

A Fast Approach to Creative Telescoping

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Introduction

Last week, Manuel Kauers presented

- complicated theory and deep results
- which, unfortunately, is completely useless (no applications)!

This week, I will present

- no complicated theory
- no deep results
- but something that is very useful and has lots of applications!



Some Notation

The following operator symbols will be used:

- shift operator S_v : $S_v f(v) = f(v + 1)$
- partial derivative D_v : $D_v f(v) = \frac{d}{dv} f(v)$
- arbitrary operator: ∂_v any of the two above

All operators are considered to live in an Ore algebra of the form

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

i.e., polynomials in the ∂ 's with rational function coefficients.

Remark: $\mathbb{Q}$ is some field of characteristic 0 containing $\mathbb{Q}$.



Creative Telescoping

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

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

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

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

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

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

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

where $\Delta_i = S_{w_i} - 1$ or $\Delta_i = D_{w_i}$ (depending on the problem).

- 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 *principal part* or the *telescoper*
- the $Q_i(\mathbf{v}, \mathbf{w}, \partial_{\mathbf{v}}, \partial_{\mathbf{w}})$ are called the *delta parts*
- they can be viewed as certificates for the correctness of the principal part



What is a Function?

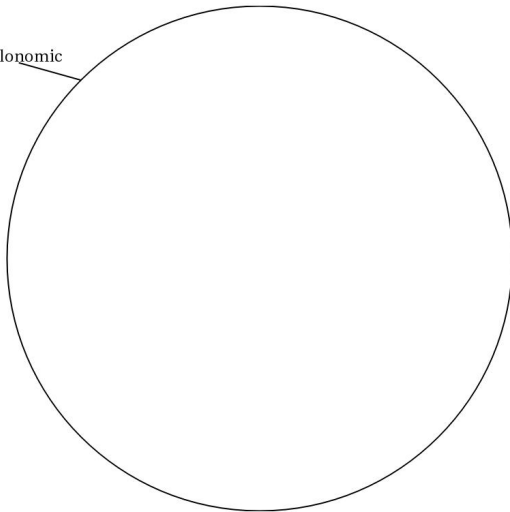
The functions that we consider here must have the following two properties:

- **∂ -finite:** Any shift and derivative of a function $f(\mathbf{v})$ is expressible as a finite $\mathbb{Q}(\mathbf{v})$ -linear combination of “basis functions” (shifts and derivatives of f).
In terms of ideals: the annihilating left ideal of $f(\mathbf{v})$ is zero-dimensional in $\mathbb{Q}(\mathbf{v})\langle\partial_{\mathbf{v}}\rangle$.
- **holonomic:** there is an annihilating ideal in the polynomial algebra $\mathbb{Q}\langle\mathbf{v}, \partial_{\mathbf{v}}\rangle$ which has the elimination property, i.e., for each choice of $n + 1$ among the $2n$ generators $v_1, \dots, v_n, \partial_{v_1}, \dots, \partial_{v_n}$ we find an element in the ideal that depends only on those.

