Rigorous Numerical Evaluation of D-Finite Functions in SageMath

Marc Mezzarobba
CNRS, Sorbonne Université

OPSFA, Hagenberg
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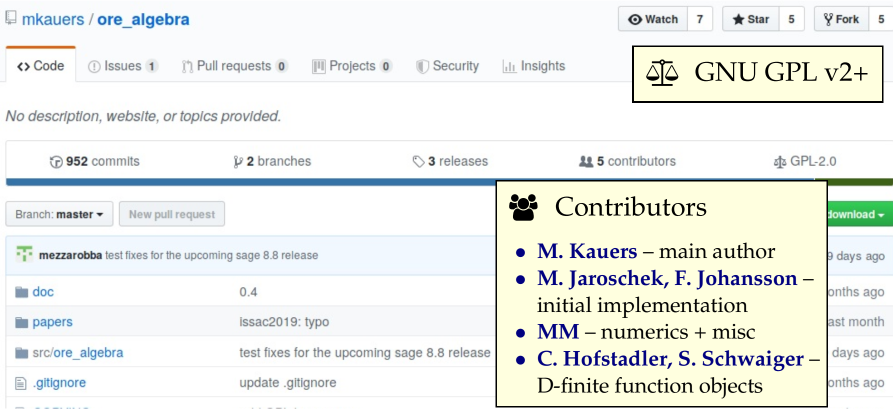
Try it yourself

Sage notebook: `http://marc.mezzarobba.net/opsfa.ipynb`
Online: `http://marc.mezzarobba.net/opsfa.binder`

ore_algebra



⚖ GNU GPL v2+

Contributors

- **M. Kauers** – main author
- **M. Jaroschek, F. Johansson** – initial implementation
- **MM** – numerics + misc
- **C. Hofstadler, S. Schwaiger** – D-finite function objects

```
$ sage -pip install \
        git+https://github.com/mkauers/ore_algebra.git
```

ore_algebra: An Implementation of Ore Polynomials

$$\mathsf{K}(z)\langle \mathsf{D}_z\rangle = \{\text{skew polynomials in } \mathsf{D}_z \text{ over } \mathsf{K}(z) \text{ subject to } \mathsf{D}_z\, z = z\, \mathsf{D}_z + 1\} \cong \{\text{differential operators}\}$$

Example

$$y''(z) + z\, y'(z) + y(z) = 0$$

$$\Updownarrow$$

$$(\mathsf{D}_z^2 + z\,\mathsf{D}_z + 1)\cdot y = 0$$

Features

- Basic arithmetic (diff, shift, qdiff, qshift, custom)
- Gcrd, lclm, D-finite closure (incl. multivariate)
- Creative telescoping
- Polynomial, rational, gen. series solutions
- **Numerical connection** (diff.)

  ⇨ THIS TALK
- Desingularization
- Guessing
- …

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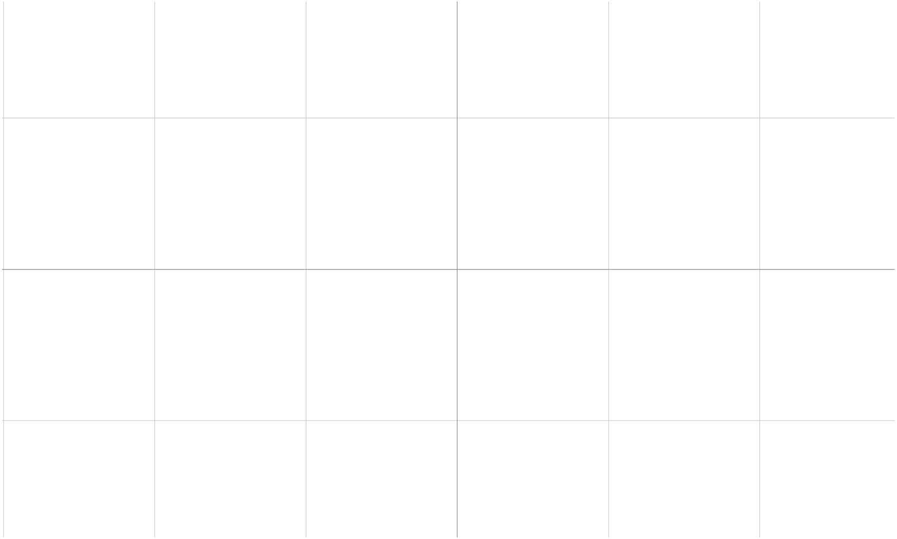
Analytic Continuation

