Two Facets of Computational Mathematics: Numerics and Symbolics

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Numerics and Symbolics

“Numerics” (Numerical Analysis): finite element method, PDEs, variational formulation, simulations, approximate solution

“Symbolics” (Symbolic Computation): Gröbner basis, operator algebra, symbolic summation, exact computation

Long-term collaborations in Linz (JKU, RICAM):

- SFB F13 “Numerical and Symbolic Scientific Computing” (1998 – 2008)
- DK W1214 “Computational Mathematics” (2008 – present)

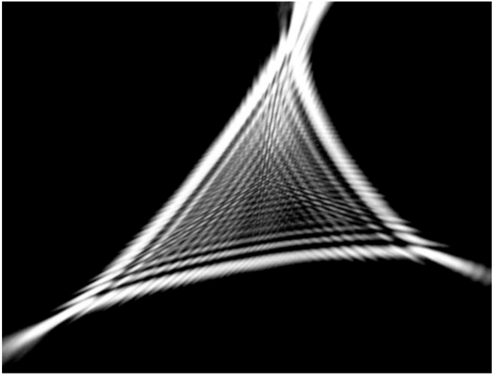
Initiators: Bruno Buchberger, Heinz Engl, Bert Jüttler, Ulrich Langer, Peter Paule, Joachim Schöberl, . . .

Outline

1. **Theory:** holonomic functions
   Application: finite elements
2. **Theory:** creative telescoping
   Application: special functions
3. **Theory:** symbolic determinants
   Application: inverse inequalities

Part 1: Theory

Holonomic Functions



Holonomic Functions

Definition: A function $f(x)$ is called **holonomic** if it satisfies a linear ordinary differential equation with polynomial coefficients:

$$p_r(x)f^{(r)}(x) + \cdots + p_1(x)f'(x) + p_0(x)f(x) = 0,$$

$p_0, \ldots, p_r \in \mathbb{K}[x]$ (not all zero).

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$\longrightarrow$ In both cases, one needs only **finitely many** initial conditions.

Closure Properties

If functions $f(x)$ and $g(x)$ are holonomic, then also:

- $f(x) + g(x)$
- $f(x) \cdot g(x)$
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A sequence is holonomic iff its generating function is holonomic.

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Generalize the finiteness property to

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- mixed setting: functions in several continuous and discrete variables $f(x_1, \ldots, x_s, n_1, \ldots, n_r)$

Legendre polynomials are orthogonal polynomials w.r.t. the L^2 inner product $\int_{-1}^{1} f(x)g(x)\,\mathrm{d}x$, and a solution of the ODE

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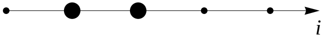

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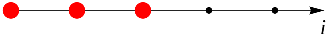

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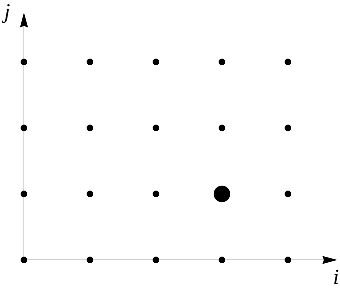

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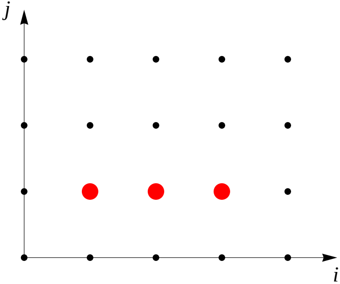

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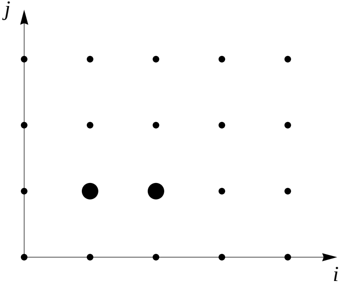

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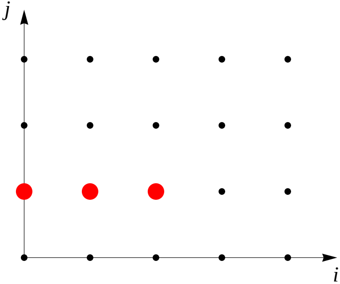

