Computing D-Finite Symmetric Scalar Products in Order to Count Regular Graphs

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Based on joint past and ongoing works with
Hadrien Brochet, Hui Huang, Manuel Kauers, Pierre Lairez,
Marni Mishna, and Bruno Salvy

General Theme

Count combinatorial classes related to symmetries by obtaining an ODE for a related generated function

- graphs on n vertices with degree constraints,
- non-negative integer $n \times n$ matrices with contrained line sums,
- standard Young tableaux of size n with repeated entries.

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Example: for 3-regular graphs, an ODE is

$$9t^3(t^4+2t^2-2)U''(t)+3(t^{10}+6t^8+3t^6-6t^4-26t^2+8)U'(t)-t^3(t^4+2t^2-2)^2U(t) = 0$$

and a (minimal order) recurrence relation is

$$\begin{gathered}12(3n+10)(n+8)(3n+16)u(n+8) - 9(3n+10)(n+6)(3n^2+40n+136)u(n+6) \\ + (-108n^3 - 1710n^2 - 8628n - 14048)u(n+4) \\ - (3n+22)(9n^2+60n+76)u(n+2) + (3n+22)(3n+16)u(n) = 0.\end{gathered}$$

Known ODEs for *k*-Regular Graphs

k	reference	order	degree
3	(Read, 1958, 1960)	2	11
4	(Read, Wormald, 1980)	2	14
	(Gessel, 1990)		
	(Chyzak, Mishna, Salvy, 2005)		
5	(Chyzak, Mishna, 2024)	6	125
6	(Chyzak, Mishna, 2024)	6	145
7	(Chyzak, Mishna, 2024)	20	1683
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Most difficult cases in a matter of hours of computer calculations.

+ many more results for generalized classes, see
`https://files.inria.fr/chyzak/kregs/`

Symmetric Functions

Indeterminates $x_1, x_2, x_3, \dots,$ exponents $\alpha_i \in \mathbb{N} = \{0, 1, 2, \dots\},$

coefficients $c_\alpha \in \mathbb{Q},$ permutation π of $\mathbb{N} \setminus \{0\}.$

Algebra of symmetric functions
(Macdonald 1979, 1995; Goulden, Jackson, 1983; Stanley, 1999)

$$\hat{\Lambda} = \left\{ \sum_{|\alpha|<\infty} c_\alpha x^\alpha \;\middle|\; c_\alpha = c_{\pi(\alpha)} \text{ for all } \pi \text{ and } \alpha \right\}$$

Ex: $\alpha = (2, 1, 0, 5, 0, 1, 0, \dots) \to$ same coefficients of $x_1^2 x_2^1 x_4^5 x_6^1$ and $x_6^1 x_7^5 x_8^2 x_9^1$

Weak composition α of n: if $\alpha_i \geq 0$ and $|\alpha| = \sum_i \alpha_i = n$.

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Partition λ of n

$\lambda \vdash n$ if $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_\ell > 0$ and $|\lambda| = \sum_i \lambda_i = n$.

Facts and Formulas about Symmetric Functions

Several vectorial bases, several sets of generators as a ring

$$\Lambda = \bigoplus_\lambda \mathbb{Q} m_\lambda = \bigoplus_\lambda \mathbb{Q} p_\lambda = \bigoplus_\lambda \mathbb{Q} e_\lambda = \bigoplus_\lambda \mathbb{Q} h_\lambda$$
$$= \mathbb{Q}[p_1, p_2, \dots] = \mathbb{Q}[e_1, e_2, \dots] = \mathbb{Q}[h_1, h_2, \dots] \subseteq \mathbb{Q}[[x_1, x_2, \dots]]$$

$$p_n = \sum_{i \in \mathbb{N}} x_i^n, \quad n \in \mathbb{N}, \qquad p_\lambda = p_{\lambda_1} p_{\lambda_2} \cdots, \quad \lambda \text{ a partition,}$$

and similar definitions for e and h.

$$m_\lambda = \sum_{\alpha \in \{\pi(\lambda)\}} x^\alpha, \quad \lambda \text{ a partition,} \qquad h_k = \sum_{\lambda \vdash k} \frac{p_\lambda}{z_\lambda}, \quad k \in \mathbb{N}.$$

