

# Selected Applications of Symbolic Summation and Integration

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Johann Radon Institute for Computational and Applied Mathematics (RICAM)  
Austrian Academy of Sciences

November 5, 2012  
Radon Seminar, Linz



## Short Curriculum Vitae

- 1999 – 2005 Undergraduate studies in computer science and mathematics, University of Erlangen-Nürnberg, Germany.
- 2005 – 2009 Ph.D. studies in symbolic computation at RISC, Johannes Kepler University Linz, Austria.
- 2009 – 2010 Postdoc at Tulane University, New Orleans, USA.
- 2010 – 2011 Postdoc at the Research Institute for Symbolic Computation (RISC), Linz.
- 2011 – 2012 Postdoc at “Institut National de Recherche en Informatique et en Automatique” (INRIA), Paris, France.
- 2012 – Postdoc at the Radon Institute for Computational and Applied Mathematics (RICAM), Linz.

## Research Interests and Scientific Results

- Algorithmic manipulation of holonomic/ $\partial$ -finite functions
  - Data structure: o.d.e.'s and recurrences plus initial values
  - Linear (homogeneous) equations with polynomial coefficients
  - Closure properties
  - Symbolic summation and integration
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- Applications of the holonomic systems approach
  - Combinatorics
  - Numerical analysis (FEM)
  - Quantum Topology
  - Physics

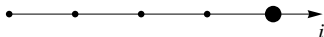
## Example: the Legendre Polynomials $P_n(x)$ are $\partial$ -Finite

This family of (orthogonal) polynomials is a solution of the differential equation

$$(x^2 - 1)P_n''(x) + 2xP_n'(x) - n(n + 1)P_n(x) = 0.$$

Consider the set  $\{P_n^{(i)}(x) : i \geq 0\}$ .

$$P_n^{(4)}(x) =$$



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$$\begin{aligned} P_n^{(4)}(x) = & \\ & \frac{n^2x^2 - n^2 + nx^2 - n + 18x^2 + 6}{(x^2 - 1)^2} P_n''(x) \\ & - \frac{6(n-1)(n+2)x}{(x^2 - 1)^2} P_n'(x) \end{aligned}$$



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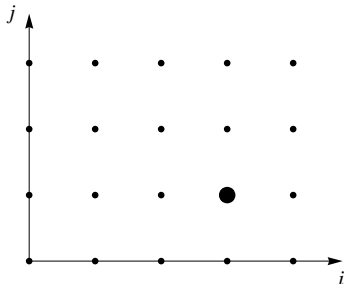
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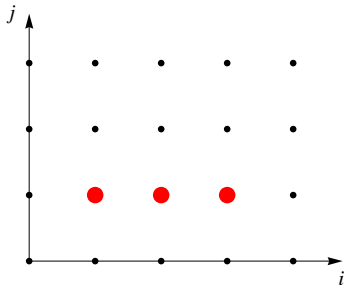
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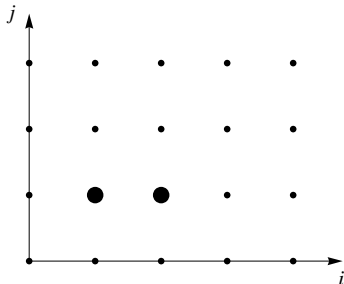
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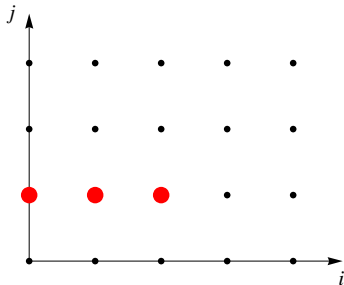
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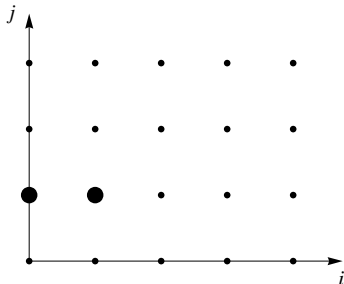
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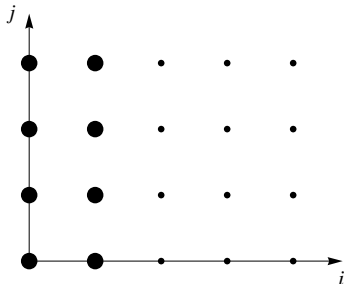
$$P_{n+1}^{(3)}(x) = \frac{(n^2x^2 - n^2 + 3nx^2 - 3n + 8x^2)}{(x^2 - 1)^2} P_{n+1}'(x) - \frac{4(n^2x + 3nx + 2x)}{(x^2 - 1)^2} P_{n+1}(x)$$