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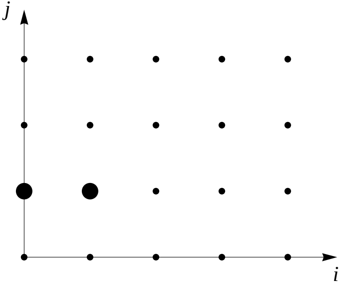

$$P_{n+1}^{(3)}(x) = \frac{(n^2x^2-n^2+3nx^2-3n+8x^2)}{(x^2-1)^2}P_{n+1}'(x) - \frac{4(n^2x+3nx+2x)}{(x^2-1)^2}P_{n+1}(x)$$

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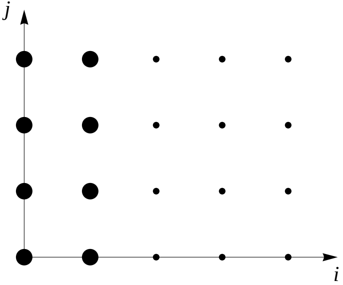

The **Legendre polynomials** can be defined recursively:

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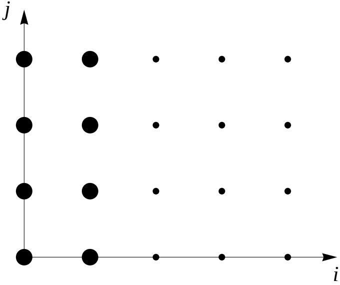

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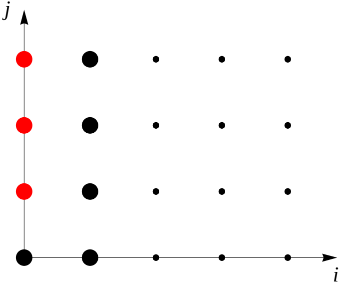

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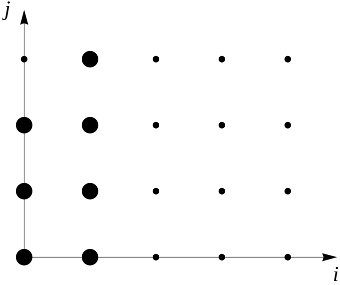

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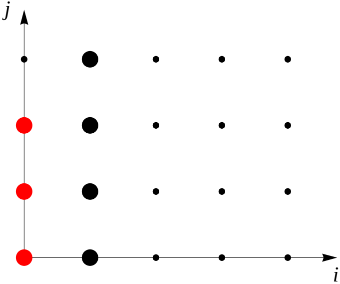

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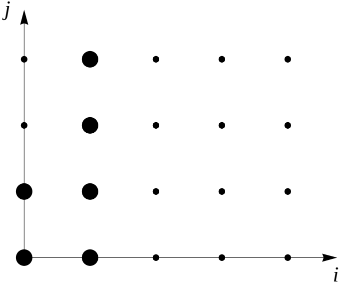

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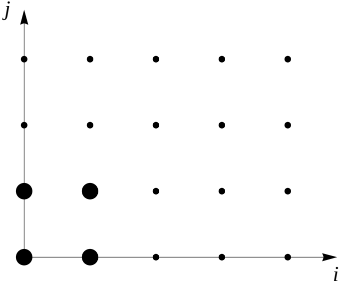

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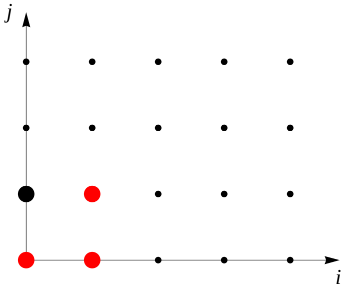

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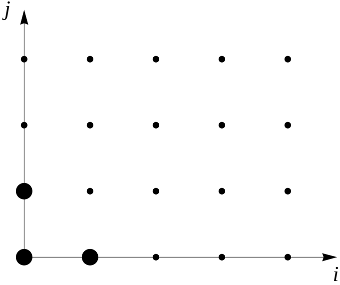

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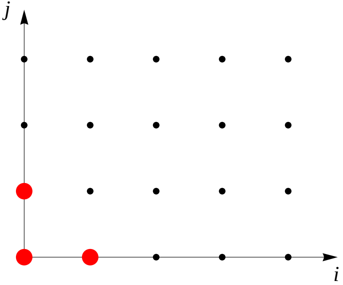

$$(n+1)P_{n+1}(x) + (1-x^2)P_n'(x) - (n+1)xP_n(x) = 0$$

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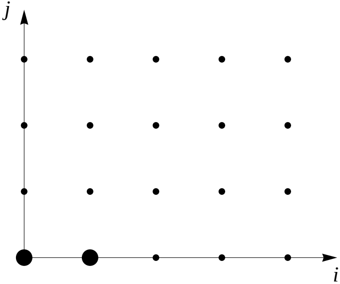

$\longrightarrow$ $P_n(x)$ is **holonomic** w.r.t. n and x (of rank 2).