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Scalar product on Λ (extends to $\hat{\Lambda}$ when sums converge)

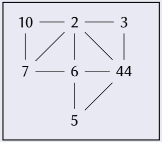
$$\langle m_\lambda, h_\mu \rangle = \begin{cases} 1 \text{ if } \lambda = \mu, \\ 0 \text{ otherwise.} \end{cases} \qquad \langle p_\lambda, p_\mu \rangle = \begin{cases} z_\lambda \text{ if } \lambda = \mu, \\ 0 \text{ otherwise.} \end{cases}$$

where $z_\lambda = 1^{r_1} r_1! \, 2^{r_2} r_2! \, 3^{r_3} r_3! \cdots$ for $r_n = \#\{\lambda_i = n\}$.

The Generating Function of Simple Graphs

Weight of a graph (by examples)

(arbitrary graph of size 7)

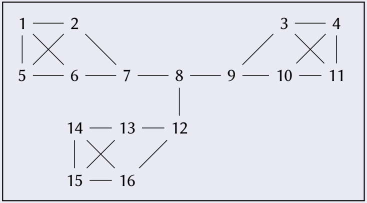
$g =$ 

$$w(g) = x_2^5 x_3^2 x_5^2 x_6^4 x_7^3 x_{10}^2 x_{44}^4$$

$$\downarrow$$

$$m_{5,4,4,3,2,2,2}$$

(3-regular graph of size 16)

$g =$ 

$$w(g) = x_1^3 x_2^3 x_3^3 \cdots x_{16}^3$$

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Generating function for vertex-labelled simple graphs

$$F = \sum_{g \text{ a simple graph}} w(g) = \prod_{i<j} (1 + x_i x_j) = \exp\left(\sum_{m \geq 1} (-1)^{m+1} \frac{p_m^2 - p_{2m}}{2m} \right)$$

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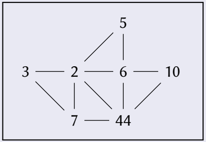
$g =$ 

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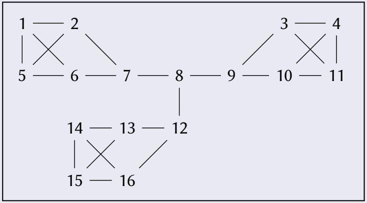
$g =$ 

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D-Finiteness of the Coefficient Extraction

$$[x^\lambda]F = [m_\lambda]F = \langle F, h_\lambda \rangle$$

Fundamental example: extracting the subseries of regular objects

$$[x_1^3 x_2^3 x_3^3 x_4^3]F = [m_{3,3,3,3}]F = \langle F, h_{3,3,3,3} \rangle = \langle F, h_3^4 \rangle = \left\langle F, \left(\frac{p_1^3}{6} + \frac{p_1 p_2}{2} + \frac{p_3}{3} \right)^4 \right\rangle$$

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(Classical multivariate) D-finiteness (Lipshitz, 1989)

A formal power series $f(u_1, \dots, u_r) \in \mathbb{Q}[[u_1, \dots, u_r]]$ is D-finite with respect to $(u_1, \dots, u_r)$ if the family of the derivatives $\partial_{u_1}^{\alpha_1} \cdots \partial_{u_r}^{\alpha_r} \cdot f$ over all $\alpha_i \geq 0$ generates a finite-dimensional vector space over $\mathbb{Q}(u_1, \dots, u_r)$.

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Theorem (Gessel, 1990) *[via a generalization to infinitely many variables]*

For each k, the generating function $\langle F, \exp(h_k t) \rangle$ of k-regular simple graphs is D-finite w.r.t. t.

Setting to Enumerate k-Regular Graphs

Number $r_n^{(k)}$ of k-regular simple graphs on n labelled vertices

The EGF $$\sum_{n=0}^{\infty} r_n^{(k)} \frac{t^n}{n!} = \langle F(p), G(p,t) \rangle,$$

where

$$F(p) = \exp\left(\sum_{m=1}^{\lfloor k/2 \rfloor} (-1)^m \frac{p_{2m}}{2m} - \sum_{m=1}^{k} (-1)^m \frac{p_m^2}{2m} \right) \quad \in \mathbb{Q}[[p_1, \dots, p_k]],$$

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Generalizations, by changing F and G accordingly

- allowed degrees in a finite set $\{k_1, \dots, k_\ell\}$ instead of $\{k\}$,
- multigraphs and variants: loops allowed, multiple edges allowed,
- marking valencies instead of degrees.

