A Rational Perspective on Holonomic Functions

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CASTA
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Notation

In Prof. Takayama's lecture, the following notation was used:

$$\begin{array}{ccccccccc} R_n & = & \mathbb{C}(& x_1, & \ldots, & x_n &)\langle & \partial_1, & \ldots, \partial_n \rangle \\ \downarrow & & \downarrow & \downarrow & & \downarrow & & \downarrow & \downarrow \\ \mathbb{O} & = & \mathbb{K}(& x, & \ldots, & z &)\langle & D_x, & \ldots, D_z \rangle \end{array}$$

- $\mathbb{K}$: computable field of characteristic 0 (i.e., $\mathbb{Q} \subseteq \mathbb{K}$).
- Here ∂_x will denote a generic operator symbol, related to the variable x.
- D_n will not appear here.

Ore Algebras

$\longrightarrow$ **Generalization** of the ring of differential operators

Let $\mathbb{A}$ be a ring,

- $\sigma \colon \mathbb{A} \to \mathbb{A}$ an automorphism on $\mathbb{A}$, and
- $\delta \colon \mathbb{A} \to \mathbb{A}$ be a σ-derivation, i.e.,

$$\delta(ab) = \sigma(a)\delta(b) + \delta(a)b \quad \text{for all } a, b \in \mathbb{A}.$$

Then the polynomial ring $\mathbb{O} = \mathbb{A}[\partial; \sigma, \delta] = \mathbb{A}\langle\partial\rangle$ whose non-commutative multiplication is defined by

$$\partial a = \sigma(a)\partial + \delta(a)$$

is called an **Ore algebra**.

Example: Let $\mathbb{A} = \mathbb{K}(x)$, $\sigma = \mathrm{id}$, and $\delta = \frac{\mathrm{d}}{\mathrm{d}x}$. In this case we denote $\partial = D_x$ and get $\mathbb{O} = \mathbb{K}(x)\langle D_x\rangle$.

Examples of Ore Algebras

Ore operator	∂	σ	δ
Differential operator	D_x	$\sigma = \mathrm{id}$	$\delta = \frac{\mathrm{d}}{\mathrm{d}x}$
Euler operator	θ_x	$\sigma = \mathrm{id}$	$\delta = x\frac{\mathrm{d}}{\mathrm{d}x}$
Shift operator	S_n	$\sigma(n) = n + 1$	$\delta = 0$
Difference operator	Δ_n	$\sigma(n) = n + 1$	$\delta(n) = 1$
q-Shift operator	$S_{z,q}$	$\sigma(z) = qz$	$\delta = 0$
q-Difference operator	$\Delta_{z,q}$	$\sigma(z) = qz$	$\delta(z) = (q-1)z$

Multivariate Ore Algebras

The construction of Ore algebras can be iterated:

$$\mathbb{A}[\partial_1; \sigma_1, \delta_1] \cdots [\partial_r; \sigma_r, \delta_r] = \mathbb{A}\langle \partial_1, \ldots, \partial_r \rangle$$

In this case, one must ensure that the ∂_i's commute: $\partial_i \partial_j = \partial_j \partial_i$.

In this talk $\mathbb{A}$ is always a **rational** function field:

$$\mathbb{A} = \mathbb{K}(v_1, \ldots, v_r) = \mathbb{K}(\boldsymbol{v}).$$

Each ∂_i is related to exactly one variable, say v_i, i.e., $\partial_i v_j = v_j \partial_i$ for $i \neq j$; write ∂_{v_i} for ∂_i.

Summarizing, Ore algebras in this talk are always of the form

$$\mathbb{O} = \mathbb{K}(v_1, \ldots, v_r)\langle \partial_{v_1}, \ldots, \partial_{v_r} \rangle = \mathbb{K}(\boldsymbol{v})\langle \boldsymbol{\partial_v} \rangle.$$

Action!

Define how operators act on functions.

Let $\mathcal{F}$ be an appropriate space of functions / sequences, $f \in \mathcal{F}$.

Differential operator:	$D_x \bullet f(x) = \frac{\mathrm{d}}{\mathrm{d}x} f(x)$
Euler operator:	$\theta_x \bullet f(x) = x \frac{\mathrm{d}}{\mathrm{d}x} f(x)$
Shift operator:	$S_n \bullet f(n) = f(n+1)$
Difference operator:	$\Delta_n \bullet f(n) = f(n+1) - f(n)$
q-Shift operator:	$S_{z,q} \bullet f(z) = f(qz)$
q-Difference operator:	$\Delta_{z,q} \bullet f(z) = f(qz) - f(z)$

$\longrightarrow$ The action $\bullet$: $\mathbb{O} \times \mathcal{F} \to \mathcal{F}$ turns $\mathcal{F}$ into a left $\mathbb{O}$-module.

Definitions

1. The **annihilator** of a function f w.r.t. an Ore algebra $\mathbb{O}$:

$$\operatorname{ann}_{\mathbb{O}}(f) = \left\{P \in \mathbb{O} \mid P \bullet f = 0\right\}$$

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2. A function is called **∂-finite w.r.t. $\mathbb{O}$** ("holonomic") if

$$\dim_{\mathbb{K}(\boldsymbol{v})} \left(\mathbb{O}/\operatorname{ann}_{\mathbb{O}}(f)\right) < \infty$$

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4. The definitions **∂-finite** and **holonomic** differ only by some technical conditions.

Example: Legendre Polynomials $P_n(x)$

Important family of orthogonal polynomials $P_0(x), P_1(x), \ldots$:

$$\deg(P_n(x)) = n, \qquad \text{and} \qquad \frac{2n+1}{2}\int_{-1}^{1} P_m(x)P_n(x)\,\mathrm{d}x = \delta_{m,n}.$$

They are a particular solution of the Legendre differential equation:

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

Corresponding operator: $(x^2-1)D_x^2 + 2xD_x - n(n+1)$.

Legendre polynomials also satisfy the three-term recurrence

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

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

These operators live in the Ore algebra

$$\mathbb{K}(x,n)\langle D_x, S_n\rangle = \mathbb{K}(x,n)[D_x; 1, \tfrac{\mathrm{d}}{\mathrm{d}x}][S_n; \sigma_n, 0].$$

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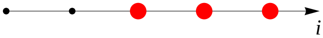

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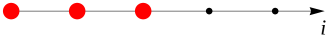

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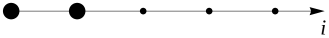

$\longrightarrow$ $P_n(x)$ is ∂-finite w.r.t. $\mathbb{K}(x)\langle D_x\rangle$.

