Computer Algebra Tools for Summation and Integration

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RISC

(Research Institute for Symbolic Computation)

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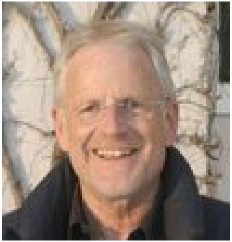

Founded by Bruno Buchberger in 1989

Overview of this talk

Introduction to

- holonomic and ∂-finite functions
- creative telescoping
- our Mathematica package `HolonomicFunctions`

Applications in

- numerical analysis
- combinatorics
- quantum topology
- particle physics

Some notation

- $\mathbb{K}$: computable field, usually $\mathbb{K} = \mathbb{Q}$
- D_x operator "partial derivative w.r.t. x",
  i.e., $D_x(f(x)) = f'(x)$
- x is called a *continuous variable*.
- S_n: shift operator in n,
  i.e., $S_n(f(n)) = f(n+1)$
- n is called a *discrete variable*.
- $\mathbb{O}$: an *Ore algebra* (operator algebra)
- $\operatorname{Ann}_{\mathbb{O}} f = \{P \in \mathbb{O} : P(f) = 0\}$: annihilator of the function f

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Note: noncommutative multiplication

$$D_x x = x D_x + 1 \quad \text{and} \quad S_n n = n S_n + S_n$$

or more general

$$D_x \cdot a(x) = a(x) D_x + a'(x) \quad \text{and} \quad S_n a(n) = a(n+1) S_n$$

∂-finite functions

Definition: Let

- $n_1, \ldots, n_a$ be a set of discrete variables
- $x_1, \ldots, x_b$ be a set of continuous variables
- $\mathbb{F} = \mathbb{K}(n_1, \ldots, n_a, x_1, \ldots, x_b)$
- $\mathbb{O} = \mathbb{F}[S_{n_1}, \ldots, S_{n_a}, D_{x_1}, \ldots, D_{x_b}]$ be the Ore algebra containing the corresponding operators.

Then a function $f(n_1, \ldots, n_a, x_1, \ldots, x_b)$ is called ∂-finite w.r.t. $\mathbb{O}$ if $\mathbb{O}/\operatorname{Ann}_{\mathbb{O}} f$ is a finite-dimensional $\mathbb{F}$-vector space.

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In other words, f is ∂-finite if all its derivatives and shifts span a finite-dimensional $\mathbb{F}$-vector space.

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We omit the more complicated definition for the closely related concept of *holonomic functions*.

∂-finite functions: Example

All derivatives (w.r.t. x and y) of $\sin\left(\frac{x+y}{x-y}\right)$ are of the form

$$r_1(x,y)\sin\left(\frac{x+y}{x-y}\right) + r_2(x,y)\cos\left(\frac{x+y}{x-y}\right), \quad r_1, r_2 \in \mathbb{Q}(x,y)$$

e.g.,

$$D_x^3 D_y^2 \bullet \sin\left(\frac{x+y}{x-y}\right) = \frac{32\left(3x^4+12yx^3-30y^2x^2-4y^3x+9y^4\right)}{(x-y)^9}\sin\left(\frac{x+y}{x-y}\right) - \frac{16\left(6x^5-33yx^4+80y^3x^2-54y^4x+3y^5\right)}{(x-y)^{10}}\cos\left(\frac{x+y}{x-y}\right)$$

Annihilating ideals

All operators that annihilate a function f form a *left ideal* in the corresponding operator algebra $\mathbb{O}$.

We represent such left ideals by their *Gröbner bases*; this allows us

- to decide the equality of two ideals
- to decide ideal membership
- to eliminate certain operators or variables

A function is ∂-finite w.r.t. $\mathbb{O}$ if $\operatorname{Ann}_{\mathbb{O}} f$ is a zero-dimensional left ideal in $\mathbb{O}$.