Multivariate Holonomic Functions

Definition:
Let $f(x_1,\ldots,x_s,n_1,\ldots,n_r)$ be a function in the continuous variables $x_1,\ldots,x_s$ and in the discrete variables $n_1,\ldots,n_r$.
If there is a finite set of basis functions of the form

$$\frac{\mathrm{d}^{i_1}}{\mathrm{d}x_1^{i_1}}\cdots\frac{\mathrm{d}^{i_s}}{\mathrm{d}x_s^{i_s}}f(x_1,\ldots,x_s,n_1+j_1,\ldots,n_r+j_r)$$

with $i_1,\ldots,i_s,j_1,\ldots,j_r\in\mathbb{N}$ such that any shifted partial derivative of f (of the above form) can be expressed as a $\mathbb{K}(x_1,\ldots,x_s,n_1,\ldots,n_r)$-linear combination of the basis functions (plus some further, technical assumptions), then f is **holonomic**.

$\longrightarrow$ Finitely many initial conditions suffice.

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Example 1: The Legendre differential equation

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Example 2: The three-term recurrence

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

translates to the operator

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

Operator Algebra

Noncommutative multiplication:

$$D_x x = x D_x + 1, \quad S_n n = n S_n + S_n, \quad \text{etc.}$$

Operator Algebra

Noncommutative multiplication:

$$D_x x = x D_x + 1, \quad S_n n = n S_n + S_n, \quad \text{etc.}$$

Such operators form an **Ore algebra**

$$\mathbb{O} = \mathbb{K}(v, w, \ldots)\langle \partial_v, \partial_w, \ldots \rangle,$$

i.e., multivariate polynomials in the ∂'s with coefficients being rational functions in $v, w, \ldots$, where $\mathbb{K}$ is a field ($\mathrm{char}(\mathbb{K}) = 0$).

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One can employ the theory of (noncommutative) **Gröbner bases**.

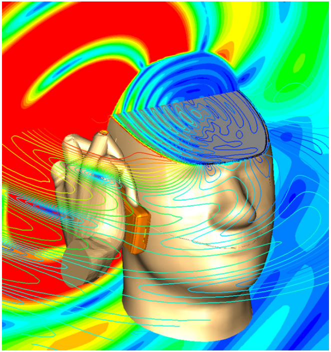
Example: The operators that we encountered with the Legendre polynomials live in the Ore algebra $\mathbb{K}(x, n)\langle D_x, S_n \rangle$.

Many Functions are Holonomic

ArcCsc, KelvinBei, HypergeometricPFQ, ExpIntegralE, ArcTanh, HankelH2, AngerJ, JacobiP, ChebyshevT, AiryBi, AiryAi, Sinc, Multinomial, CatalanNumber, QBinomial, CosIntegral, ArcSech, SphericalHankelH2, HermiteH, ExpIntegralEi, Beta, AiryBiPrime, SphericalBesselJ, Binomial, ParabolicCylinderD, Erfc, EllipticK, Fibonacci, QFactorial, Cos, Hypergeometric2F1, Erf, KelvinKer, HypergeometricPFQRegularized, Log, Factorial, BesselY, Cosh, CoshIntegral, ArcTan, ArcCoth, LegendreP, LaguerreL, EllipticE, SinhIntegral, Sinh, BetaRegularized, SphericalHankelH1, ArcSin, EllipticThetaPrime, Root, LucasL, AppellF1, FresnelC, LegendreQ, ChebyshevU, GammaRegularized, Erfi, HarmonicNumber, BesselI, KelvinKei, ArithmeticGeometricMean, Exp, ArcCot, EllipticTheta, Hypergeometric0F1, EllipticPi, GegenbauerC, ArcCos, WeberE, FresnelS, EllipticF, ArcCosh, Subfactorial, QPochhammer, Gamma, StruveH, WhittakerM, ArcCsch, Hypergeometric1F1, SinIntegral,

Part 1: Application

Finite Elements



(joint work with Joachim Schöberl and Peter Paule)

Problem Setting

Simulate the propagation of electromagnetic waves according to

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

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

Define basis functions (2D case):

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

using 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).