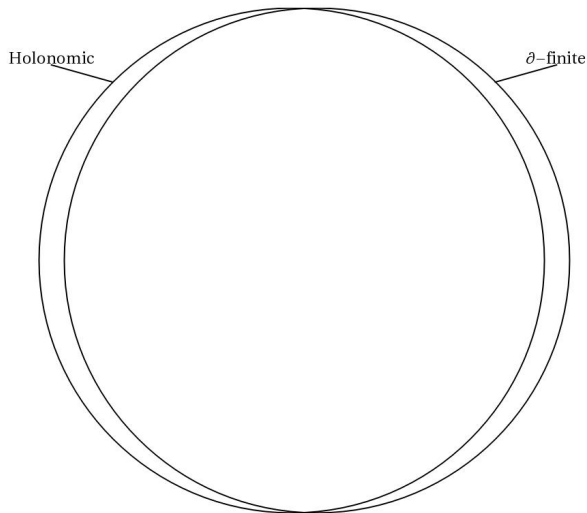


Holonomic and ∂ -Finite Functions

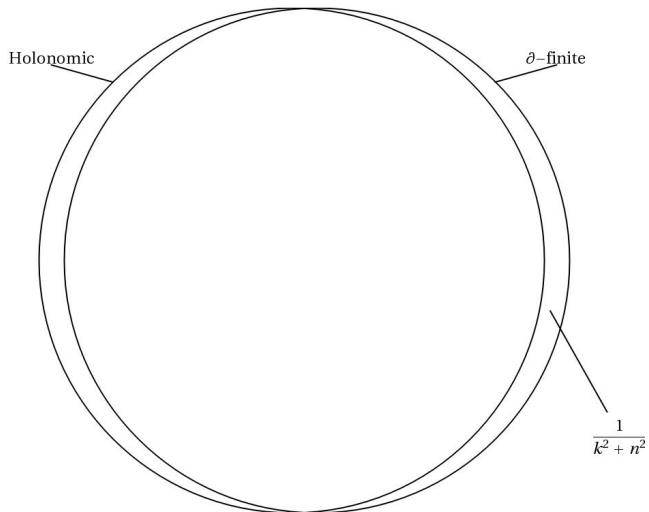
Holonomic



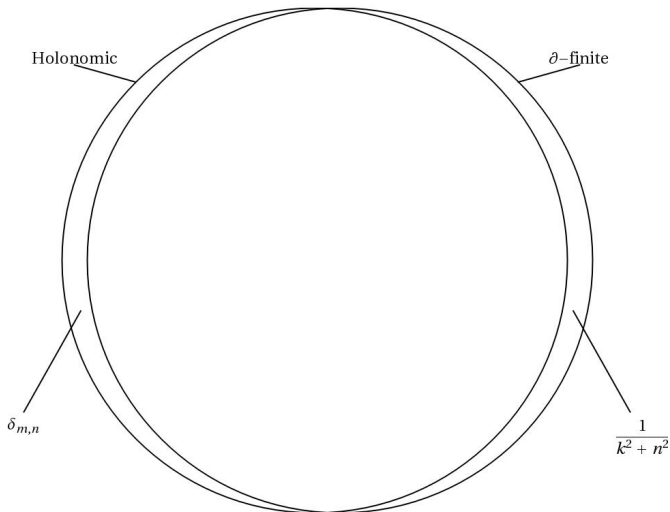
Holonomic and ∂ -Finite Functions



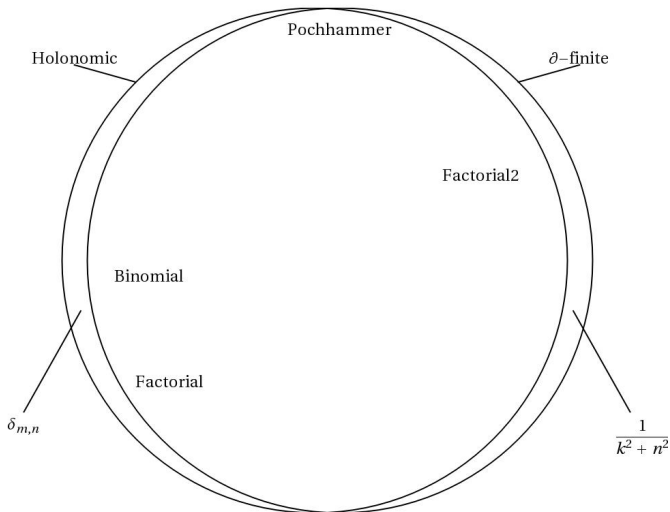
Holonomic and ∂ -Finite Functions



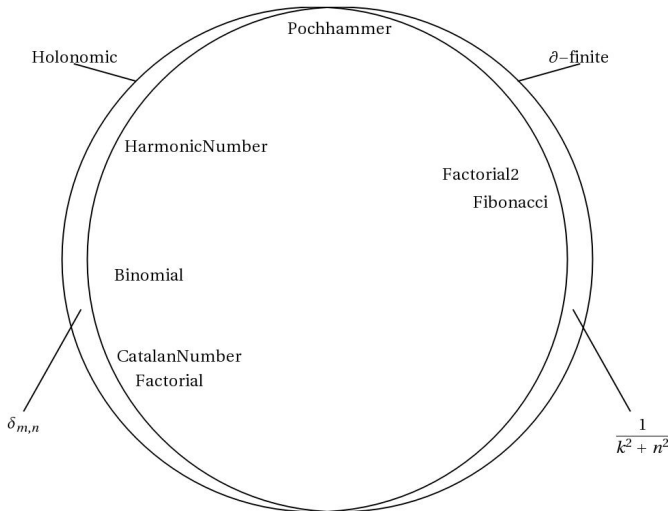
Holonomic and ∂ -Finite Functions



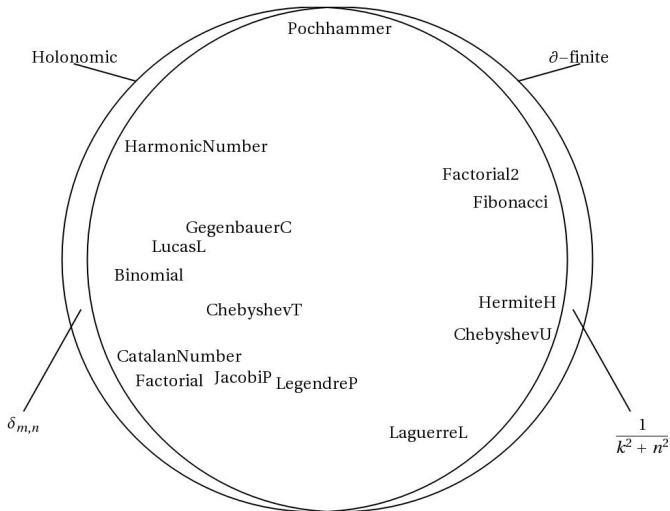
Holonomic and ∂ -Finite Functions



