Rigorous Numerics for Differentially Finite Functions

Marc Mezzarobba
CNRS, Sorbonne Université

Computing with D-Modules II, Leipzig
September 3, 2019

Try the implementation!

With Sage: `http://marc.mezzarobba.net/leipzig2019.ipynb`
Online: `http://marc.mezzarobba.net/oaademo`

Introduction

ODE Solving from a Computer Algebra Perspective

Problem

Starting from a linear differential equation

$$p_r(z)\, y^{(r)}(z) + \cdots + p_1(z)\, y'(z) + p_0(z)\, y(z) = 0$$

with polynomial coefficients $p_0, \ldots, p_r$ and initial values,
compute the solution at a given point.

I.e.: Evaluate a (univariate) holonomic function.

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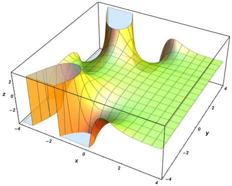
I.e.: Evaluate a (univariate) holonomic function.

Our requirements:

- Complex variables: $z \in \mathbb{C}$
- Arbitrary precision
- Rigorous error bounds (↝ use in algebraic algorithms, in proofs)
- **Singular cases**

Applications

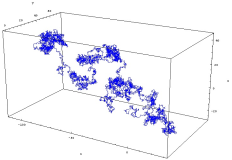
- **Special functions**



- **Combinatorics**

  via **generating functions** and **singularity analysis**

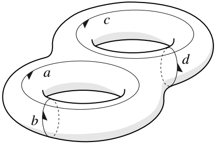
  random walks on lattices,
  asymptotics of P-recursive sequences…



- **Numerical (Real) Algebraic Geometry**

  via **Picard-Fuchs equations**

  periods of surfaces [Sertöz 2019, …],
  volumes of semi-algebraic sets [Lairez, M., Safey 2019]…



- **"Numerical differential Galois theory"**

  via **connection / monodromy / Stokes matrices**

  operator factoring, heuristic diff. Galois groups
  [van der Hoeven 2007, …]

$$\mathfrak{g} = \mathcal{L}(\hat{\mathfrak{B}}(\hat{\mathfrak{g}}))$$

Applications

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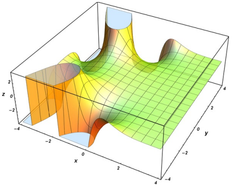
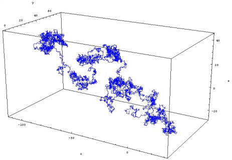
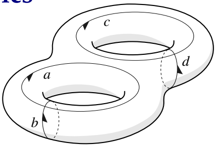
Math. physics





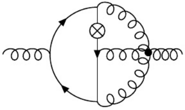


$$\mathfrak{g} = \mathcal{L}(\hat{\mathcal{B}}(\hat{\mathfrak{g}}))$$

Iterated Integrals

arising from Feynman diagram calculations

[Ablinger, Blümlein, Raab, Schneider, 2014]



$$\int_0^1 \frac{x_5\,dx_5}{x_5-1} \int_{x_5}^1 \frac{dx_4}{x_4\sqrt{x_4-\frac{1}{4}}} \int_{x_4}^1 \frac{dx_3}{x_3\sqrt{x_3-\frac{1}{4}}} \int_{x_3}^1 \frac{dx_2}{1-x_2} \int_{x_2}^1 \frac{dx_1}{1-x_1} = ?$$

(with suitable branch choices)

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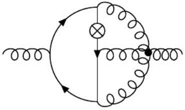

$$I(x) = \int_x^1 \frac{x_5\, dx_5}{x_5 - 1} \int_{x_5}^1 \frac{dx_4}{x_4 \sqrt{x_4 - \frac{1}{4}}} \int_{x_4}^1 \frac{dx_3}{x_3 \sqrt{x_3 - \frac{1}{4}}} \int_{x_3}^1 \frac{dx_2}{1 - x_2} \int_{x_2}^1 \frac{dx_1}{1 - x_1} = ?$$

(with suitable branch choices)

$$\begin{aligned}
&(4x^9 - 13x^8 + 15x^7 - 7x^6 + x^5)\, I^{(6)}(x) \\
+\,&(54x^8 - 140x^7 + 120x^6 - 36x^5 + 2x^4)\, I^{(5)}(x) \\
+\,&(202x^7 - 397x^6 + 228x^5 - 34x^4 + x^3)\, I^{(4)}(x) \\
+\,&(222x^6 - 303x^5 + 90x^4 + 3x^3 - 3x^2)\, I^{(3)}(x) \\
+\,&(48x^5 - 37x^4 + x^3 - 6x^2 + 6x)\, I''(x) \\
+\,&(-x^2 + 6x - 6)\, I'(x) = 0
\end{aligned}$$

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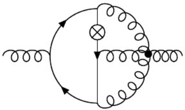

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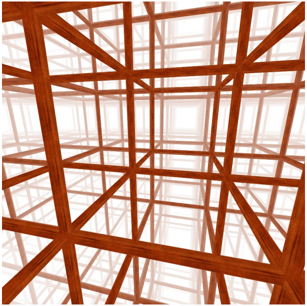
```
sage: iint_value(dop, myini, 1e-500)
[0.9708046956249312405 ... 59027603834204946 +/- 9.05e-501]
```

Pólya Walks



For a random walk on $\mathbb{Z}^d$ ($d \geqslant 3$) starting at 0:

$$\text{return probability} = 1 - \frac{1}{w(1/2d)}$$

where

$$w(z) = \sum_{n=0}^{\infty} w_n z^n$$

#walks of length n
ending at origin

satisfies an LODE with polynomial coefficients

Examples:

$d=3$ $\quad z^2(4z^2-1)(36z^2-1)D^3 + (1296z^5 - 240z^3 + 3z)D^2$
$\quad + (2592z^4 - 288z^2 + 1)D + 864z^3 - 48z$

$d=4$ $\quad (1024z^7 - 80z^5 + z^3)D^4 + (14336z^6 - 800z^4 + 6z^2)D^3$
$\quad + (55296z^5 - 2048z^3 + 7z)D^2 + (61440z^4 - 1344z^2 + 1)D$
$\quad + 12288z^3 - 128z$

...

(thanks to B. Salvy)

First return after n steps:

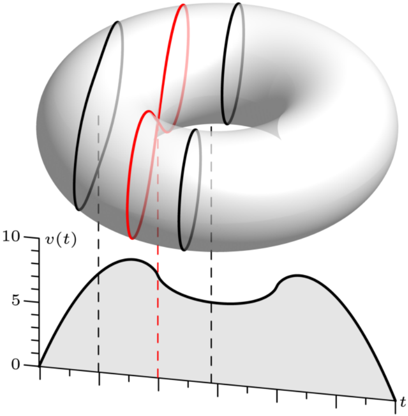
$$f(z) = \sum_{n=0}^{\infty} f_n z^n$$

$$f\left(\frac{1}{2d}\right) = \sum_{n=0}^{\infty} \frac{f_n}{(2d)^n}$$

$$w(z) = 1 + f(z)\,w(z)$$

Volumes of Compact Semi-Algebraic Sets

[Lairez, M., Safey El Din, 2019]