Ansatz

More precisely, one needs a relation of the form (ansatz)

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

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

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

Approach:

1. Work in the Ore algebra $\mathbb{O} = \mathbb{Q}(i,j,x,y)\langle S_i, S_j, D_x\rangle$.
2. Compute a Gröbner basis G of the annihilator of $\varphi_{i,j}(x,y)$.
3. Choose index sets A and B.
4. Reduce the above ansatz with G and obtain a normal form.
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

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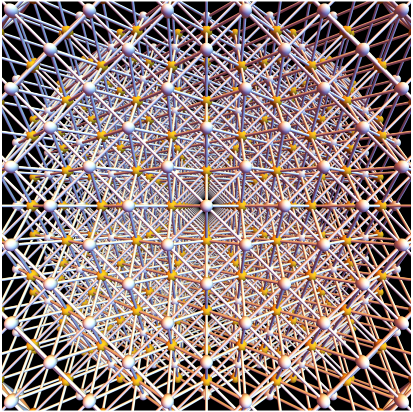
&(2i+j+5)(2i+2j+5)\tfrac{\mathrm{d}}{\mathrm{d}x}\varphi_{i+1,j+2}(x,y)+\\
&2(i+j+3)(2i+2j+5)(2i+2j+7)\varphi_{i,j+2}(x,y)+\\
&2(i+j+3)(2i+2j+5)(2i+2j+7)\varphi_{i+1,j+1}(x,y)=0
\end{aligned}$$

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

$\longrightarrow$ The use of these (previously unknown) formulas caused a considerable speed-up in the numerical simulations.

Part 2: Theory

Creative Telescoping



What is Creative Telescoping?

Creative telescoping is a method

- to deal with parametrized symbolic sums and integrals
- that yields differential/recurrence equations for them
- that became popular in computer algebra in the past 25 years

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$$\sum_{k=1}^{\infty} \frac{1}{k(k+n)}$$

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$$\sum_{k=1}^{\infty} \frac{1}{k(k+n)} = \frac{\gamma + \psi(n)}{n}$$

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Example:

$$\sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6}$$

Bad: no parameter!

$$f_n := \sum_{k=1}^{\infty} \frac{1}{k(k+n)} \rightsquigarrow (n+2)^2 f_{n+2} = (n+1)(2n+3) f_{n+1} - n(n+1) f_n$$

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Creative telescoping can be performed in different settings:

- difference fields (Carsten Schneider, RISC, JKU)
- differential fields (Clemens Raab, Institute for Algebra, JKU)
- holonomic functions (here)

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 $F(n) = \sum_{k=a}^{b} \bigl(g(n,k+1) - g(n,k)\bigr) = g(n,b+1) - g(n,a)$.

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Creative Telescoping: write

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

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

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

Creative Telescoping

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

Consider the following integration problem: $F(x) := \int_a^b f(x,y)\,\mathrm{d}y$

Telescoping: write $f(x,y) = \frac{\mathrm{d}}{\mathrm{d}y} g(x,y)$.

Then $F(n) = \int_a^b \left(\frac{\mathrm{d}}{\mathrm{d}y} g(x,y)\right) \mathrm{d}y \qquad = g(x,b) - g(x,a)$.

Creative Telescoping: write

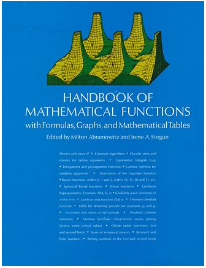
$$c_r(x) \frac{\mathrm{d}^r}{\mathrm{d}x^r} f(x,y) + \cdots + c_0(x) f(x,y) \; = \frac{\mathrm{d}}{\mathrm{d}y} g(x,y).$$

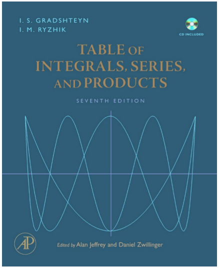
Integrating from a to b yields a differential equation for $F(x)$:

$$c_r(x) \frac{\mathrm{d}^r}{\mathrm{d}x^r} F(x) + \cdots + c_0(x) F(x) \; = g(x,b) - g(x,a)$$

Part 2: Application

Special Function Identities


HANDBOOK OF MATHEMATICAL FUNCTIONS
with Formulas, Graphs, and Mathematical Tables
Edited by Milton Abramowitz and Irene A. Stegun