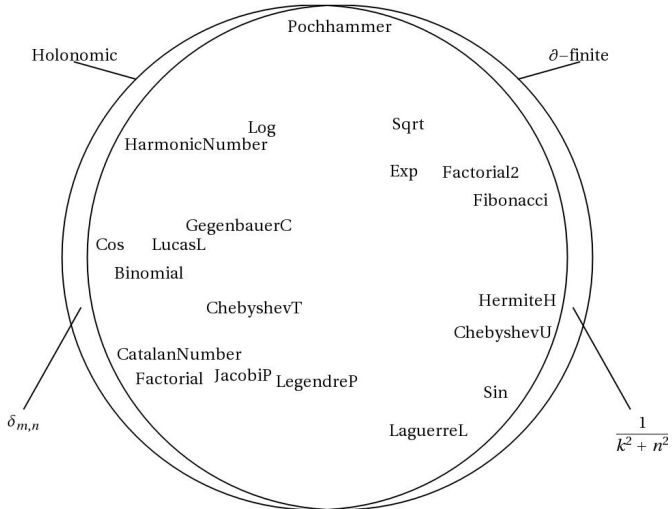
Holonomic and ∂ -Finite Functions



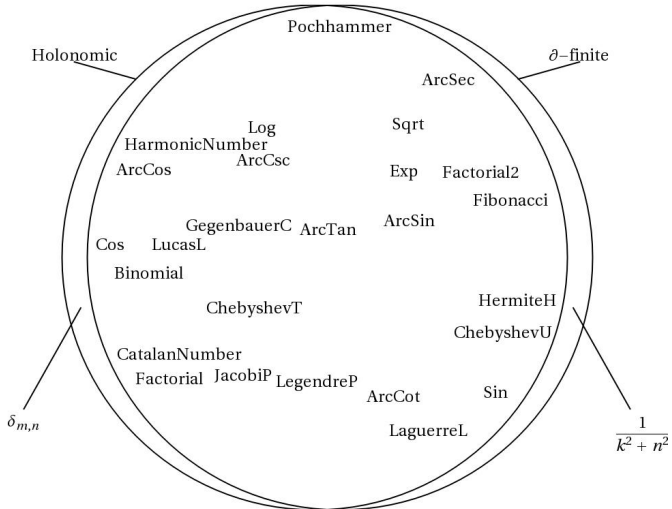
Holonomic and ∂ -Finite Functions



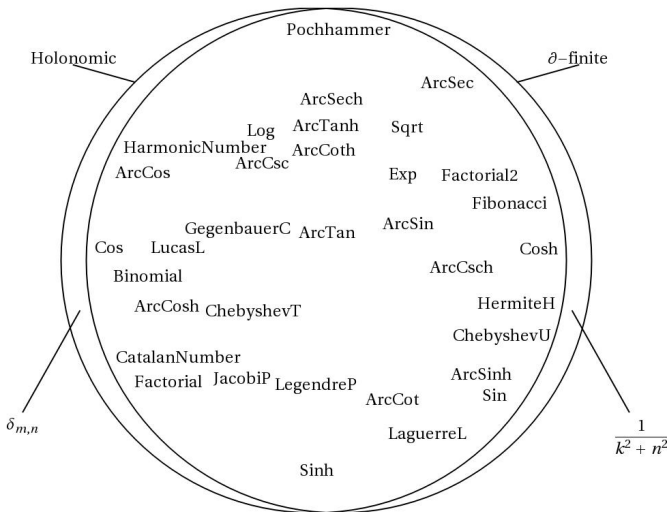
Holonomic and ∂ -Finite Functions



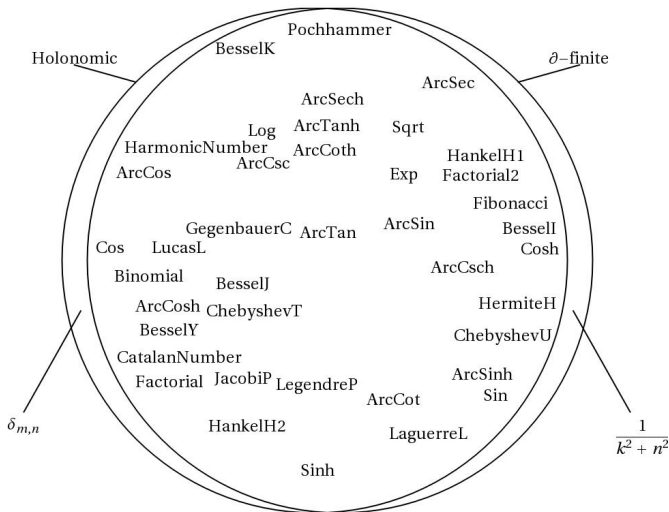
Holonomic and ∂ -Finite Functions



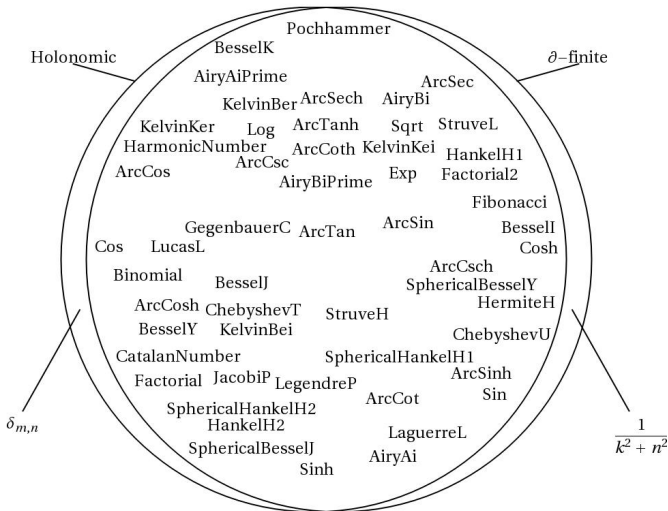
Holonomic and ∂ -Finite Functions



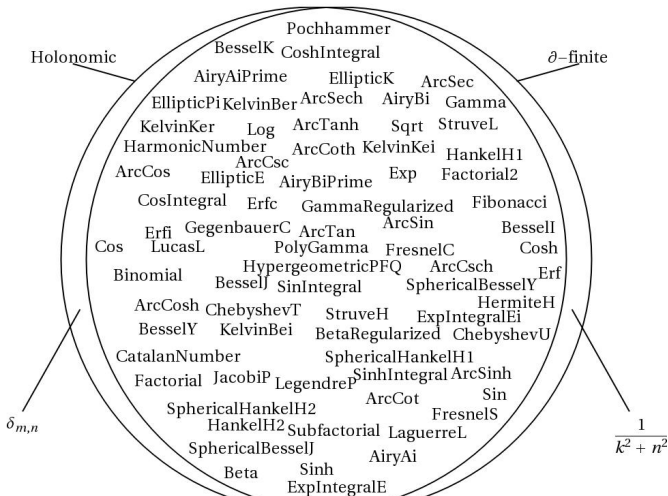
Holonomic and ∂ -Finite Functions



Holonomic and ∂ -Finite Functions



Holonomic and ∂ -Finite Functions



Example of a ∂ -finite function

The Legendre polynomials are ∂ -finite.

Their annihilating left ideal is generated by

$$\{(n+1)S_n + (1-x^2)D_x - (n+1)x, \\ (x^2-1)D_x^2 + 2xD_x - n(n+1)\}.$$

This is a Gröbner basis ($S_n > D_x$) with finitely many (namely 2) monomials under the stairs: $\mathfrak{U} = \{1, D_x\}$.