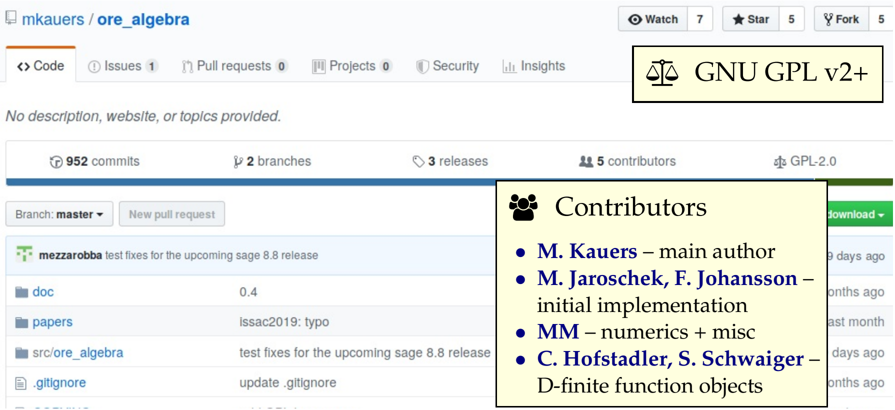
- The **"slice volume"** function satisfies a Picard-Fuchs eqn
- Except at critical values of the projection, it is analytic

➙ Compute initial values by recursive calls, integrate the equation

Cost for p digits $= \tilde{O}(p)$

Implementation

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

Ore polynomials are **skew polynomials**
that can be used to model linear functional operators.

Examples

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

  $$\big[z\,f(z)\big]' = z\,f'(z) + f(z)$$

- $K(n)\langle S\rangle = \{$skew polynomials in S over $K(n)$ subject to $S\,n = (n+1)\,S\}$
  $\cong \{$**recurrence operators**$\}$

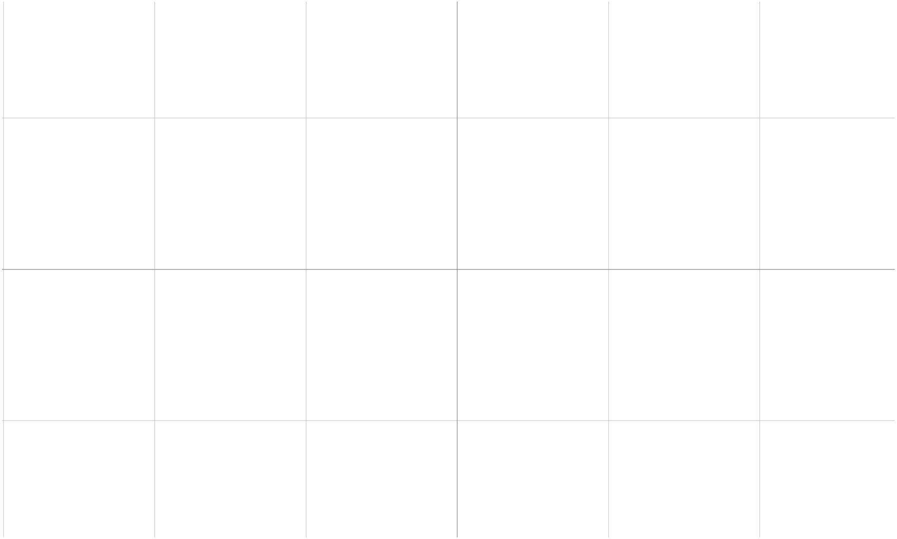
  $$\big[n\,u(n)\big]_{k+1} = [(n+1)\,u(n+1)]_k$$

Features

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

Analytic Continuation

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



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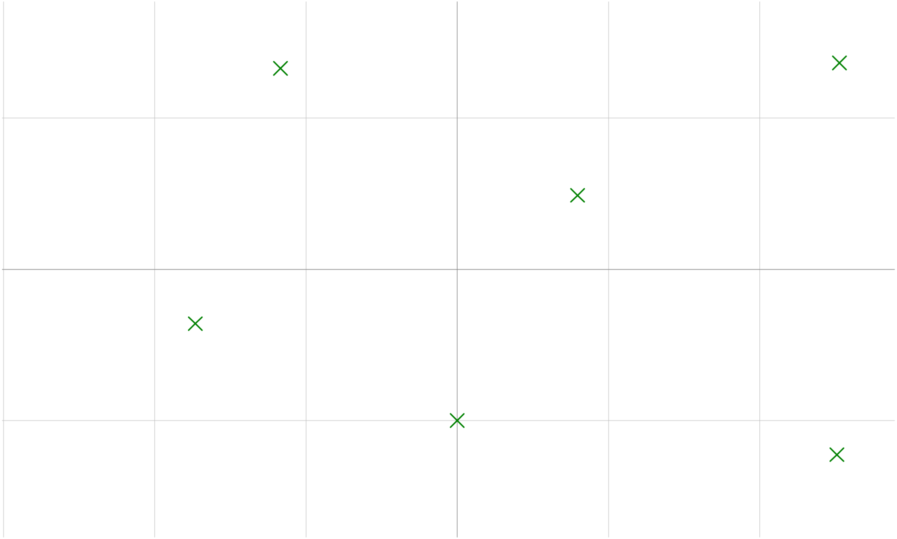

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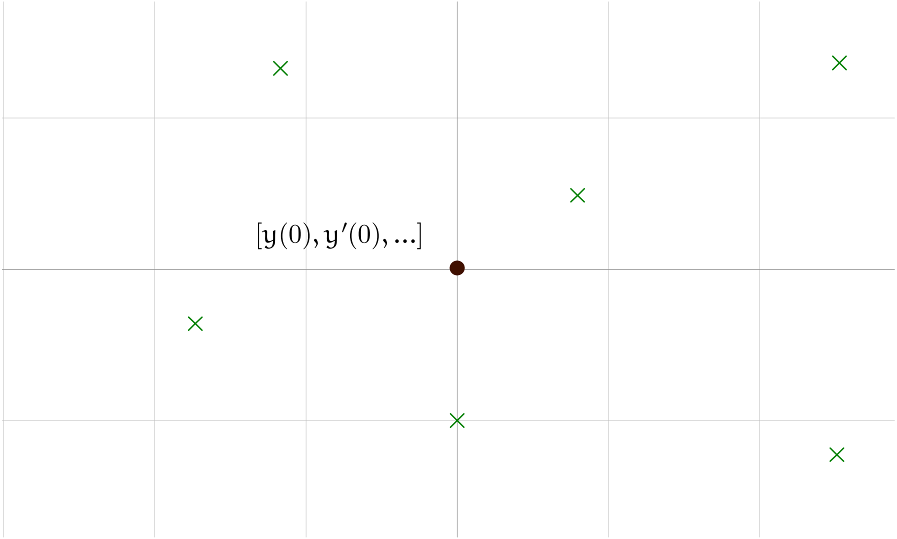

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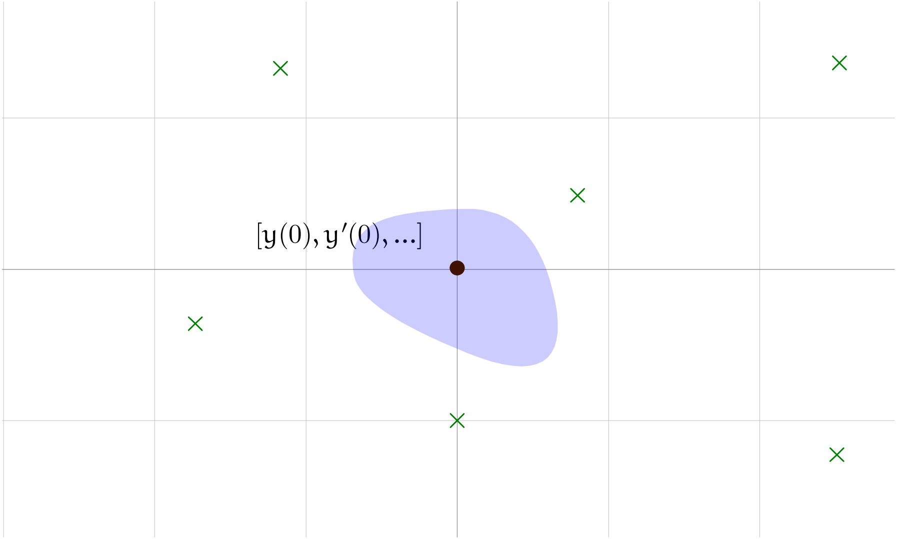