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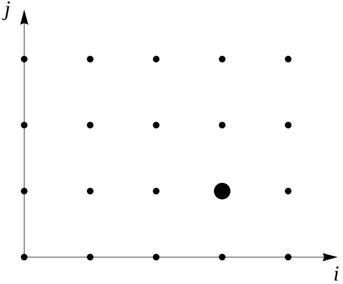

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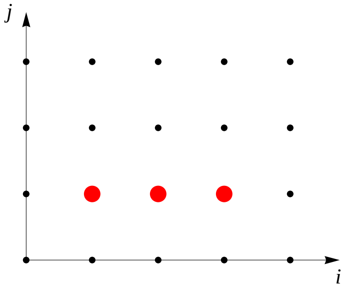

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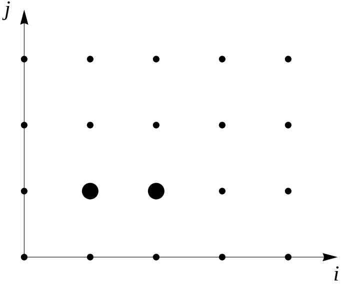

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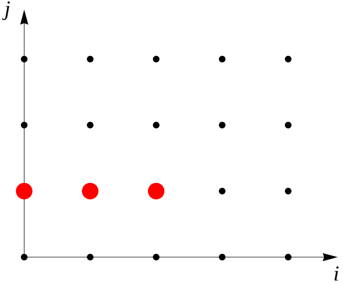

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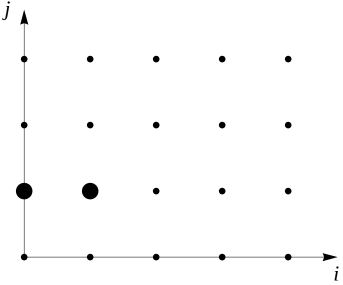

$$P_{n+1}^{(3)}(x) =$$
$$\frac{(n^2x^2-n^2+3nx^2-3n+8x^2)}{(x^2-1)^2}P_{n+1}'(x)$$
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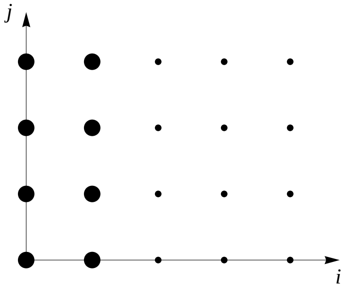

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The Legendre polynomials can be defined recursively:

$$P_0(x) = 1$$
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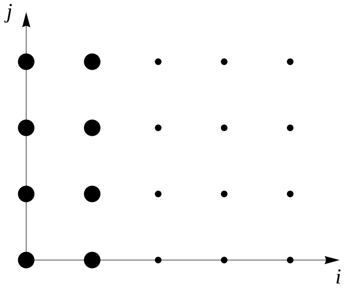

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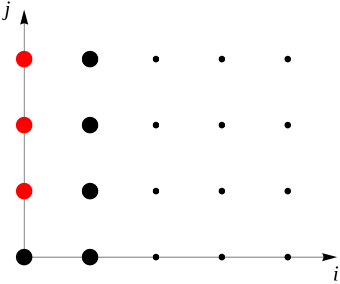

$$P_{n+3}(x) =$$
$$\frac{(2n+5)x}{n+3} P_{n+2}(x) - \frac{n+2}{n+3} P_{n+1}(x)$$

$$(n+3)P_{n+3}(x) - (2n+5)xP_{n+2}(x) + (n+2)P_{n+1}(x) = 0$$

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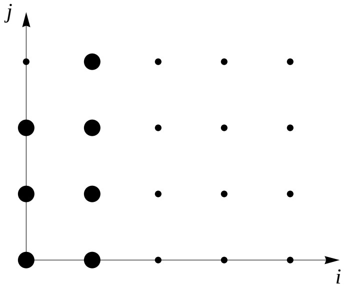

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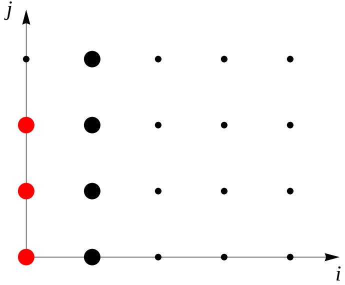

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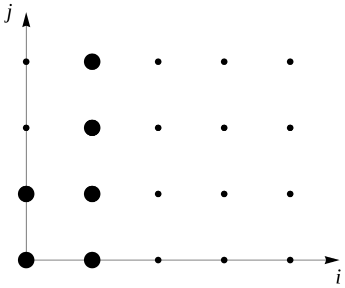

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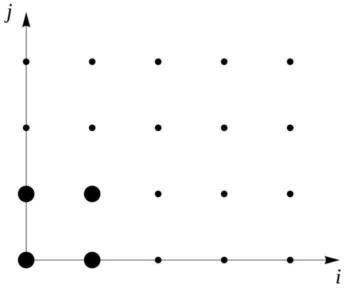

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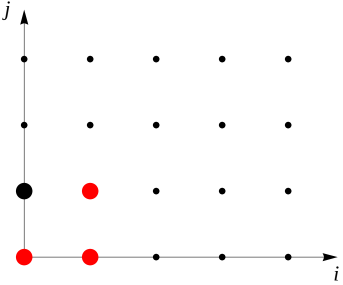

$P'_{n+1}(x) - xP'_n(x) - (n+1)P_n(x) = 0$

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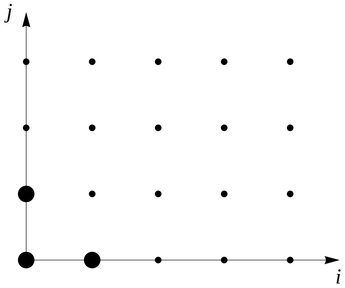

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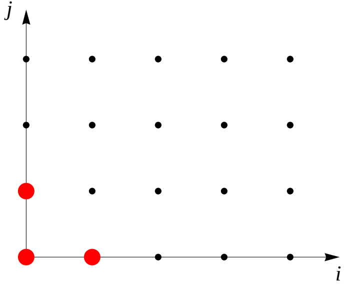


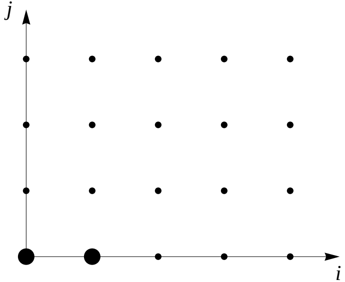
$(n+1)P_{n+1}(x) + (1-x^2)P_n'(x) - (n+1)xP_n(x) = 0$

Example: Legendre Polynomials $P_n(x)$

The Legendre polynomials can be defined recursively:

$$P_0(x) = 1$$
$$P_1(x) = x$$
$$nP_n(x) = (2n-1)xP_{n-1}(x) - (n-1)P_{n-2}(x).$$

Consider the set $\left\{P_{n+j}^{(i)}(x) : i, j \geq 0\right\}$.



$\longrightarrow$ $P_n(x)$ is ∂-finite w.r.t. $\mathbb{K}(n,x)\langle S_n, D_x\rangle$ (of rank 2).

(Incomplete) List of ∂-Finite Functions

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, BesselJ, StruveL, ArcSec, Factorial2, KelvinBer, BesselK, ArcSinh, HankelH1, Sqrt, PolyGamma, HypergeometricU, AiryAiPrime, Sin,

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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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 $F(x)$:

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

The Right-Hand Side

$$\begin{aligned} c_r(n)f(n+r,k) + \cdots + c_0(n)f(n,k) &= g(n,k+1) - g(n,k) \\ &= (S_k - 1) \cdot g(n,k). \end{aligned}$$

Where should we look for a suitable $g(n,k)$?
Note that there are trivial solutions like:

$$g(n,k) := \sum_{i=0}^{k-1} \big(c_r(n)f(n+r,i) + \cdots + c_0(n)f(n,i) \big)$$

A reasonable choice for where to look for g is $\mathbb{O} \cdot f$.

Then the task is to find $P(n, S_n) = c_r(n)S_n^r + \cdots + c_0(n)$ and $Q \in \mathbb{O}$ such that

$$\big(P - (S_k - 1)Q\big) \cdot f = 0 \quad \iff \quad P - (S_k - 1)Q \in \mathrm{ann}_{\mathbb{O}}(f).$$

Integrals

For an integral $\int_a^b f(x,y)\,\mathrm{d}y$ where the integrand f is ∂-finite, the creative telescoping problem is the following: find

$$P \in \mathbb{K}(x)\langle D_x \rangle \quad \text{and} \quad Q \in \mathbb{O} = \mathbb{K}(x,y)\langle D_x, D_y \rangle$$

such that $P - D_y Q \in \operatorname{ann}_{\mathbb{O}}(f)$.