Example: A Gröbner basis for the annihilator of $\sin\left(\frac{x+y}{x-y}\right)$ in $\mathbb{O} = \mathbb{Q}(x, y)[D_x, D_y]$ is given by

$$\{xD_x + yD_y, (x-y)^4 D_y^2 - 2(x-y)^3 D_y + 4x^2\}.$$

Closure properties of ∂-finite functions

Closure properties:

- sum
- product
- application of an Ore operator
- algebraic substitution (of a continuous variable)
- subsequence / $\mathbb{Q}$-linear substitution (of a discrete variable)
- definite summation and integration

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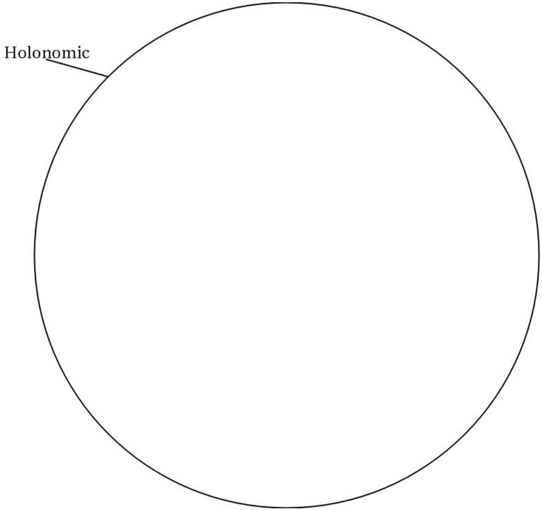
In contrast to holonomic closure properties, the closure properties for ∂-finite functions can be computed quite easily (using linear algebra and an FGLM-like algorithm).

The Universe of Holonomic Functions



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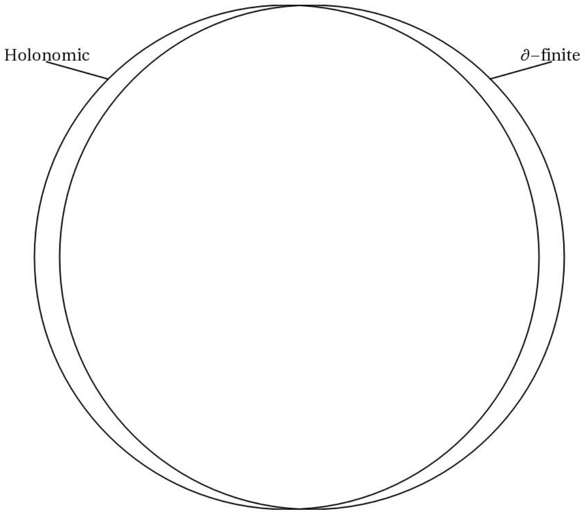

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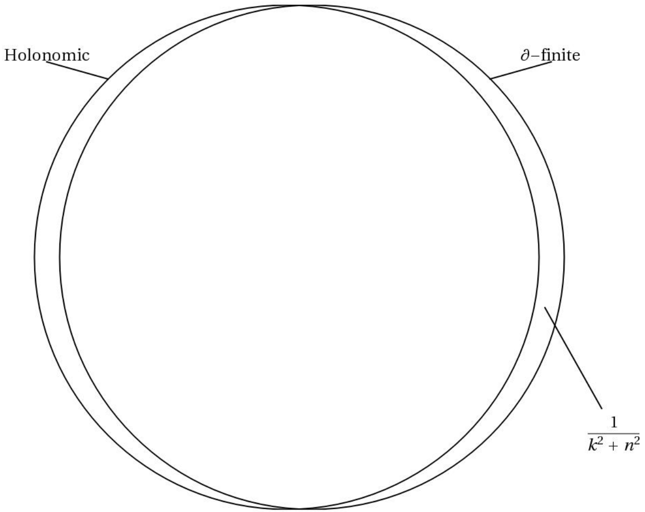

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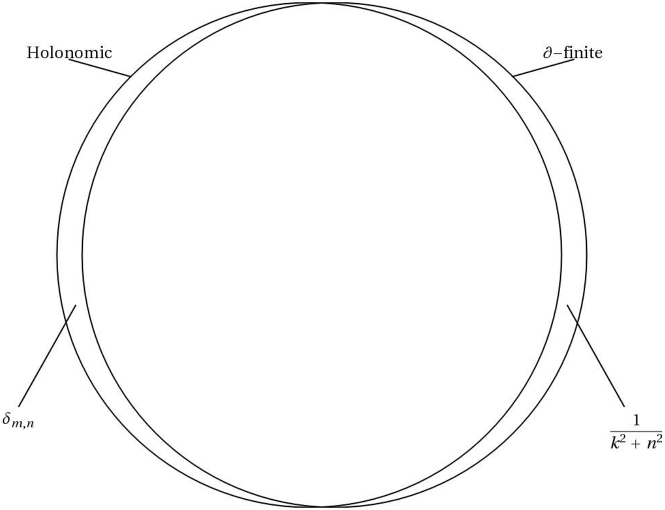

