∂-finite functions revisited

Christoph Koutschan

Research Institute for Symbolic Computation
Johannes Kepler Universität Linz, Austria

20 April 2009
INRIA Paris-Rocquencourt

What is this talk about?

Starting point: Algorithmic framework for the automatic treatment of ∂-finite functions, as described in Frédéric Chyzak's PhD thesis

Now: some new ideas, exemplified on two applications:

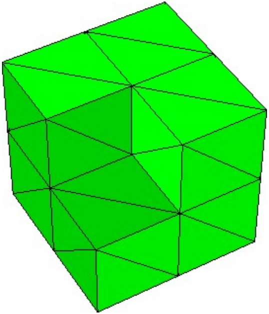
- Part I: Simulation of electromagnetic waves
- Part II: TSPP

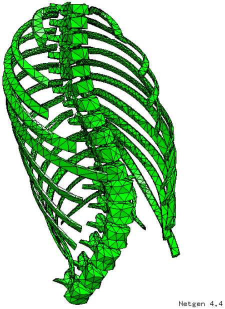
Simulation of electromagnetic waves

- joint work by Joachim Schöberl (RWTH Aachen), Peter Paule and CK
- wide range of applications in constructing antennas, mobile phones, etc.
- merchandised by the company CST (Computer Simulation Technology)
- simulation with finite element methods
- significant contributions from Symbolic Computation using CK's package `HolonomicFunctions`
- symbolically derived formulae allow a considerable speed-up

Finite Element Method (FEM)

Numerical method for finding approximate solutions to partial differential equations on non-trivial domains:





- divide the domain into small finite elements (triangles in 2D, tetrahedra in 3D)
- approximate the solution by certain basis functions that are defined on each finite element
- locally supported piecewise polynomial basis functions

Our 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 basis (i.e., as linear combinations of shifts of the $\varphi_{i,j}(x,y)$ itself)

Recall: ∂-finite functions

Definition: A function $f(x_1, \ldots, x_n)$ is called ∂-finite w.r.t. an Ore algebra $\mathbb{O} = \mathbb{K}(x_1, \ldots, x_n)[\partial_1; \sigma_1, \delta_1] \cdots [\partial_n; \sigma_n, \delta_n]$ if $\mathbb{O}/\operatorname{Ann}_{\mathbb{O}} f$ is a finite-dimensional $\mathbb{K}(x_1, \ldots, x_n)$-vector space.

In other words, f is ∂-finite if all its "derivatives" span a finite-dimensional $\mathbb{K}(x_1, \ldots, x_n)$-vector space.

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.,

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

First try

```
phi[i_,j_,x_,y_] :=
 LegendreP[i,2*y/(1-x)-1]*(1-x)^i*JacobiP[j,2*i+1,0,2*x-1]
ann = Annihilator[phi[i,j,x,y], {Der[x], S[i], S[j]}]
```

$\langle$*quite big output*$\rangle$

In order to see better the structure of the output, we look only at the support of each operator:

```
Support[ann]
```

$$\{\{S_j^2, S_j, 1\}, \{S_i S_j, D_x, S_i, S_j, 1\}, \{S_i^2, D_x, S_i, S_j, 1\}, \{D_x S_j, D_x, S_i, S_j, 1\}, \{D_x S_i, D_x, S_i, S_j, 1\}, \{D_x^2, D_x, S_i, S_j, 1\}\}$$

$\longrightarrow$ second and third operator match exactly our needs!

Second try

BUT: The numerists need a relation that is free of x and y! In change, they allow also shifted derivatives.

- "switch" to the Ore algebra $\mathbb{Q}(i,j)[x,y][D_x;1,D_x][S_i;S_i,0][S_j;S_j,0]$
- compute 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

Third try

Recall: We are looking for a relation of the following form

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

where $A, B \subset \mathbb{N}^2$ are finite index sets.

- make an ansatz!
- let $\mathbb{O} = \mathbb{Q}(i,j,x,y)[D_x;1,D_x][S_i;S_i,0][S_j;S_j,0]$
- choose index sets A and B
- reduce the ansatz with the Gröbner basis of $\operatorname{Ann}_{\mathbb{O}} \varphi$
- do coefficient comparison w.r.t. x and y
- solve the resulting linear system for $a_{k,l}, b_{m,n} \in \mathbb{Q}(i,j)$

Result

With this method, we find in short time a (similar) relation:

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

Joachim Schöberl's answer: "jetzt bin ich echt beeindruckt... Genau so eine Relation brauche ich!"