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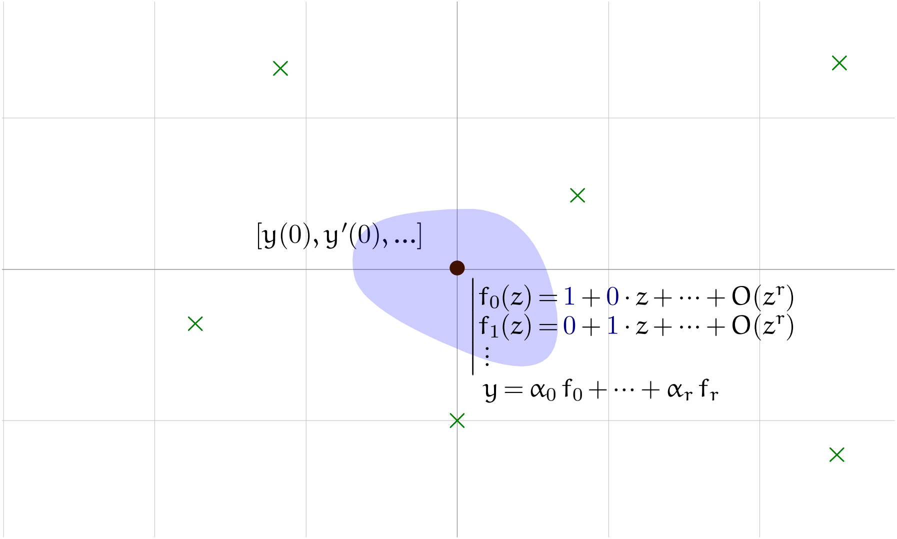

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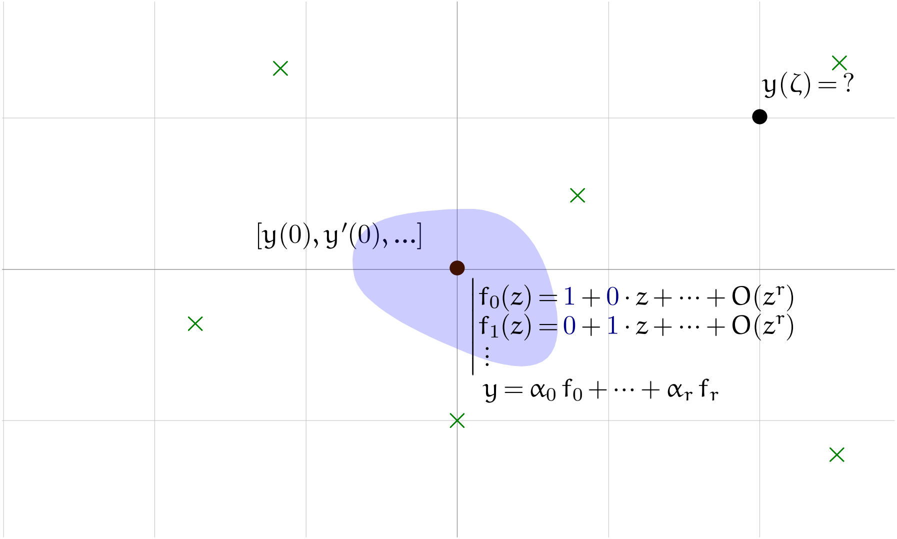

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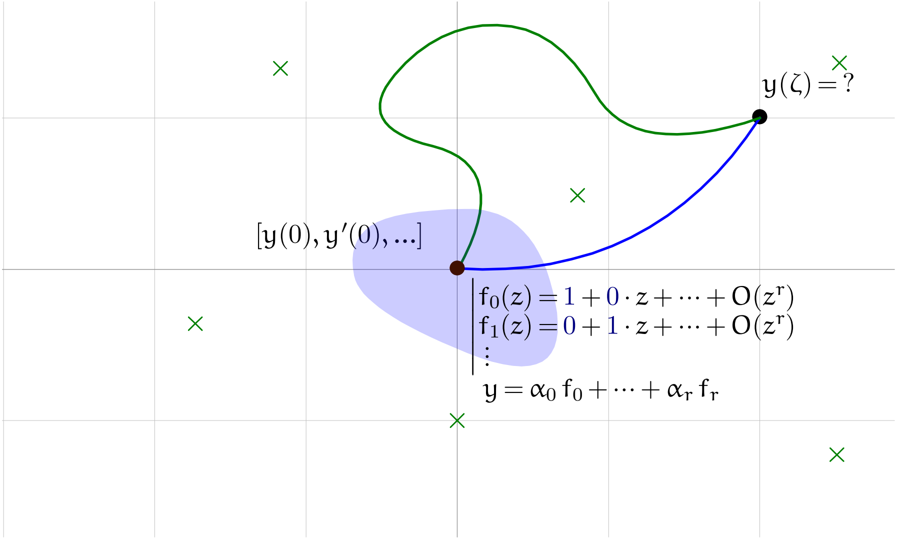
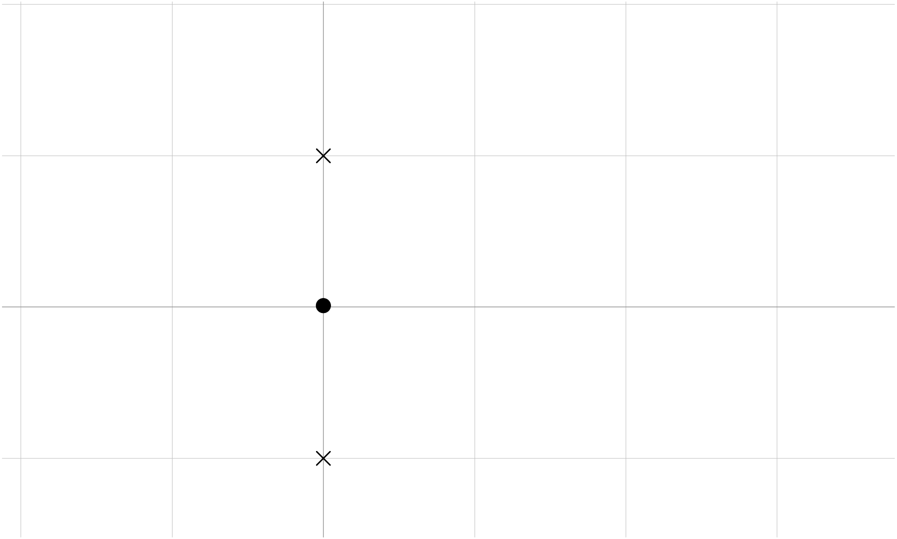


