Faster Multivariate Integration in D-modules

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A symbolic integration problem

Let $I(t) = \oiiint \frac{dx\, dy\, dz}{1-(1-xy)z-txyz(1-x)(1-y)(1-z)}$ (g.f. of Apéry numbers)

The objective is to compute a linear differential equation (LDE) for I:

$$t^2(t^2-34t+1)\frac{\partial^3 I}{\partial t^3}+3t(2t^2-51t+1)\frac{\partial^2 I}{\partial t^2}+(7t^2-112t+1)\frac{\partial I}{\partial t}+(t-5)I=0.$$

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With this LDE it is possible to

1. compute a series expansion at any points,
2. evaluate the integral numerically to arbitrary precision,
3. prove identities involving $I(t)$.

The method of Creative Telescoping

Write $\mathbf{x} = x_1, \ldots, x_n$ and let $I(t) = \oint f(\mathbf{x}, t) d\mathbf{x}$.

Creative telescoping (multivariate integration w.r.t $\mathbf{x}$)

Find $\ell \in \mathbb{N}$, $a_1, \ldots, a_\ell \in \mathbb{K}(t)$ and functions $g_1, \ldots, g_n$ s.t.

$$a_\ell(t) \frac{\partial^\ell f(\mathbf{x}, t)}{\partial t^\ell} + \cdots + a_1(t) \frac{\partial f(\mathbf{x}, t)}{\partial t} + a_0(t) f(\mathbf{x}, t) = \sum_{i=1}^{n} \frac{\partial g_i(\mathbf{x}, t)}{\partial x_i}.$$

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After integration, we obtain

$$a_\ell(t) \frac{\partial^\ell I(t)}{\partial t^\ell} + \cdots + a_1(t) \frac{\partial I(t)}{\partial t} + a_0(t) I(t) = \underbrace{\sum_{i=1}^{n} \oint \frac{\partial g_i(\mathbf{x}, t)}{\partial x_i} d\mathbf{x}}_{\text{equals } 0}.$$

Algebra of Differential Operators: Weyl algebra

The n-th Weyl algebra W_n over $\mathbb{K}$ is

- generated by the variables $x_1, \ldots, x_n, \partial_1, \ldots, \partial_n$ and
- subject to the relations $[\partial_i, x_i] = 1$ and $[x_i, x_j] = [x_i, \partial_j] = [\partial_i, \partial_j] = 0$ for $i \neq j$

The homogeneous linear differential equation with *polynomial* coefficients

$$x_1 \frac{\partial^2 y}{\partial x_1 \partial x_2} + (x^2 + 1)\frac{\partial y}{\partial x_1} + y = 0$$

is represented in W_2 by

$$x_1 \partial_1 \partial_2 + (x^2 + 1)\partial_1 + 1.$$

Holonomy

Holonomic function

A function $f(\mathbf{x})$ is holonomic if for each ∂_i if it satisfies a LODE with polynomial coefficients in $\mathbb{K}[\mathbf{x}]$.

Annihilator of f

The set $\operatorname{ann}(f) \stackrel{\text{def}}{=} \{L \in W_n \mid L \cdot f = 0\}$ is a left ideal of W_n.

Link between functions and operators

f is characterized by its annihilator: $W_n \cdot f \simeq W_n / \operatorname{ann}(f)$.

Input of the algorithm

Let $I(t) = \oint f(\mathbf{x}, t) d\mathbf{x}$

Assumptions

1. f is holonomic
2. The integration domain has no boundary
3. f has no singularities on the integration domain

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Data-structure for f: (separate ∂_t from $\partial_1, \ldots, \partial_n$)

Assume we know generators of $\operatorname{ann}(f)$ in the algebra W_n over $\mathbb{K}(t)$ and a derivation map $\partial_t : W_n \to W_n$ satisfying

$$\partial_t(\lambda m) = \frac{\partial \lambda}{\partial t} m + \lambda \partial_t(m) \quad \text{for } \lambda \in \mathbb{K}(t) \text{ and } m \in W_n$$

Example of Input

Example

Let $f(x,t) = \frac{1}{x-t}$, which is annihilated by

$$\partial_t + \partial_x \quad \text{and} \quad \partial_x(x-t).$$

Then f is represented by the ideal in W_1:

$$W_1(\partial_x(x-t)),$$

and the derivation map $\partial_t : W_1 \to W_1$ is defined by

$$\partial_t(x^a\partial_x^b) = -x^a\partial_x^{b+1}.$$

Algebraic analog of creative telescoping

Recall: creative telescoping

Look for a LHS such that there exists functions $g_1, \ldots, g_n \in W_n \cdot f$ satisfying

$$a_\ell(t) \frac{\partial^\ell f(\mathbf{x}, t)}{\partial t^\ell} + \cdots + a_0(t) f(\mathbf{x}, t) = \sum_{i=1}^{n} \frac{\partial_i g_i(\mathbf{x}, t)}{\partial x_i}.$$

Algebraic formulation

Find coefficients $a_\ell, \ldots, a_0 \in \mathbb{K}(t)$ satisfying

$$a_\ell(t) \partial_t^\ell(1) + \cdots + a_0(t) \in \operatorname{ann}(f) + \sum_{i=1}^{n} \partial_i W_n.$$

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Theorem (Kashiwara)

If f is holonomic, then $W_n/(\operatorname{ann}(f) + \boldsymbol{\partial} W_n)$ is a finite-dimensional vector space.