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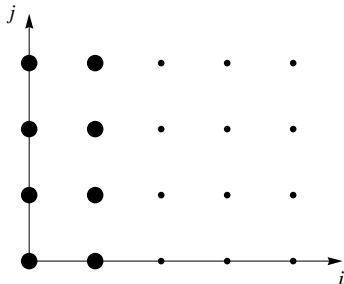
The Legendre polynomials can be defined recursively:

$$P_0(x) = 1$$

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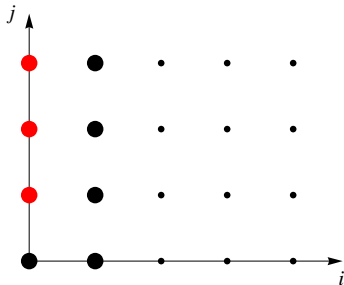
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$$P_{n+3}(x) =$$

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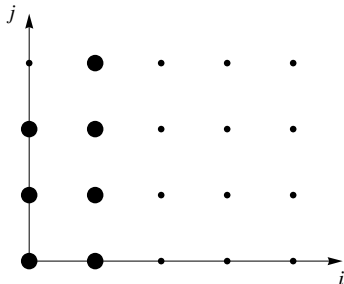
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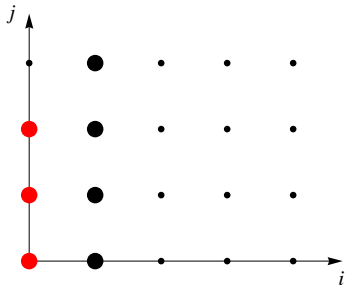
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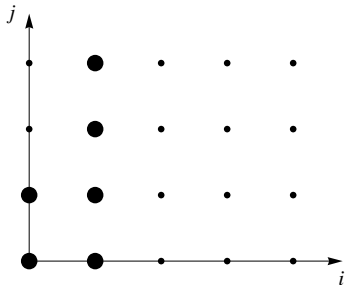
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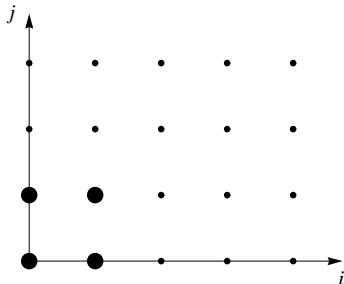
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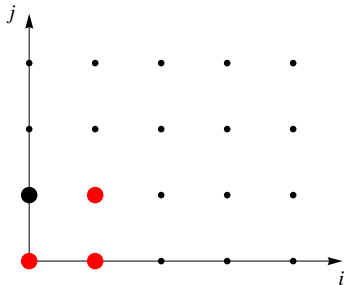
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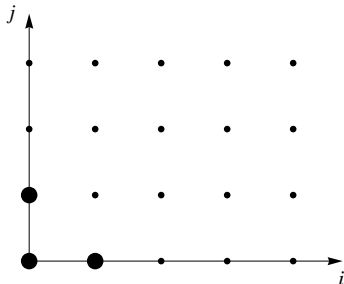
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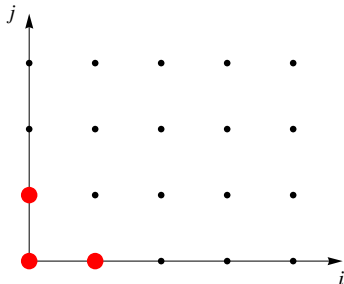
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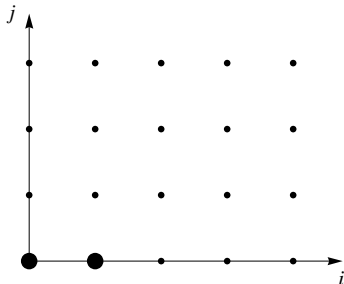
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→  $P_n(x)$  is  $\partial$ -finite w.r.t.  $n$  and  $x$  (of rank 2).

## Algebraic Setting

Write differential/difference equations in operator notation:

- shift operator  $S_v$ :  $S_v f(v) = f(v + 1)$
- partial derivative  $D_v$ :  $D_v f(v) = \frac{d}{dv} f(v)$
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**Example 2:** The three-term recurrence

$$nP_n(x) = (2n - 1)xP_{n-1}(x) - (n - 1)P_{n-2}(x)$$

is written as

$$(n + 2)S_n^2 - (2n + 3)xS_n + (n + 1).$$

# Operator Algebra

Noncommutative multiplication

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

or more general

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

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Such operators form an **Ore algebra**

$$\mathbb{K}(v, w, \dots) \langle \partial_v, \partial_w, \dots \rangle,$$

i.e., multivariate polynomials in the  $\partial$ 's with coefficients being rational functions in  $v, w, \dots$ , where  $\mathbb{K}$  is a computable field of characteristic 0 (i.e., containing  $\mathbb{Q}$ ).