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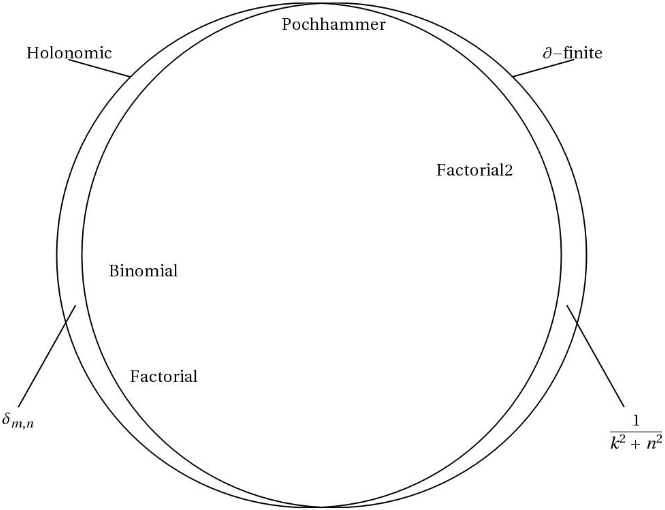

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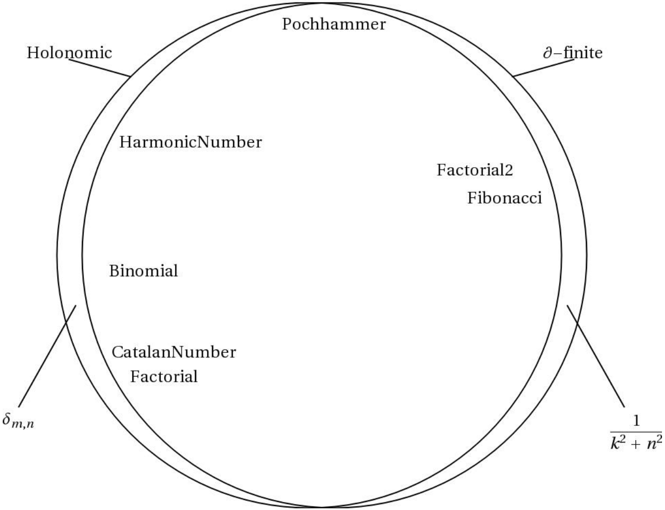

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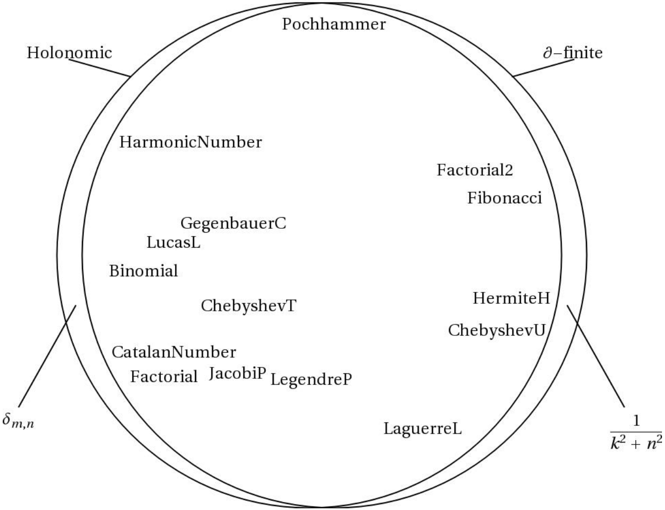