I. S. GRADSHTEYN
I. M. RYZHIK
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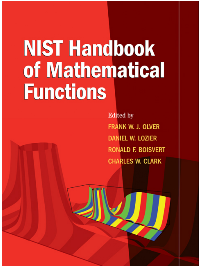
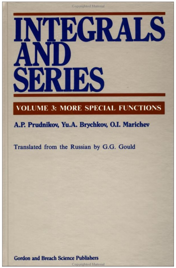
SEVENTH EDITION
CD INCLUDED
Edited by Alan Jeffrey and Daniel Zwillinger


NIST Handbook of Mathematical Functions
Edited by
FRANK W. J. OLVER
DANIEL W. LOZIER
RONALD F. BOISVERT
CHARLES W. CLARK


INTEGRALS AND SERIES
VOLUME 3: MORE SPECIAL FUNCTIONS
A.P. Prudnikov, Yu.A. Brychkov, O.I. Marichev
Translated from the Russian by G.G. Gould
Gordon and Breach Science Publishers

Special Function Identities

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

$$\int_{0}^{\infty}\frac{1}{\left(x^{4}+2ax^{2}+1\right)^{m+1}}\,\mathrm{d}x=\frac{\pi P_{m}^{\left(m+\frac{1}{2},-m-\frac{1}{2}\right)}(a)}{2^{m+\frac{3}{2}}(a+1)^{m+\frac{1}{2}}} \tag{2}$$

$$e^{-x}x^{a/2}n!\,L_{n}^{a}(x)=\int_{0}^{\infty}e^{-t}t^{\frac{a}{2}+n}J_{a}\left(2\sqrt{tx}\right)\mathrm{d}t \tag{3}$$

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

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

Computer-Assisted Proof

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

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

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

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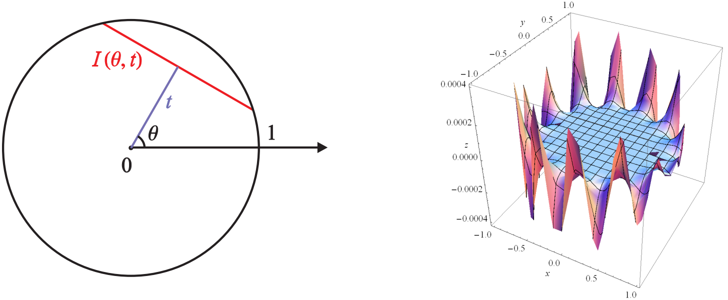
&\ 2xS_a^2 + (2ax+2x^2+2x)D_x + (-a^2+ax-a+2nx+2x)\}
\end{aligned}$$

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

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

Part 2: Application

Harmonic Interpolation from Radon Projections



(joint work with Irina Georgieva, Clemens Hofreither, Veronika Pillwein, Thotsaporn Thanatipanonda)

Harmonic Interpolation

We use the basis of harmonic polynomials

$$\begin{aligned} \phi_0(x,y) &= 1, \\ \phi_{k,1}(x,y) &= \operatorname{Re}(x+i\,y)^k, \\ \phi_{k,2}(x,y) &= \operatorname{Im}(x+i\,y)^k. \end{aligned}$$

to interpolate a harmonic function from the values of finitely many line integrals along chords.

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to interpolate a harmonic function from the values of finitely many line integrals along chords.

Theorem. If the chords form a regular polygon, then this interpolation problem has a unique solution.

Symbolic Summation

To prove the theorem we have to evaluate the following integrals:

$$\int_{I(\theta,t)} \phi_{k,1} = \sum_{\ell=0}^{\lfloor k/2 \rfloor} \binom{k}{2\ell} (-1)^{\ell} \sum_{p=0}^{k-2\ell} \sum_{q=0}^{2\ell} \binom{k-2\ell}{p} \binom{2\ell}{q} t^{p+q}$$

$$\times (\cos\theta)^{2\ell+p-q} (\sin\theta)^{k-2\ell-(p-q)} \frac{(-1)^{k-2\ell-p}}{k-p-q+1}$$

$$\times (1-t^2)^{\frac{1}{2}(k-p-q+1)} \left(1-(-1)^{k-p-q+1}\right)$$

and a similar one for $\phi_{k,2}$.

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$$\times (\cos\theta)^{2\ell+p-q} (\sin\theta)^{k-2\ell-(p-q)} \frac{(-1)^{k-2\ell-p}}{k-p-q+1}$$
$$\times (1-t^2)^{\frac{1}{2}(k-p-q+1)} \left(1-(-1)^{k-p-q+1}\right)$$

and a similar one for $\phi_{k,2}$.

$\longrightarrow$ This can be achieved with creative telescoping.

