Faster Multivariate Integration in D-modules

Hadrien Brochet

Joint work with Frédéric Chyzak and Pierre Lairez

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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,
2. evaluate the integral numerically,
3. prove identities involving $I(t)$.

Other examples of parametric integrals

The method of creative telescoping can deal with:

- orthogonal polynomials

$$A_n(p) = \int_{-1}^{1} \frac{e^{-px}\, T_n(x)}{\sqrt{1-x^2}}\, dx,$$

- special functions

$$B(c) = \int_0^\infty \int_0^\infty \mathrm{J}_1(x)\, \mathrm{J}_1(y)\, \mathrm{J}_2(c\,\sqrt{xy})\, \frac{dxdy}{e^{x+y}},$$

- semi-algebraic integration domains

$$C_{n,s}(r) = \iint\limits_{x^2+y^2 \le r^2} y^s\, \mathrm{J}_n(x) dxdy.$$

Motivating examples of applications

- Computation of volumes of compact semi-algebraic sets up to a prescribed precision 2^{-p} (2019: Lairez-Mezzarobba-Safey El Din)
- Computation of the generating functions of some walks with small steps in the quarter plane (2017: Bostan-Chyzak-van Hoeij-Kauers-Pech)
- Computation of Feynman integrals for theoretical physics (e.g. 2015: Ablinger-Behring-Blümlein-De Freitas-von Manteuffel-Schneider)
- Counting k-regular graphs (2005: Chyzak-Mishna-Salvy, 2025: Chyzak-Mishna)

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NEW! Counting k-regular graphs for k up to 8 (at the end)

The method of Creative Telescoping

Let $I(t) = \int_a^b f(x,t)dx$.

Creative telescoping (univariate integration w.r.t x)

Find $\ell \in \mathbb{N}, a_0, \ldots, a_\ell \in \mathbb{K}(t)$ and a function g s.t.

$$a_\ell(t)\frac{\partial^\ell f(x,t)}{\partial t^\ell} + \cdots + a_1(t)\frac{\partial f(x,t)}{\partial t} + a_0(t)f(x,t) = \frac{\partial g(x,t)}{\partial x}.$$

After integration, we obtain

$$a_\ell(t)\frac{\partial^\ell I(t)}{\partial t^\ell} + \cdots + a_1(t)\frac{\partial I(t)}{\partial t} + a_0 I(t) = \underbrace{g(b,t) - g(a,t)}_{\text{often zero}}.$$

The method of Creative Telescoping

Write $\mathbf{x} = x_1, \ldots, x_n$.

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.

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

Let $I(t) = \int_\gamma f(\mathbf{x}, t) d\mathbf{x}$. After integration, we obtain

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

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

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

Algebra of Differential Operators: rational Weyl algebra

The n-th rational Weyl algebra R_n over $\mathbb{K}(x_1, \ldots, x_n)$ is

- generated by the variables $\partial_1, \ldots, \partial_n$ 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 equations with rational coefficients

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

is represented in R_2 by

$$\frac{x_1}{x_2^2 + 1} \partial_1 \partial_2 + (x^2 + 1) \partial_1 + 1.$$

D-finite functions

Definition

A function f is D-finite if for each ∂_i it satisfies a LODE with polynomial coefficients.

Proposition

f is D-finite if and only if $R_n / \operatorname{ann}_{R_n}(f)$ is a finite-dimensional vector space,
where $\operatorname{ann}_{R_n}(f) = \{P \in R_n \mid P \cdot f = 0\}$.

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Example

The function $f = \mathrm{J}_0(x - y)$ is D-finite as its annihilator is generated by

$$(x-y)\partial_x^2 + \partial_x + (x-y), \qquad \partial_y + \partial_x$$

which implies

$$R_n / \operatorname{ann}_{R_n}(f) \simeq \mathbb{Q}(x,y) f \oplus \mathbb{Q}(x,y)\partial_x \cdot f.$$

Holonomy

Holonomic module

A module W_n/S is holonomic if its module dimension is exactly n. Or equivalently if for every choice of $n+1$ variables $I \subset \{x_1 \ldots, x_n, \partial_1, \ldots \partial_n\}$, $\mathbb{K}\langle I \rangle \cap S$ is non-empty.