Transition Matrices

$$(z^2+1)\,y''(z)+2\,z\,y'(z)=0$$



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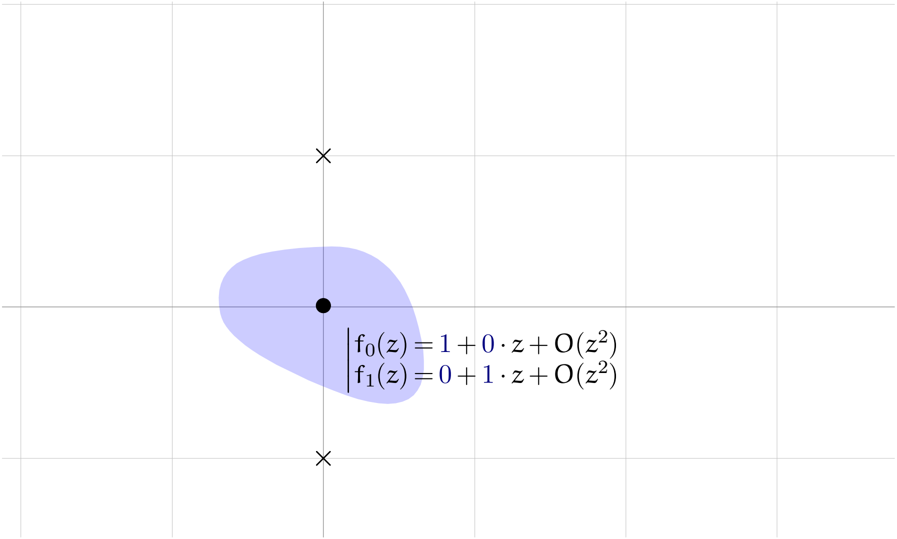

$$\left|\begin{array}{l} f_0(z)=1+0\cdot z+O(z^2) \\ f_1(z)=0+1\cdot z+O(z^2) \end{array}\right.$$

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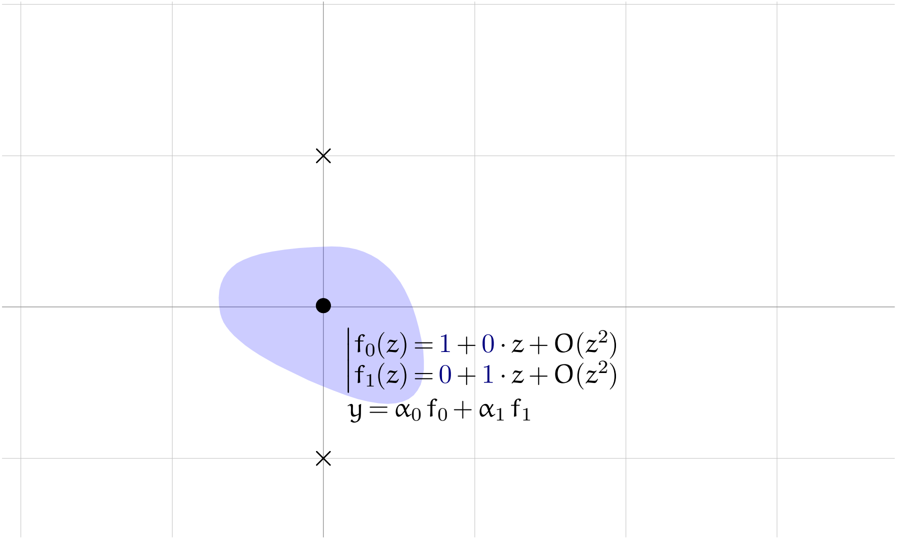

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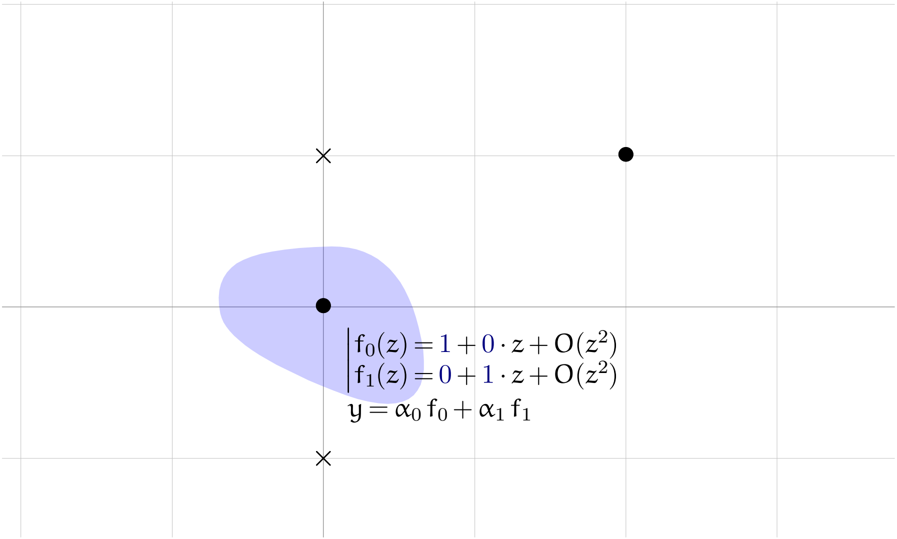

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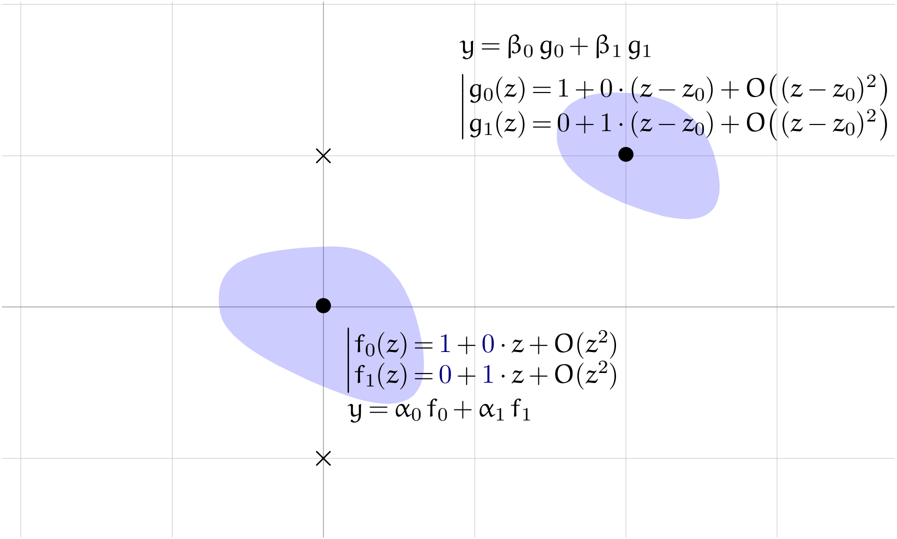