- P is called **telescoper**.
- Q is called **certificate**.

Observation: Since f is ∂-finite we can restrict the search space for Q to $\mathbb{O}/\operatorname{ann}_{\mathbb{O}}(f)$.

How to Find (P, Q)?

Make an ansatz for P and Q.

Fix an integer r and set

$$P = \sum_{i=0}^{r} p_i(x) D_x^i \qquad \text{with } p_i \in \mathbb{K}(x) \text{ unknown coefficients.}$$

Let $\mathfrak{U}$ denote the set of monomials under the stairs of a Gröbner basis for $\operatorname{ann}_{\mathbb{O}}(f)$, or some other vector space basis of $\mathbb{O}/\operatorname{ann}_{\mathbb{O}}(f)$.

Since $Q \in \mathbb{O}/\operatorname{ann}_{\mathbb{O}}(f)$ we can set

$$Q = \sum_{u \in \mathfrak{U}} q_u(x, y)\, u \qquad \text{with } q_u \in \mathbb{K}(x, y) \text{ unknown.}$$

Chyzak's Algorithm

Put things together:

$$\begin{aligned} P - D_y Q &= \sum_{i=0}^{r} p_i(x) D_x^i - D_y \sum_{u \in \mathfrak{U}} q_u(x,y)\, u \\ &= \sum_{i=0}^{r} p_i(x) D_x^i - \sum_{u \in \mathfrak{U}} \left(q_u(x,y) D_y + \tfrac{\mathrm{d}}{\mathrm{d}y} q_u(x,y) \right) u \end{aligned}$$

Since we want $P - D_y Q \in \operatorname{ann}_{\mathbb{O}}(f)$ we reduce the above expression with a Gröbner basis of $\operatorname{ann}_{\mathbb{O}}(f)$ and equate (D_x, D_y)-coefficients to zero.

This yields a coupled first-order linear system of differential equations for the q_u's with parameters $p_0, \ldots, p_r$.
$\longrightarrow$ There are algorithms to find **rational** solutions of such systems.

Finally: loop over the (a priori) unknown order r of the telescoper.
$\longrightarrow$ This is Chyzak's algorithm (analogously in other Ore algebras).

Creative Telescoping in Full Generality

Let $\boldsymbol{v} = v_1, \ldots, v_n$, $\boldsymbol{w} = w_1, \ldots, w_m$, and $\mathbb{O} = \mathbb{K}(\boldsymbol{v}, \boldsymbol{w})\langle \boldsymbol{\partial_v}, \boldsymbol{\partial_w} \rangle$.

In general, a creative telescoping operator has the form

$$P(\boldsymbol{v}, \boldsymbol{\partial_v}) + \Delta_1 Q_1(\boldsymbol{v}, \boldsymbol{w}, \boldsymbol{\partial_v}, \boldsymbol{\partial_w}) + \cdots + \Delta_m Q_m(\boldsymbol{v}, \boldsymbol{w}, \boldsymbol{\partial_v}, \boldsymbol{\partial_w})$$

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
- $\boldsymbol{w} = w_1, \ldots, w_m$ are the summation/integration variables
- $\boldsymbol{v} = v_1, \ldots, v_n$ are the surviving parameters
- $P(\boldsymbol{v}, \boldsymbol{\partial_v}) \in \mathbb{K}(\boldsymbol{v})\langle \boldsymbol{\partial_v} \rangle$ is called the **telescoper**
- the $Q_i(\boldsymbol{v}, \boldsymbol{w}, \boldsymbol{\partial_v}, \boldsymbol{\partial_w}) \in \mathbb{O}$ are called the **certificates**
- the Q_i's "certify" the correctness of the telescoper

Ansatz with Specific Denominators

For finding CT operators, we proposed an ansatz of the form

$$\sum_{\boldsymbol{\alpha}} p_{\boldsymbol{\alpha}}(\boldsymbol{v})\boldsymbol{\partial}_{\boldsymbol{v}}^{\boldsymbol{\alpha}} + \sum_{i=1}^{m} \Delta_i \sum_{u\in\mathfrak{U}} \frac{\sum_{\boldsymbol{\beta}} q_{i,j,\boldsymbol{\beta}}(\boldsymbol{v})\boldsymbol{w}^{\boldsymbol{\beta}}}{d_{i,j}(\boldsymbol{v},\boldsymbol{w})}\, u$$

with unknowns $p_{\boldsymbol{\alpha}}$ and $q_{i,j,\boldsymbol{\beta}}$, and with specific denominators $d_{i,j}$.

- input: a (non-commutative) Gröbner basis G of $\operatorname{ann}_{\mathbb{O}}(f)$
- denote by $\mathfrak{U}$ the (finitely many) monomials under its stairs
- reduce the ansatz with G and equate coefficients to zero
- new: coefficient comparison w.r.t. $\boldsymbol{w}$
- this leads to a **linear** system of equations over $\mathbb{K}(\boldsymbol{v})$
- the denominators $d_{i,j}$ can be roughly predicted from the leading coefficients of the Gröbner basis G
- implemented in `HolonomicFunctions` (Mathematica)
- current research: optimize shape of this ansatz, bounds.

Examples: Some Special Function Identities

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

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

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

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

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

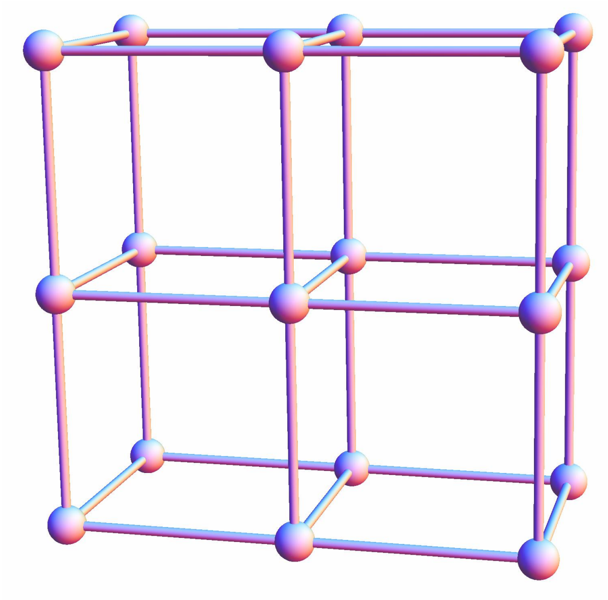
$$\frac{\sin\left(\sqrt{z^2 + 2tz}\right)}{z} = \sum_{n=0}^{\infty} \frac{(-t)^n y_{n-1}(z)}{n!} \tag{6}$$

Application

Study **random walks** on lattices. Here:

- unrestricted lattices in $\mathbb{R}^d$ for some dimension d
- steps are allowed only to nearest neighbors
- probabilities of all steps are the same
- consider the **face-centered cubic** lattice (fcc)