Annihilator of the Scalar Product by Elimination

Differential operators = skew polynonomials in ∂_u such that $\partial_u u = u\partial_u + 1$.

Adjoints

$$\langle p_m F, G\rangle = \langle F, m\partial_{p_m} \cdot G\rangle \qquad \langle \partial_{p_m} \cdot F, G\rangle = \langle F, m^{-1} p_m G\rangle$$

$$p_m^\dagger = m\partial_{p_m} \qquad \partial_{p_m}^\dagger = m^{-1} p_m$$

$$\langle P \cdot F, G\rangle = \langle F, P^\dagger \cdot G\rangle$$

$$P(p_1, p_2, \dots, \partial_{p_1}, \partial_{p_2}, \dots)^\dagger = P(1\partial_{p_1}, 2\partial_{p_2}, \dots, 1^{-1} p_1, 2^{-2} p_2, \dots)$$

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Consequence:

- If $P \cdot F = 0$, then $\langle P \cdot F, G\rangle = \langle F, P^\dagger \cdot G\rangle = 0$. $\qquad P = P(p, \partial_p)$
- If $Q \cdot G = 0$, then $\langle F, Q \cdot G\rangle = 0$. $\qquad Q = Q(p, \partial_p, t, \partial_t)$

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Consequence:

- If $P \cdot F = 0$, then for all R, $\langle F, P^\dagger R^\dagger \cdot G\rangle = 0$. $\quad P = P(p, \partial_p)$
- If $Q \cdot G = 0$, then for all R, $\langle F, RQ \cdot G\rangle = 0$. $\quad Q = Q(p, \partial_p, t, \partial_t)$

An analogue of creative telescoping

The scalar product $\langle F, G\rangle$ is cancelled by any element of

$$\big(\mathrm{ann}(F)^\dagger \mathbb{Q}(t)\langle\partial_t\rangle + \mathrm{ann}(G)\big) \cap \mathbb{Q}(t)\langle\partial_t\rangle.$$

Idea 1: Plain Linear Algebra (Chyzak, Mishna, Salvy, 2005)

Main idea

Filter each of $\operatorname{ann}(F)^\dagger$ and $\operatorname{ann}(G)$ up to total degree N before eliminating (p, ∂_p) by $\mathbb{Q}(t)$-linear algebra.

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Given annihilators of F and of G:

1. Compute:
   1. a (right) Gröbner basis $(P_1, P_2, \dots)$, with $P_i = P_i(p, \partial_p)$,
   2. a (left) Gröbner basis $(Q_1, Q_2, \dots)$, with $Q_i = Q_i(p, \partial_p, t, \partial_t)$,

   such that $\quad P_1^\dagger \cdot F = P_2^\dagger \cdot F = \cdots = 0, \qquad Q_1 \cdot G = Q_2 \cdot G = \cdots = 0.$
2. For increasing integer $N \geq 0$:
   - Consider all $P_i p^\alpha \partial_p^\beta \partial_t^\gamma$ and all $p^\alpha \partial_p^\beta Q_i$ of total degree at most N.
   - Decompose them in the basis of the $p^\alpha \partial_p^\beta \partial_t^\gamma$ over $\mathbb{Q}(t)$ and form a matrix (one operator per row, one basis element per column).
   - Order the columns so that those corresponding to the ∂_t^γ are right-most and perform a row echelon form computation.
   - If a row represents a non-zero element of $\mathbb{Q}(t)\langle \partial_t \rangle$, return it.