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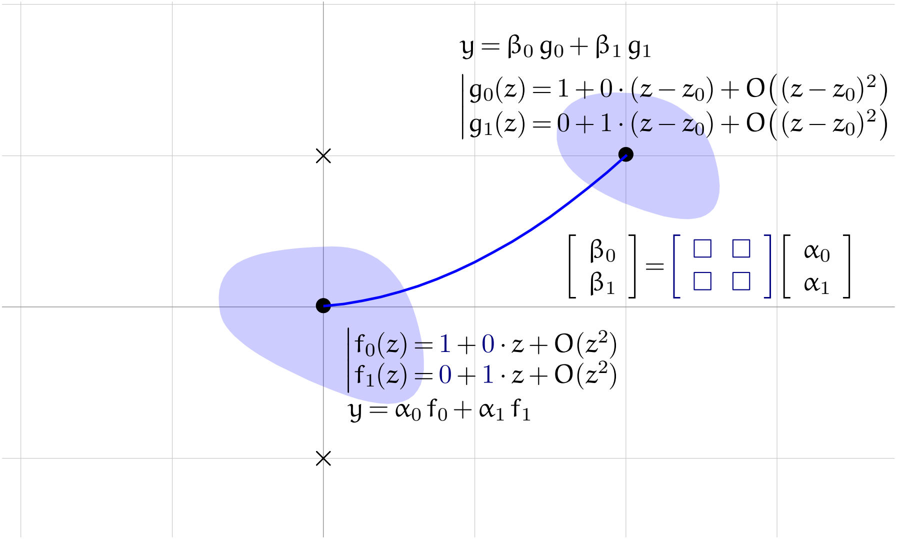

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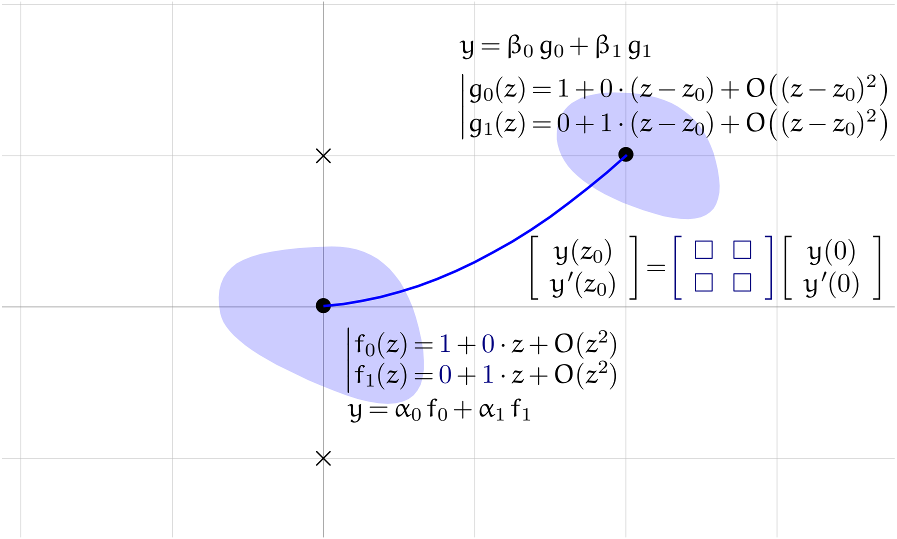

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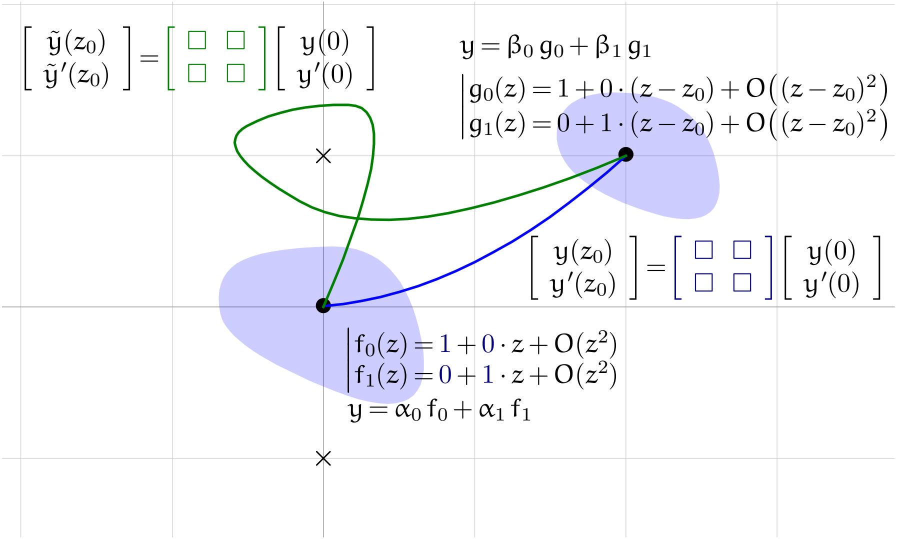

$$\begin{bmatrix} \tilde{y}(z_0) \\ \tilde{y}'(z_0) \end{bmatrix} = \begin{bmatrix} \square & \square \\ \square & \square \end{bmatrix} \begin{bmatrix} y(0) \\ y'(0) \end{bmatrix}$$

$$y = \beta_0\, g_0 + \beta_1\, g_1$$

$$\left| \begin{array}{l} g_0(z) = 1 + 0 \cdot (z - z_0) + O\big((z-z_0)^2\big) \\ g_1(z) = 0 + 1 \cdot (z - z_0) + O\big((z-z_0)^2\big) \end{array} \right.$$

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$$y = \alpha_0\, f_0 + \alpha_1\, f_1$$

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 $D \backslash \mathbb{R}_{\leqslant 0}$ of the form

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

Thus $y(z)=\sum_{\nu\in\Lambda}\sum_{k=0}^{t} \boldsymbol{y_{\nu,k}}\, z^{\nu}\frac{\log^k z}{k!}$ where $\Lambda=(\lambda_1+\mathbb{N})\cup\cdots\cup(\lambda_\ell+\mathbb{N})\subset\mathbb{C}$

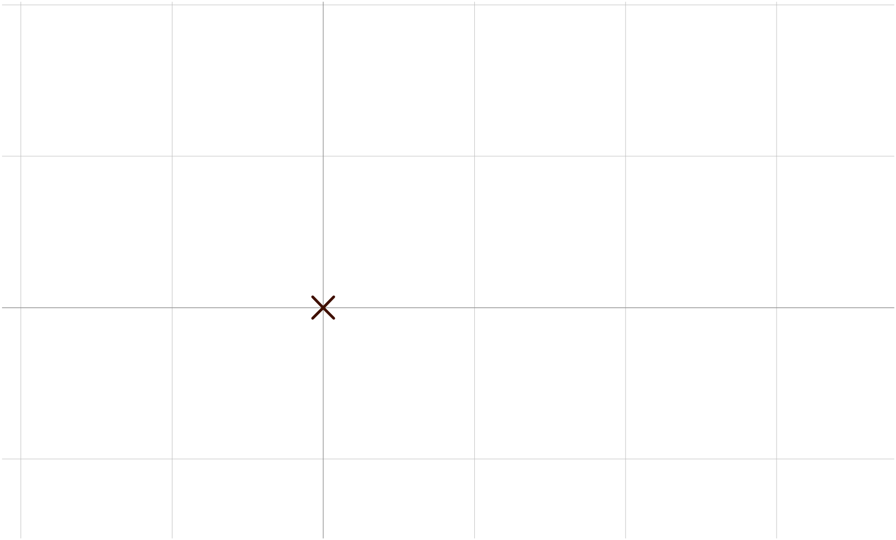
"Canonical" basis: $\left[z^{\nu}\frac{\log^k z}{k!}\right]^{\vee}$, ν root of mult. $>k$ of indicial polynomial

(compare $[z^n]^{\vee}$, $0\leqslant n<r$, at ordinary points)

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

Initial Conditions at Regular Singular Points

$\mathcal{L} = z\,\mathrm{D}_z^2 + \mathrm{D}_z + z \quad (\mathrm{J}_0, \mathrm{Y}_0)$