## Annihilating Ideals

Let now  $\mathbb{D}$  be such an Ore algebra. The set

$$\text{Ann}_{\mathbb{D}} f := \{P \in \mathbb{D} : P(f) = 0\}$$

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- $r(x) \cdot \text{Eq}_1$  corresponds to  $r(x) \cdot P$
- $\frac{d}{dx} \text{Eq}_1$  corresponds to  $D_x \cdot P$
- $\text{Eq}_1|_{n \rightarrow n+1}$  corresponds to  $S_n \cdot P$

are also valid equations for  $f$ .

## Annihilating Ideals

Let now  $\mathbb{O}$  be such an Ore algebra. The set

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- $\text{Eq}_{q_1} + \text{Eq}_{q_2}$  corresponds to  $P + Q$
- $r(x) \cdot \text{Eq}_{q_1}$  corresponds to  $r(x) \cdot P$
- $\frac{d}{dx} \text{Eq}_{q_1}$  corresponds to  $D_x \cdot P$
- $\text{Eq}_{q_1}|_{n \rightarrow n+1}$  corresponds to  $S_n \cdot P$

are also valid equations for  $f$ . More generally,

$$\begin{aligned} P, Q \in \text{Ann}_{\mathbb{O}} f &\implies P + Q \in \text{Ann}_{\mathbb{O}} f \\ L \in \mathbb{O}, P \in \text{Ann}_{\mathbb{O}} f &\implies L \cdot P \in \text{Ann}_{\mathbb{O}} f \end{aligned}$$

which states that  $\text{Ann}_{\mathbb{O}} f$  is a **left ideal** in  $\mathbb{O}$ .

## Definition: $\partial$ -Finite Function

Let  $\mathbb{D} = \mathbb{K}(v, w, \dots) \langle \partial_v, \partial_w, \dots \rangle$  be an Ore algebra.

A function  $f$  is  $\partial$ -finite w.r.t.  $\mathbb{D}$  if all its shifts and derivatives

$$\mathbb{D}(f) = \{P(f) : P \in \mathbb{D}\}$$

form a finite-dimensional  $\mathbb{K}(v, w, \dots)$ -vector space.

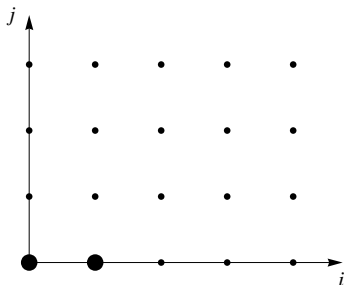
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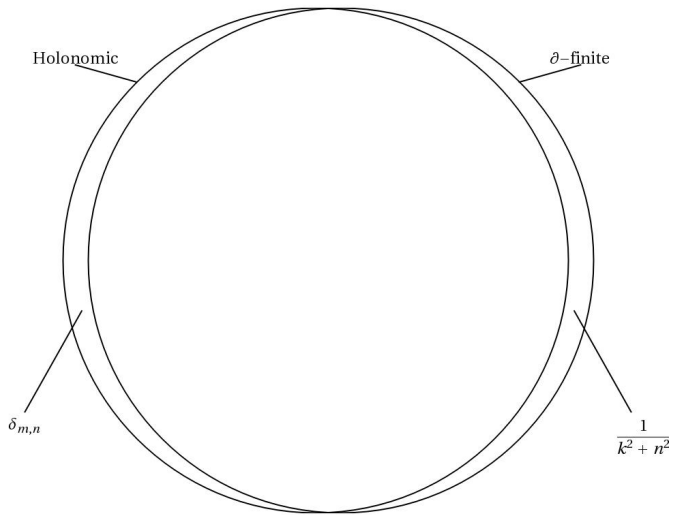
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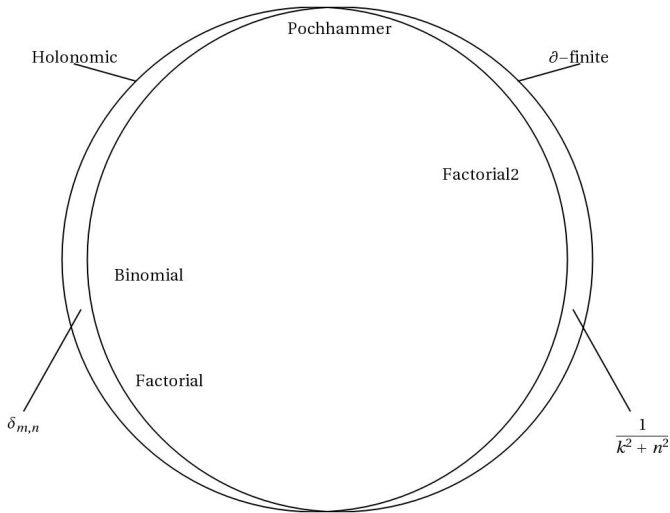
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The definition of “holonomic” is a bit technical, so we skip it here.