The fcc Lattice in 3D



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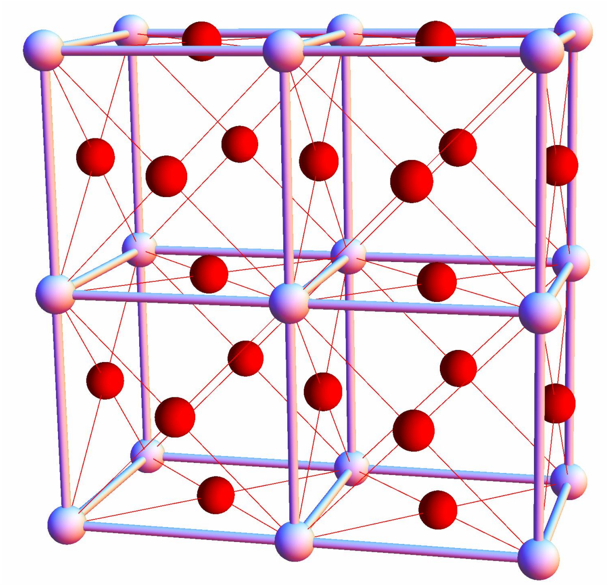

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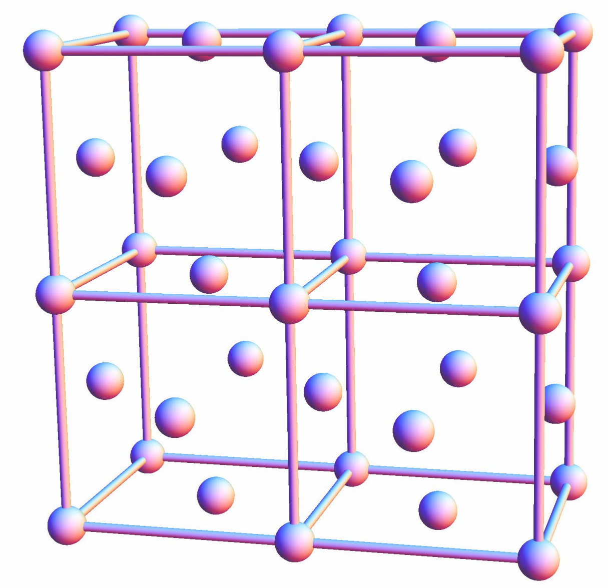

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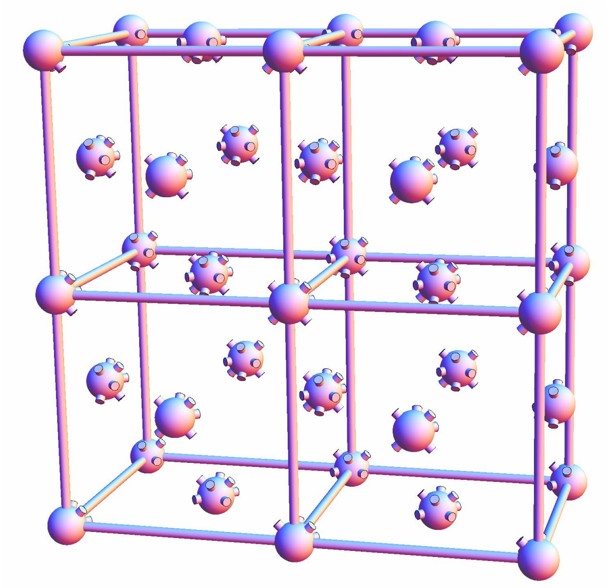

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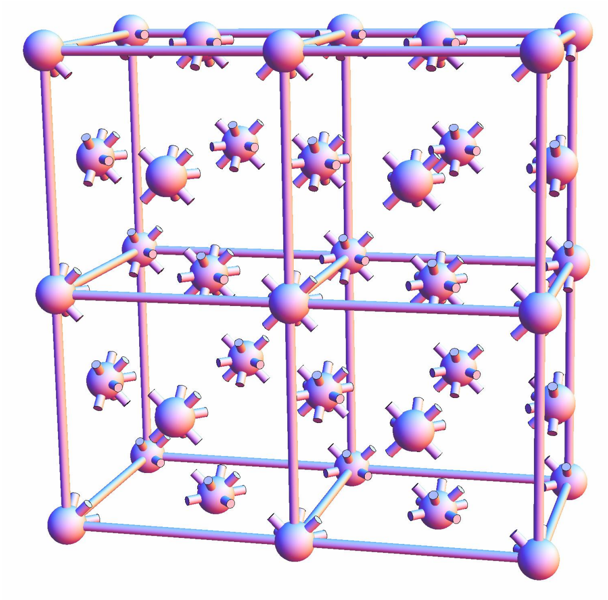

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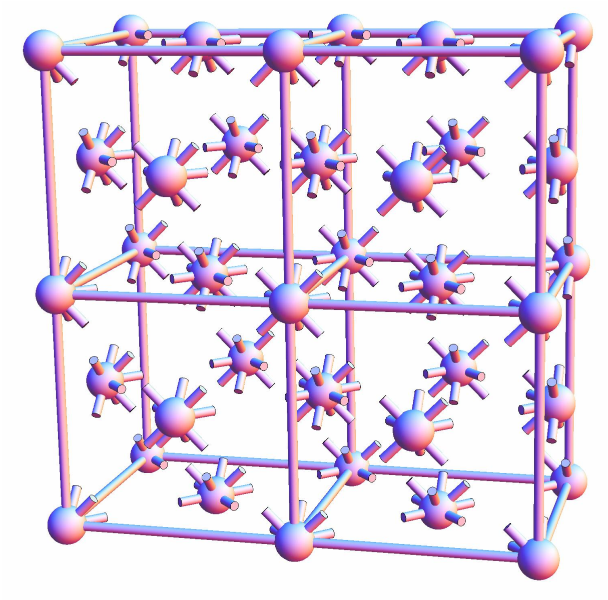

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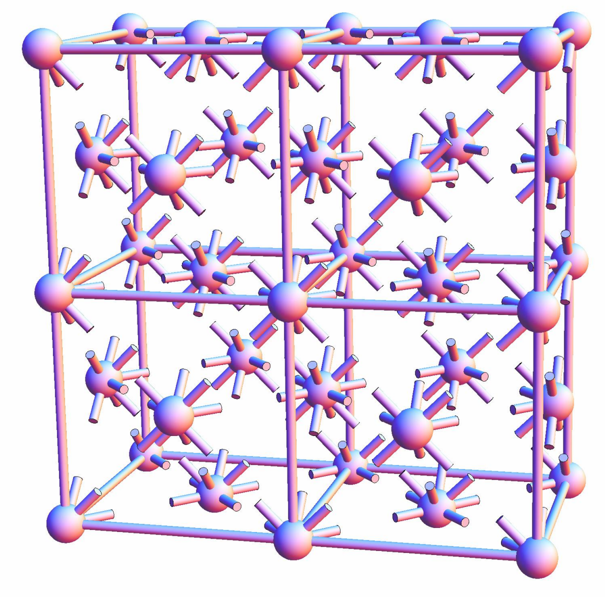

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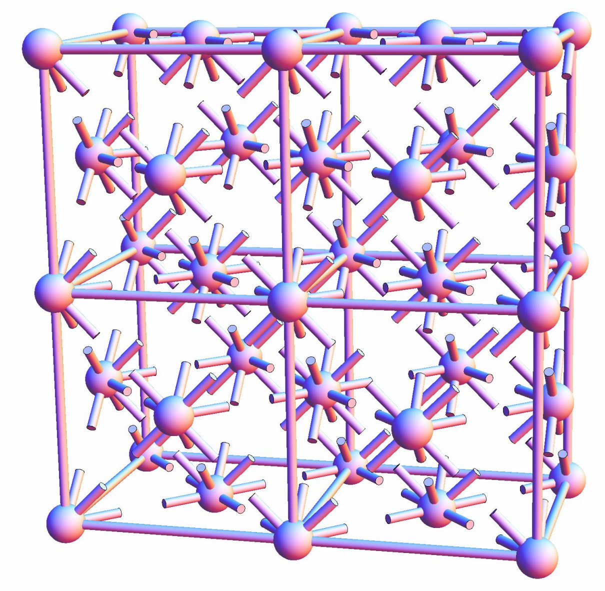