Changing the monomial order to $D_x > S_n$ we obtain a different Gröbner basis

$$\{(x^2-1)D_x - (n+1)S_n + (n+1)x, \\ (n+2)S_n^2 - (2n+3)xS_n + (n+1)\}$$

with $\mathfrak{U} = \{1, S_n\}$ under the stairs.



How to Find CT Operators

The general strategy is:

1. make an ansatz with undetermined coefficients
2. extract equations for these coefficients
3. solve these equations

Remarks:

- step 2 is done by reduction modulo the annihilating ideal
- using a Gröbner basis ensures the equivalence

$$(\text{remainder is zero}) \iff (\text{operator is in the ideal})$$

- equating all coefficients (in the Ore algebra sense) of the remainder to zero yields a system of equations
- depending on the ansatz, a coefficient comparison w.r.t. some variables is performed



Different Ansätze

There are plenty of ways to obtain CT operators:

1. k -free ansatz (in our terminology: w -free)
2. polynomial ansatz
3. ansatz with undetermined rational functions
4. ansatz with generic denominators
5. ansatz with specific denominators

Since we are usually interested in the principal part of “smallest order”, the main loop is over its support (trial and error).



k -Free Ansatz

Ansatz of the form

$$\sum_{\alpha} \sum_{\beta} c_{\alpha,\beta}(\mathbf{v}) \partial_{\mathbf{v}}^{\alpha} \partial_{\mathbf{w}}^{\beta}$$

where none of the summation/integration variables $\mathbf{w}$ appear in the unknown coefficients $c_{\alpha,\beta}$.

- existence of such an operator is guaranteed by holonomy
- rewriting to the form $P(\mathbf{v}, \partial_{\mathbf{v}}) + \sum_i \Delta_i Q_i(\mathbf{v}, \partial_{\mathbf{v}}, \partial_{\mathbf{w}})$ is straight-forward
- coefficient comparison w.r.t. $\mathbf{w}$ is necessary
- leads to a linear system for the $c_{\alpha,\beta}$
- known as Sister Celine's algorithm



Polynomial Ansatz

Ansatz of the form

$$\sum_{\alpha} c_{\alpha}(v) \partial_v^{\alpha} + \sum_{i=1}^m \Delta_i \sum_{\alpha} \sum_{\beta} \sum_{\gamma} c_{i,\alpha,\beta,\gamma}(v) w^{\gamma} \partial_v^{\alpha} \partial_w^{\beta}$$

- existence of such an operator is guaranteed by holonomy (a fortiori: generalization of the k -free ansatz)
- coefficient comparison w.r.t. w is necessary
- leads to a linear system
- implemented in Wegschaider's MultiSum package (for hypergeometric summands only)



Ansatz with Undetermined Rational Functions

Ansatz of the form

$$\sum_{\alpha} c_{\alpha}(\mathbf{v}) \partial_{\mathbf{v}}^{\alpha} + \Delta_w \sum_{j=1}^{|\mathfrak{U}|} \varphi_j(\mathbf{v}, w) U_j$$

with unknowns $c_{\alpha} \in \mathbb{Q}(\mathbf{v})$ and $\varphi_j \in \mathbb{Q}(\mathbf{v}, w)$, where $\mathfrak{U} = \{U_1, U_2, \dots\}$ are the monomials under the stairs.

- existence is guaranteed (reduce the delta part of the previous ansatz to normal form)
- two different kinds of unknowns
- leads to a coupled linear first-order system of differential or difference equations in the unknowns φ_j with parameters c_{α}
- only a single summation/integration is possible
- this ansatz was proposed by Chyzak
- implemented in Mgfund (Maple) and HolonomicFunctions (Mathematica)



Ansatz with Generic Denominators

Ansatz of the form

$$\sum_{\alpha} c_{\alpha}(\mathbf{v}) \partial_{\mathbf{v}}^{\alpha} + \sum_{i=1}^m \Delta_i \sum_{j=1}^{|\mathcal{U}|} \frac{\sum_{\alpha} c_{1,i,j,\alpha}(\mathbf{v}) \mathbf{w}^{\alpha}}{\sum_{\alpha} c_{2,i,j,\alpha}(\mathbf{v}) \mathbf{w}^{\alpha}} U_j$$

- coefficient comparison w.r.t. $\mathbf{w}$ is necessary
- leads to a nonlinear system of equations
- nobody ever proposed to use this ansatz!