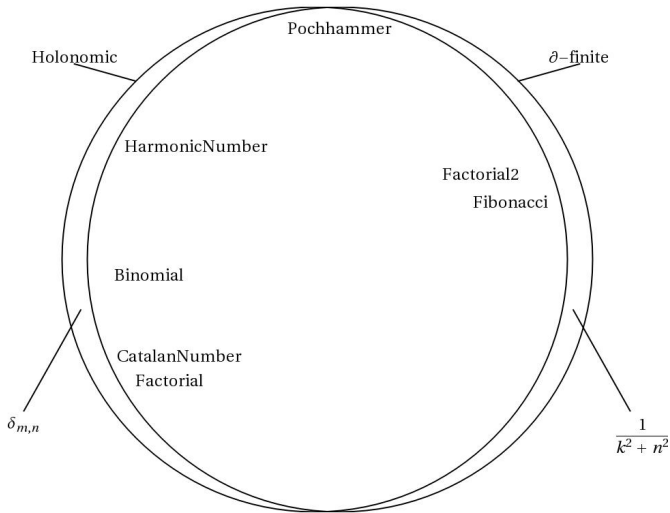
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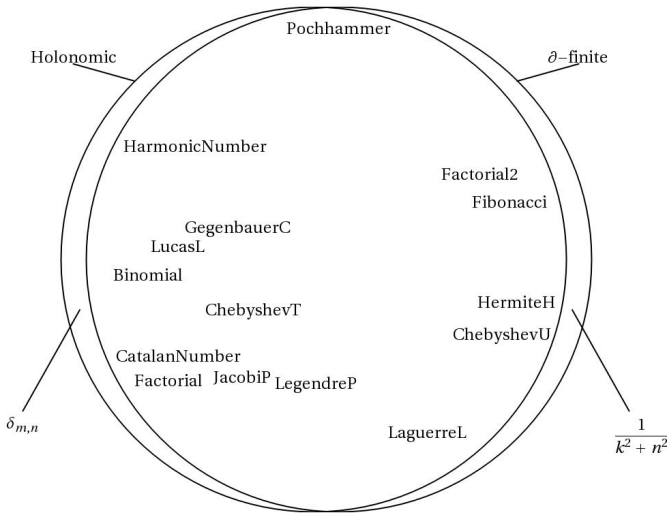
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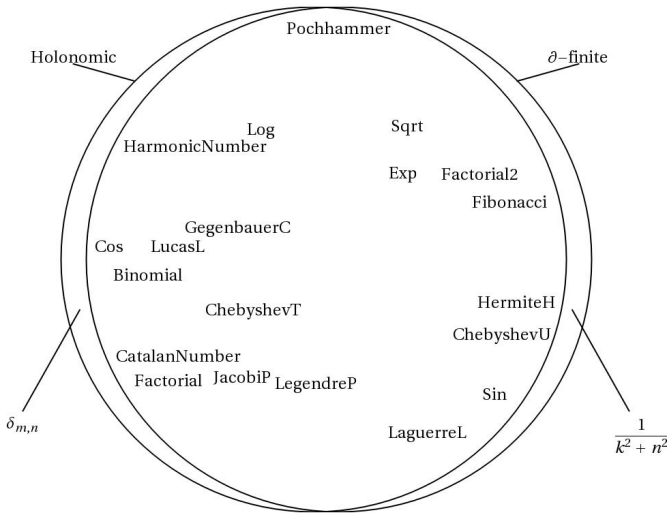
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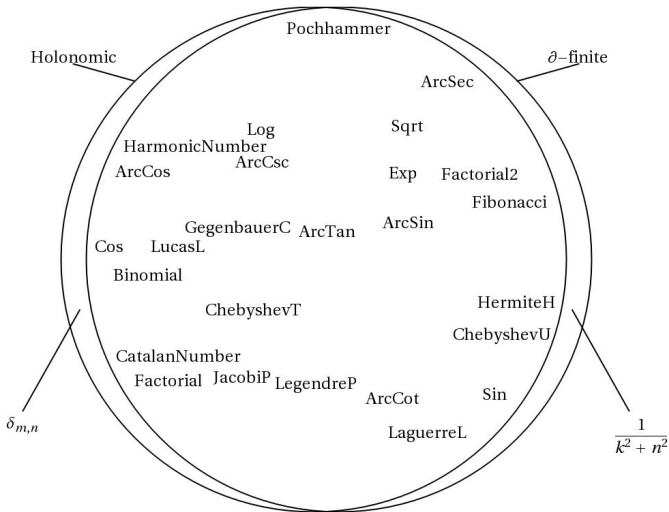
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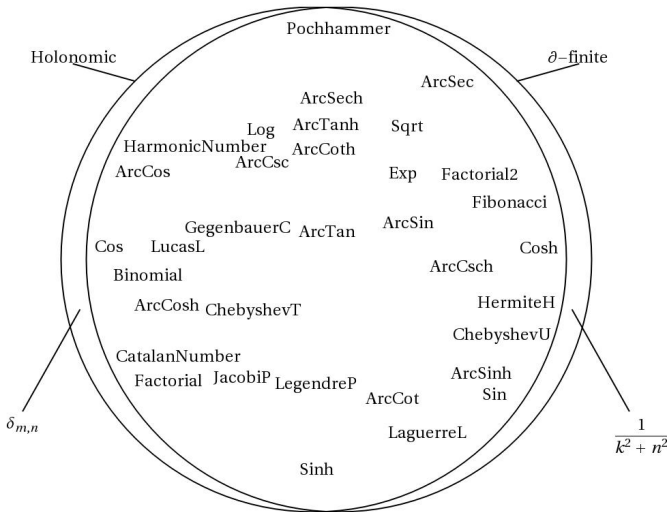