Part 3: Theory

Symbolic Determinants

$$\det_{1\leqslant i,j\leqslant n} \frac{1}{i+j-1} = \frac{1}{(2n-1)!}\prod_{k=1}^{n-1}\frac{(k!)^2}{(k+1)_{n-1}}$$

$$\det_{0\leqslant i,j\leqslant n-1} \binom{2i+2a}{j+b} = 2^{n(n-1)/2}\prod_{k=0}^{n-1}\frac{(2k+2a)!k!}{(k+b)!(2k+2a-b)!}$$

$$\det_{0\leqslant i,j\leqslant n-1} \sum_k \binom{i}{k}\binom{j}{k}2^k = 2^{n(n-1)/2}$$

The HOLONOMIC ANSATZ II.
Automatic DISCOVERY(!) and PROOF(!!)
of Holonomic Determinant Evaluations
(D. Zeilberger, *Annals of Combinatorics* **11**:241–247, 2007)

The HOLONOMIC ANSATZ II. Automatic DISCOVERY(!) and PROOF(!!) of Holonomic Determinant Evaluations

(D. Zeilberger, *Annals of Combinatorics* **11**:241–247, 2007)

Algorithmic method to prove determinant evaluations of the form

$$\det A_n = b_n \qquad (n \geqslant 1)$$

where

- $A_n = (a_{i,j})_{1 \leqslant i,j \leqslant n}$ is an $n \times n$ matrix,
- $a_{i,j}$ is a bivariate holonomic sequence, not depending on n,
- $b_n \neq 0$ for all $n \geqslant 1$.

$$\begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n} \end{pmatrix}$$

$$\begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n} \end{pmatrix} \begin{pmatrix} (A_n^{-1})_{1,n} \\ (A_n^{-1})_{2,n} \\ (A_n^{-1})_{3,n} \\ \vdots \\ (A_n^{-1})_{n,n} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n} \end{pmatrix} \begin{pmatrix} (-1)^{n+1}\frac{\det A_n^{(n,1)}}{\det A_n} \\ (-1)^{n+2}\frac{\det A_n^{(n,2)}}{\det A_n} \\ (-1)^{n+3}\frac{\det A_n^{(n,3)}}{\det A_n} \\ \vdots \\ (-1)^{2n}\frac{\det A_n^{(n,n)}}{\det A_n} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

- $A_n^{(i,j)}$: matrix A_n with row i and column j deleted

$$\begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n} \end{pmatrix} \begin{pmatrix} (-1)^{n+1}\dfrac{M_{n,1}}{\det A_n} \\ (-1)^{n+2}\dfrac{M_{n,2}}{\det A_n} \\ (-1)^{n+3}\dfrac{M_{n,3}}{\det A_n} \\ \vdots \\ \dfrac{M_{n,n}}{\det A_n} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}$$

- $A_n^{(i,j)}$: matrix A_n with row i and column j deleted
- $M_{i,j} = \det A_n^{(i,j)}$ is the (i,j)-minor of A_n

$$\begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\ \vdots & \vdots & \vdots & & \vdots \\ a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n} \end{pmatrix} \begin{pmatrix} (-1)^{n+1}\frac{M_{n,1}}{M_{n,n}} \\ (-1)^{n+2}\frac{M_{n,2}}{M_{n,n}} \\ (-1)^{n+3}\frac{M_{n,3}}{M_{n,n}} \\ \vdots \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ \frac{\det A_n}{M_{n,n}} \end{pmatrix}$$

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Problem: Prove that $\det A_n = \det\limits_{1 \leqslant i,j \leqslant n} a_{i,j} = b_n$ for all $n \in \mathbb{N}$.

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Now use $c_{n,j}$ to do Laplace expansion of A_n w.r.t. the last row:

$$\det A_n = \sum_{j=1}^{n} (-1)^{n+j} M_{n,j} a_{n,j} = \sum_{j=1}^{n} M_{n,n} c_{n,j} a_{n,j}.$$