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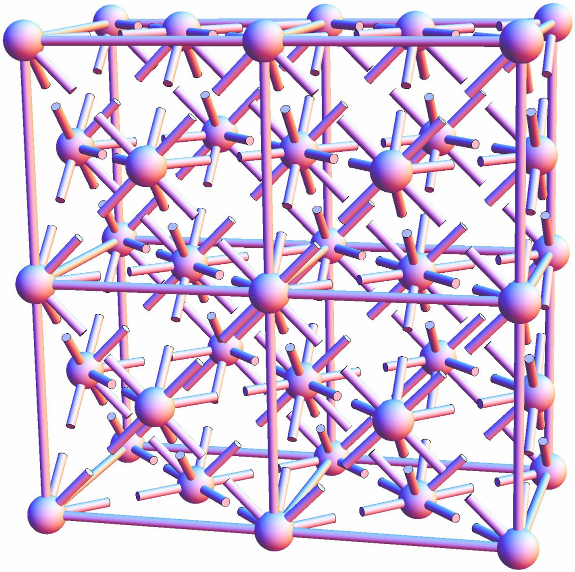

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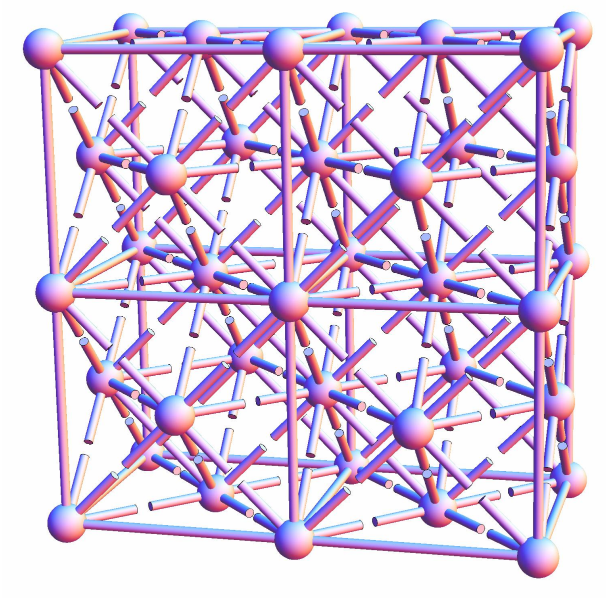

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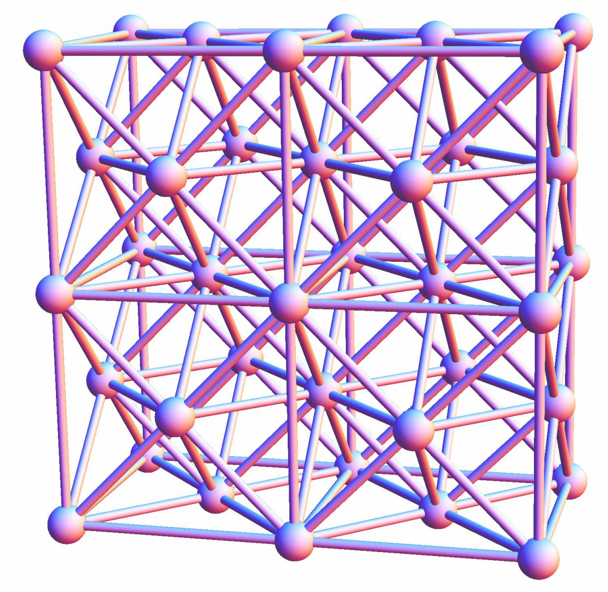

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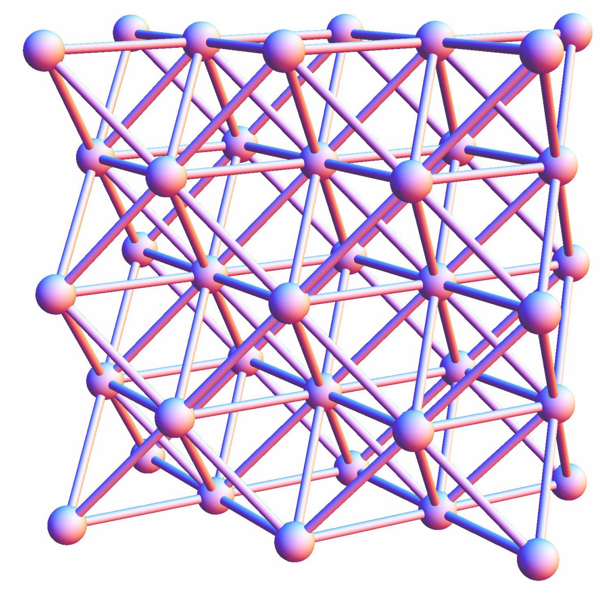

Lattice Green's Functions

The **lattice Green's function** is the probability generating function

$$G(\boldsymbol{x}; z) = \sum_{n=0}^{\infty} p_n(\boldsymbol{x}) z^n$$

where $p_n(\boldsymbol{x})$ is the probability of being at point $\boldsymbol{x}$ after n steps.

Of particular interest is

$$G(\mathbf{0}; z) = \sum_{n=0}^{\infty} p_n(\mathbf{0}) z^n = \frac{1}{\pi^d} \int_0^{\pi} \cdots \int_0^{\pi} \frac{\mathrm{d}k_1 \ldots \mathrm{d}k_d}{1 - z\lambda(\boldsymbol{k})}.$$

that encodes the **return probabilities**.

Here $\lambda(\boldsymbol{k})$ is called the **structure function** of the lattice; it is given by the discrete Fourier transform of the single-step probabilities:

$$\lambda(\boldsymbol{k}) = \sum_{\boldsymbol{x} \in \mathbb{R}^d} p_1(\boldsymbol{x}) e^{i\boldsymbol{x}\cdot\boldsymbol{k}} \qquad \text{(a finite sum, actually).}$$

Example in 2D

Square lattice $\mathbb{Z}^2$ with step set $\{(-1,0),(1,0),(0,-1),(0,1)\}$:

The structure function is

$$\lambda(k_1,k_2) = \tfrac{1}{4}\left(e^{-ik_1}+e^{ik_1}+e^{-ik_2}+e^{ik_2}\right) = \tfrac{1}{2}\left(\cos k_1 + \cos k_2\right).$$

The lattice Green's function is

$$G(0,0;z) = \frac{1}{\pi^2}\int_0^\pi\int_0^\pi \frac{\mathrm{d}k_1\,\mathrm{d}k_2}{1-\frac{z}{2}\left(\cos k_1+\cos k_2\right)} = \frac{2}{\pi}\mathbf{K}(z^2)$$

where $\mathbf{K}(z)$ is the complete elliptic integral of the first kind:

$$\mathbf{K}(z) = \int_0^1 \frac{\mathrm{d}t}{\sqrt{(1-t^2)(1-z^2t^2)}}.$$

Solution with Creative Telescoping

The lattice Green's function of the 2D fcc lattice is given by

$$G(z) = \frac{1}{\pi^2} \int_0^{\pi} \int_0^{\pi} \frac{\mathrm{d}k_1 \, \mathrm{d}k_2}{1 - z \cos(k_1) \cos(k_2)}.$$

Unfortunately, the integrand is not ∂-finite/holonomic
(no ODE w.r.t. k_1 for example).