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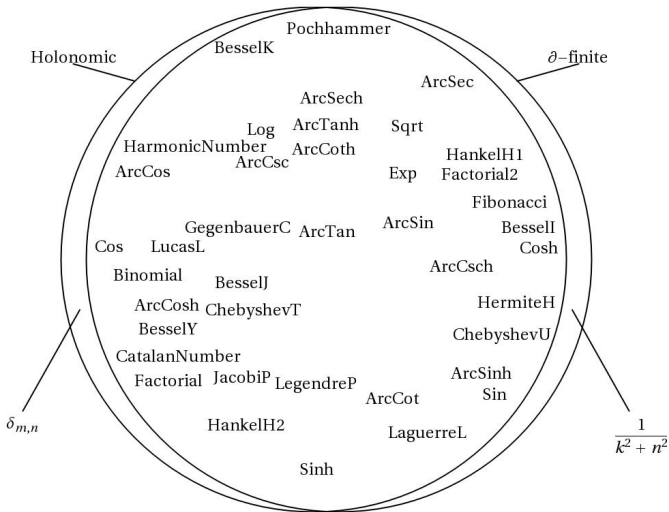
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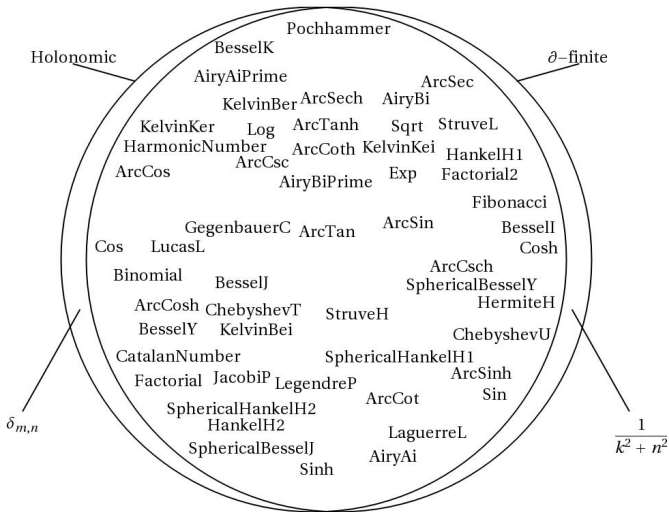
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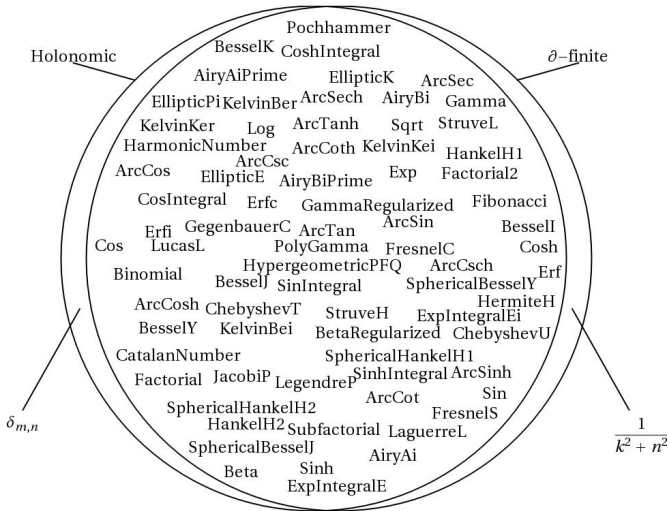
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3. These operations (closure properties) can be executed algorithmically.
4. Many elementary and special functions are covered.