Holonomic function

A function f is holonomic if the module $W_n / \operatorname{ann}_{W_n}(f)$ is holonomic, where $\operatorname{ann}_{W_n}(f) = \{P \in W_n \mid P \cdot f = 0\}$.

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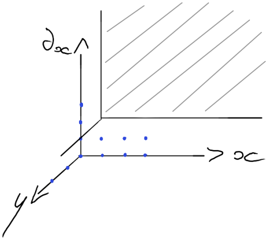
Example

The same function $f = \mathrm{J}_0(x-y)$ is also holonomic as the dimension of $W_n/\operatorname{ann}_{W_n}(f)$ is 2. A basis of this quotient is given by the image of the monomials $x^a\partial_x^b y^c$ such that $x\partial_x^2 \nmid x^a\partial_x^b$.



D-finiteness vs Holonomy

Theorem

A function is D-finite if and only if it is holonomic.

D-finiteness

- ⊕ Fast computation
- ⊖ Lacks expressivity
- ⊖ No general multivariate integration algorithm known

Holonomy

- ⊕ Useful for proofs of existence and termination
- ⊕ Extends to holonomic distribution $\Longrightarrow$ allows integration over semi-algebraic sets
- ⊖ Slow computation

Today: Mixed approach

Operators with coefficients in $\mathbb{Q}(t)[\mathbf{x}]$

Previous work (non-exhaustive)

Ansatz-based approaches (D-finite)

- Univariate integration of hyperexponential functions (Almkvist-Zeilberger 1990)
- Univariate integration of D-finite functions (Chyzak 2000)
- Fast heuristic for univariate integration of D-finite functions (Koutschan 2010)

Gröbner basis approaches (holonomy)

- Integration of holonomic functions (Takayama 1990,Oaku-Takayama 1997, Chyzak-Salvy 1998)
- Integration of holonomic functions over semi-algebraic sets (Oaku 2013)

Reduction-based approaches (D-finite)

- Univariate integration of bivariate rational functions (Bostan-Chen-Chyzak-Li 2010)
- Multivariate integration of rational functions (Bostan-Lairez-Salvy 2013, Lairez 2016)
- Univariate integration of D-finite functions (van der Hoeven 2018, Bostan-Chyzak-Lairez-Salvy 2018, Chen-Du-Kauers 2023)

Input of the algorithm

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

Assumptions

1. f is holonomic
2. γ has natural boundaries, i.e., for any i and $a \in W_n$, $\int_\gamma \partial_i a \cdot f(\mathbf{x}, t) d\mathbf{x} = 0$.

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Data-structure

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:

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

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

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

Integral of the module $W_n/\operatorname{ann}(f)$

Definition

The integral of the module $M = W_n/\operatorname{ann}(f)$ is

$$M/\sum_{i=1}^{n} \partial_i M \quad \simeq \quad W_n/(\operatorname{ann}(f) + \sum_{i=1}^{n} \partial_i W_n).$$

This yields the following commutative diagram:

$$\begin{tikzcd}
W_n \cdot f \arrow[r, "\simeq"] \arrow[d] & M \arrow[d] \\
\dfrac{W_n \cdot f}{\sum_{i=1}^{n} \partial_i W_n \cdot f} \arrow[r, "\simeq"'] & \dfrac{M}{\sum_{i=1}^{n} \partial_i M}
\end{tikzcd}$$

Integral of the module $W_n/\operatorname{ann}(f)$

Definition

The integral of the module $M = W_n/\operatorname{ann}(f)$ is

$$M/\partial M \simeq W_n/(\operatorname{ann}(f) + \partial W_n).$$

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\dfrac{W_n \cdot f}{\partial W_n \cdot f} \arrow[r, "\simeq"'] & \dfrac{M}{\partial M}
\end{tikzcd}$$

Algebraic analog of creative telescoping

Recall: creative telescoping

Look for a LHS such that there exists functions $g_1, \dots, g_n \in W_n \cdot f$ 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 $a_0, \dots, a_\ell \in \mathbb{K}(t)$ satisfying

$$a_\ell(t)\partial_t^\ell(1) + \cdots + a_0(t) \in \operatorname{ann}(f) + \boldsymbol{\partial} W_n.$$

Computing in the quotient $M/\partial M$

Recall $M/\partial M \simeq W_n/(\mathrm{ann}(f) + \partial W_n)$.