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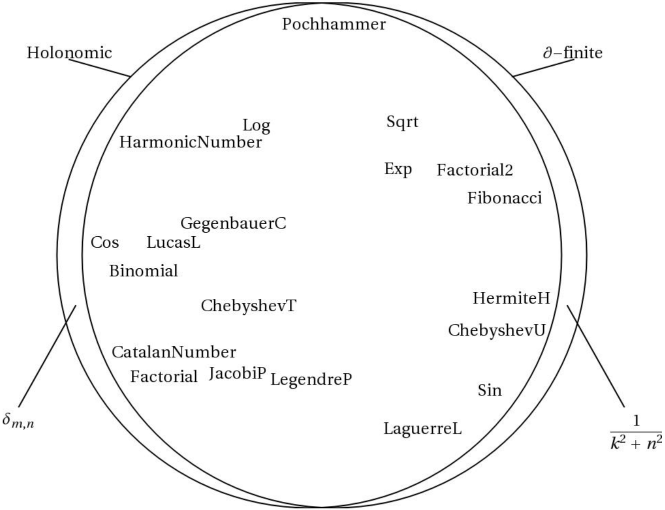

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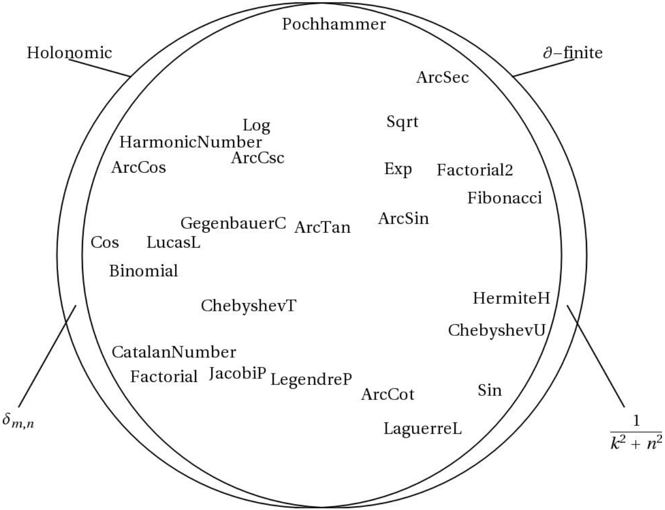

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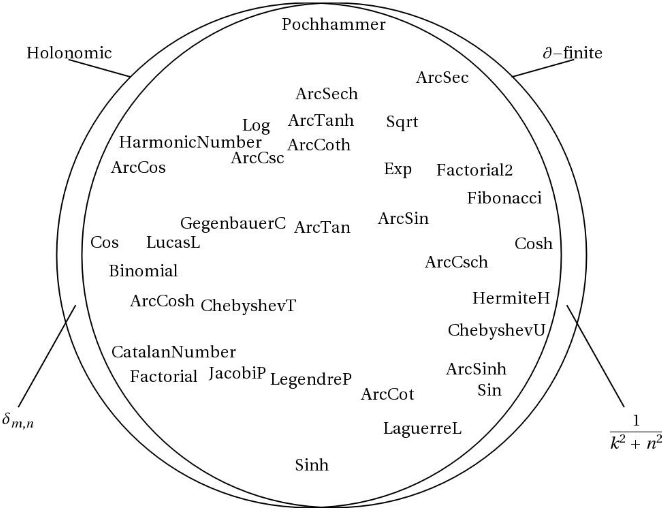

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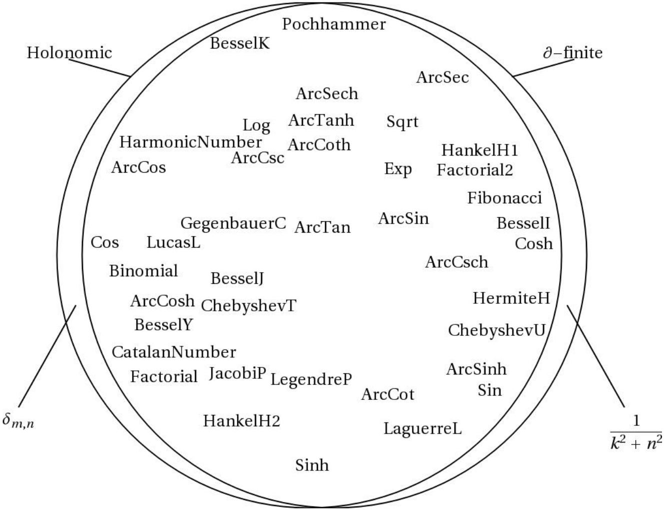