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3. Integrals and sums are treated by the method of creative telescoping.
4. The output is always given as an annihilating ideal, not as a closed form.

## Application 1

# Finite Elements

Joint work with Joachim Schöberl and Peter Paule

## Problem Setting

Simulate the propagation of electromagnetic waves using the Maxwell equations

$$\frac{dH}{dt} = \text{curl } E, \quad \frac{dE}{dt} = -\text{curl } H$$

where  $H$  and  $E$  are the magnetic and the electric field respectively.

Define basis functions (this is the 2D case):

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

using the Legendre and Jacobi polynomials.

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

## Make an Ansatz!

More precisely, we need a relation of the form

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

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

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### Sketch of the algorithm:

1. Work in the Ore algebra  $\mathbb{D} = \mathbb{Q}(i, j, x, y) \langle S_i, S_j, D_x \rangle$ .
2. Compute a Gröbner basis  $G$  of  $\text{Ann}_{\mathbb{D}} \varphi_{i,j}(x, y)$ .
3. Choose index sets  $A$  and  $B$ .
4. Reduce the above ansatz with  $G$ .
5. Do coefficient comparison with respect to  $x$  and  $y$ .
6. Solve the resulting linear system for  $a_{k,l}, b_{m,n} \in \mathbb{Q}(i, j)$ .
7. If there is no solution, go back to step 3.

## Result

With this method, we find the relation

$$\begin{aligned} & (2i + j + 3)(2i + 2j + 7) \frac{d}{dx} \varphi_{i,j+1}(x, y) + \\ & 2(2i + 1)(i + j + 3) \frac{d}{dx} \varphi_{i,j+2}(x, y) - \\ & (j + 3)(2i + 2j + 5) \frac{d}{dx} \varphi_{i,j+3}(x, y) + \\ & (j + 1)(2i + 2j + 7) \frac{d}{dx} \varphi_{i+1,j}(x, y) - \\ & 2(2i + 3)(i + j + 3) \frac{d}{dx} \varphi_{i+1,j+1}(x, y) - \\ & (2i + j + 5)(2i + 2j + 5) \frac{d}{dx} \varphi_{i+1,j+2}(x, y) + \\ & 2(i + j + 3)(2i + 2j + 5)(2i + 2j + 7) \varphi_{i,j+2}(x, y) + \\ & 2(i + j + 3)(2i + 2j + 5)(2i + 2j + 7) \varphi_{i+1,j+1}(x, y) = 0 \end{aligned}$$

and a similar one for  $\frac{d}{dy} \varphi_{i,j}(x, y)$ .

→ These formulae caused a speed-up of 20%  
in the numerical simulations.

# Creative Telescoping

Method for doing integrals and sums  
(aka Feynman's differentiating under the integral sign)

Consider the following summation problem:  $F(n) = \sum_{k=a}^b f(n, k)$

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**Telescoping:** write  $f(n, k) = g(n, k + 1) - g(n, k)$ . Then

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**Creative Telescoping:** write

$$c_d(n)f(n + d, k) + \cdots + c_0(n)f(n, k) = g(n, k + 1) - g(n, k).$$

Summing from  $a$  to  $b$  yields a recurrence for  $F(n)$ :

$$c_d(n)F(n + d) + \cdots + c_0(n)F(n) = g(n, b + 1) - g(n, a).$$

## Creative Telescoping (Example 1)

Let  $F(n)$  denote the double sum over the trinomial coefficients

$$F(n) = \sum_{j=0}^n \sum_{i=0}^n \binom{n}{i, j, n-i-j} = \sum_{j=0}^n \sum_{i=0}^n \frac{n!}{i!j!(n-i-j)!}.$$

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Then the creative telescoping operator

$$CT = S_n - 3 + (S_i - 1) \frac{i}{n-i-j+1} + (S_j - 1) \frac{j}{n-i-j+1}$$

with  $CT \left( \binom{n}{i, j, n-i-j} \right) = 0$  implies that

$$F(n+1) = 3F(n).$$

## Creative Telescoping (Example 2)

The lattice Green's function of the square lattice is given by

$$P(z) = \int_0^1 \int_0^1 \frac{1}{(1 - xyz)\sqrt{1 - x^2}\sqrt{1 - y^2}} dx dy.$$