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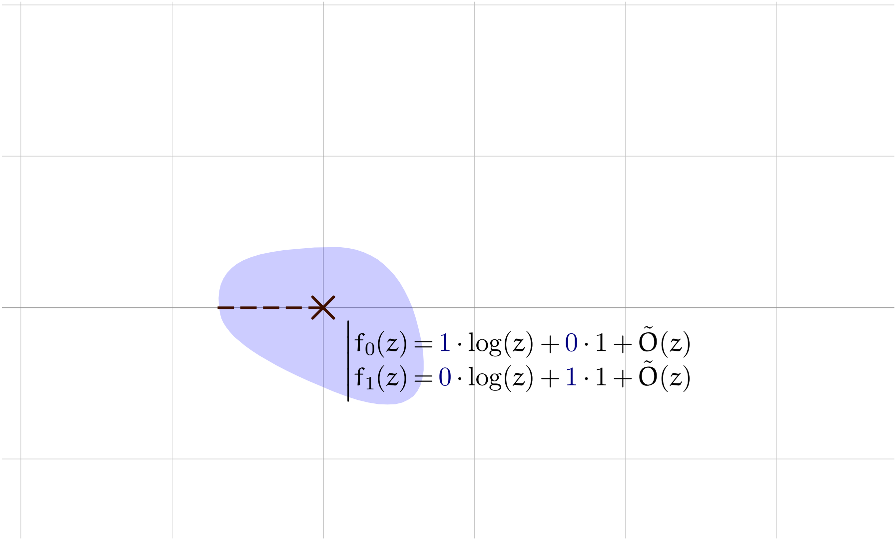

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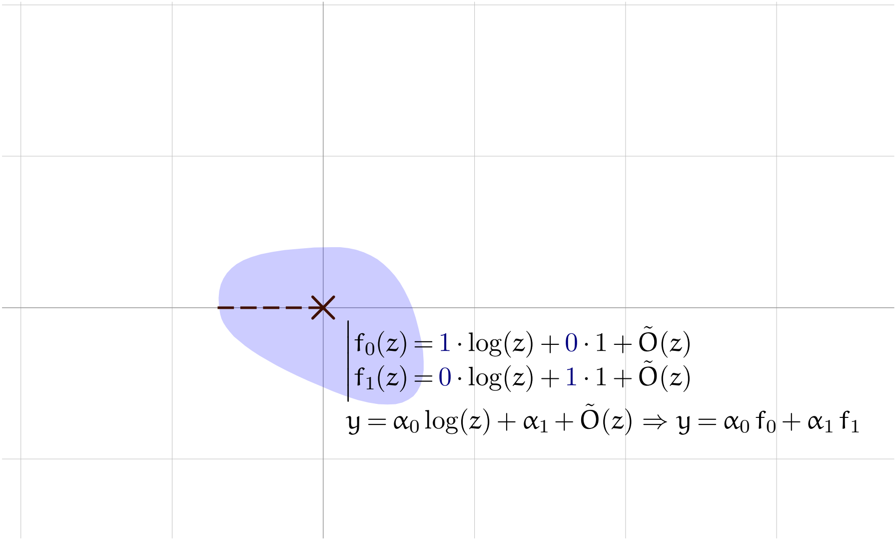

$$\left|\begin{array}{l} f_0(z) = 1 \cdot \log(z) + 0 \cdot 1 + \tilde{O}(z) \\ f_1(z) = 0 \cdot \log(z) + 1 \cdot 1 + \tilde{O}(z) \end{array}\right.$$

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

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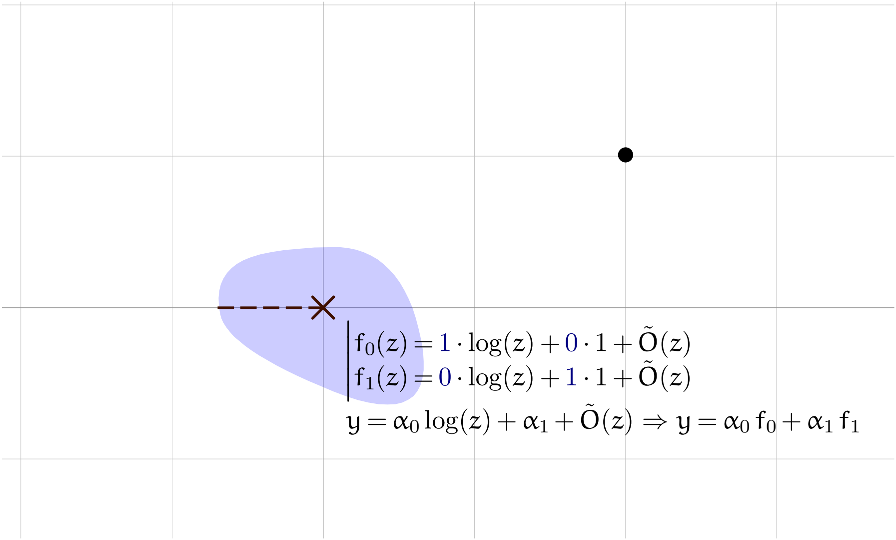

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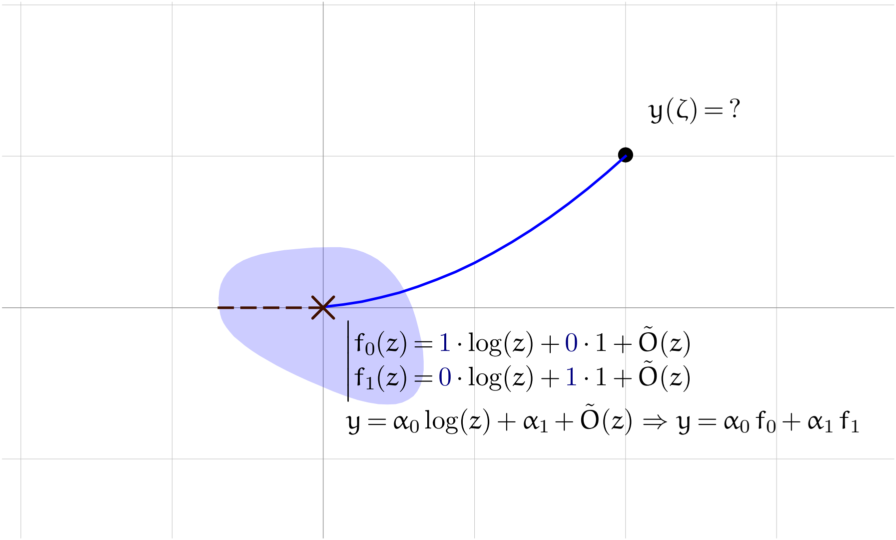
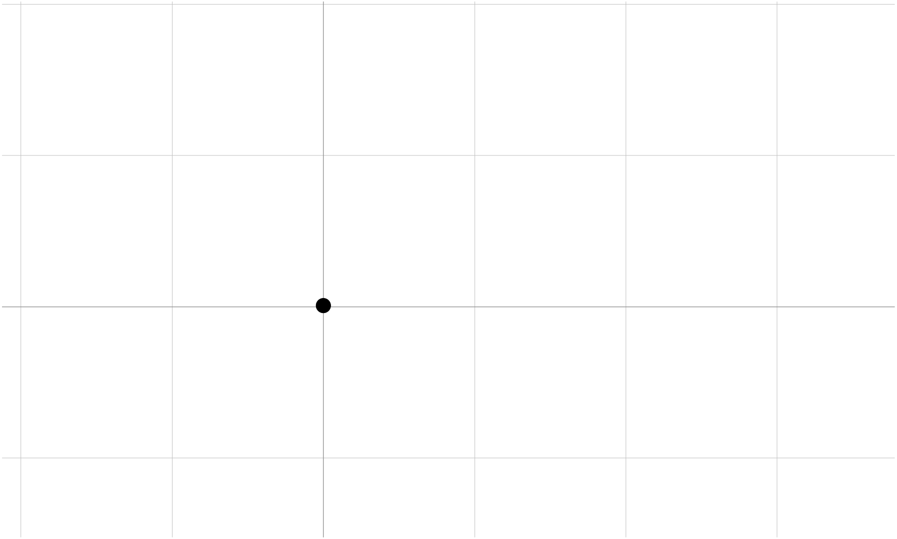