Theorem (Kashiwara)

If f is holonomic, $M/\partial M$ is a finite-dimensional vector space.

Difficulties:

- $\mathrm{ann}(f) + \partial W_n$ is the sum of a left and a right module $\implies$ no module structure
- Even though $M/\partial M$ 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 $M/\boldsymbol{\partial} M$ 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.

- $a - [a] \in \operatorname{ann}(f) + \partial W_n$ (reduction)
- $[a] = 0$ iff $a \in \operatorname{ann}(f) + \partial W_n$ (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: $p_\ell \equiv [\partial_t^{\ell+1}(1)] \mod \operatorname{ann}(f) + \boldsymbol{\partial} W_n$

  $\ell \leftarrow \ell + 1$

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

Always terminates as $M/\boldsymbol{\partial} M$ is finite-dimensional!

"Naïve" reduction

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

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

repeat
  $a \leftarrow a \mod \partial W_n$
  $a \leftarrow a \mod \mathrm{ann}(f)$
until no term in a can be further reduced
return a

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

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 $\mathrm{ann}(f)$ for $\mathrm{grevlex}(x, y, z) > \mathrm{grevlex}(\partial_x, \partial_y, \partial_z)$ 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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$$4\underline{z^2\partial_z} + 2z - \partial_x^2, \qquad \underline{x\partial_x} - 2z\partial_z$$

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 reduction $[.]_\eta$

⚠ $[\mathrm{ann}(f) + \boldsymbol{\partial} W_n]$ 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

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

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 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 reduction $[.]_\eta$

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

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

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

How to choose η ?

The reduction $[\,.\,]_\eta$ does not compute a normal form.

$\rightsquigarrow$ Find a finite-dimensional vector space stable under $[\partial_t(\,.\,)]_\eta$.

Confinement

A confinement (η, B) for ∂_t is a monomial η and a set of monomials B such that

1. $1 \in B$;
2. the support of $[\partial_t(m)]_\eta$ is included in B for any $m \in B$.

This property is only about monomials, not coefficients!

Computation of a confinement

An algorithm when $\preccurlyeq$ is a total degree order

1 $q \leftarrow 1$
2 $\eta \leftarrow$ largest monomial of degree q
3 $Q \leftarrow 1, B \leftarrow \varnothing$
4 **while** $Q \setminus B \neq \varnothing$
5     $m \leftarrow$ an element of $Q \setminus B$
6   **if** $\deg m > q$
7         $q \leftarrow q + 1$
8   **goto** line 2
9     $Q \leftarrow Q \cup \operatorname{supp}([\partial_t(m)]_\eta)$
10     $B \leftarrow B \cup \{m\}$
11 **return** (η, B)

Final algorithm

Creative telescoping algorithm

$\eta, \_ \leftarrow$ compute a confinement for ∂_t

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

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

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

$\quad \ell \leftarrow \ell + 1$

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.

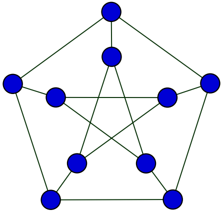
Application: counting k-regular graphs

k-regular graph: every vertex has degree k

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



Petersen's graph is 3-regular

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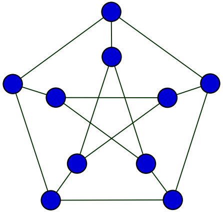

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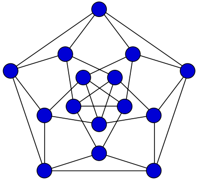

A 4-regular graph

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 polynomial 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[12]	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`