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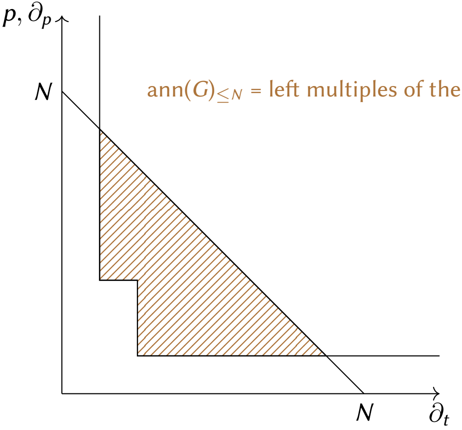

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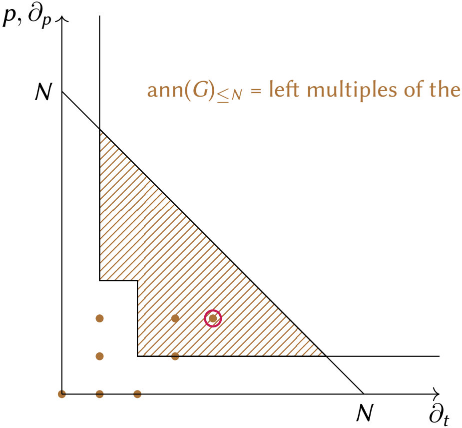

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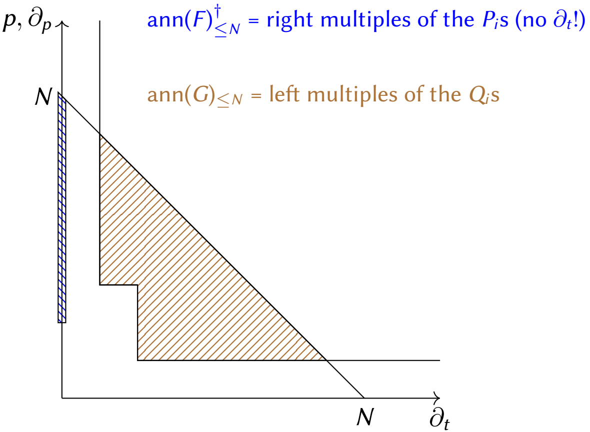

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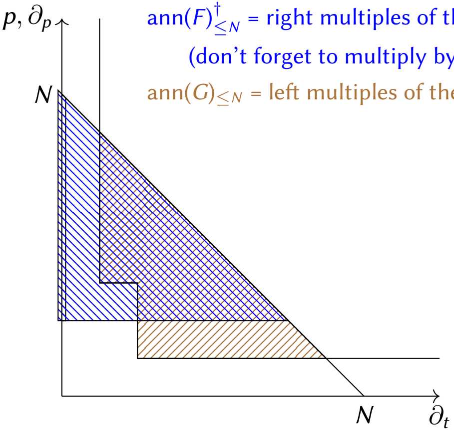
$\mathrm{ann}(F)^\dagger_{\leq N}$ = right multiples of the P_is (no ∂_t!)

(don't forget to multiply by $\partial_t, \partial_t^2, \ldots$)

$\mathrm{ann}(G)_{\leq N}$ = left multiples of the Q_is



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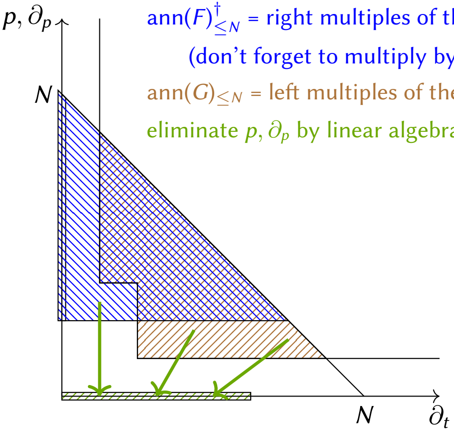

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eliminate p, ∂_p by linear algebra (RREF)

Idea 2: Hammond Series (Chyzak, Mishna, Salvy, 2005)

Main idea

Use Hammond series to make a change of variables, observe an explicit chain rule, then perform elimination of the new variables.