$\longrightarrow$ these formulae caused a speed-up of 20 percent (!) in the numerical simulations

3D case

We would like to do the same thing in 3D.

Problems:

- now the basis functions

$$\begin{aligned}\varphi(i,j,k,x,y,z) := \quad & P_i\left(\tfrac{2z}{(1-x)(1-y)}-1\right)(1-x)^i(1-y)^i \\ & P_j^{(2i+1,0)}\left(\tfrac{2y}{1-x}-1\right)(1-x)^j \\ & P_k^{(2i+2j+2,0)}(2x-1)\end{aligned}$$

  contain 6 variables
- computations become too big and too slow
- need some optimizations

Optimizations (1)

Of course,

$$\mathrm{nf}\left(\sum_k a_k \boldsymbol{\partial}^{\boldsymbol{\alpha}_k}\right) = \sum_k a_k \,\mathrm{nf}\left(\boldsymbol{\partial}^{\boldsymbol{\alpha}_k}\right)$$

- reduce each monomial $\boldsymbol{\partial}^{\boldsymbol{\alpha}_k}$ separately
- use previously computed normal forms

Optimizations (2)

Idea: Can we use homomorphic images for finding a good ansatz?

- surely we can compute in $\mathbb{Z}_p(i,j,x,y)[D_x;1,D_x][S_i;S_i,0][S_j;S_j,0]$
- this does not help much
- better: try to reduce polynomial arithmetic
- have to keep x, y and z symbolically (coefficient comparison)
- what about i, j and k?

Recall: normal form computation

Input: $p \in \mathbb{O}$, a Gröbner basis $G = \{g_1, \ldots, g_n\} \subseteq \mathbb{O}$
Output: normal form of p modulo ${}_{\mathbb{O}}\langle G \rangle$

while exists $1 \leq i \leq n$ such that $\mathrm{lm}(g_i) \mid \mathrm{lm}(p)$
    $g := (\mathrm{lm}(p)/\mathrm{lm}(g_i)) \cdot g_i$
    $p := p - (\mathrm{lc}(p)/\mathrm{lc}(g)) \cdot g$
end while

Modular normal form computation

Input: $p \in \mathbb{O}$, a Gröbner basis $G = \{g_1, \ldots, g_n\} \subseteq \mathbb{O}$
Output: normal form of p modulo ${}_{\mathbb{O}}\langle G \rangle$

while exists $1 \leq i \leq n$ such that $\operatorname{lm}(g_i) \mid \operatorname{lm}(p)$
$\quad g := h((\operatorname{lm}(p)/\operatorname{lm}(g_i)) \cdot g_i)$
$\quad p := p - (\operatorname{lc}(p)/\operatorname{lc}(g)) \cdot g$
end while

where h is an insertion homomorphism, in our example

$$\begin{aligned} h :\ \mathbb{Q}(i,j,k,x,y,z) &\to \mathbb{Q}(x,y,z) \\ f(i,j,k,x,y,z) &\mapsto f(i_0,j_0,k_0,x,y,z), \quad \text{for } i_0,j_0,k_0 \in \mathbb{Z} \end{aligned}$$

A first result for 3D

One of the supports looks as follows:

$$
\begin{aligned}
&\{S_j S_k^4, S_j^2 S_k^3, S_j^3 S_k^2, S_j^4 S_k, D_x S_j S_k^3, D_x S_j^2 S_k^2, D_x S_j^3 S_k, D_x S_j^4, S_j S_k^5,\\
&S_j^2 S_k^4, S_j^3 S_k^3, S_j^4 S_k^2, S_i S_k^5, S_i S_j S_k^4, S_i S_j^2 S_k^3, S_i S_j^3 S_k^2, D_x S_j S_k^4, D_x S_j^2 S_k^3,\\
&D_x S_j^3 S_k^2, D_x S_j^4 S_k, D_x S_i S_k^4, D_x S_i S_j S_k^3, D_x S_i S_j^2 S_k^2, D_x S_i S_j^3 S_k, S_j S_k^6,\\
&S_j^2 S_k^5, S_j^3 S_k^4, S_j^4 S_k^3, S_i S_k^6, S_i S_j S_k^5, S_i S_j^2 S_k^4, S_i S_j^3 S_k^3, D_x S_j S_k^5, D_x S_j^2 S_k^4,\\
&D_x S_j^3 S_k^3, D_x S_j^4 S_k^2, D_x S_i S_k^5, D_x S_i S_j S_k^4, D_x S_i S_j^2 S_k^3, D_x S_i S_j^3 S_k^2, S_j S_k^7,\\
&S_j^2 S_k^6, S_j^3 S_k^5, S_j^4 S_k^4, S_i S_k^7, S_i S_j S_k^6, S_i S_j^2 S_k^5, S_i S_j^3 S_k^4, D_x S_j S_k^6, D_x S_j^2 S_k^5,\\
&D_x S_j^3 S_k^4, D_x S_j^4 S_k^3, D_x S_i S_k^6, D_x S_i S_j S_k^5, D_x S_i S_j^2 S_k^4, D_x S_i S_j^3 S_k^3, S_j S_k^8,\\
&S_j^2 S_k^7, S_j^3 S_k^6, S_j^4 S_k^5, D_x S_j S_k^7, D_x S_j^2 S_k^6, D_x S_j^3 S_k^5, D_x S_j^4 S_k^4, D_x S_i S_k^7,\\
&D_x S_i S_j S_k^6, D_x S_i S_j^2 S_k^5, D_x S_i S_j^3 S_k^4, D_x S_j S_k^8, D_x S_j^2 S_k^7, D_x S_j^3 S_k^6,\\
&D_x S_j^4 S_k^5, D_x S_i S_k^8, D_x S_i S_j S_k^7, D_x S_i S_j^2 S_k^6, D_x S_i S_j^3 S_k^5, D_x S_j S_k^9,\\
&D_x S_j^2 S_k^8, D_x S_j^3 S_k^7, D_x S_j^4 S_k^6\}
\end{aligned}
$$

Joachim Schöberl was impressed but not too happy about these results...

Divide

Next idea: Write $\varphi = u \cdot v \cdot w$ with

$$\begin{aligned} u &= P_i\left(\tfrac{2z}{(1-x)(1-y)} - 1\right)(1-x)^i(1-y)^i \\ v &= P_j^{(2i+1,0)}\left(\tfrac{2y}{1-x} - 1\right)(1-x)^j \\ w &= P_k^{(2i+2j+2,0)}(2x-1) \end{aligned}$$

and use the product rule

$$\frac{\mathrm{d}\varphi}{\mathrm{d}x} = \frac{\mathrm{d}u}{\mathrm{d}x}vw + u\frac{\mathrm{d}v}{\mathrm{d}x}w + uv\frac{\mathrm{d}w}{\mathrm{d}x}$$

We now want to find a relation between e.g. uvw and $\frac{\mathrm{d}u}{\mathrm{d}x}vw$.

. . .

Task: find relation between uvw and $\frac{\mathrm{d}u}{\mathrm{d}x}vw$

How does this fit into our framework?

Usually we have something like

$$\mathrm{op} \bullet f = 0.$$

Now we search for a relation of the form

$$\mathrm{op}_1 \bullet f = \mathrm{op}_2 \bullet g.$$

Trivial solution: $\mathrm{op}_1 \in \mathrm{Ann}\, f$ and $\mathrm{op}_2 \in \mathrm{Ann}\, g$. But since f and g are closely related we expect that there exists something "better".

The natural way to express a relation like

$$\mathrm{op}_1 \bullet f = \mathrm{op}_2 \bullet g$$

is by using operator vectors in $M = \mathbb{O} \times \mathbb{O}$ which we let act on $\mathcal{F} \times \mathcal{F}$ by

$$P \bullet F = (P_1, P_2) \bullet (f, g) := P_1 \bullet f + P_2 \bullet g, \quad \text{where } P \in M, F \in \mathcal{F} \times \mathcal{F}$$

But how to compute a Gröbner basis for the ideal of relations between f and g, i.e. the annihilator $\mathrm{Ann}_M(f, g)$?

Closure properties

Let $f = uvw$ and $g = \frac{\mathrm{d}u}{\mathrm{d}x}vw$.

We start with u and $u' = \frac{\mathrm{d}u}{\mathrm{d}x}$:
$\mathrm{Ann}_M(u, u') =$

$$_{\mathbb{O}}\Big\langle \big\{(p,0)|p \in \mathrm{Ann}_{\mathbb{O}}\, u\big\} \cup \big\{(0,p)|p \in \mathrm{Ann}_{\mathbb{O}}\, u'\big\} \cup \big\{(D_x, -1)\big\} \Big\rangle$$

After computing a Gröbner basis of the above, we can perform the closure property "multiplication by vw" in a very similar fashion as usual (using an FGLM-like approach).