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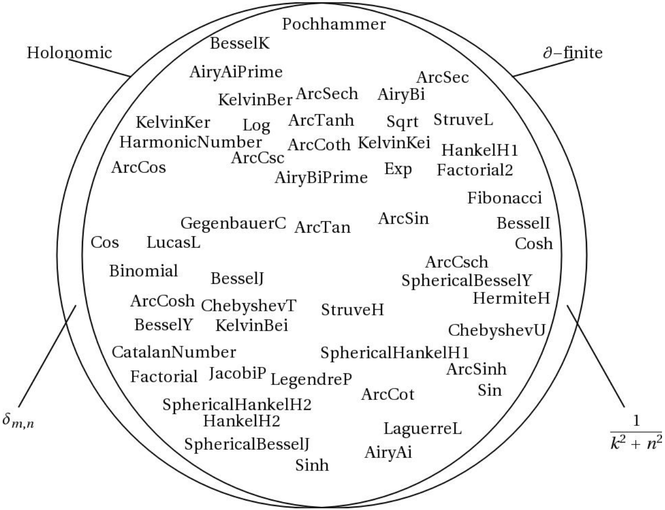

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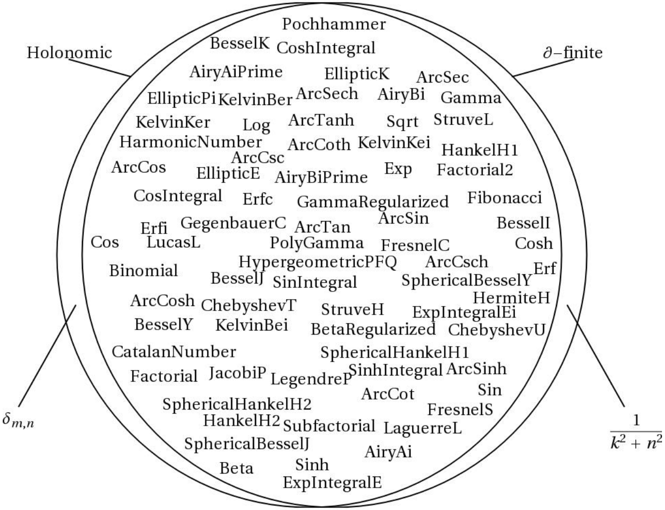

Application 1

Relations for speeding up FEM

Problem setting

Simulate the propagation of electromagnetic waves using the Maxwell equations

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \operatorname{curl} E, \quad \frac{\mathrm{d}E}{\mathrm{d}t} = -\operatorname{curl} H$$

where H and E are the magnetic and the electric field respectively. Define basis functions (in 2D) in order to approximate the solution:

$\varphi_{i,j}(x,y) :=$

$(1-x)^i P_j^{(2i+1,0)}(2x-1) P_i\left(\frac{2y}{1-x} - 1\right)$

Problem: need to represent the partial derivatives of $\varphi_{i,j}(x,y)$ in the original basis (i.e., as linear combinations of shifts of the $\varphi_{i,j}(x,y)$ itself)

The Gröbner approach

The numerists need a relation of the form

$$\sum_{(k,l)\in A} a_{k,l}(i,j)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i+k,j+l}(x,y) = \sum_{(m,n)\in B} b_{m,n}(i,j)\varphi_{i+m,j+n}(x,y),$$

that is free of x and y (and similarly for $\frac{\mathrm{d}}{\mathrm{d}y}$).

