,n) + \sum_k \Delta_k R(k,n,S_k,S_n) f(k,n) \end{aligned}$$

Hence $Q(n,S_n)F(n) = 0$ (in the case of "natural boundaries")

The operator Q can be computed with Takayama's algorithm (noncommutative Gröbner bases over modules). The theory of holonomy guarantees that such an operator exists.

Irresistible integral (Boros / Moll, 7.2.1)

Task: Compute the definite integral

$$F(a,m) = \int_0^\infty \frac{\mathrm{d}x}{(x^4 + 2ax^2 + 1)^{m+1}}, \quad a \in \mathbb{C}, m \in \mathbb{N}$$

$\longrightarrow$ Find an x-free annihilator of the integrand.

$\longrightarrow$ Or use Takayama's algorithm! Annihilator for the integral:

$$\{(4m+4)S_m - 2aD_a - 4m - 3, (4a^2-4)D_a^2 + (8ma+12a)D_a + 4m + 3\}$$

Solution:

$$F(a,m) = -\frac{(1+i)(-i)^m 2^{-m-1}\left(a^2-1\right)^{-\frac{m}{2}-\frac{1}{4}}\sqrt{\pi}Q_m^{m+\frac{1}{2}}(a)}{\Gamma(m+1)}$$

Jacobi Polynomials (1)

The Jacobi polynomials are defined by

$$P_n^{(a,b)}(x) = \sum_{k=0}^{\infty} \frac{(a+1)_n(-n)_k(n+a+b+1)_k}{n!(a+1)_k k!} \left(\frac{1-x}{2}\right)^k$$

The summand is both hypergeometric and hyperexponential.
Applying Takayama's algorithm gives an annihilator for $P_n^{(a,b)}(x)$:

$$\begin{aligned}
&\{(-2n^2 - 2an - 2bn - 4n - 2a - 2b - 2)S_n \\
&\quad +(ax^2 + bx^2 + 2nx^2 + 2x^2 - a - b - 2n - 2)D_x \\
&\quad +xa^2 + a^2 + na + 2bxa + 3nxa + 3xa + a - b^2 - b - bn \\
&\quad +b^2x + 2n^2x + 3bx + 3bnx + 4nx + 2x, \\
&\ (-a - b - n - 1)S_b + (x-1)D_x + (a + b + n + 1), \\
&\ (a + b + n + 1)S_a + (-x-1)D_x + (-a - b - n - 1), \\
&\ (1 - x^2)D_x^2 + (-xa - a + b - bx - 2x)D_x + (n^2 + an + bn + n)\}.
\end{aligned}$$

Jacobi polynomials (2)

Task: Prove (or even better: find!):

$$\begin{aligned}(2n+a+b)P_n^{(a,b-1)}(x) &= (n+a+b)P_n^{(a,b)}(x)\\ &\quad +(n+a)P_{n-1}^{(a,b)}(x),\\ (1-x)\frac{d}{dx}P_n^{(a,b)}(x) &= aP_n^{(a,b)}(x)-(n+a)P_n^{(a-1,b+1)}(x).\end{aligned}$$

Solution: Use Gröbner bases for elimination. We get:

$$(a+b+n+2)S_bS_n+(a+n+1)S_b-(a+b+2n+3)S_n,$$

$$(1-x)D_xS_a+(a+n+1)S_b-(a+1)S_a$$

∂-finite functions

Definition: Let $\mathbb{O}$ be an Ore algebra over some $\mathbb{K}$-algebra $\mathbb{A}$ (typically here $\mathbb{A} = \mathbb{K}(\mathbf{x})$. A left ideal I in $\mathbb{O}$ is called ∂-finite w.r.t. $\mathbb{O}$, if $\mathbb{O}/I$ is a finite dimensional vector space over $\mathbb{A}$.
A function $f \in \mathcal{F}$ is called ∂-finite w.r.t. $\mathbb{O}$ if it is annihilated by a ∂-finite ideal. We have $\mathbb{O}/\operatorname{Ann}_{\mathbb{O}} f \cong \mathbb{O} \cdot f$.

Example:

$$f(k,n) = \frac{1}{k^2 + n^2}$$

$f(n,k)$ is ∂-finite w.r.t. $\mathbb{Q}(k,n)[S_k; S_k, 0][S_n; S_n, 0]$.

$$I = \langle (k^2+n^2+2n+1)S_n - (k^2+n^2), (k^2+2k+n^2+1)S_k - (k^2+n^2) \rangle$$

Note: The sequence $f(k,n)$ is not holonomic!