Ansatz with Specific Denominators

Topic of our talk: ansatz of the form

$$\sum_{\alpha} c_{\alpha}(\mathbf{v}) \partial_{\mathbf{v}}^{\alpha} + \sum_{i=1}^m \Delta_i \sum_{j=1}^{|\mathcal{U}|} \frac{\sum_{\alpha} c_{i,j,\alpha}(\mathbf{v}) \mathbf{w}^{\alpha}}{d_{i,j}(\mathbf{v}, \mathbf{w})} U_j$$

with unknowns c_{α} and $c_{i,j,\alpha}$, and with specific denominators $d_{i,j}$.

- coefficient comparison w.r.t. $\mathbf{w}$
- leads to a linear system of equations
- the denominators $d_{i,j}$ can be somehow predicted
- implemented in `HolonomicFunctions`
- partly available in `MultiSum` (the hypergeometric case only), see also Wilf/Zeilberger (1992) and Apagodu/Zeilberger (2005)



Comparison

Let's compare the classical method (Chyzak) with our new approach:

- several summations/integrations possible in one step
- no guarantee for termination or for finding the operator with minimal principal part
- coupled diff. system with few unknowns vs. linear system with many unknowns
- perfectly suited for homomorphic images
- no expensive uncoupling required
- memory requirements can be confined to a minimum
- better controllability



Optimization 1: Homomorphic Images

Homomorphic images (i.e., modular arithmetic) play a crucial role in our approach.

- the unknown coefficients have to be determined in $\mathbb{Q}(v)$
- but for testing whether a certain principal part admits a solution: use homomorphic images
- plug in concrete values for $v_1, v_2, \dots$
- compute in $\mathbb{Z}_p$ instead of $\mathbb{Q}$ for some prime p
- caveat: Gröbner basis reduction; first compute the necessary products $\partial_v^\alpha \partial_w^\beta g_i$ where $\{g_1, g_2, \dots\}$ is the Gröbner basis, then do the substitution!



Denominators

$$\sum_{\alpha} c_{\alpha}(\mathbf{v}) \partial_{\mathbf{v}}^{\alpha} + \sum_{i=1}^m \Delta_i \sum_{j=1}^{|\mathcal{U}|} \frac{\sum_{\alpha} c_{i,j,\alpha}(\mathbf{v}) \mathbf{w}^{\alpha}}{d_{i,j}(\mathbf{v}, \mathbf{w})} U_j$$

- candidates for denominators: leading coefficients of the Gröbner basis
 - in case of summation, also shifts need to be included
 - find a candidate d such that $d_{i,j} \mid d$ for all i, j
 - heuristic: take the common denominator that occurs during the reduction of the ansatz
 - works well in more than 90% of the examples
- better understanding needed!



Optimization 2

$$\sum_{\alpha} c_{\alpha}(\mathbf{v}) \partial_{\mathbf{v}}^{\alpha} + \sum_{i=1}^m \Delta_i \sum_{j=1}^{|\mathcal{U}|} \frac{\sum_{\alpha} c_{i,j,\alpha}(\mathbf{v}) \mathbf{w}^{\alpha}}{d_{i,j}(\mathbf{v}, \mathbf{w})} U_j$$

For computing a candidate d for the common denominator:

- don't do the reduction with symbolic $\mathbf{v}$
- perform modular reduction
- identify the true factors from their homomorphic images
- consider only factors that depend on some of the $\mathbf{w}$



Optimization 3

$$\sum_{\alpha} c_{\alpha}(\mathbf{v}) \partial_{\mathbf{v}}^{\alpha} + \sum_{i=1}^m \Delta_i \sum_{j=1}^{|\mathcal{U}|} \frac{\sum_{\alpha} c_{i,j,\alpha}(\mathbf{v}) \mathbf{w}^{\alpha}}{d_{i,j}(\mathbf{v}, \mathbf{w})} U_j$$

Still, for fixed support of the principal part and denominators $d_{i,j}$, the degree of $\mathbf{w}^{\alpha}$ in the delta parts is yet unknown.

- start with small degree
- increase the degree until it becomes “unreasonably” large (heuristic!)
- need not to build the whole matrix in each step
- just add a few columns (and probably rows)
- this is very fast, and thus the heuristic bound can be generous
- problematic for multiple summations/integrations



Optimization 4

$$\sum_{\alpha} c_{\alpha}(\mathbf{v}) \partial_{\mathbf{v}}^{\alpha} + \sum_{i=1}^m \Delta_i \sum_{j=1}^{|\mathcal{U}|} \frac{\sum_{\alpha} c_{i,j,\alpha}(\mathbf{v}) \mathbf{w}^{\alpha}}{d_{i,j}(\mathbf{v}, \mathbf{w})} U_j$$

Minimize the common denominator d .