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- consider the operators D_x, S_i, and S_j
- basis functions $\varphi_{i,j}(x,y)$ are ∂-finite with respect to them
- compute generators of an annihilating left ideal for $\varphi_{i,j}(x,y)$
- represent them in the algebra $\mathbb{Q}(i,j)[x,y][D_x;1,D_x][S_i;S_i,0][S_j;S_j,0]$
- compute a Gröbner basis in order to eliminate x and y

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- compute a Gröbner basis in order to eliminate x and y
- takes very long, interrupt as soon as a desired operator is found
- result is quite big (2 pages of output)
- because of "extension/contraction" we can not be sure that we obtain the smallest operator

The ansatz approach

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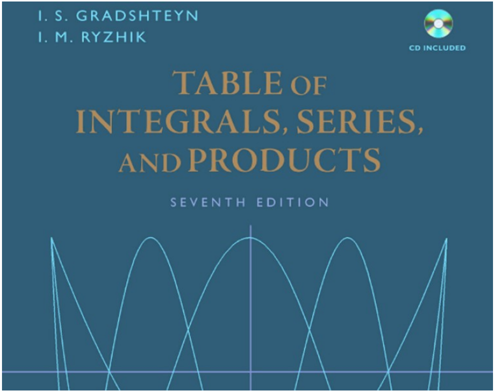
that is free of x and y (and similarly for $\frac{\mathrm{d}}{\mathrm{d}y}$).

- work in the algebra $\mathbb{Q}(i,j,x,y)[D_x;1,D_x][S_i;S_i,0][S_j;S_j,0]$
- compute a Gröbner basis G of a ∂-finite annihilating ideal for $\varphi_{i,j}(x,y)$
- choose index sets A and B
- reduce the above ansatz with G
- do coefficient comparison with respect to x and y
- solve the resulting linear system for $a_{k,l}, b_{m,n} \in \mathbb{Q}(i,j)$
- can find the "smallest" relation
- certain optimizations (e.g., using homomorphic images) reduce the computation time to a few seconds

Application 2

Special Function Identities



Creative telescoping

- can treat symbolic sums and integrals
- delivers a recurrence / differential equation / annihilating ideal
- for summation of $f(k, n_1, \ldots, n_a)$ w.r.t. k find an operator of the form

$$Q(n_1, \ldots, n_a, S_{n_1}, \ldots, S_{n_a}) + (S_k - 1) R(k, n_1, \ldots, n_a, S_k, S_{n_1}, \ldots, S_{n_a})$$

- for integrating $f(t, x_1, \ldots, x_b)$ w.r.t. t find an operator of the form

$$Q(x_1, \ldots, x_b, D_{x_1}, \ldots, D_{x_b}) + D_t R(t, x_1, \ldots, x_b, D_t, D_{x_1}, \ldots, D_{x_b})$$

Chyzak's extension of Zeilberger's fast algorithm

Example: integrate a function in two continuous variables.

Given: $\mathrm{Ann}_{\mathbb{O}}\, f$, the annihilator of a ∂-finite function $f(x, y)$ in the Ore algebra $\mathbb{O} = \mathbb{K}(x, y)[D_x, D_y]$.
Find: Operators $Q(y, D_y)$ and $R(x, y, D_x, D_y)$ such that $Q + D_x \cdot R \in \mathrm{Ann}_{\mathbb{O}}\, f$.

1. compute a Gröbner basis G of $\mathrm{Ann}_{\mathbb{O}}\, f$ in order to know the set $U = \{u_1, \ldots, u_k\}$ of monomials that can not be reduced by $\mathrm{Ann}_{\mathbb{O}}\, f$, i.e., the elements under the stairs of G
2. make an ansatz for $Q(y, D_y) = \sum_{i=0}^{d} \eta_i(y) D_y^i$ and $R(x, y, D_x, D_y) = \sum_{j=1}^{k} \phi_j(x, y) u_j$
3. reduce $Q + D_x \cdot R$ with G and set all coefficients to zero
4. solve the corresponding coupled system of differential equations (for rational solutions)
5. if there is no solution, increase d