$\mathcal{L} = a_r(z)\, D_z^r + \cdots + a_1(z)\, D_z + a_0(z)$



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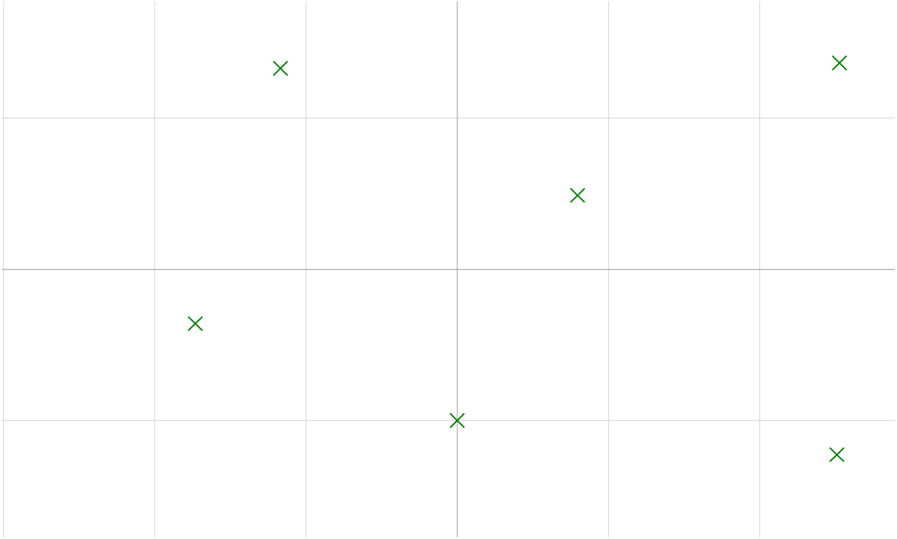

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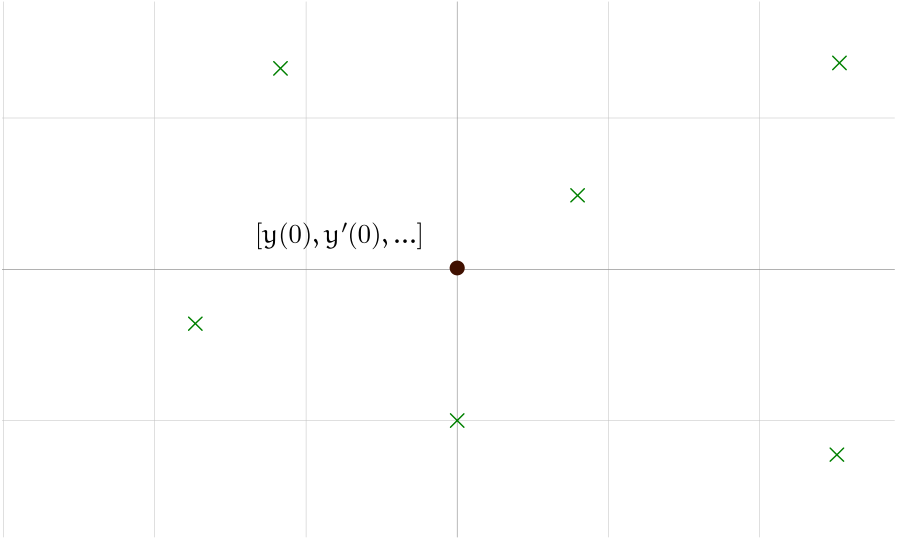

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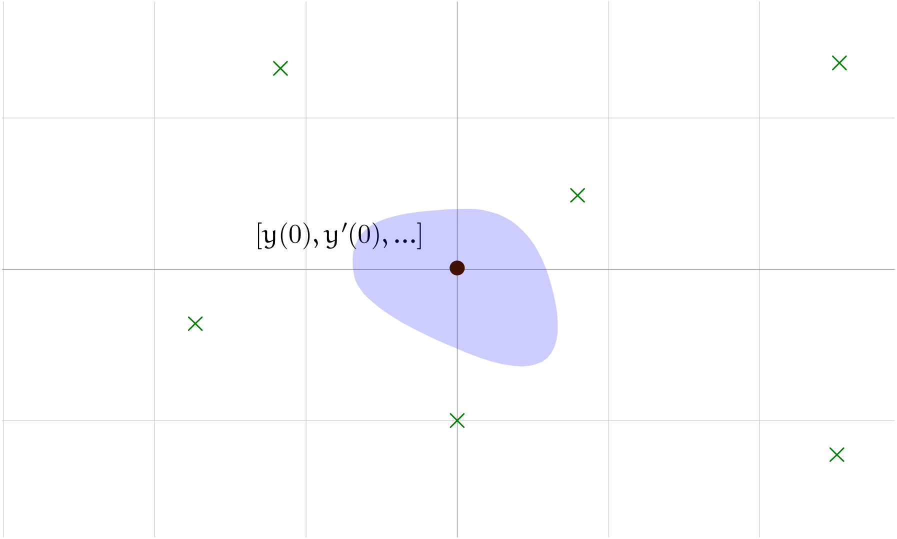

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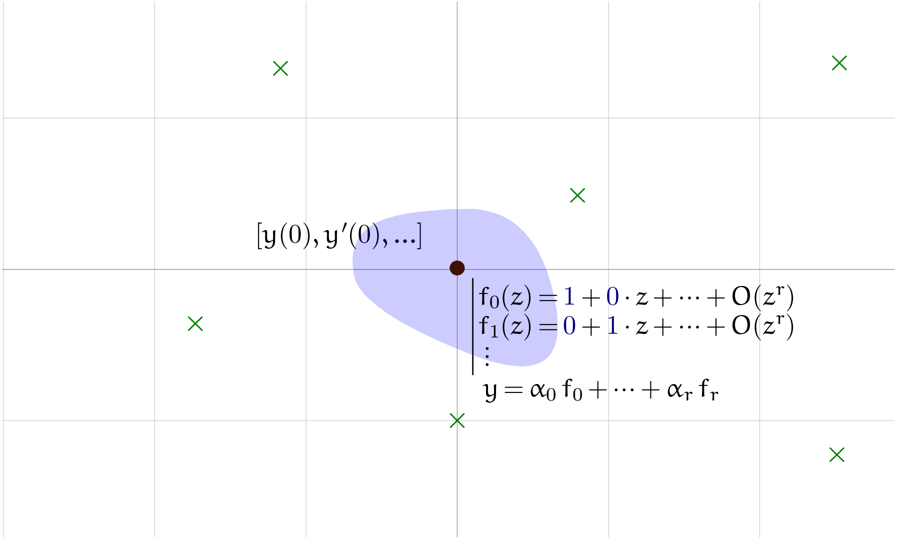