Result

Finally we can use the ansatz technique as before in order to find an $\{x, y, z\}$-free operator:

$$-2(1+2i)(2+j)(3+2i+j)(7+2i+2j)(5+i+j+k)$$
$$(7+i+j+k)(8+i+j+k)(8+2i+2j+k)(9+2i+2j+k)$$
$$(11+2i+2j+2k)(15+2i+2j+2k)f(i,j+1,k+3)+$$

$$\vdots$$

$\langle$ 31 similar terms $\rangle$

$$\vdots$$

$$-2(4+2i+j)(5+2i+j)(5+2i+2j)(5+i+j+k)$$
$$(6+i+j+k)(8+i+j+k)(10+2i+2j+k)$$
$$(11+2i+2j+k)(11+2i+2j+2k)(15+2i+2j+2k)$$
$$g(i+1,j+2,k+3)=0$$

where $f = uvw$ and $g = \frac{\mathrm{d}u}{\mathrm{d}x}vw$.

Part II
Totally Symmetric Plane Partitions

(joint work with M. Kauers and D. Zeilberger)

Plane Partitions

Definition: A *plane partition* π is an array

$$\pi = (\pi_{ij}), \quad i, j \geq 1, \quad \pi_{ij} \geq 1$$

with finite sum $|\pi| = \sum \pi_{ij}$, which is weakly decreasing in rows and columns, i.e.,

$$\pi_{i+1,j} \leq \pi_{ij} \quad \text{and} \quad \pi_{i,j+1} \leq \pi_{ij} \quad \text{for all } i, j \geq 1.$$

Example:

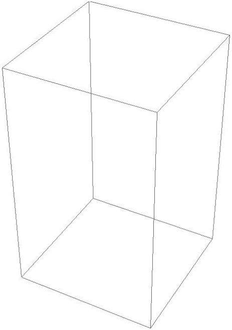
5	4	1
3	2	1
1		

3D Ferrers diagram

By stacking π_{ij} unit cubes on top of the ij location, one gets the corresponding 3D Ferrers diagram, which is a left-, up-, and bottom-justified structure of unit cubes, and we can refer to the locations (i, j, k) of the individual unit cubes.