Some special function identities

$$\sum_{k=0}^{n} \binom{n}{k}^2 \binom{k+n}{k}^2 = \sum_{k=0}^{n} \binom{n}{k} \binom{k+n}{k} \sum_{j=0}^{k} \binom{k}{j}^3 \tag{1}$$

$$\int_0^\infty \frac{1}{(x^4+2ax^2+1)^{m+1}}\,\mathrm{d}x = \frac{\pi P_m^{(m+\frac{1}{2},-m-\frac{1}{2})}(a)}{2^{m+\frac{3}{2}}(a+1)^{m+\frac{1}{2}}} \tag{2}$$

$$e^{-x}x^{a/2}n!L_n^a(x) = \int_0^\infty e^{-t}t^{\frac{a}{2}+n}J_a\left(2\sqrt{tx}\right)\,\mathrm{d}t \tag{3}$$

$$\int_{-\infty}^{\infty}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{H_m(x)H_n(x)r^m s^n e^{-x^2}}{m!n!}\,\mathrm{d}x = \sqrt{\pi}e^{2rs} \tag{4}$$

$$\int_{-1}^{1}\left(1-x^2\right)^{\nu-\frac{1}{2}} e^{iax}C_n^{(\nu)}(x)\,\mathrm{d}x = \frac{\pi 2^{1-\nu}i^n\Gamma(n+2\nu)a^{-\nu}J_{n+\nu}(a)}{n!\Gamma(\nu)} \tag{5}$$

$$\frac{\sin\left(\sqrt{z^2+2tz}\right)}{z} = \sum_{n=0}^{\infty}\frac{(-t)^n y_{n-1}(z)}{n!} \tag{6}$$

Computer proof of a special function identity

We consider identity (3):

$$e^{-x}x^{a/2}n!L_n^a(x) = \int_0^\infty e^{-t}t^{\frac{a}{2}+n}J_a\left(2\sqrt{tx}\right)\,\mathrm{d}t.$$

```
Annihilator[Exp[-x]*x^(a/2)*n!*LaguerreL[n, a, x],
            {S[a], S[n], Der[x]}]
```

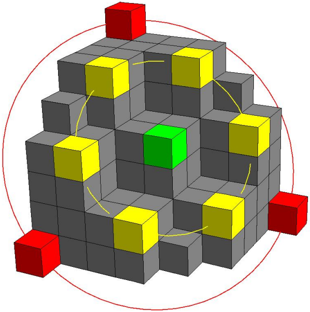
$$\{2S_n - 2xD_x + (-a-2n-2),\\ 4x^2D_x^2 + (4x^2+4x)D_x + (-a^2+2ax+4nx+4x),\\ 2xS_a^2 + (2ax+2x^2+2x)D_x + (-a^2+ax-a+2nx+2x)\}$$

```
CreativeTelescoping[Exp[-t]*t^(a/2+n)*BesselJ[a,2*Sqrt[t*x]
                    Der[t], {S[a], S[n], Der[x]}]
```

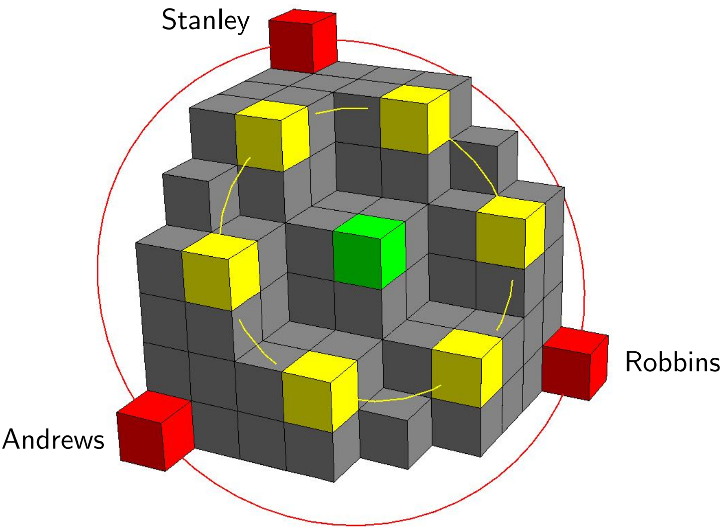
$$\{\{-2S_n + 2xD_x + (a+2n+2),\\ 4x^2D_x^2 + (4x^2+4x)D_x + (-a^2+2ax+4nx+4x),\\ 2xS_a^2 + (2ax+2x^2+2x)D_x + (-a^2+ax-a+2nx+2x)\},\\ \{-2t, -4tx, -2tx\}\}$$