$$\alpha = \sigma(\lambda) \longleftarrow \lambda \longleftrightarrow r = \tau(\lambda) = (\#\text{ of 1's}, \#\text{ of 2's}, \dots)$$

$$F(x) := \sum_{\alpha} \tilde{c}_\alpha x^\alpha = \sum_{\lambda} c_\lambda m_\lambda \longleftrightarrow \sum_{\lambda} c_\lambda \frac{y^r}{r_1!\, r_2! \cdots} =: \mathcal{H}(F)(y)$$

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$$x_1^k \cdots x_n^k + \cdots = m_{\underbrace{k, \dots, k}_{n \text{ times}}} \longleftrightarrow \frac{y_k^n}{n!} = \mathcal{H}(F)(m_{k,\dots,k})$$

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Use Hammond series to make a change of variables, observe an explicit chain rule, then perform elimination of the new variables.

Observation

$$\left\langle F, \exp(h_k t) \right\rangle = \mathcal{H}(F)(\underbrace{0, \ldots, 0}_{k-1}, t, 0, 0, \ldots)$$

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Thm (Hammond, 1883; MacMahon, 1915; Goulden, Jackson, Reilly, 1983)

$$\mathcal{H}\left(\frac{dF}{dp_i}\right) = \sum_{1\alpha_1+2\alpha_2+\cdots=i} (-1)^{|\alpha|-1} \frac{|\alpha|-1}{\alpha!} \partial_y^\alpha \cdot \mathcal{H}(F),$$

$$\mathcal{H}(p_i F) = \left(y_i + \sum_{j\geq 1} y_{i+j} \partial_{y_j}\right) \cdot \mathcal{H}(F).$$

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$$\mathcal{H}\left(\frac{dF}{dp_i}\right) = E_i(y, \partial_y) \cdot \mathcal{H}(F),$$

$$\mathcal{H}(p_i F) = C_i(y, \partial_y) \cdot \mathcal{H}(F).$$

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Observation

$$\left\langle F, \exp(h_k t) \right\rangle = \mathcal{H}(F)(\underbrace{0, \dots, 0}_{k-1}, t, 0, 0, \dots)$$

Given the annihilator of F:

1. Compute a (right) Gröbner basis $(P_1(p, \partial_p), P_2(p, \partial_p), \dots)$ such that $P_1^\dagger \cdot F = P_2^\dagger \cdot F = \cdots = 0$.
2. Substitute $C_i(y, \partial_y)$ for p_i and $E_i(y, \partial_y)$ for ∂_{p_i}, $1 \leq i \leq k$.
3. For i from 1 to $k - 1$ eliminate ∂_{y_i} and set $y_i = 0$ in the resulting polynomials.
4. Make $y_k = t$ and $\partial_{y_k} = \partial_t$ in the final set and return the single operator it contains.

Idea 3: Polynomial Reductions (Chyzak, Mishna, 2024)

Main idea

Reduce each $\partial_t^i \cdot \langle F, G\rangle$ to some $\langle F, sG\rangle$ where $s \in \mathbb{Q}(t)[p]$ is confined to finite dimension, then find a linear dependency over $\mathbb{Q}(t)$.

Specifics: $F = \exp(f(p))$ and $G = \exp(tg(p))$ for polynomials f and g.

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Reduction

Taking inspiration from (Bostan, Chyzak, Lairez, Salvy, 2018):

$$\begin{cases} P \cdot F = 0 \\ h \in \mathbb{Q}(t)[p] \end{cases} \quad \Rightarrow \quad 0 = \langle P \cdot F, hG \rangle = \langle F, P^\dagger \cdot (hG) \rangle = \langle F, (P^\sharp \cdot h)\, G \rangle$$

"Dominant" operator $\rightarrow$ reducible monomials:

$$P^\sharp = x^\mu + \sum_{|\alpha|-|\beta|<|\mu|} u_{\alpha,\beta} x^\alpha \partial_x^\beta \quad \Rightarrow \quad \forall \sigma \geq \mu,\ x^\sigma = \mathrm{lm}(P^\sharp \cdot x^{\sigma-\mu})$$

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Computational observations

- $\operatorname{ann}(F)^\sharp$ has a Gröbner bases made of dominant operators.
- The corresponding leading monomials x^μ generate a 0-dimensional ideal in $\mathbb{Q}(t)[p]$.