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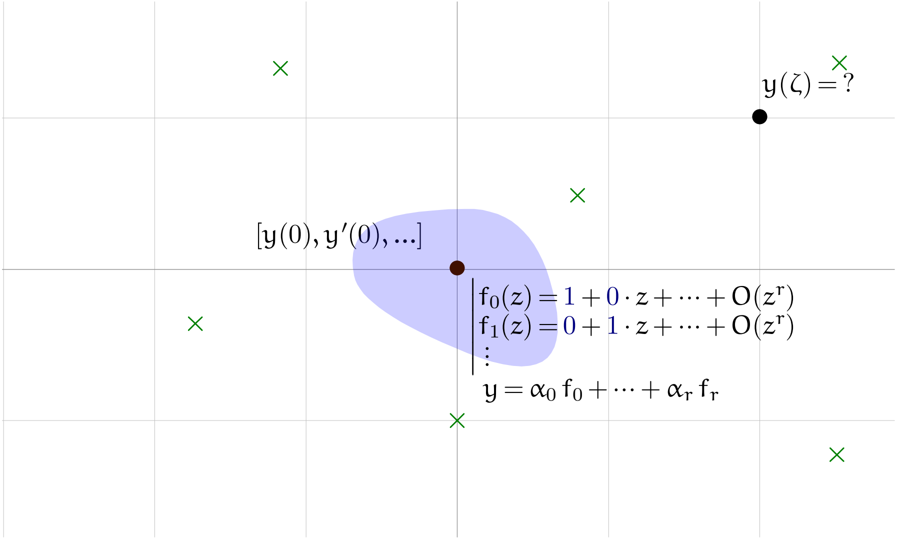

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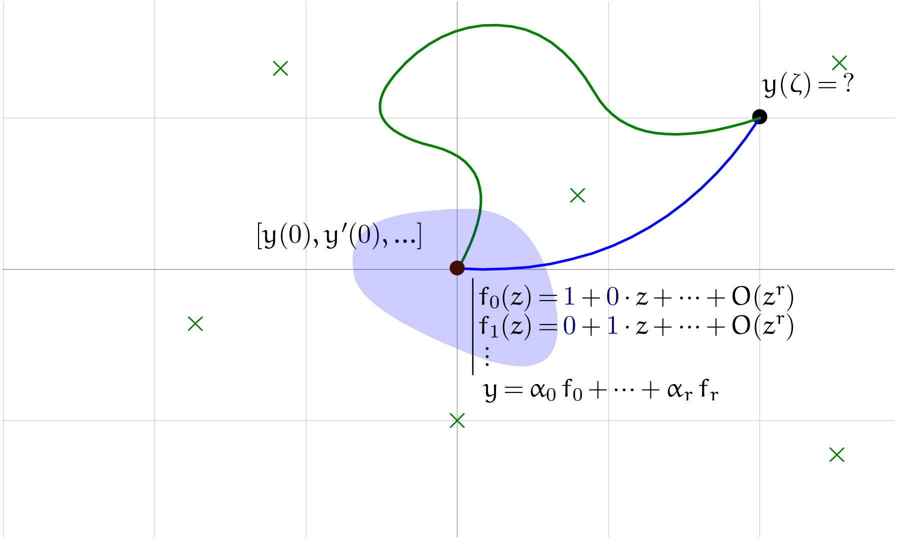


Regular Singular Points

Theorem **[Fuchs, 1866]**

Assume that 0 is a regular singular point. Then, for some neighborhood D of 0, there exists a basis of solutions defined on $D\setminus\{0\}$ of the form

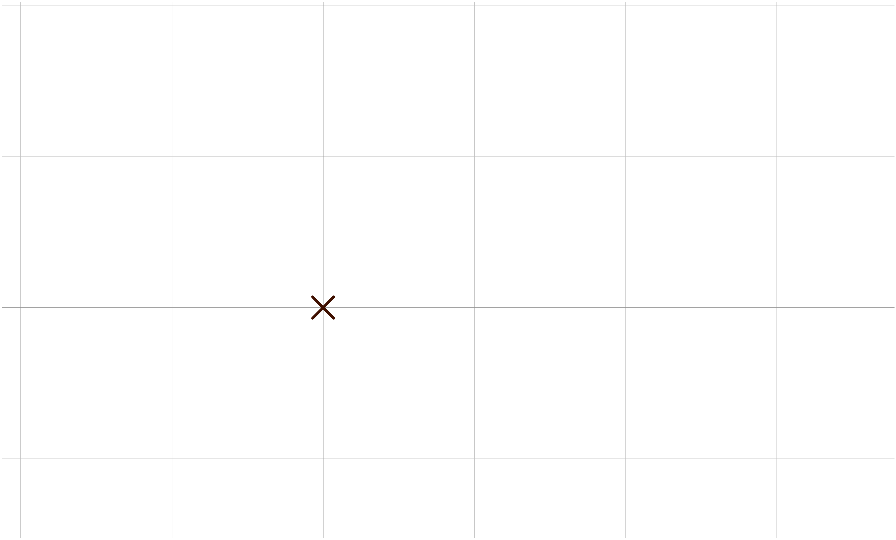
$$z^{\lambda}\left(y_0(z)+y_1(z)\log z+\cdots+y_t(z)\log^t z\right),\qquad \lambda\in\bar{\mathbb{Q}},\qquad y_i \text{ analytic } \textbf{on D}.$$