Computing in $W_n/(\mathrm{ann}(f) + \partial W_n)$

Main difficulties:

- $\mathrm{ann}(f) + \partial W_n$ is the sum of a left and a right module $\implies$ no module structure $\Rightarrow$ no natural module structure on the sum
- Even though $W_n/(\mathrm{ann}(f) + \partial W_n)$ is finite-dimensional, W_n and $\mathrm{ann}(f) + \partial W_n$ are not!

Takayama's algorithm

💡 Work in W_n by increasing degree:

$$F_q = \bigoplus_{|\alpha|+|\beta|\leq q} \mathbb{K}\cdot \mathbf{x}^{\alpha}\boldsymbol{\partial}^{\beta}.$$

Takayama's algorithm 1990 (without parameters)

Fix q and approximate the quotient $W_n/(\mathrm{ann}(f) + \boldsymbol{\partial} W_n)$ by

$$F_q/(\mathrm{ann}(f) \cap F_q + \boldsymbol{\partial} F_{q-1})$$

which is a quotient of two finite-dimensional $\mathbb{K}(t)$-vector spaces.

Termination criterion

A bound on q to get a basis of $W_n/(\mathrm{ann}(f) + \boldsymbol{\partial} W_n)$ can be deduced from the roots of the b-function (Oaku-Takayama 1997). However, it is costly to compute.

Reduction-based creative telescoping

Goal: Construct a $\mathbb{K}(t)$-linear map $[\,.\,] : W_n \to W_n$ s.t.

- $a - [a] \in \operatorname{ann}(f) + \boldsymbol{\partial} W_n$ (reduction)
- $[a] = 0$ iff $a \in \operatorname{ann}(f) + \boldsymbol{\partial} W_n$ (normal form)

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Creative telescoping algorithm

$p_0 \leftarrow [1]; \quad \ell \leftarrow 0$

while there is no $\mathbb{K}(t)$-linear relation $\sum_{i=0}^{\ell} \lambda_i p_i = 0$

    $p_{\ell+1} \leftarrow [\partial_t(p_\ell)]$ # invariant: $p_\ell \equiv [\partial_t^\ell(1)] \mod \operatorname{ann}(f) + \partial W_n$

    $\ell \leftarrow \ell + 1$

return $\sum_{i=0}^{\ell} \lambda_i \partial_t^i$

➕ Always terminates as $W_n/(\operatorname{ann}(f) + \partial W_n)$ is finite-dimensional!

A first reduction

Use more structure of $\operatorname{ann}(f) + \partial W_n$

Reduction procedure $[.] : W_n \mapsto W_n$

```
repeat
    a ← a mod ∂W_n
    a ← a mod ann(f)
until no term in a can be further reduced
return a
```

- The reduction $[.]$ does not reduce all $\operatorname{ann}(f) + \partial W_n$ to zero
- But $\dim([(\operatorname{ann}(f) + \partial W_n)] \cap F_q) \ll \dim((\operatorname{ann}(f) + \partial W_n) \cap F_q)$

Critical pairs

What does $[\mathrm{ann}(f) + \partial W_n]$ look like ?

It is generated by terms $a + d$ with $\mathrm{lt}(a) = -\mathrm{lt}(d)$ and $a \in \mathrm{ann}(f), d \in \partial W_n$

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Example

Take $f = e^{x^2 z - y^3}$, a Gröbner basis of $\text{ann}(f)$ for $\text{grevlex}(x, y, z) > \text{grevlex}(\partial_x, \partial_y, \partial_z)$ is

$$2\underline{xz} - \partial_x, \qquad 3\underline{y^2} + \partial_y, \qquad \underline{x^2} - \partial_z$$
$$4\underline{z^2\partial_z} + 2z - \partial_x^2, \qquad \underline{x\partial_x} - 2z\partial_z$$

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For example z is irreducible by $[.]$ but

$$z = \underbrace{-\frac{1}{6}(4\underline{z^2\partial_z} + 2z - \partial_x^2)}_{\in \mathrm{ann}(f)} + \underbrace{\frac{1}{6}(4\underline{\partial_z z^2} - \partial_x^2)}_{\in \boldsymbol{\partial} W_n}$$

The family of reduction $[.]_\eta$

⚠ $[\mathrm{ann}(f) + \partial W_n]$ may not be a finite-dimensional vector space

Fix a monomial order $\preccurlyeq$ on W_n and let η be a monomial of W_n.