But this is easily repaired by the substitutions $\cos(k_i) \mapsto x_i$:

$$G(z) = \frac{1}{\pi^2} \int_0^{1} \int_0^{1} \frac{\mathrm{d}x_1 \, \mathrm{d}x_2}{(1 - z x_1 x_2)\sqrt{1 - x_1^2}\sqrt{1 - x_2^2}}.$$

Indeed, the integrand is annihilated by the operators:

$$\begin{aligned}
&(x_1 x_2 z - 1) D_z + x_1 x_2, \\
&(x_2^2 - 1)(x_1 x_2 z - 1) D_{x_2} + (2 x_1 x_2^2 z - x_1 z - x_2), \\
&(x_1^2 - 1)(x_1 x_2 z - 1) D_{x_1} + (2 x_1^2 x_2 z - x_1 - x_2 z).
\end{aligned}$$

Solution with Creative Telescoping

$$G(z) = \frac{1}{\pi^2} \int_0^1 \int_0^1 \frac{1}{(1 - zx_1x_2)\sqrt{1-x_1^2}\sqrt{1-x_2^2}} \, \mathrm{d}x_1 \, \mathrm{d}x_2.$$

The creative telescoping operator

$$\underbrace{(z^3 - z)D_z^2 + (3z^2 - 1)D_z + z}_{P(z,D_z)} + D_{x_1} \underbrace{\frac{x_2(1-x_1^2)}{x_1x_2z - 1}}_{Q_1} + D_{x_2} \underbrace{\frac{x_2z(1-x_2^2)}{x_1x_2z - 1}}_{Q_2}$$

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

$$z(z^2 - 1)G''(z) + (3z^2 - 1)G'(z) + zG(z) = 0.$$

Result for the 3D fcc Lattice

In 3D we have to compute the 3-fold integral $G(z) =$

$$\frac{1}{\pi^3}\int_0^1\int_0^1\int_0^1 \frac{\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3}{\left(1-\frac{z}{3}(x_1x_2+x_1x_3+x_2x_3)\right)\sqrt{1-x_1^2}\sqrt{1-x_2^2}\sqrt{1-x_3^2}}$$

Iterative application of creative telescoping yields the differential equation

$$\begin{aligned}2(z-1)z^2(z+3)^2G^{(3)}(z)+3z(5z^2+5z-6)(z+3)G''(z)+\\ 6(4z^3+12z^2+3z-3)G'(z)+6z(z+2)G(z)=0.\end{aligned}$$

Result for the 4D fcc Lattice

With this machinery, we find (and prove!) that the LGF $G(z)$ of the 4D fcc lattice satisfies the differential equation

$$
\begin{aligned}
&(z-1)(z+2)(z+3)(z+6)(z+8)(3z+4)^2 z^3 G^{(4)}(z)+\\
&2(3z+4)(21z^6+356z^5+2079z^4+4920z^3+3676z^2-\\
&\qquad 2304z-3456)z^2G^{(3)}(z)+\\
&6(81z^7+1286z^6+7432z^5+19898z^4+25286z^3+11080z^2-\\
&\qquad 5248z-5376)zG''(z)+\\
&12(45z^7+604z^6+2939z^5+6734z^4+7633z^3+3716z^2+\\
&\qquad 224z-384)G'(z)+\\
&12(9z^5+98z^4+382z^3+702z^2+632z+256)zG(z)=0.
\end{aligned}
$$

Result for the 5D fcc Lattice

$$16(z-5)(z-1)(z+5)^2(z+10)(z+15)(3z+5)(15678z^6+144776z^5+449735z^4+933650z^3-1053375z^2+3465000z-675000)z^4G^{(6)}(z)+8(z+5)(3057210z^{12}+97471734z^{11}+1048560285z^{10}+3939663705z^9-4878146975z^8-87265479875z^7-304623830625z^6-266627903125z^5+254876515625z^4-1289447109375z^3-503550000000z^2+1774828125000z-354375000000)z^3G^{(5)}(z)+10(27279720z^{13}+923795772z^{12}+11725276842z^{11}+68439921540z^{10}+148313757125z^9-382134335775z^8-3351125770500z^7-7801785421250z^6-3779011321875z^5-7716298734375z^4-39702348750000z^3+3393646875000z^2+23905125000000z-5568750000000)z^2G^{(4)}(z)+5(255864960z^{13}+7892060544z^{12}+92744995638z^{11}+524857986060z^{10}+1350059072325z^9-465440555100z^8-13545524756500z^7-26918293320000z^6-3649915059375z^5-77498059625000z^4-190176960000000z^3+40530375000000z^2+45343125000000z-13162500000000)zG^{(3)}(z)+5(496679040z^{13}+13819981248z^{12}+149186684934z^{11}+810956145330z^{10}+2287368823475z^9+1646226060075z^8-8282515456375z^7-6199228765625z^6+13367806743750z^5-110925736437500z^4-133825053750000z^3+44457862500000z^2+5055750000000z-3240000000000)G''(z)+10(167064768z^{12}+4143853440z^{11}+40678130502z^{10}+209673119160z^9+607021304825z^8+689643286650z^7-135661728250z^6+3711617481250z^5+2664478321875z^4-21210430812500z^3-7268326875000z^2+4816462500000z-189000000000)G'(z)+30(7525440z^{11}+163913184z^{10}+1443544710z^9+6925739310z^8+19123388575z^7+21336230625z^6+36477006875z^5+187923165625z^4-55567000000z^3-346865625000z^2+84037500000z+27000000000)G(z)=0$$

Result for the 6D fcc Lattice

$$
\begin{aligned}
&(z-3)(z-1)(z+4)(z+5)(z+9)(z+15)^2(z+24)(2z+3)(2z+15)(4z+\\
&15)(7z+60)(242161043152z^{25}+51659233261888z^{24}+3764987488054392z^{23}+\\
&149102740118852712z^{22}+3823803744461234343z^{21}+69321047461074869130z^{20}+\\
&931032563834500230663z^{19}+9465736161794804567892z^{18}+72864795413899911011922z^{17}+\\
&412843760981101392072948z^{16}+1557656993073750677220582z^{15}+2189507486524206284827296z^{14}-\\
&16970927000980381863663141z^{13}-152346950611719661239440526z^{12}-\\
&693159300555093708939611829z^{11}-2157072153972513398276826924z^{10}-\\
&4872861027995366524279994100z^{9}-7971869741181425686355371200z^{8}-\\
&8883487977021576719907033600z^{7}-5337917399156522389289280000z^{6}+\\
&7534597696291106962430400000z^{5}+3920543674198265211436800000z^{4}+\\
&2878395143123986146432000000z^{3}+1348035643913347353600000000z^{2}+\\
&242306901961056460800000000z+19280523023769600000000000)z^{6}G^{(8)}(z)+2(z+\\
&15)(800100086574208z^{36}+2273899880575263336z^{35}+2599684057220488851 2z^{34}+\\
&171934241162782875 7728z^{33}+763180860604907919 60792z^{32}+24622880211526068853 58700z^{31}+\\
&606187150389376704730 18584z^{30}+11751544341781190416717007 40z^{29}+\\
&18309889884984684630822323370z^{28}+232115671681854334221586338585z^{27}+\\
&2406227015296631910854902756563z^{26}+20337622679657217515316342764256z^{25}+\\
&138105907223379522203625428215332z^{24}+724749378242590885585485419445843z^{23}+\\
&2620577206027992337931632885352217z^{22}+3221036141212186087856769990927054z^{21}-\\
&35907063701591969077649893288537878z^{20}-331259809437872111827650003935308209z^{19}-\\
&1638945569143497023502201509481372411z^{18}-5466573829106434312238352307226140764z^{17}-\\
&11704453530273493922795299130700457200z^{16}-7977590414255123112276744122571399783z^{15}+\\
&51498237061832672183443454747804923575z^{14}+253995260187409794081727430934766869450z^{13}+\\
&661181529544504134786063620152764386400z^{12}+1138666598560461678104890857545212608000z^{11}+\\
&1251150937075501602577084871183562120000z^{10}+564704048394845939194551470638922400000z^{9}-\\
&682640121106346995555734719308248000000z^{8}-1460286146960184444033629739148560000000z^{7}-\\
&1074498717874767393664900393675200000000z^{6}-1450218746083946510596388474880000000000z^{5}+\\
&3447189729571578013712505600000000000000z^{4}+3144130563959386258385101824000000000000z^{3}+\\
&1403603566598885837201141760000000000000z^{2}+250840098120631904501760000000000000000z+\\
&19733923803196565913600000000000000000000)z^{5}G^{(7)}(z)+
\end{aligned}
$$