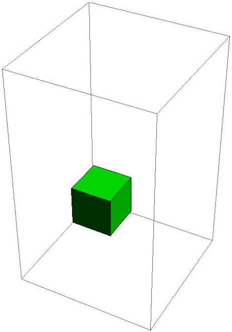
3D Ferrers diagram

5	4	1
3	2	1
1		



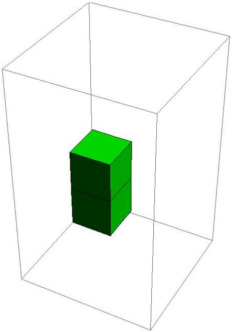
3D Ferrers diagram

5	4	1
3	2	1
1		



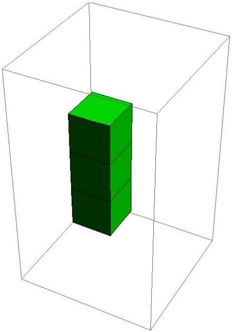
3D Ferrers diagram

5	4	1
3	2	1
1		



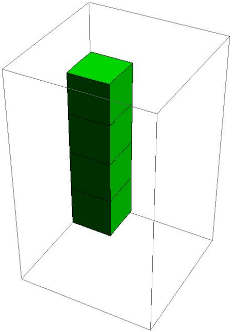
3D Ferrers diagram

5	4	1
3	2	1
1		



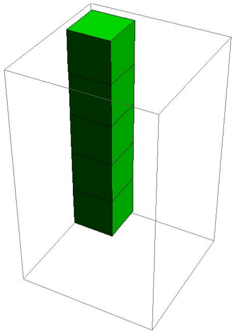
3D Ferrers diagram

5	4	1
3	2	1
1		



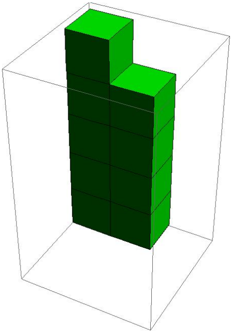
3D Ferrers diagram

5	4	1
3	2	1
1		



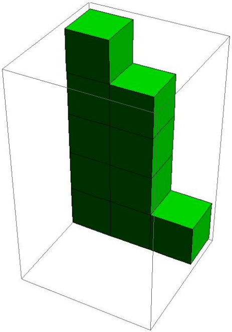
3D Ferrers diagram

5	4	1
3	2	1
1		



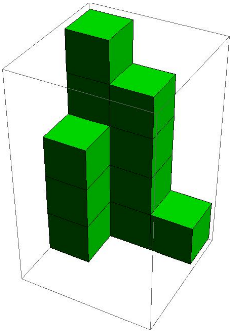
3D Ferrers diagram

5	4	1
3	2	1
1		



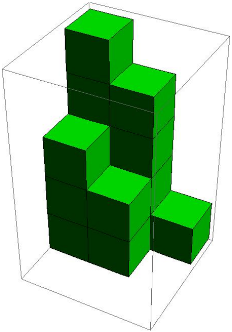
3D Ferrers diagram

5	4	1
3	2	1
1		



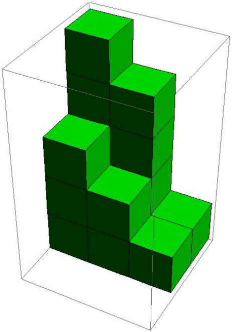
3D Ferrers diagram

5	4	1
3	2	1
1		



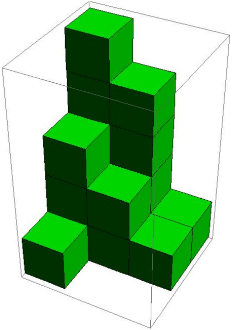
3D Ferrers diagram

5	4	1
3	2	1
1		



3D Ferrers diagram

5	4	1
3	2	1
1		

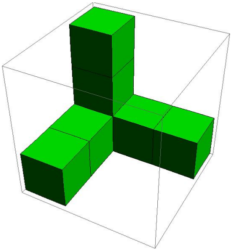


Totally Symmetric Plane Partitions (1)

Definition: A plane partition is *totally symmetric* iff whenever (i, j, k) is occupied (i.e. $\pi_{ij} \geq k$), it follows that all its (up to 5) permutations: $\{(i,k,j),(j,i,k),(j,k,i),(k,i,j),(k,j,i)\}$ are also occupied.

Example:

3	1	1
1		
1		



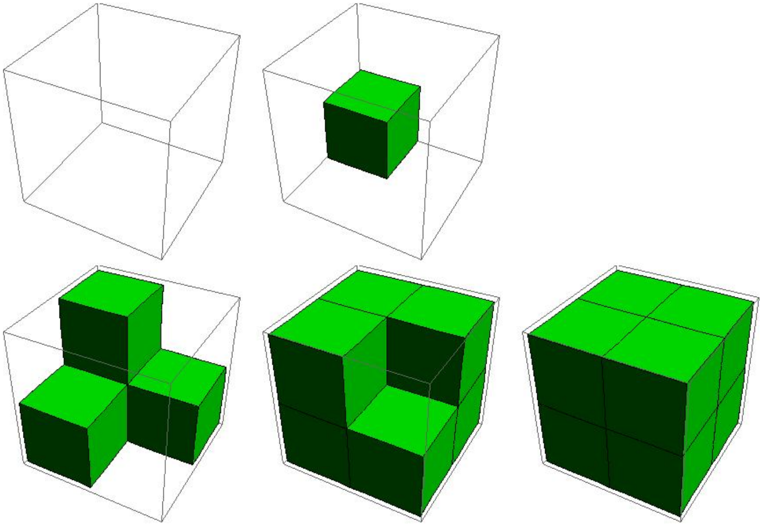
The TSPP Problem

Conjecture: (Ian Macdonald)
The number of totally symmetric plane partitions (TSPPs) whose 3D Ferrers diagram is bounded inside the cube $[0, n]^3$ is given by the nice product-formula

$$\prod_{1 \leq i \leq j \leq k \leq n} \frac{i+j+k-1}{i+j+k-2}.$$

Totally Symmetric Plane Partitions (2)

Example: All TSPPs for $n = 2$:



The TSPP Problem

Ian Macdonald's conjecture was proven in 1995 by John Stembridge.

Ten years later George Andrews, Peter Paule, and Carsten Schneider came up with a computer-assisted proof, that, however required lots of human ingenuity and ad hoc tricks, in addition to a considerable amount of computer time.