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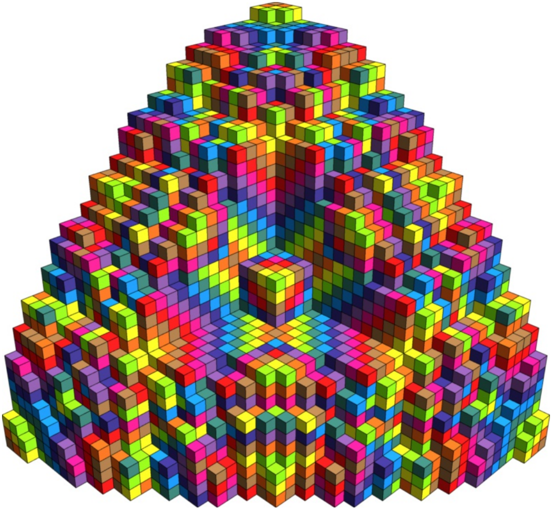
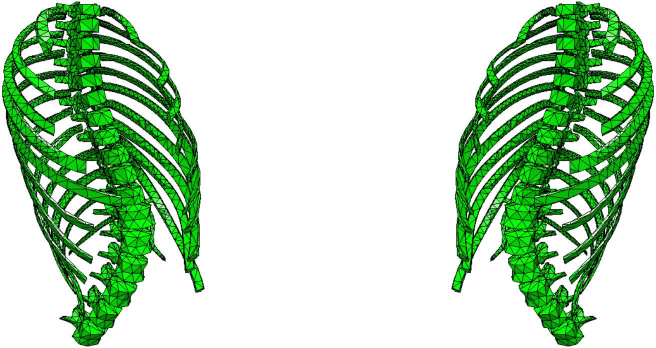
- The values of $c_{n,j}$ can be computed for concrete $n, j \in \mathbb{N}$.
- If recurrences exist they can be **guessed** automatically

Totally Symmtric Plane Partitions



Part 3: Application

Inverse Inequalities



(joint work with Martin Neumüller and Silviu Radu)

Inverse Inequalities

We consider inequalities of the form

$$||v_n||_{X(\Omega)} \leqslant c_1(h,n)\,||v_n||_{Y(\Omega)} \qquad \text{for all } v_n \in V_n$$

where

- $\Omega \subset \mathbb{R}^d, d \in \mathbb{N}$
- V: some infinite-dimensional space of functions defined on Ω
- $||\cdot||_{X(\Omega)}$, $||\cdot||_{Y(\Omega)}$: norms that are used in the analysis of numerical methods
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Dependence on h is easily obtained by a scaling argument:
$\longrightarrow$ Transform the problem to a reference element $\hat{\Omega}$.

Inverse Inequalities

We obtain for c_1:

$$\hat{c}_1(n) = \sup_{v_n \in \hat{V}_n} \frac{||v_n||_{X(\hat{\Omega})}}{||v_n||_{Y(\hat{\Omega})}} = \sqrt{\sup_{v_n \in \hat{V}_n} \frac{(v_n, v_n)_{X(\hat{\Omega})}}{(v_n, v_n)_{Y(\hat{\Omega})}}}$$

Let $(\varphi_k)_{1 \leqslant k \leqslant n}$ be a basis of $\hat{V}_n$. Then:

$$\big(\hat{c}_1(n)\big)^2 = \sup_{\vec{v}_n \in \mathbb{R}^n} \frac{(K_n \vec{v}_n, \vec{v}_n)_{\ell^2}}{(M_n \vec{v}_n, \vec{v}_n)_{\ell^2}}$$

for certain symmetric and positive (semi-) definite matrices

$$K_n(i,j) := (\varphi_j, \varphi_i)_{X(\hat{\Omega})}, \text{ and } M_n(i,j) := (\varphi_j, \varphi_i)_{Y(\hat{\Omega})}.$$

This can be reformulated as a generalized eigenvalue problem

$$K_n \vec{x}_n = \lambda_n M_n \vec{x}_n$$

where the largest eigenvalue λ_n gives the desired $\big(\hat{c}_1(n)\big)^2$.

Inverse Inequalities

In this work, we consider the reference domain $\hat{\Omega} = (-1,1)^2$ with

$$(u,v)_{X(\hat{\Omega})} = \int_{\hat{\Omega}} \partial_x u(x,y) \partial_x v(x,y) \,\mathrm{d}x\,\mathrm{d}y,$$
$$(u,v)_{Y(\hat{\Omega})} = \int_{\hat{\Omega}} u(x,y) v(x,y) \,\mathrm{d}x\,\mathrm{d}y,$$

for $u, v \in \hat{V}_n$, where $\hat{V}_n$ is the space of polynomials of degree less than n, i.e.

$$\hat{V}_n = \left\{ x^i y^j : 0 \leqslant i, j < n \right\}.$$

Problem Statement

The interest in inverse inequalities leads to the following problem:

Find the largest eigenvalue λ_n of the generalized eigenvalue problem

$$B_n\vec{x}_n = \lambda_n A_n\vec{x}_n$$

where A_n and B_n are certain $n \times n$ matrices.