Result for the 6D fcc Lattice

$$(3588245473009075 2z^{37} + 1061260405161448665 6z^{36} + 127653260094221277516 8z^{35} + 893939801294330320963 20z^{34} + 4221606838983473228197008z^{33} + 145494567985766484898923048z^{32} + 3840828004490920060950969480z^{31} + 80160062388267727172211985080z^{30} + 1350855094398006902682870922050z^{29} + 18631082892630536824222949409585z^{28} + 211815796834464054711973645322142z^{27} + 1986708322085667572665525016037411z^{26} + 15263082383031406770429022758762048z^{25} + 94068732852089205756130773605094705z^{24} + 441055376229095921513357130918811338z^{23} + 1319636945498761264973744224282378779z^{22} - 1376268096732267953995912640790411 12z^{21} - 31072001737970299221405533198706303141z^{20} - 226886176666918560987240200768631693150z^{19} - 1033954017266382248984767586852072344191z^{18} - 3356732946224373601649087937349109785896z^{17} - 7573126212785007618891225542456994124245z^{16} - 9076459539413303184641722134776573895810z^{15} + 10278671248090335377408918358815408788425z^{14} + 85149274357043292385925033653294291853550z^{13} + 240689360358498296007939096187740586134000z^{12} + 429409878921957648790555775268242743350000z^{11} + 495779225046771906420255540348281344800000z^{10} + 287121363379312616871562346484465378000000z^{9} - 119682652007548350954457856750250720000000z^{8} - 395683465592680867401293480616198000000000z^{7} - 327383462755042385949747691240824000000000z^{6} - 86642575450501391066787202019520000000000z^{5} + 59704683972170679548931977222400000000000z^{4} + 72511610277412390990839363072000000000000z^{3} + 33882896755872071956886261760000000000000z^{2} + 6311156771304917325766656000000000000000z + 512323021813756999680000000000000000000)z^{4}G^{(6)}(z) + 3(1302400208721812 48z^{37} + 38072220474786769152z^{36} + 448027411720532102 3232z^{35} + 30598839345549153729 0240z^{34} + 1407922464408792532952 3520z^{33} + 47273961310349397765869 2800z^{32} + 1216240227880266706589 6636880z^{31} + 2475013840209218674125 86484240z^{30} + 406856488897300388082085 3550310z^{29} + 547503407981479263289212 45513135z^{28} + 607255705204278811351245 801585018z^{27} + 5552646100941335755747908 121811397z^{26} + 4151115361654006666990381 5109576752z^{25} + 2478645988143028466901774 15162792735z^{24} + 1112001535696035843878120 629687073790z^{23} + 3006740720618245361400876 608130182349z^{22} - 3066274907647801401815807 099801425704z^{21} - 9314995626746750472522568 0596497523339z^{20} - 6359544758873132951922410 42199635547930z^{19} - 2858027882158570016919188 514224326558185z^{18} - 9468529098949077023394535 618861256937240z^{17} - 2319141939177098517148023 7991217872142915z^{16} - 3833047896416257055664594 9941637505810110z^{15} - 2345933906719328778816514 40557275751112 25z^{14} + 8721398883369638261455202 77387192809598 50z^{13} + 3498036082650454616124890 699366751798000 00z^{12} + 6965545936547576658667199 66270600171130000z^{11} +$$

Result for the 6D fcc Lattice

$$865953342265454601104437816976581680000000z^{10}+586378944861718695144037906690882422000000z^9-448918716637412377029136427636037600000000z^8-526332032930456915428235817813056400000000z^7-518937227107573341964843985332680000000000z^6-226302972537833147253780811598400000000000z^5+104974053097834899670129395840000000000000z^4+64135781486584141753707277824000000000000z^3+34708946736814927353542983680000000000000z^2+69940922143484645330042880000000000000000z+5958126994426655477760000000000000000000)z^3G^{(5)}(z)+15(14618777852999936 0z^{37}+422326808984872512 00z^{36}+485766573409896369 0240z^{35}+3231657913197024840 35520z^{34}+1446760113658410970 7654400z^{33}+4725344663866749805 33072704z^{32}+11827310475440684698 801079376z^{31}+2342059941824389437 69949245108z^{30}+3746772515516029997 311378363446z^{29}+4905651728844870193 4966949399201z^{28}+5289607375382209621 99232165726700z^{27}+4693678127508685757 3297047931182 74z^{26}+3392552092805670737 99490422451549 48z^{25}+1942257848193764334 18854177036400765z^{24}+8158659849976308923 3752606179754773 0z^{23}+1820210924970374403 47705989836829241 4z^{22}-5626714951506760337 6847848842931473 02z^{21}-8728863653905123753 154193816918161099 7z^{20}-5486179466041628296 176173489985231870 24z^{19}-2396582727922965009 354571656000074347578z^{18}-7949778754688875639 594299226888542864672z^{17}-2028488721982924201 0855806602752336703097z^{16}-3847633539306011937 98207417591264024511 66z^{15}-4718521118600910684 853587633117806112249 0z^{14}-1022276043692715561 636466920839572905426 0z^{13}+1074135280419217295 29347960434391761302800z^{12}+2792662410803344697 933159416141029695640 00z^{11}+3799750928054678691 635506264129937592000 00z^{10}+2763426791468873224 122207598834979976000 00z^9+6337926159808918213 308690816700464000000z^8-2149651298091206908 272829027314686400000 00z^7-2424557018759285535 178443324933024000000 00z^6-1402612474157728856 915464074355200000000 00z^5-3677270682836095894 427452388352000000000 00z^4+7747728379627393494 726545203200000000000 0z^3+7522568512298824734 532104192000000000000 0z^2+1776029394112720931 570319360000000000000 00z+1618181751862118404 915200000000000000000 0)z^2G^{(4)}(z)+90(6910694985054515 2z^{37}+1972812595897802803 2z^{36}+2215666629279250997 248z^{35}+1433873610843605435 57376z^{34}+6235802763945868063 424352z^{33}+1977632824563633074 38541552z^{32}+4805890762274729535 435673296z^{31}+9239099911481490590 7317974392z^{30}+1434485821162175237 888091472086z^{29}+1821323042813317967 4440523308931z^{28}+1901226745537869226 19563973540916z^{27}+1627987793820686707 319681442965532z^{26}+1128371420896299825 7330503635013918z^{25}+6107042528947862305 6319494081223364z^{24}+2321174912190547504 36300759063832796z^{23}+3351623330065771909 980786248324667 45z^{22}-$$