Application 3

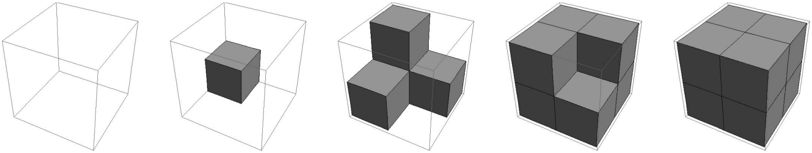
Proof of the q-TSPP conjecture



q-TSPP



Let $T(n)$ denote set of TSPPs with largest part at most n.



q^0 $\quad$ q^1 $\quad$ q^2 $\quad$ q^3 $\quad$ q^4

Andrews-Robbins q-TSPP conjecture:

$$\sum_{\pi \in T(n)} q^{|\pi/S_3|} = \prod_{1 \leq i \leq j \leq k \leq n} \frac{1 - q^{i+j+k-1}}{1 - q^{i+j+k-2}}$$

For $q = 1$:

$$|T(n)| = \prod_{1 \leq i \leq j \leq k \leq n} \frac{i+j+k-1}{i+j+k-2}$$ (Stembridge)

The determinant

Reduction by Soichi Okada:

The q-TSPP conjecture is true if

$$\det(a_{i,j})_{1\le i,j\le n} = \prod_{1\le i\le j\le k\le n} \left(\frac{1-q^{i+j+k-1}}{1-q^{i+j+k-2}} \right)^2 =: b_n$$

where

$$a_{i,j} := q^{i+j-1} \left(\begin{bmatrix} i+j-2 \\ i-1 \end{bmatrix}_q + q \begin{bmatrix} i+j-1 \\ i \end{bmatrix}_q \right) + (1+q^i)\delta_{i,j} - \delta_{i,j+1}$$

where

$$\begin{bmatrix} n \\ k \end{bmatrix}_q := \frac{(1-q^n)(1-q^{n-1})\cdots(1-q^{n-k+1})}{(1-q^k)(1-q^{k-1})\cdots(1-q)}.$$

The holonomic ansatz

Second reduction by Doron Zeilberger:

"Pull out of the hat" a discrete function $c_{n,j}$ and prove

$$c_{n,n} = 1 \qquad (n \geq 1),$$

$$\sum_{j=1}^{n} c_{n,j} a_{i,j} = 0 \qquad (1 \leq i < n),$$

$$\sum_{j=1}^{n} c_{n,j} a_{n,j} = \frac{b_n}{b_{n-1}} \qquad (n \geq 1).$$

Then $\det(a_{i,j})_{1 \leq i,j \leq n} = b_n$ holds.

The result. . .

. . . is about 7GB large (corresponding to some million printed pages).

A short version will soon appear in PNAS (Proceedings of the National Academy of Sciences of the United States of America):

Christoph Koutschan, Manuel Kauers, Doron Zeilberger:
A proof of George Andrews' and David Robbins' q-TSPP conjecture

Application 4

Quantum Topology and Knot Theory

A multiple sum

While studying invariants of such knots, Stavros Garoufalidis asked me to evaluate the following sum:

$$\sum_{k=0}^{2n}(2k+1)\left((1-)^k a(k,n)\right)^s$$

with

$$a(k,n) = \sum_{j=\max(3n,k+2n)}^{\min(4n,k+3n)} (-1)^j \binom{j+1}{k+2n+1}\binom{k}{j-3n}^2\binom{2n-k}{4n-j}.$$

The package `HolonomicFunctions` can compute the recurrence for the sum up to $s = 6$. This recurrence has order 12, coefficient degrees about 500 and integer coefficients with several hundred decimal digits.

Application 5

Particle Physics

A Feynman integral

Johannes Blümlein and his colleagues from DESY are studying integrals like the following:

$$\int_0^1 \int_0^1 \frac{w^{-1-\varepsilon/2}(1-z)^{\varepsilon/2} z^{-\varepsilon/2}}{(z+w-wz)^{1-\varepsilon}} \left(1 - w^{n+1} - (1-w)^{n+1}\right) \mathrm{d}w \, \mathrm{d}z$$

The physicists are interested in a recurrence in n for this integral. Such a recurrence can be obtained by means of creative telescoping.