"Canonical" basis: $\left[z^{\nu}\frac{\log^k z}{k!}\right]^{\vee}$, ν root of mult. $> k$ of indicial polynomial

✓ $y(z)\sim z^{-3/2}\log z$ ✓ $y(z)\sim z^{i\sqrt{2}}$ ✗ $y(z)\sim e^{\pm 1/z}$

Initial Conditions at Regular Singular Points

$\mathcal{L} = z\,D_z^2 + D_z + z \quad (J_0, Y_0)$



Initial Conditions at Regular Singular Points

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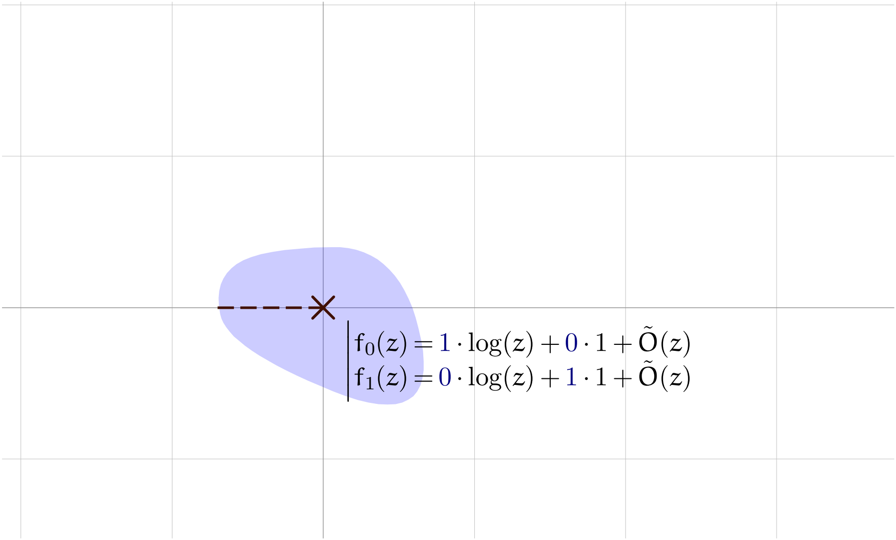

$$\begin{aligned} \mathrm{f}_0(z) &= 1 \cdot \log(z) + 0 \cdot 1 + \tilde{\mathrm{O}}(z) \\ \mathrm{f}_1(z) &= 0 \cdot \log(z) + 1 \cdot 1 + \tilde{\mathrm{O}}(z) \end{aligned}$$

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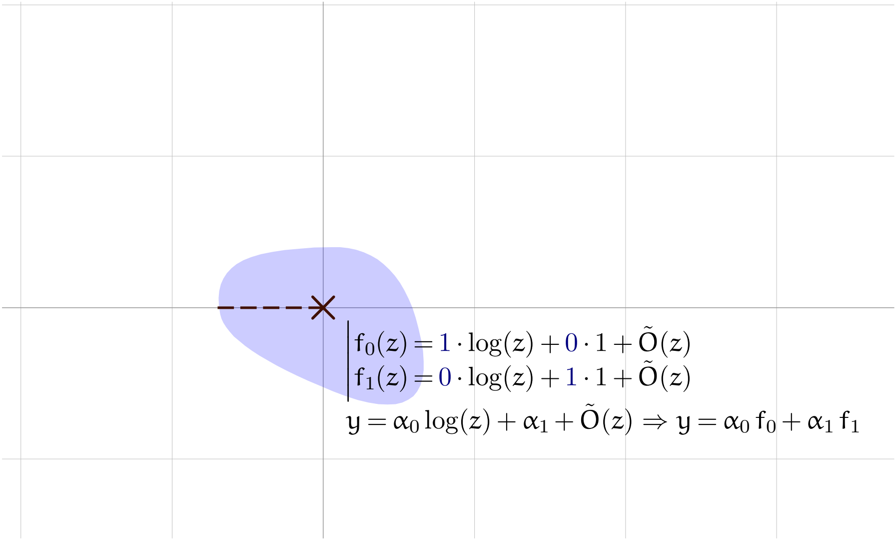

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$$y = \alpha_0 \log(z) + \alpha_1 + \tilde{O}(z) \Rightarrow y = \alpha_0\, f_0 + \alpha_1\, f_1$$