Regular Singular Transition Matrices



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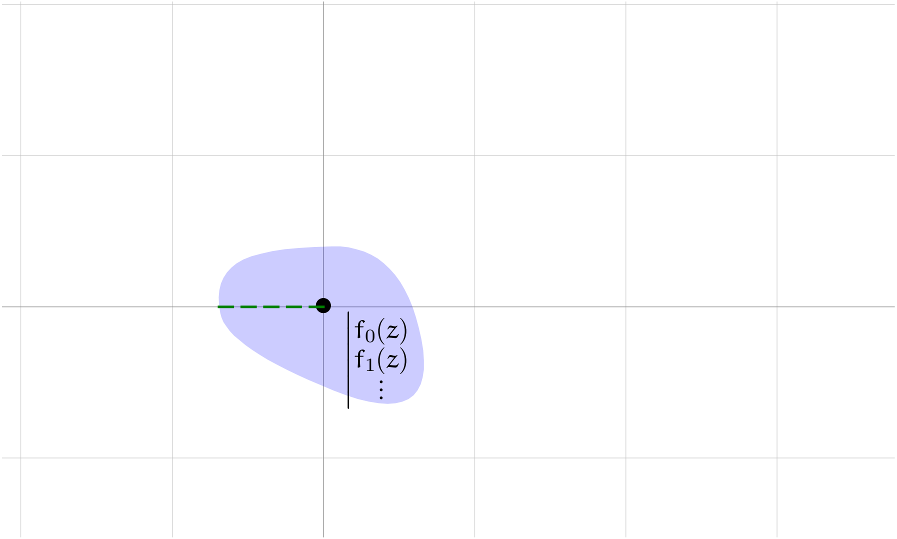

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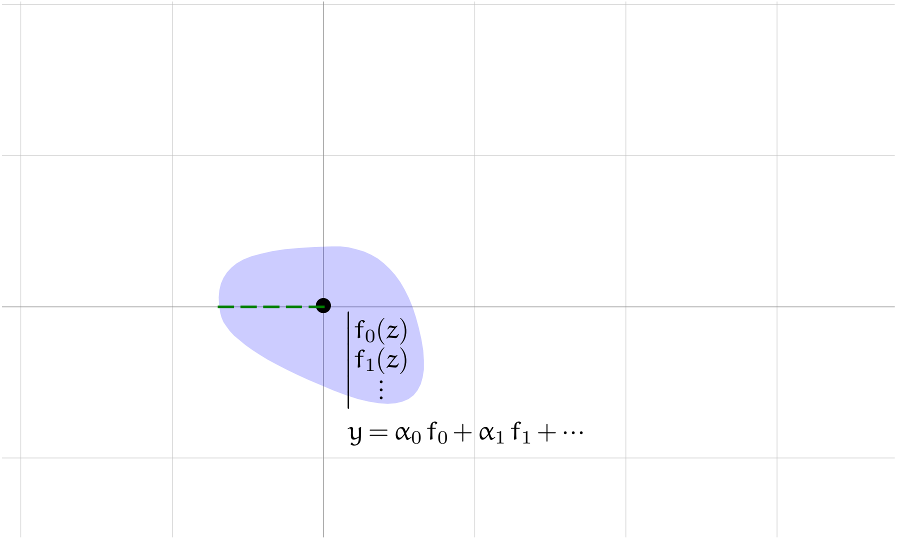
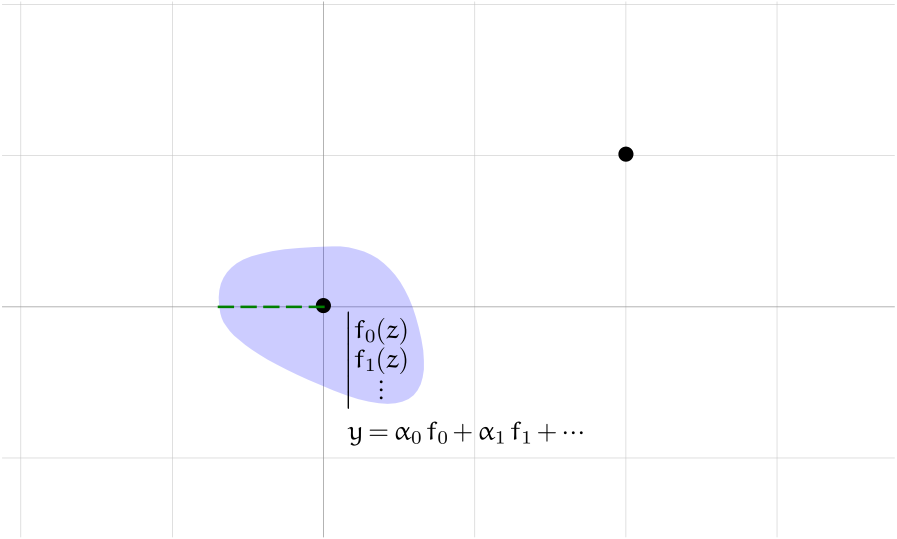
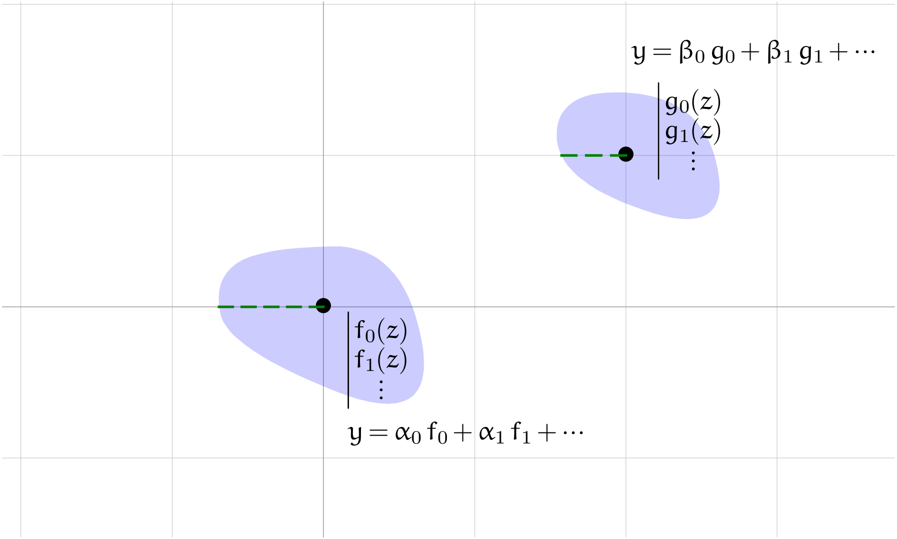