- write d as a product of irreducible factors
- delete one factor
- reduce the degree bound according to the $\mathbf{w}$ -degree of this factor
- check whether still a solution is found
- if so, this factor can be omitted in the ansatz



Optimization 5

$$\sum_{\alpha} c_{\alpha}(\mathbf{v}) \partial_{\mathbf{v}}^{\alpha} + \sum_{i=1}^m \Delta_i \sum_{j=1}^{|\mathcal{U}|} \frac{\sum_{\alpha} c_{i,j,\alpha}(\mathbf{v}) \mathbf{w}^{\alpha}}{d_{i,j}(\mathbf{v}, \mathbf{w})} U_j$$

Minimize denominators $d_{i,j}$.

- is done in the same way as before
- sometimes it pays off, sometimes not



Optimization 6

Delete zero-components from the ansatz.

Use modular computations to reduce the number of rows in the matrix.

With the refined ansatz, we may either

- start the final computation (non-modular) or
- perform many modular computations, allowing for interpolating and reconstructing the solution



Example: Three Gegenbauer Polynomials (1)

$$\int_{-1}^1 C_l^{(\lambda)}(x) C_m^{(\lambda)}(x) C_n^{(\lambda)}(x) (1-x^2)^{\lambda-1/2} dx =$$
$$\frac{\pi 2^{1-2\lambda} \Gamma\left(2\lambda + \frac{1}{2}(l+m+n)\right)}{\Gamma(\lambda)^2 \left(\frac{1}{2}(l+m+n) + \lambda\right)}$$
$$\times \frac{(\lambda)_{(m+n-l)/2} (\lambda)_{(l+n-m)/2} (\lambda)_{(l+m-n)/2}}{\left(\frac{1}{2}(m+n-l)\right)! \left(\frac{1}{2}(l+n-m)\right)! \left(\frac{1}{2}(l+m-n)\right)! (\lambda)_{(l+m+n)/2}}$$

The identity is valid when $\lambda > -\frac{1}{2}$ and $\lambda \neq 0$, $l+m+n$ is even and the sum of any two of l, m, n is not less than the third; the integral is zero in all other cases (Andrews/Askey/Roy (6.8.10)).

Trying Chyzak's algorithm:

- with HolonomicFunctions: 20 minutes to find one relation (a Mathematica bug prevents us from finding all of them)
- with Mgfuns: out of memory after a few minutes



Example: Three Gegenbauer Polynomials (2)

But the result is strikingly simple: there are three CT operators whose principal parts are

$$\begin{aligned} & (l + m - n + 1)(l - m + n + 2\lambda - 1)S_m - \\ & \quad (l - m + n + 1)(l + m - n + 2\lambda - 1)S_n, \\ & (l + m - n + 1)(l - m - n - 2\lambda + 1)S_l - \\ & \quad (l - m - n - 1)(l + m - n + 2\lambda - 1)S_n, \\ & (l - m - n - 2)(l - m + n + 2)(l + m - n + 2\lambda - 2) \\ & \quad \times (l + m + n + 2\lambda + 2)S_n^2 - \\ & \quad (l + m - n)(l - m - n - 2\lambda)(l - m + n + 2\lambda)(l + m + n + 4\lambda). \end{aligned}$$

With our new approach, it is computed within 10 seconds!



Examples from Thierry Combet (1)

Let $P_n(x) = \frac{1}{x^2 - 1} \frac{d^{n-1}}{dx^{n-1}} (x^2 - 1)^n$.

Now consider (for specific values of k) the integral

$$\int_{-1}^1 P_n(x)^{k+1} (x^2 - 1)^k dx.$$

Our results using the ansatz with denominators:

- found recurrence in n for $2 \leq k \leq 7$
- the integrand has $k + 2$ monomials under the stairs
- the cases with even k are harder: $k = 6$ took 10848s while $k = 7$ took only 2293s
- the recurrence for $k = 6$ has order 6 (with even exponents only) and degree 92
- the recurrence for $k = 7$ has order 4 and degree 70



Examples from Thierry Combot (2)

Consider the integral

$$\int (x^2 - 1)^2 P_n(x) Q_n(x)^2 \left(\int (x^2 - 1)^2 P_n(x)^3 dx \right) dx$$

where $Q_n(x)$ is annihilated by the same operators as $P_n(x)$.