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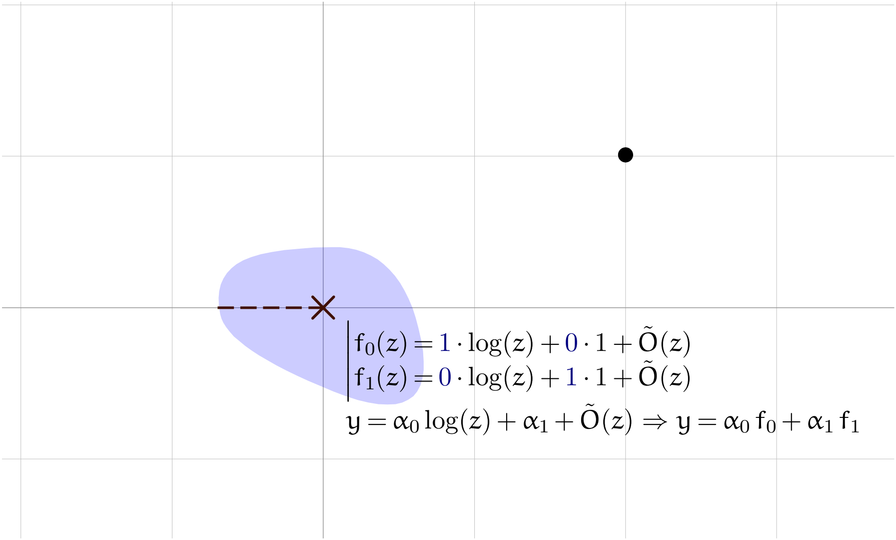

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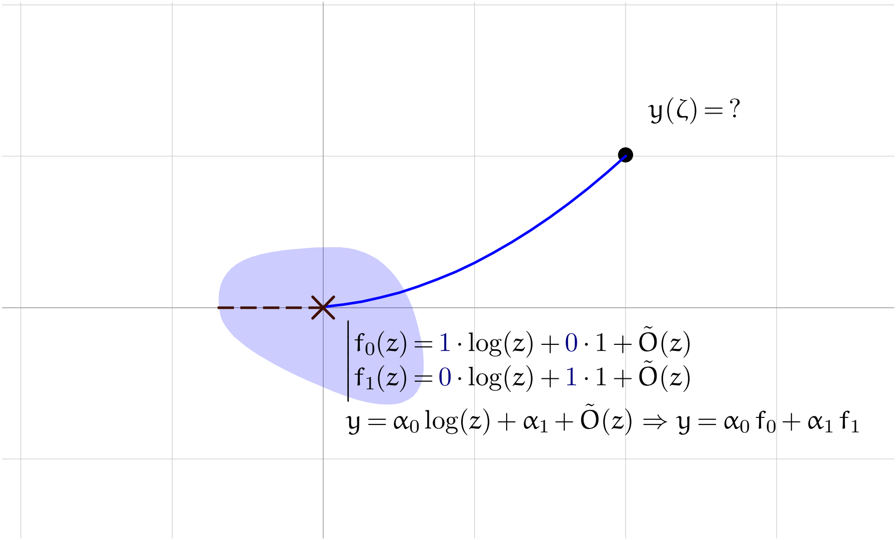
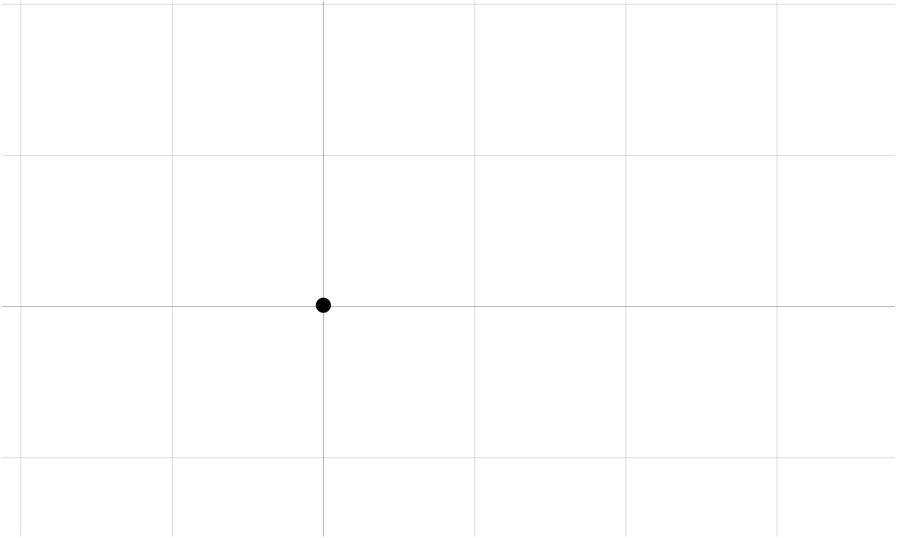