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Given the annihilator of F:

1. Compute a (right) Gröbner basis $\operatorname{ann}(F)^\sharp$, viewed as a right $\mathbb{Q}(t)[p]$-module and for an ordering that makes $\partial_p^0 \succeq \partial_p^\alpha$.
2. Fail if cannot verify: *(never happened for k-regular graphs)*
   - that the operators are dominant,
   - that their leading monomials do not involve ∂_p,
   - that they generate a zero-dimensional ideal I: $\dim \mathbb{Q}(t)[p]/I < \infty$.
3. Set $s_0 = 1$, then for successive $r = 1, 2, \dots$: $(\partial_t^i \leftrightarrow s_i)$
   - write $\partial_t^r \cdot \langle F, G \rangle = \partial_t \cdot \langle F, s_{r-1} G \rangle = \left\langle F, \left(\frac{ds_{r_1}}{dt} + s_{r-1} g \right) G \right\rangle$,
   - reduce to get $\partial_t^r \cdot \langle F, G \rangle = \langle F, s_r G \rangle$ with confinement of s_r,
   - if $\exists (a_i)$, $a_0 s_0 + \dots + a_r s_r = 0$, output $a_0 + a_1 \partial_t + \dots + a_r \partial_t^r$.

Idea 4: Residues (Brochet, Chyzak, Lairez, 2025)

Main idea

Use Laplace transform to get a residue representation of the scalar product.

Hadrien Brochet - Faster multivariate integration in D-modules

SS10 (AAADIOS), Tuesday, 9am

Idea 4: Residues (Brochet, Chyzak, Lairez, 2025)

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Use Laplace transform to get a residue representation of the scalar product.

Hadrien Brochet - Faster multivariate integration in D-modules

$$F = \exp(f(p)), \qquad G = \exp(tg(p))$$

Define the formal Laplace transform and the formal residue:

$$\mathcal{L}(p_1^{r_1} \dots p_k^{r_k}) = \frac{r_1!}{p_1^{r_1+1}} \dots \frac{r_k!}{p_k^{r_k+1}} \quad \text{and} \quad \operatorname{res}\left(\sum_{r\in\mathbb{Z}^k} c_r p^r\right) = c_{-1,\dots,-1}.$$

Residue representation

$$\langle F, G\rangle = \operatorname{res}_p \left(\exp\left(f(p_1, \dots, p_k)\right)\mathcal{L}\left(\exp\left(tg(1p_1, 2p_2, \dots, kp_k)\right)\right)\right)$$

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Composition of holonomy-preserving operations

- $\exp(t\tilde{g}(p))$: a manifestly holonomic system

$$\partial_{p_i} - t\frac{d\tilde{g}}{dp_i}\ (1 \leq i \leq k), \quad \partial_t - \tilde{g}$$

- $\mathcal{L}(\ldots)$: change $p_i \to -\partial_{p_i}$ and $\partial_{p_i} \to p_i$, and think modulo $\ker(\mathrm{res}_p)$
- $\exp(f(p)) \times \ldots$: change $\partial_{p_i} \to \partial_{p_i} - \frac{df}{dp_i}$
- $\mathrm{res}_p(\ldots)$: compute the integral of a (holonomic) module

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$$\mathrm{res}_p(h(t,p)) = \frac{1}{(2i\pi)^k} \oint \cdots \oint \frac{h(t,p)}{p_1 \cdots p_k} dp_1 \cdots dp_k$$

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holonomic system in $\partial_t, \partial_{p_1}, \ldots, \partial_{p_k}$ $\to$ $\boxed{\dfrac{M}{\partial M}}$ $\longrightarrow$ ODE in ∂_t

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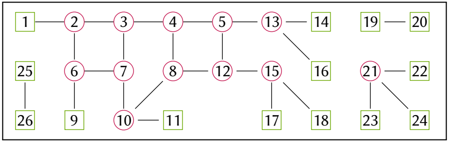
holonomic system in $\partial_t, \partial_{p_1}, \ldots, \partial_{p_k}$ $\to$ [Hadrien Brochet] $\longrightarrow$ ODE in ∂_t

Bonus: Vertices and Edges (Chyzak, Huang, Kauers, 20??)