$\rightsquigarrow$ Compute instead a basis of

$$\begin{aligned} E_{\preccurlyeq \eta} &:= \{[a+d] \mid a \in \mathrm{ann}(f), d \in \partial W_n, max(\mathrm{lm}(a), \mathrm{lm}(d)) \preccurlyeq \eta\} \\ &= \{[a] \mid a \in \mathrm{ann}(f), \mathrm{lm}(a) \preccurlyeq \eta\} \end{aligned}$$

Critical pair criterion

Let $a \in \mathrm{ann}(f)$. If there exists $b \in \mathrm{ann}(f)$ and i s.t. $\mathrm{lm}(a) = \mathrm{lm}(\partial_i b)$, then $[a] \in E_{\prec \eta}$.

The family of reduction $[.]_\eta$

Algorithm for computing $E_{\preccurlyeq\eta}$

$B \leftarrow \emptyset$
for each monomial $\eta' \preccurlyeq \eta$ in $\mathrm{lm}(\mathrm{ann}(f)) \cap \mathrm{lm}(\boldsymbol{\partial} W_{\boldsymbol{n}})$
    if there exists i and $b \in \mathrm{ann}(f)$ s.t. $\eta' = \mathrm{lm}(\partial_i b)$
        continue
    pick $a \in \mathrm{ann}(f)$ s.t. $\mathrm{lm}(a) = \eta'$
    $B \leftarrow B \cup \{[a]\}$
return Echelon(B)

The family of reduction $[.]_\eta$

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Define: $[a]_\eta := [a] \mod E_{\preccurlyeq\eta}$

Final algorithm

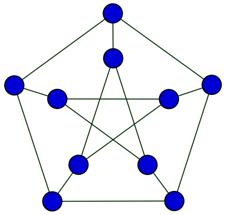
Creative telescoping algorithm

Choose η smartly (not presented today!)
$p_0 \leftarrow [1]_\eta; \quad \ell \leftarrow 0$
while there is no $\mathbb{K}(t)$-linear relation $\sum_{i=0}^{\ell} \lambda_i p_i = 0$
    $p_{\ell+1} \leftarrow [\partial_t(p_\ell)]_\eta$ # invariant: $p_\ell \equiv [\partial_t^\ell(1)]_\eta \mod \operatorname{ann}(f) + \boldsymbol{\partial} W_n$
    $\ell \leftarrow \ell + 1$
return $\sum_{i=0}^{\ell} \lambda_i \partial_t^i$

- ➕ Always terminates even though $[.]_\eta$ is not a normal form.
- ➖ The returned LDE may not be of minimal order.

Application: counting k-regular graphs

k-regular graph: every vertex has degree k



Petersen's graph is 3-regular

Problem statement

$c_n^{(k)}$: number of k-regular graphs on n vertices.

Goal: compute a LDE for $\sum_{n=0}^{\infty} \frac{c_n^{(k)}}{n!} t^n$ for fixed k

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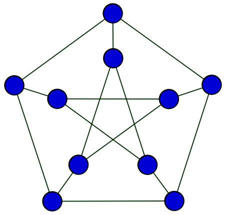

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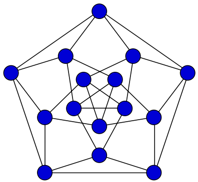

A 4-regular graph

Previous work

- Read (1959): up to $k = 3$
- McKay, Wormald ($\approx$ 1959): $k = 4$
- Chyzak, Mishna, Salvy (2005): $k = 4$ using C.T.[1]
- Chyzak, Mishna (2025): up to $k = 7$ using red.-based C.T.[1]

[1] It is actually a variant of creative telescoping for scalar products of symmetric functions

Application: counting k-regular graphs

$\rightsquigarrow$ Building on Chyzak-Mishna-Salvy (2005) we obtained

$$\sum_{n=0}^{\infty} \frac{c_n^{(k)}}{n!} t^n = \operatorname{res}_{\mathbf{x}} F(t, \mathbf{x})$$

where F is a series in $\mathbb{K}[[\mathbf{x}]][\mathbf{x}^{-1}]((t))$ implicitly represented by an ideal $I \subset \mathbb{K}(t)[\mathbf{x}]\langle \partial_t, \boldsymbol{\partial}_{\mathbf{x}} \rangle$ satisfying for any $L \in I$, $\operatorname{res}_{\mathbf{x}} L(F) = 0$.

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Example

For $k = 2$, I is generated by

$$(t-1)x_1 - t\partial_1, \qquad x_2 - t$$
$$2(t-1)^2\partial_t - \partial_1^2 + 2(t-1)^2\partial_2 + t^2(t-1)$$

and we obtain the LDE

$$2(t-1)d_t + t^2.$$

Benchmarks

Because of the polynomials in the ideal I, no creative telescoping algorithms over $\mathbb{Q}(t, \mathbf{x})$ work here!

k	2	3	4	5	6	7	8
Tak-Macaulay2	0.02s	1.7s	535s	$>$90m	-	-	-
Tak-Singular	$<$1s	$<$1s	25s	$>$90m	-	-	-
Ch/Mi-Maple[1]	0.04	0.08	0.2	1.96	52.3s	9h	-
Our algo-Julia[1,2]	7.2s	7.6s	8.7s	7.9s	8.5s	363s	7h28min

[1] Results available at `https://files.inria.fr/chyzak/kregs/`

[2] Code available at `https://github.com/HBrochet/MultivariateCreativeTelescoping.jl`