Transition Matrices



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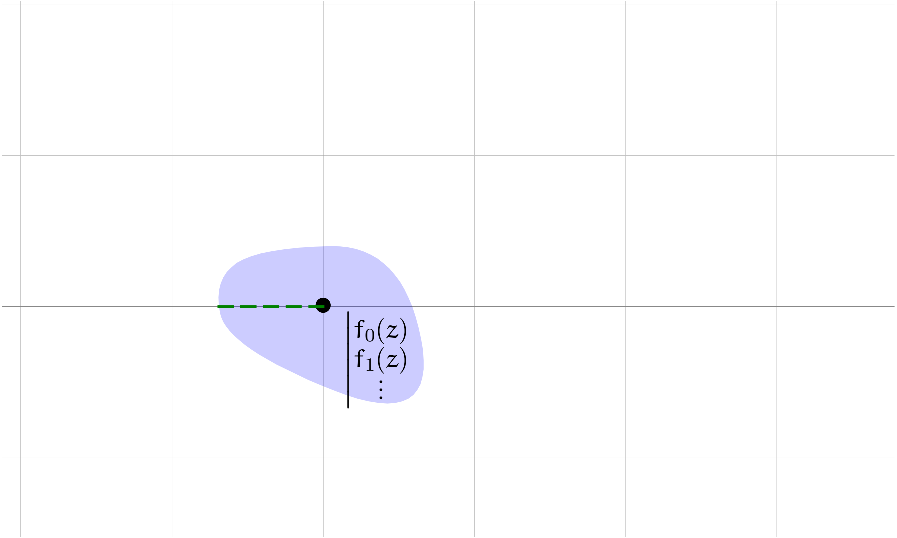

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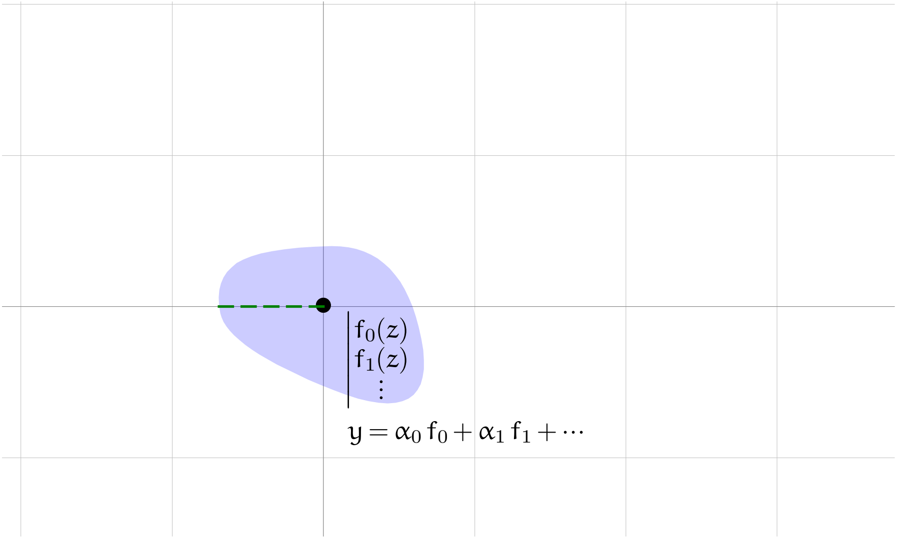

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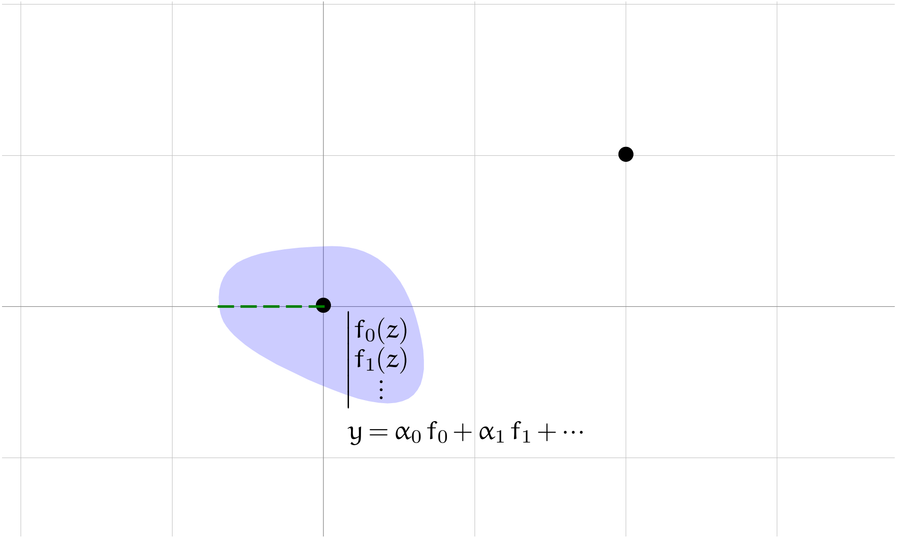