∂-finite functions

Closure properties:

- sum
- product
- application of Ore operators
- algebraic substitution (only in the differential case!)

$\longrightarrow$ These closure properties can be executed effectively (using an extended version of the FGLM algorithm).

Remark: The annihilator of a ∂-finite function is usually not very difficult to compute.

holonomic vs. ∂-finite

Let

$$\begin{aligned} \mathbb{O}_r &= \mathbb{K}(x)[D_x; 1, D_x] \\ \mathbb{O}_p &= \mathbb{K}[x][D_x; 1, D_x]. \end{aligned}$$

Theorem (Kashiwara): An ideal I in $\mathbb{O}_r$ is ∂-finite if and only if $\mathbb{O}_p/(I \cap \mathbb{O}_p)$ is a holonomic module.

Remark: This applies only to the differential case.

Rational Resolution

Given a function f that is ∂-finite w.r.t. an Ore algebra $\mathbb{O}$.
Any function in $\mathbb{O} \cdot f$ can be written in normal form

$$\left(\sum_{\alpha \in V} \varphi_\alpha \partial^\alpha \right) \cdot f.$$

Task: Find an operator $Q \in \operatorname{Ann}_{\mathbb{O}} f$ with certain properties, e.g., such that $\partial Q - 1 = 0$ (indefinite integration).

Algorithm:

- compute a Gröbner basis G for $\operatorname{Ann}_{\mathbb{O}} f$
- make an ansatz for Q with undetermined coefficients
- reduce the ansatz with G, i.e., compute the normal form
- all coefficients of the normal form must be zero
- solve the resulting system

Integrated Jacobi polynomials (1)

Define

$$\begin{aligned} p_n^a(x) &= \sum_{k=0}^{\infty} \frac{(a+1)_n(-n)_k(n+a+1)_k}{n!(a+1)_k k!} \left(\frac{1-x}{2}\right)^k, \\ \hat{p}_n^a(x) &= \int_{-1}^{x} p_{n-1}^a(y)\mathsf{d}y. \end{aligned}$$

Task: Express $\hat{p}_n^a(x)$ in terms of $p_{n-1}^a(x)$ and $p_n^{a-2}(x)$.

Ansatz: $\hat{p}_{n+1}^{a+2}(x) = Q \cdot p_n^a(x)$ with $Q = \varphi_1(x)S_a^2 + \varphi_2(x)S_n$.

Integrated Jacobi polynomials (2)

Ansatz: $\hat{p}_{n+1}^{a+2}(x) = Q \cdot p_n^a(x)$ with $Q = \varphi_1(x) S_a^2 + \varphi_2(x) S_n$.

Solution:

- compute a Gröbner basis G for $\operatorname{Ann} p_n^a$
- $\frac{\mathrm{d}}{\mathrm{d}x} \hat{p}_{n+1}^{a+2} = p_n^{a+2}$ translates to $0 = D_x Q - S_a^2 =: Z$
- compute the normal form of Z by reducing it with G
- all coefficients of the normal form must be zero
- solve the system of coupled differential equations for rational solutions: use `OreSys` (by S. Gerhold) for uncoupling.

We find

$$(a+1)\hat{p}_{n+1}^{a+2}(x) = (1-x) p_n^{a+2}(x) + 2 p_{n+1}^a(x).$$

Jacobi polynomials (3)

Task: Prove (or even better: find!):

$$\begin{aligned}(2n+a+b)P_n^{(a,b-1)}(x) &= (n+a+b)P_n^{(a,b)}(x)\\ &\quad +(n+a)P_{n-1}^{(a,b)}(x),\\ (1-x)\frac{d}{dx}P_n^{(a,b)}(x) &= aP_n^{(a,b)}(x)-(n+a)P_n^{(a-1,b+1)}(x).\end{aligned}$$

Solution: Make the following ansaetze:

$$\varphi_1 S_b + \varphi_2 S_n + \varphi_3 S_b S_n = 0$$
$$\varphi_1 S_a + \varphi_2 S_b + \varphi_3 S_a D_x = 0$$

Thanks for your attention!