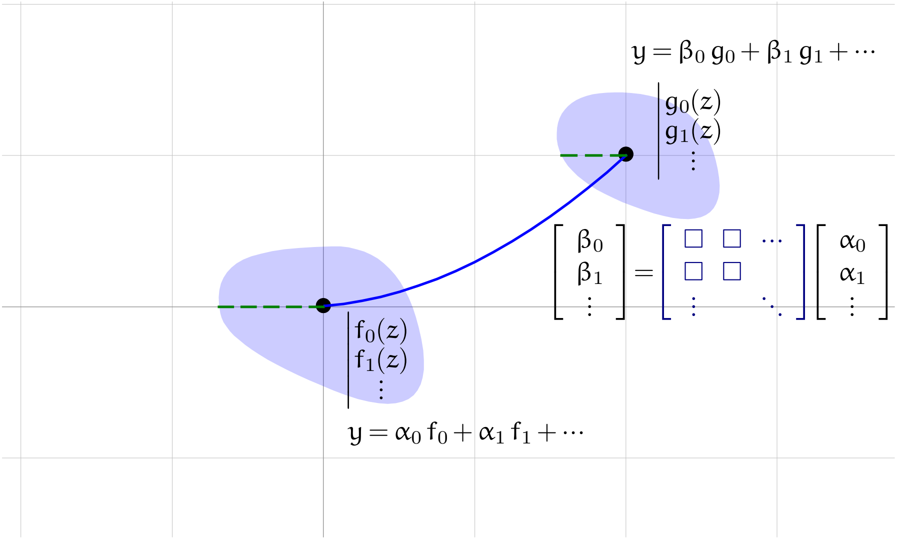
Regular Singular Transition Matrices



Regular Singular Transition Matrices

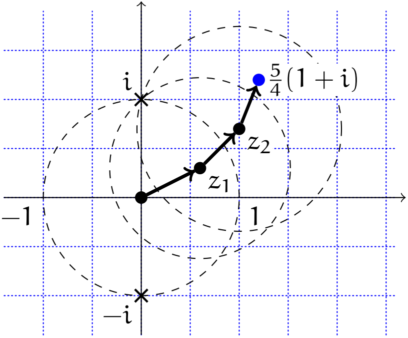


Regular Singular Transition Matrices



Algorithms

A Taylor Series Method



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

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

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

$\ldots$

- Locally, the solutions are given by **convergent power series** (Cauchy)
- **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.)

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Proof.

$$\begin{aligned}
y &= \sum_{n=-\infty}^{\infty} y_n z^n & &\leftrightarrow & Y &= (y_n)_{n\in\mathbb{Z}}\\
\mathbf{D}\cdot y &= \sum_{n=-\infty}^{\infty} (n+1)\, y_{n+1} z^n & &\leftrightarrow & &(\mathbf{S}\,\mathbf{n})\cdot Y\\
\mathbf{z}\cdot y &= \sum_{n=-\infty}^{\infty} y_{n-1} z^n & &\leftrightarrow & &\mathbf{S}^{-1}\cdot Y
\end{aligned}$$

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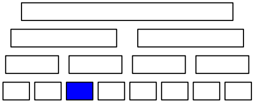
(And conversely, for D-finite formal power series.)

- Easy to generate
- Leads to **fast algorithms**

  Best **boolean** complexity:

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

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



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

Recurrences

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

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

- Easy to generate
- Leads to **fast algorithms**

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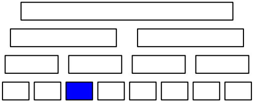


[Schroeppel 1972; Brent 1976; Chudnovsky & Chudnovsky 1988; van der Hoeven 1999, 2001; M. 2010, 2012]

Error Bounds

Rounding Errors

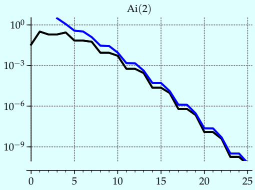
Real & complex arithmetic based on **Arb** [Johansson 2012–]

(`{Real,Complex}BallField` in Sage) [Heuberger, M. & others]

- More generally: takes care of error propagation
- Arb supports truncated power series (→ derivatives, reg. sing. points)
- 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]

Summary

Numerical solution of linear ODEs with polynomial coefficients

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

Based on: Taylor series, an. continuation, recurrences, ball arithmetic, majorants…

Code available at

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

Perspectives

- Irregular singular case
- Performance improvements (algorithms, code optimization)
- Convenience features (singularity analysis, monodromy…)

Bug reports, feature requests, examples welcome!

The Method of Majorants

[Cauchy 1842]

- Instead of directly bounding $|\sum_{n \geqslant N} u_n \, \zeta^n|$, compute a **majorant series**:

$$\sum \hat{u}_n \, z^n \in \mathbb{R}_{\geqslant 0}[[z]] \qquad \text{s.t.} \qquad \forall n, \quad |u_n| \leqslant \hat{u}_n$$

- To do that, "replace" L with a simple **model equation**:

$$L(z, {}^{d}\!/_{dz}) \cdot u = 0 \qquad \underset{\text{“bounded by”}}{\ll} \qquad \hat{u}'(z) - \hat{a}(z)\, \hat{u}(z) = 0$$

for us: always 1st order

- Solve the model equation and study the solutions:

$$\hat{u}(z) = \exp \int^z \hat{a}(w)\, dw \qquad \left| \sum_{n=N}^{+\infty} u_n \, z^n \right| \leqslant \sum_{n=N}^{+\infty} \hat{u}_n \, |z|^n \leqslant \cdots$$

Adaptive Bounds

Problem. Computing majorants in a (too) naive way leads to catastrophic overestimations

Idea. Take into account the last computed / first neglected terms of the series

Analogy. Residuals of linear systems

$$A\,x = b \qquad A \in \mathrm{GL}_n(\mathbb{C}), \quad \|A^{-1}\| \leqslant \boldsymbol{M}$$

residual (≈ 1st negl. term)

$$A\,\tilde{x} = \tilde{b} \qquad \|x - \tilde{x}\| \leqslant \boldsymbol{M} \cdot \underbrace{\|b - \tilde{b}\|}_{\text{known}}$$

computed approx.

Adaptive Majorants

$L(z, D_z) \cdot u = 0$

Residual: $q(z) := L(z, D_z) \cdot \tilde{u}$

$$u(z) = \sum_{n=0}^{\infty} u_n z^n = \underbrace{\sum_{n=0}^{N-1} u_n z^n}_{\tilde{u}(z)} + \sum_{n=N}^{\infty} u_n z^n$$

- **Model equation**

$$\begin{aligned} q(z) \quad &\lll \quad \hat{q}(z) \\ L(z, D_z) \cdot (\tilde{u} - u) = q \quad &\lll \quad \hat{L}(z, D_z) \cdot v = \hat{q} \end{aligned}$$

- **Majorant property:**

$$(\forall n \leqslant n_0) \quad |u_n| \leqslant v_n \qquad \Rightarrow \qquad (\forall n) \quad |u_n| \leqslant v_n$$

- **Solving the model equation**

$$v(z) = h(z) \left(\underset{\substack{\nearrow \\ \text{choose cst} = 0}}{\mathrm{cst}} + \int^z \underset{\substack{\nwarrow \\ = O(z^N)}}{\frac{t^{-1}\, \hat{q}(t)}{h(t)}}\, dt \right) \qquad \text{where } h(z) = \exp \int^z t^{-1}\, \hat{a}(t)\, dt$$

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