New problem: Conjecture 16 in (Kauers, Koutschan, 2023)

Sequence A339987 of the OEIS, which counts (3,1)-regular graphs having one more vertex than edges by number of vertices, satisfies an explicit, guessed recurrence relation of order 5, valid for all $n \geq 0$.



26 vertices, 25 edges

Bonus: Vertices and Edges (Chyzak, Huang, Kauers, 20??)

Main idea

A diagonal is a residue, too.

Bonus: Vertices and Edges (Chyzak, Huang, Kauers, 20??)

Marking edges by $x_i x_j \to q x_i x_j$, or equivalently $p_i \to q^{i/2} p_i$, leads to:

Number $r_{m,n}^{(k)}$ of k-regular simple graphs on n labelled vertices with m edges

The EGF $$\sum_{m,n=0}^{\infty} r_{m,n}^{(k)} q^m \frac{t^n}{n!} = \langle F(p,q), G(p,t) \rangle,$$

where

$$F(p,q) = \exp\left(\sum_{m=1}^{\lfloor k/2 \rfloor} (-q)^m \frac{p_{2m}}{2m} - \sum_{m=1}^{k} (-q)^m \frac{p_m^2}{2m} \right) \qquad \in \mathbb{Q}[p_1, \dots, p_k][[q]],$$

$$G(p,t) = \exp(h_k t) \qquad \in \mathbb{Q}[p_1, \dots, p_k][[t]],$$

is D-finite w.r.t. q and t.

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Marking edges by $x_i x_j \to q x_i x_j$, or equivalently $p_i \to q^{i/2} p_i$, leads to:

Number $r_{m,n}^{(3,1)}$ of (3, 1)-regular simple graphs on n labelled vertices with m edges

The EGF $$\sum_{m,n=0}^{\infty} r_{m,n}^{(3,1)} q^m \frac{t^n}{n!} = \langle F(p,q), G(p,t) \rangle,$$

where
$$F(p,q) = \exp\left(-\frac{p_2}{2} - \frac{p_1^2}{2} + \frac{p_2^2}{4} - \frac{p_3^2}{6}\right) \qquad \in \mathbb{Q}[p_1,p_2,p_3][[q]],$$
$$G(p,t) = \exp((h_3 + h_1)t) \qquad \in \mathbb{Q}[p_1,p_2,p_3][[t]],$$

is D-finite w.r.t. q and t.

1. 'Idea 3: polynomial reductions' works, and delivers a *system* of linear PDEs w.r.t. q and t.
2. For $r_{n-1,n}^{(3,1)}$, next compute the diagonal of $q\langle F(p,q), G(p,t)\rangle$.

Bonus: Vertices and Edges (Chyzak, Huang, Kauers, 20??)

Better yet:

EGF of (3,1)-regular simple graphs on n labelled vertices with $n-1$ edges

$$\operatorname{diag}_{q,t}\left(q\langle F(p,q), G(p,t)\rangle\right) = \operatorname{res}_{q,p}\left(q\exp\big(f(p_1,p_2,p_3)\big)\mathcal{L}\Big(\exp\big(q^{-1}tg(1p_1,2p_2,3p_3)\big)\Big)\right)$$

Proof: for any $h = \sum_{m,n} h_{m,n}q^m t^n$,

$$\operatorname{diag}_{q,t}(h(q,t)) = \sum_n h_{n,n}t^n = \operatorname{res}_q\left(q^{-1}h(q,q^{-1}t)\right).$$

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Use D-module integration and Hadrien Brochet's implementation again.

Conclusions

Evolution of efficiency

- 'Idea 1, plain linear algebra': very slow because it enumerates monomials *above* the stairs [Maple]
- 'Idea 2, Hammond series': slow, probably because elimination is done too incrementally (variable after variable) [Maple]
- 'Idea 3, polynomial reductions': reasonable, because it does not compute the 'certificates' s_i in expansion [Maple]
- 'Idea 4, residues': faster, because the implementation adds evaluation-interpolation technique [Julia]

Methodological remarks

- Plain linear algebra: reminiscent of Takayama's algorithm for integration
- Hammond series: elimination-and-setting-variables-to-0 is really a D-module 'restriction' and so should work as fast as residues