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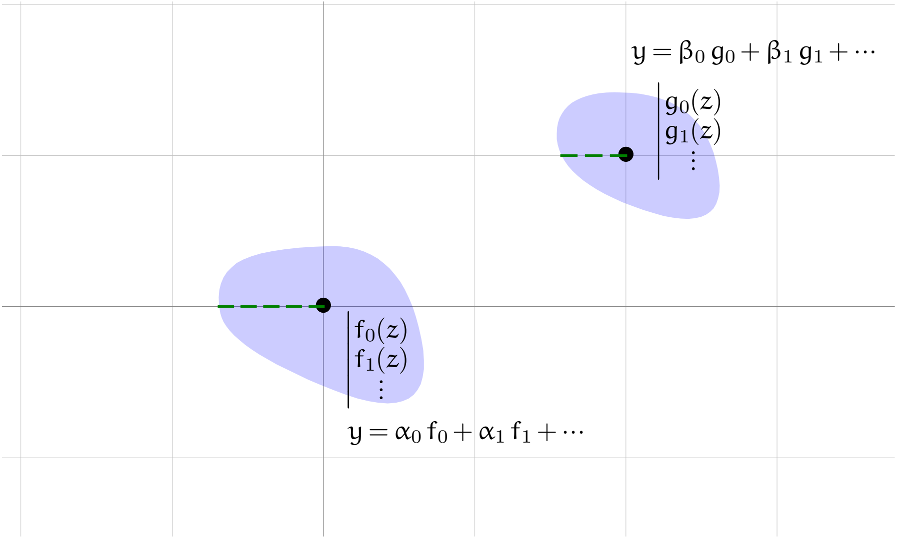

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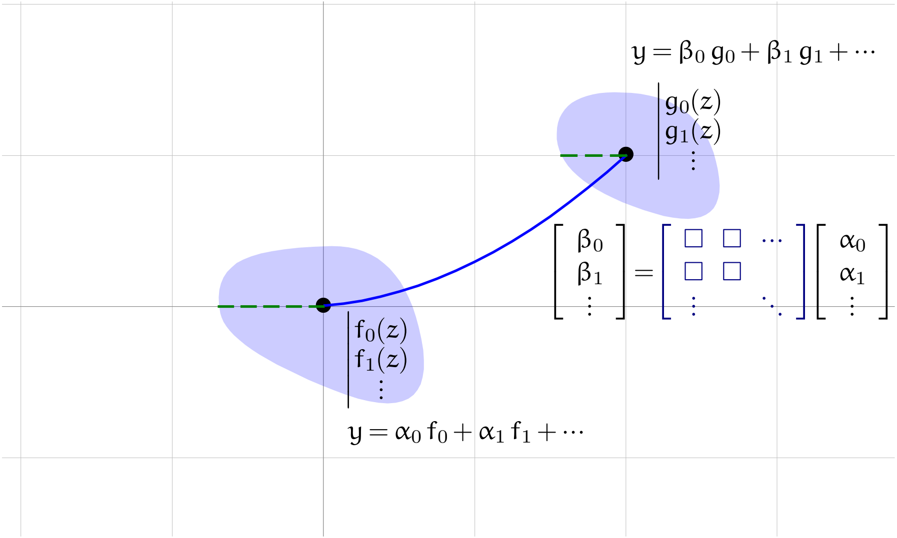
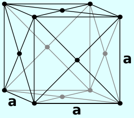


“Large” Computations

Face-centered cubic lattice in dimension 11

[Hassani, Koutschan, Maillard, Zenine 2016]

order	**22**	int. size	**~1 900** bits	singular	**both**
degree	**300**	accuracy	**~340** bits	time	**8 hours**



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$\mathcal{L} = \mathbf{D}_x\, x\,(x-1)\,(x-\varepsilon)\,\mathbf{D}_x + x$

After A. Bostan, based on an idea of M. Kontsevich, via D. van Straten

order	**2**	int. size	**~19 000** bits	singular	**both**
degree	**3**	accuracy	**~2.3 M** bits	time	**a few days**

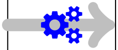
Timings on a single core.

Many optimization opportunities remaining!

Code Generation for Special Functions

[Lauter-M.]

$$x^2\,Y_1'' + x\,Y_1' + (x^2 - 1)\,Y_1 = 0$$
$$Y_1(x) \sim -\frac{2}{\pi x} + \frac{x \ln x}{\pi} + \cdots$$
as $x \to 0$



```
double BesselY1 (double x) {
    // generated code
}
```

Specification:

$$\left|\frac{\mathtt{implem}(x) - f(x)}{f(x)}\right| \leqslant \varepsilon \text{ for all } x \in [a, b] \cap \mathtt{double}$$

Working prototype (“Sagenstein”, 2017)

https://scm.gforge.inria.fr/anonscm/git/metalibm/sagenstein.git

Project stalled due to lack of time : - (

Summary

Numerical solution of linear ODEs with polynomial coefficients

- full support for regular singular points (incl. algebraic, resonant…)
- arbitrary precision
- rigorous error bounds

Code available at

`https://github.com/mkauers/ore_algebra/`

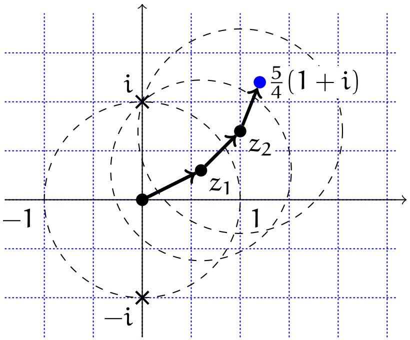
Perspectives

Features: irregular singular connection, automatic singularity analysis, D-finite functions as objects…

Speed: automatic path optimization, better handling of apparent singularities, some lower-level code…

Bug reports, feature requests, examples welcome!