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Equivalent formulation:

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Relaxed problem: find expressions $b_1(n)$ and $b_2(n)$ such that

$$b_1(n) < \lambda_n < b_2(n)$$

(“as accurate as possible”).

The Matrices

$$a_{i,j} := \frac{1-(-1)^{i+j-1}}{i+j-1}, \quad b_{i,j} := (i-1)(j-1)\frac{1-(-1)^{i+j-3}}{i+j-3}$$

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$$|B_6 - \lambda A_6| = \begin{vmatrix} -2\lambda & 0 & -\frac{2}{3}\lambda & 0 & -\frac{2}{5}\lambda & 0 \\ 0 & 2-\frac{2}{3}\lambda & 0 & 2-\frac{2}{5}\lambda & 0 & 2-\frac{2}{7}\lambda \\ -\frac{2}{3}\lambda & 0 & \frac{8}{3}-\frac{2}{5}\lambda & 0 & \frac{16}{5}-\frac{2}{7}\lambda & 0 \\ 0 & 2-\frac{2}{5}\lambda & 0 & \frac{18}{5}-\frac{2}{7}\lambda & 0 & \frac{30}{7}-\frac{2}{9}\lambda \\ -\frac{2}{5}\lambda & 0 & \frac{16}{5}-\frac{2}{7}\lambda & 0 & \frac{32}{7}-\frac{2}{9}\lambda & 0 \\ 0 & 2-\frac{2}{7}\lambda & 0 & \frac{30}{7}-\frac{2}{9}\lambda & 0 & \frac{50}{9}-\frac{2}{11}\lambda \end{vmatrix}$$

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Hence we get: $\det(B_n - \lambda A_n) = 2^n \det\left(A^{(1)}_{\lceil n/2 \rceil}\right) \cdot \det\left(A^{(0)}_{\lfloor n/2 \rfloor}\right).$

The Determinant

By a variation of the **holonomic ansatz** we can prove:

Theorem.

$$\det A_n^{(0)} = \underbrace{\left(-\tfrac{1}{2}\right)^n \prod_{i=1}^{n} \frac{\big((i-1)!\big)^2}{\left(i+\frac{1}{2}\right)_n}}_{\text{“hyperholonomic” part}} \underbrace{\sum_{j=0}^{n} (-4)^{j-n} \frac{(2n-2j+1)_{2n}}{(2j)!} \lambda^j}_{\text{holonomic part}},$$

$$\det A_n^{(1)} = \left(-\tfrac{1}{2}\right)^n \prod_{i=1}^{n} \frac{\big((i-1)!\big)^2}{\left(i-1+\frac{1}{2}\right)_n} \sum_{j=0}^{n-1} \frac{(2n-2j-1)_{2n-1}}{(-4)^{n-j-1}(2j+1)!} \lambda^j.$$

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We use this explicit evaluation to estimate the largest eigenvalue.

Final Result

For all $n \in \mathbb{N}$ we have the estimate $b_1(n) < \lambda_n < b_2(n)$ with

$$b_1(n) := \frac{m_1(n)}{2}\left(1 + \sqrt{1 - \frac{2}{3}\frac{(n-2)(n-3)(n+3)(n+4)}{n(n-1)(n+1)(n+2)}}\right),$$

$$b_2(n) := m_1(n)\left(\frac{1}{3} + \left(r_1(n) + \sqrt{r_2(n)}\right)^{1/3} + \left(r_1(n) - \sqrt{r_2(n)}\right)^{1/3}\right),$$

where m_1, r_1, and r_2 are given by

$$m_1(n) := \frac{n(n-1)(n+1)(n+2)}{8},$$

$$r_1(n) := \frac{2(n^8 + 4n^7 + 8n^6 + \cdots - 4733n^2 - 5130n + 16200)}{135n^2(n-1)^2(n+1)^2(n+2)^2},$$

$$r_2(n) := \frac{(n-2)(n-3)(n+4)(n+3)(7n^{12} + 42n^{11} + \dots)}{145800n^4(n-1)^4(n+1)^4(n+2)^4}.$$

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Outlook

There are many other collaborations between the symbolic computation group and other research groups in Linz:

1. analysis of pedestrian dynamics
2. performance evaluation of wireless communication systems
3. special function inequalities (Veronika Pillwein)
4. Feynman integrals in particle physics (Carsten Schneider)
5. . . .