We aim at a complete computer proof (which works analogously for the q-version of TSPP).

The qTSPP Problem

Conjecture: (independently by George Andrews and Dave Robbins, around 1983)
A q-analogue of the TSPP problem leads to the nice formula

$$\prod_{1\leq i\leq j\leq k\leq n} \frac{1-q^{i+j+k-1}}{1-q^{i+j+k-2}}.$$

This conjecture is still open.

Okada's Determinant (1)

Soichi Okada reduced the problem to a determinant evaluation: He proved that the q-TSPP conjecture is true if

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

Analogously, in the $q=1$ case we have to show

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

Okada's Determinant (2)

where

$$\bar{a}(i,j) = q^{i+j-1}\left(\begin{bmatrix} i+j-2 \\ i-1 \end{bmatrix} + q\begin{bmatrix} i+j-1 \\ i \end{bmatrix}\right) + (1+q^i)\delta(i,j) - \delta(i,j+1)$$

where

$$\begin{bmatrix} a \\ b \end{bmatrix} = \frac{(1-q^a)(1-q^{a-1})\cdots(1-q^{a-b+1})}{(1-q^b)(1-q^{b-1})\cdots(1-q)}.$$

Remark: In the ordinary TSPP case ($q=1$) we have

$$a(i,j) = \binom{i+j-2}{i-1} + \binom{i+j-1}{i} + 2\delta(i,j) - \delta(i,j+1)$$

Zeilberger's Ansatz (1)

In his article

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

Doron Zeilberger proposes the following method:

We want to prove for all $n \geq 0$ that

$$\det(a(i,j))_{1 \leq i,j \leq n} = \mathrm{Nice}(n),$$

for some explicit expressions $a(i,j)$ and $\mathrm{Nice}(n)$.

Zeilberger's Ansatz (2)

Now a magician's trick is used: Pull out of the hat another "explicit" discrete function $B(n, j)$:

Zeilberger's Ansatz (3)

Check the identities

$$\sum_{j=1}^{n} B(n,j)a(i,j) = 0, \qquad (1 \leq i < n < \infty),$$

$$B(n,n) = 1, \qquad (1 \leq n < \infty).$$

Then by uniqueness, it follows that $B(n,j)$ equals the co-factor of the (n,j) entry of the $n \times n$ determinant divided by the $(n-1) \times (n-1)$ determinant.

Finally one has to check the identity

$$\sum_{j=1}^{n} B(n,j)a(n,j) = \mathrm{Nice}(n)/\mathrm{Nice}(n-1) \quad (1 \leq n < \infty).$$

Zeilberger's Ansatz (4)

If the suggested function $B(n, j)$ does satisfy all these identities then the determinant identity follows as a consequence. So in a sense, the explicit description of $B(n, j)$ plays the role of a certificate for the determinant identity.

Some results on TSPP

Result of guessing: 65 recurrences for $B(n,j)$, their total size being about 5MB.

∂-finite description: We succeeded to compute a Gröbner basis of the annihilating ideal of $B(n,j)$ (using CK's noncommutative `OreGroebnerBasis` implementation).
The Gröbner basis consists of 5 polynomials (their total size being about 1.6MB). Their leading monomials $S_j^4, S_j^3 S_n, S_j^2 S_n^2, S_j S_n^3, S_n^4$ form a staircase of regular shape.

How to proceed

We want to prove

$$\sum_{j=1}^{n} B(n,j)a(n,j) = \mathrm{Nice}(n)/\mathrm{Nice}(n-1)$$

where

$$a(n,j) = \binom{n+j-2}{n-1} + \binom{n+j-1}{n} + 2\delta(n,j) - \delta(n,j+1).$$

Hence we can consider the expression

$$\sum_{j=1}^{n} B(n,j)a'(n,j) + 2B(n,n) - B(n,n-1)$$

with $a'(n,j) = \binom{n+j-2}{n-1} + \binom{n+j-1}{n}$ being hypergeometric.

Several approaches

We unsuccessfully tried

- Gröbner basis elimination
- Takayama's algorithm
- Chyzak's algorithm

Finally, we succeeded by using the ansatz technique with an ansatz of the form

$$\sum_i \eta_i(n) S_n^i + (S_j - 1) \sum_{k,l,m} \varphi_{k,l,m}(n) j^k S_j^l S_n^m$$

Note: With this type of ansatz, it can happen that $\eta_i = 0$ for all i.

(The computations just came to an end on Friday evening.)