A Taylor Series Method



$$\arctan\left(\frac{5}{4}(1+i)\right)?$$

$$\begin{bmatrix} y(z_1) \\ y'(z_1) \end{bmatrix} = \begin{bmatrix} 1 & 0.57\ldots+0.22\ldots \\ 0 & 0.72\ldots-0.20\ldots \end{bmatrix} \begin{bmatrix} y(0) \\ y'(0) \end{bmatrix}$$

$$\begin{bmatrix} y(z_2) \\ y'(z_2) \end{bmatrix} = \begin{bmatrix} 1 & 0.39\ldots+0.24\ldots \\ 0 & 0.57\ldots-0.29\ldots \end{bmatrix} \begin{bmatrix} y(z_1) \\ y'(z_1) \end{bmatrix}$$

...

- Locally, the solutions are given by **convergent power series**
- **Sum the series** numerically to get "initial values" at a new point

- Large steps ($\propto$ radius of convergence)
- Extends to the regular singular case

Recurrences

The **Taylor coefficients** of a D-finite function $y(z) = \sum_{n=0}^{\infty} y_n z^n$

obey a linear **recurrence relation** with polynomial coefficients:

$$b_s(n)\, y_{n+s} + \cdots + b_1(n)\, y_{n+1} + b_0(n)\, y_n = 0.$$

(And conversely, for D-finite formal power series.)

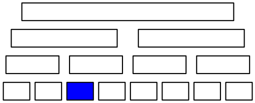
- Easy to generate
- Also leads to **fast algorithms**

[Schroeppel 1972; Brent 1976; Chudnovsky & Chudnovsky 1988; van der Hoeven 1999, 2001; M. 2010, 2012; Johansson 2014]

Best complexity:

time $\mathbf{O}(\mathbf{M}(n \log^2 n))$, space $\mathbf{O}(n)$

for fixed z and $\varepsilon = 2^{-n}$



Recurrences

The **coefficients** of a D-finite function $\sum_{\nu \in \lambda + \mathbb{Z}} \sum_{k=0}^{K} y_{\nu,k} \, z^{\nu} \frac{\log(z)^k}{k!}$
obey a linear **recurrence relation** with polynomial coefficients:

$$[b_s(\nu + S_k) \cdot S_\nu^s + \cdots + b_1(\nu + S_k) \, S_\nu + b_0(\nu + S_k)] \cdot (y_{\nu,k}) = 0.$$

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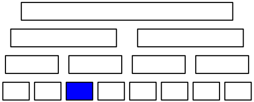

Error Bounds

Round-off errors

Real & complex arithmetic based on **Arb** [Johansson 2012–]

(`{Real,Complex}BallField` in Sage)

- More generally: takes care of error propagation
- Arb supports truncated power series (cf. autodiff)
- Manual error analysis still useful when intervals blow up

Truncation Errors

$$\sum_{n=0}^{\infty} u_n z^n = \underbrace{\sum_{n=0}^{N-1} u_n z^n}_{\text{known}} + \underbrace{\sum_{n=N}^{\infty} u_n z^n}_{|\cdot| \leqslant ?}$$

- Majorant series
- "Adaptive" bounds using residuals [M. 2019]

Asymptotics of Apéry Numbers

$$a_n = \sum_{k=0}^{n} \binom{n}{k}^2 \binom{n+k}{k}^2 \qquad b_n = \sum_{k=1}^{n} \left(\frac{a_n}{k^3} - \sum_{m=1}^{k} \frac{(-1)^m \binom{n}{k}^2 \binom{n+k}{k}^2}{2\, m^3 \binom{n}{m} \binom{n+m}{m}} \right)$$

(1, 5, 73, 1445, 33001...) (0, 6, 351/4, 62531/36, ...)

- The OGS $a(z)$ and $b(z)$ are solutions of $L = \boldsymbol{z}^2\, (\boldsymbol{z}^2 - 34\, \boldsymbol{z} + 1)\, D_x^4 + \cdots$
- Singular points: $0, \quad \boldsymbol{\alpha} = (\sqrt{2}+1)^4 \approx 33.9, \quad \boldsymbol{\alpha}^{-1} = (\sqrt{2}-1)^4 \approx 0.0294$
- Prove: $a_n, b_n = \alpha^{n+o(n)} \qquad b_n - \zeta(3)\, a_n = \alpha^{-n+o(n)}$
- Local expansion at $\boldsymbol{\alpha}^{-1}$: $a(z) = c_0\, f_0(z) + \mathbf{c}_1\, f_1(z) + c_2\, f_2(z) + c_3\, f_3(z)$

  where
  $f_0(\alpha^{-1}+t) = 1 + O(t^3) \qquad f_3(\alpha^{-1}+t) = t + O(t^3)$
  $f_1(\alpha^{-1}+t) = \sqrt{\mathbf{t}} + O(t^3) \qquad f_4(\alpha^{-1}+t) = t^2 + O(t^3)$
- Singularity analysis: $(c_1 \neq 0)$

$$a(z) \sim \mathbf{c}_1 \sqrt{z - \alpha^{-1}} \qquad \Rightarrow \qquad a_n \sim \mathbf{c}_1\, [z^n] \sqrt{z - \alpha^{-1}} \sim \frac{\mathbf{c}_1\, i}{2\sqrt{\alpha \pi}}\, \alpha^n\, n^{-3/2}$$

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