Result for the 6D fcc Lattice

$$
\begin{aligned}
&3212526847572548623801062566839102968z^{21} - 3392965866525625940881278435486638555 7z^{20} - \\
&19518317899005734964327227543512673634 0z^{19} - 8185961182051286059853304788561116790 58z^{18} - \\
&26711937663061933212590810775037397189 22z^{17} - 6879647707640439013900747488611335523490z^{16} - \\
&137913922587828958199554539989551025175 48z^{15} - 2039504216816486273624834199179924314327 5z^{14} - \\
&18559051142634901231618230067011245261730z^{13} + 34076387354025513180834306750306345480 0z^{12} + \\
&32573268392371003654841290966684606314000z^{11} + 54660627321107405540934107870983869840000z^{10} + \\
&41970729402708473923386620935623814800000z^{9} + 75772932393795193904464292935104000000 0z^{8} - \\
&34653454861369485847062964251845520000000z^{7} - 41909264304440185602876764536603200000000z^{6} - \\
&27649387021455520276766166546048000000000z^{5} - 99328789269121533702589473638400000000 00z^{4} - \\
&11120411746592534075218062336000000000000z^{3} + 28491145384085971960200192000000000000 00z^{2} + \\
&11423067813148192266682368000000000000000z + 11486155649552872980480000000000000000000)zG^{(3)}(z) + \\
&45(180741253455271936z^{37} + 5098070626763698483 2z^{36} + 5584340634105826525184z^{35} + \\
&351010067005351488224256z^{34} + 14802080405483677823943104z^{33} + 454875015831485400909097248z^{32} + \\
&10707051961496414217407305536z^{31} + 199288291693600445167066471488z^{30} + \\
&2993264774540100816050708154540z^{29} + 36707414555219468440447241903970z^{28} + \\
&369055333918742878506923895821094z^{27} + 3028085987873439981041316741040299z^{26} + \\
&19908118207277143280846917552738638z^{25} + 99771357205875220145109466450106517z^{24} + \\
&322041161855435062814533420723282482z^{23} - 374464592158210104407054773630095 0z^{22} - \\
&8583686545551708471758291210460691032z^{21} - 70294647356901524101024740972933056916z^{20} - \\
&369692934875862692678770756612360457070z^{19} - 1472149779764303912910700825119513125745z^{18} - \\
&4646227686063347368140269721102656923194z^{17} - 11757721460891217253150507437222976590963z^{16} - \\
&23667524905718087319814208022941410083354z^{15} - 36747814326347114270377987158311612338260z^{14} - \\
&40652966100310576219422839345851085154840z^{13} - 24193553263042351259117425539502701518400z^{12} + \\
&97196459408295308209885325185989534240 00z^{11} + 37297341452565155702787810516361533600000z^{10} + \\
&34764119013156176353837403619970113600000z^{9} + 67468310825627989823784956369579520000 00z^{8} - \\
&20656761408545661580810751146327680000000z^{7} - 29659078571699608256375734426214400000000z^{6} - \\
&20932834089033885270730650301440000000000z^{5} - 77843923078397261686505559244800000000 00z^{4} - \\
&14285831438642699607697907712000000000000z^{3} - 83241123892330166885744640000000000000 0z^{2} + \\
&14860150621853249942323200000000000000z + 161919374795459002368000000000000000000)G''(z) + \\
&45(880923756336619 52z^{36} + 245492997769647452 16z^{35} + 2619357527554007840768z^{34} + \\
&159628611480988435906560z^{33} + 6513463004865397861819008z^{32} + 193479386194110772817766720z^{31} +
\end{aligned}
$$

Result for the 6D fcc Lattice

$$
\begin{aligned}
&439888391418035258075220566 4z^{30} + 7901099164769596773436564113 6z^{29} + \\
&1143508859378085891069139805496z^{28} + 1347828522176737423743381389415 6z^{27} + \\
&12967481859657838184170935236331 0z^{26} + 10101156111516968661023604440438 67z^{25} + \\
&620340898816671250996736795196135 0z^{24} + 2782834220828526964581126761397575 1z^{23} + \\
&654040622871900452924735018823764 46z^{22} - 2329669581156953199668980714871155 50z^{21} - \\
&377662628741127731469461256819147846 0z^{20} - 2566599099502838134775728413297379008 6z^{19} - \\
&12330432201735600084488496344721300430 2z^{18} - 461005100390610028275047960932687009761z^{17} - \\
&1382954753973214192431623770039149437562z^{16} - 33513343533773096192036331788090102502 69z^{15} - \\
&650063614495568136954200526406770799947 0z^{14} - 980877991251518108531129271663511861734 0z^{13} - \\
&107583017503230454007080268105270059854 00z^{12} - 695503521442966141004023697462231547600 0z^{11} + \\
&698114077775776671885153675463762080000z^{10} + 734974355750387901041092183621241040000 0z^{9} + \\
&869104397596366604944729937914400160000 0z^{8} + 516578156502106727434299667345065600000 0z^{7} + \\
&401336331886317774107713318790400000000z^{6} - 222696446424871338600651835637760000000 0z^{5} - \\
&186353476702189192213117998796800000000 0z^{4} - 655267817084534423521940643840000000000z^{3} - \\
&122588504883178716188285337600000000000 0z^{2} - 843452865918902193743462400000000000000z + \\
&186207281014777852723200000000000000000)G'(z) + 90(4556502187948032z^{35} + \\
&12545029608245729 28z^{34} + 1301854737512773498 88z^{33} + 767574890318976574848 0z^{32} + \\
&302276251598295683586240z^{31} + 8653460076869413651316640z^{30} + 189382045823502675349219920z^{29} + \\
&3269391489631666671425989920z^{28} + 45371384308945745114138623620z^{27} + \\
&510811439434664402615401586970z^{26} + 4663284432121091702260620852777z^{25} + \\
&34047746401934351907977621763618z^{24} + 190773160991774404319508940400373z^{23} + \\
&717575244018720111969771948822450z^{22} + 574602465936356660227512513519630z^{21} - \\
&16377415461160421103082005421146444z^{20} - 158195048236903725948800257698582066z^{19} - \\
&924626001493256833520380233115382826z^{18} - 4044657270312306250764976742472089595z^{17} - \\
&14017460872371123201967056591950292270z^{16} - 39203789245543299948038211301310631735z^{15} - \\
&88492994651041978105789511893808827410z^{14} - 158672230290697625052364901820833352540z^{13} - \\
&217051701285403806039787021788244210200z^{12} - 204430925935804223158200138096719244000z^{11} - \\
&83930464288781215080378386513083200000z^{10} + 98749247882439137822044179686396640000z^{9} + \\
&234855990648514674287291744222356800000z^{8} + 252029928377053385449407192172320000000z^{7} + \\
&165979815868291791006070607462400000000z^{6} + 52113850317609070332668882227200000000z^{5} - \\
&96981000959420637658462494720000000000z^{4} - 122703104531082876683419238400000000000z^{3} - \\
&39322078689731206308102144000000000000z^{2} - 5786593656752716097126400000000000000z - \\
&2698656246590983372800000000000000000)G(z) = 0.
\end{aligned}
$$

Some Timings

Timings with our approach to creative telescoping, using the implementation in `HolonomicFunctions`:

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

$\longrightarrow$ With other methods (e.g., Chyzak's algorithm), the computations seem not to be feasible (at least the cases $d = 5$ and $d = 6$).

Conclusions and Outlook

- We presented a framework to deal with parametrized integrals and sums of ∂-finite/holonomic functions.
- All algorithms are supported by an implementation, in the package `HolonomicFunctions` in Mathematica.
- Many integrals / sums that appear in practice can be treated automatically in this way.
- It would be interesting to combine our methods with the holonomic gradient method.

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Description of the HolonomicFunctions package and download link