The inner integral denotes an antiderivative, whereas the outer one is a contour around infinity.

- 24 monomials under the stairs
- ansatz with 1310 unknowns
- total timing is about 50 hours



Example: Lattice Green's Functions

We study the face-centered cubic lattice in several dimensions $d = 2, \dots, 6$.

The lattice Green's function is the probability generating function

$$P(\mathbf{x}; z) = \sum_{n=0}^{\infty} p_n(\mathbf{x}) z^n.$$

Of particular interest is

$$P(\mathbf{0}; z) = \sum_{n=0}^{\infty} p_n(\mathbf{0}) z^n = \frac{1}{\pi^d} \int_0^\pi \cdots \int_0^\pi \frac{dk_1 \dots dk_d}{1 - z\lambda(\mathbf{k})}.$$

that gives the return probabilities. Here $\lambda(\mathbf{k})$ is the structure function that is given by the discrete Fourier transform of the step probabilities.



Example: Lattice Green's Functions

Thus, for the d -dimensional face-centered cubic lattice, we have to compute a d -fold integral of $\frac{1}{1-z\lambda(\mathbf{k})}$ where the structure function is

$$\lambda(\mathbf{k}) = \left(\frac{d}{2}\right)^{-1} \left(\cos(k_1) \cos(k_2) + \cdots + \cos(k_{d-1}) \cos(k_d) \right)$$

Timings with our approach

- $d = 3$: 2 seconds
- $d = 4$: 3 minutes
- $d = 5$: 4 hours
- $d = 6$: 5 days



Results for Lattice Green's Functions

In this instance it turned out to be most efficient to do all integrations separately.

In each case, the result is a linear ODE in z . From this we can compute the return probability

$$r = 1 - \frac{1}{\sum_{n=0}^{\infty} p_n(\mathbf{0})}$$

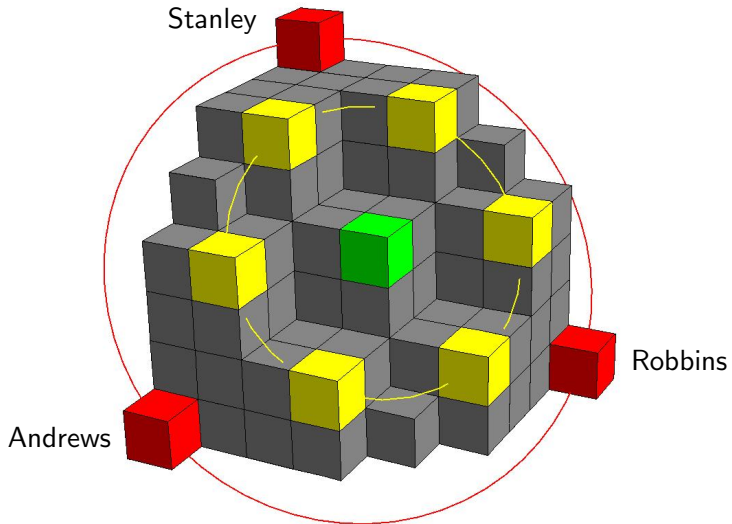
to very high accuracy using asymptotic expansions.

Some results for return probabilities:

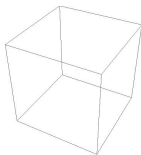
- $d = 3$: $r_3 = 1 - \frac{16 \sqrt[3]{4\pi^4}}{9(\Gamma(\frac{1}{3}))^6} \approx 0.2563182365$
- $d = 4$: $r_4 \approx 0.09571315417$
- $d = 5$: $r_5 \approx 0.04657695746$
- $d = 6$: $r_6 \approx 0.02699987828$



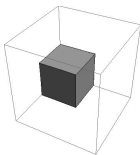
q -TSP



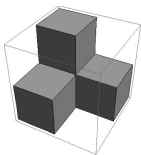
Let $T(n)$ denote set of TSPPs with largest part at most n .



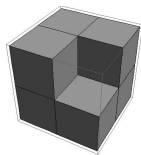
q^0



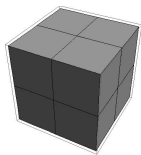
q^1



q^2



q^3



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 $q = 1$:

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



The Determinant

Reduction by Soichi Okada:

The q -TSPP conjecture is true if

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

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

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

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

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

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



The result. . .



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-TSPP conjecture