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The creative telescoping operator

$$(z^3 - z)D_z^2 + (3z^2 - 1)D_z + z + D_x \frac{y(1 - x^2)}{xyz - 1} + D_y \frac{yz(1 - y^2)}{xyz - 1}$$

that annihilates the integrand, certifies that  $P(z)$  satisfies the differential equation

$$(z^3 - z)P''(z) + (3z^2 - 1)P'(z) + zP(z) = 0.$$

## Creative Telescoping

In general, a creative telescoping operator has the form

$$P(\mathbf{v}, \partial_{\mathbf{v}}) + \Delta_1 Q_1(\mathbf{v}, \mathbf{w}, \partial_{\mathbf{v}}, \partial_{\mathbf{w}}) + \cdots + \Delta_m Q_m(\mathbf{v}, \mathbf{w}, \partial_{\mathbf{v}}, \partial_{\mathbf{w}})$$

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- Corresponds to an  $m$ -fold summation/integration problem.
- $\mathbf{w} = w_1, \dots, w_m$  are the summation/integration variables.
- $\mathbf{v} = v_1, v_2, \dots$  are the surviving parameters.
- $P(\mathbf{v}, \partial_{\mathbf{v}})$  is called the **telescoper**.
- The  $Q_i(\mathbf{v}, \mathbf{w}, \partial_{\mathbf{v}}, \partial_{\mathbf{w}})$  are called the **delta parts**.
- The delta parts can be viewed as certificates for the correctness of the telescoper.
- Research topic: develop fast algorithms to compute it!

## Application 2

# Special Function Identities

## Some Special Function Identities

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

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

$$e^{-x} x^{a/2} n! L_n^a(x) = \int_0^{\infty} e^{-t} t^{\frac{a}{2}+n} J_a(2\sqrt{tx}) dt \quad (3)$$

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

$$\int_{-1}^1 (1-x^2)^{\nu-\frac{1}{2}} e^{iax} C_n^{(\nu)}(x) dx = \frac{\pi i^n \Gamma(n+2\nu) J_{n+\nu}(a)}{2^{\nu-1} a^{\nu} n! \Gamma(\nu)} \quad (5)$$

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

## Computer Proof of a Special Function Identity

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

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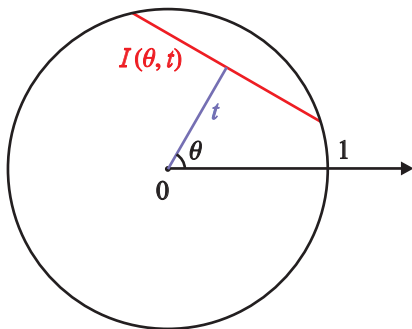
CreativeTelescoping[Exp[-t]\*t^(a/2+n)\*BesselJ[a, 2\*sqrt[t\*x]]  
Der[t], {S[a], S[n], Der[x]}]

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→ The annihilating ideals agree; complete the proof by comparing a few initial values.

## Application 3

# Radon Projections



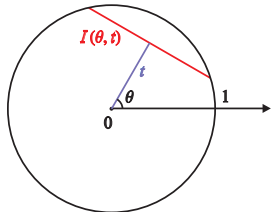
Joint work with Irina Georgieva, Clemens Hofreither,  
Veronika Pillwein, and Thotsaporn Thanatipanonda

## Radon Projection

Consider real bivariate functions  $f(x, y)$  in the unit disk in  $\mathbb{R}^2$ .

Let  $I(\theta, t)$  denote a chord of the unit circle at angle  $\theta \in [0, 2\pi)$  and distance  $t \in (-1, 1)$  from the origin.

The **Radon projection**  $\mathcal{R}_\theta(f; t)$  of  $f$  in direction  $\theta$  is defined by the line integral



$$\begin{aligned}\mathcal{R}_\theta(f; t) &:= \int_{I(\theta, t)} f(\mathbf{x}) d\mathbf{x} \\ &= \int_{-\sqrt{1-t^2}}^{\sqrt{1-t^2}} f(t \cos \theta - s \sin \theta, t \sin \theta + s \cos \theta) ds.\end{aligned}$$

## Interpolation Using Radon Projections

Find  $p \in \Pi_n^2$  (bivariate polynomials of degree  $\leq n$ ) such that

$$\int_I p \, dx = \gamma_I \quad \forall I \in \mathcal{I},$$

where

- $\mathcal{I} = \{I_1, I_2, \dots, I_{\binom{n+2}{2}}\}$  are chords of the unit circle,
- $\gamma_I \in \mathbb{R}$  are given values.

**Question:** For which configurations of chords  $\mathcal{I}$  does this problem have a unique solution?

## Radon Projections of the Harmonic Basis

Show that the matrix with the following entries is non-singular:

$$\int_{-\sqrt{1-t^2}}^{\sqrt{1-t^2}} \binom{k}{2\ell} (-1)^\ell (t \cos \theta - s \sin \theta)^{k-2\ell} (t \sin \theta + s \cos \theta)^{2\ell} ds =$$
$$\sum_{\ell=0}^{\lfloor k/2 \rfloor} \binom{k}{2\ell} (-1)^\ell \sum_{p=0}^{k-2\ell} \sum_{q=0}^{2\ell} \binom{k-2\ell}{p} \binom{2\ell}{q} t^{p+q} \times$$
$$\times (\cos \theta)^{2\ell+p-q} (\sin \theta)^{k-2\ell-(p-q)} \frac{(-1)^{k-2\ell-p}}{k-p-q+1} \times$$
$$\times (1-t^2)^{\frac{1}{2}(k-p-q+1)} \left(1 - (-1)^{k-p-q+1}\right)$$

→ Symbolic computation succeeded in simplifying these expressions drastically.

## Application 4

# Quantum Topology

Joint work with Stavros Garoufalidis

## A Multiple Sum

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

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

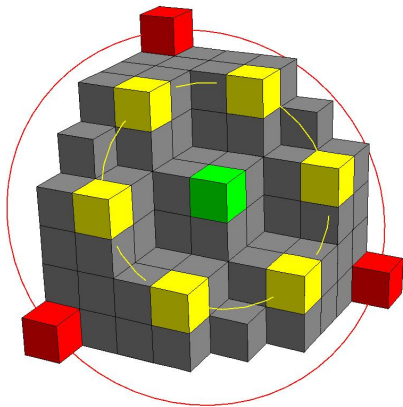
with

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

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

# Enumerative Combinatorics



Joint work with Manuel Kauers and Doron Zeilberger

# The $q$ -TSPP Conjecture

“The Holy Grail of Enumerative Combinatorics”

Last surviving open problem of the classic (Stanley, 1986)  
*A baker's dozen of conjectures concerning plane partitions*

# The $q$ -TSPP Conjecture

“The Holy Grail of Enumerative Combinatorics”

Last surviving open problem of the classic (Stanley, 1986)  
*A baker's dozen of conjectures concerning plane partitions*

Some notions from partition theory:

- partition of an integer, e.g.,  $4 = 2 + 1 + 1$
- plane partition: two-dimensional arrangement of summands,

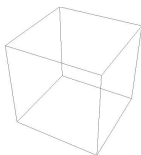
e.g., 
$$\begin{array}{cc} 2 & 1 \\ 1 & \end{array}$$

- Ferrer's diagram: three-dimensional representation of PPs,

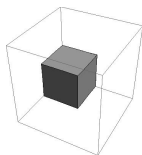
e.g., 
$$\begin{array}{cc} 2 & 1 \\ 1 & \end{array} = \begin{array}{c} \text{3D cube diagram} \end{array}$$

- totally symmetric plane partition (TSPP):  
Ferrer's diagram is symmetric w.r.t. rotation and reflection
- orbit: see the picture

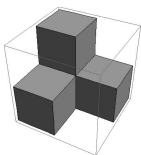
Let  $T(n)$  denote set of TSPPs with largest part  $\leq n$ , e.g.  $n = 2$ :



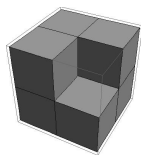
$$1 \cdot q^0$$



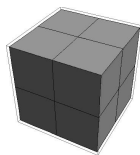
$$1 \cdot q^1$$



$$1 \cdot q^2$$

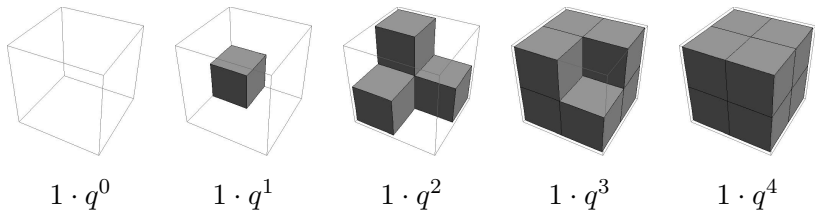


$$1 \cdot q^3$$



$$1 \cdot q^4$$

Let  $T(n)$  denote set of TSPPs with largest part  $\leq n$ , e.g.  $n = 2$ :



Andrews-Robbins  $q$ -TSPP conjecture (1983):

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

Counting formula is obtained by  $q \rightarrow 1$  (Stembridge 1995):

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

# The Determinant

First reduction by Soichi Okada:

The  $q$ -TSPP conjecture is true if

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

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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

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

is the  $q$ -binomial coefficient.

## The Holonomic Ansatz

Second reduction by Doron Zeilberger:

“Pull out of the hat” a holonomic function  $c_{n,j}$  and prove

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

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

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

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

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- $c_{n,j}$  not given explicitly
- perfect application for the holonomic systems approach
- very large computations
- feasible only due to a new algorithm

## The Result

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

A short version of this appeared in PNAS (Proceedings of the National Academy of Sciences of the USA):

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