Regular Singularities
&
Rigorous Numerics

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Periods workgroup, May 19, 2021

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http://marc.mezzarobba.net/oaademo-periodswg

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.

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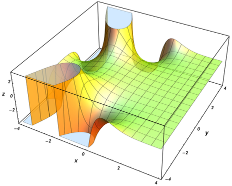
Special requirements:

- Complex variables: $z \in \mathbb{C}$
- Arbitrary precision
- Rigorous error bounds (➙ usable in computer proofs, in "exact" algorithms)
- **Singular cases**

Applications

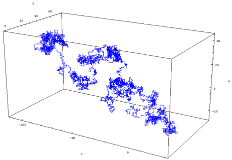
- **Special functions**



- **Combinatorics**

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

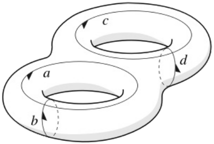
  random walks on lattices,
  asymptotics of P-recursive sequences…



- **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, …]

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

Applications

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- **Combinatorics**

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

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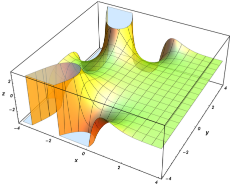
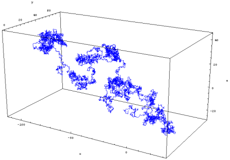
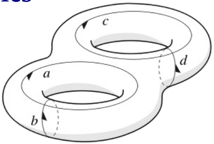
Math. physics

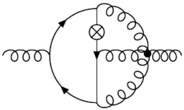






$$g = \mathcal{L}(\hat{\mathcal{B}}(\hat{g}))$$

Iterated Integrals



[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)

Iterated Integrals

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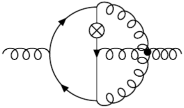

$$I(x) = \int_x^1 \frac{x_5\, dx_5}{x_5 - 1} \int_{x_5}^1 \frac{dx_4}{x_4\sqrt{x_4 - \frac{1}{4}}} \int_{x_4}^1 \frac{dx_3}{x_3\sqrt{x_3 - \frac{1}{4}}} \int_{x_3}^1 \frac{dx_2}{1 - x_2} \int_{x_2}^1 \frac{dx_1}{1 - x_1} = ?$$

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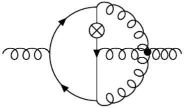
$$\begin{aligned}
&(4\,x^9 - 13\,x^8 + 15\,x^7 - 7\,x^6 + x^5)\, I^{(6)}(x) \\
+\,&(54\,x^8 - 140\,x^7 + 120\,x^6 - 36\,x^5 + 2\,x^4)\, I^{(5)}(x) \\
+\,&(202\,x^7 - 397\,x^6 + 228\,x^5 - 34\,x^4 + x^3)\, I^{(4)}(x) \\
+\,&(222\,x^6 - 303\,x^5 + 90\,x^4 + 3\,x^3 - 3\,x^2)\, I^{(3)}(x) \\
+\,&(48\,x^5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

Iterated Integrals

[Ablinger, Blümlein, Raab, Schneider, 2014]



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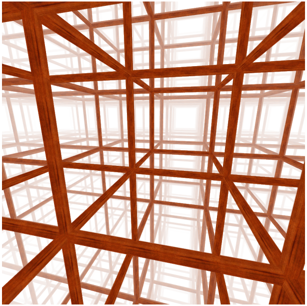
```
sage: iint_value(dop, myini, 1e-500)
[0.97080469562493124O5 ... 59027603834204946 +/- 9.05e-501]
```

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

#walks of length n ending at origin

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

satisfies an LODE with polynomial coefficients

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

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

[thanks to B. Salvy]

First return after n steps:

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

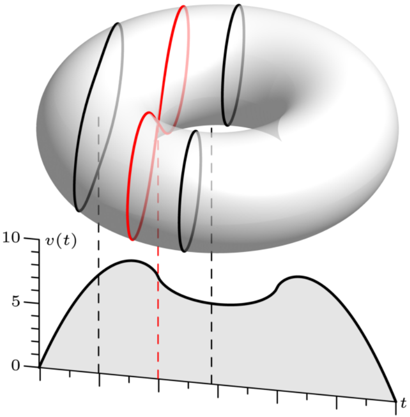
$$f\left(\frac{1}{2d}\right) = \sum_{n=0}^{\infty} \frac{f_n}{(2d)^n}$$

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

```
sage: from ore_algebra.examples import polya
sage: 1 - 1/polya.dop[10].numerical_solution([0]*9+[1], [0, 1/(2*10)], 1e-50).real()
[0.05619753597426778812097369256252412572131681661862 +/- 7.03e-51]
```

Volumes of Compact Semi-Algebraic Sets

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



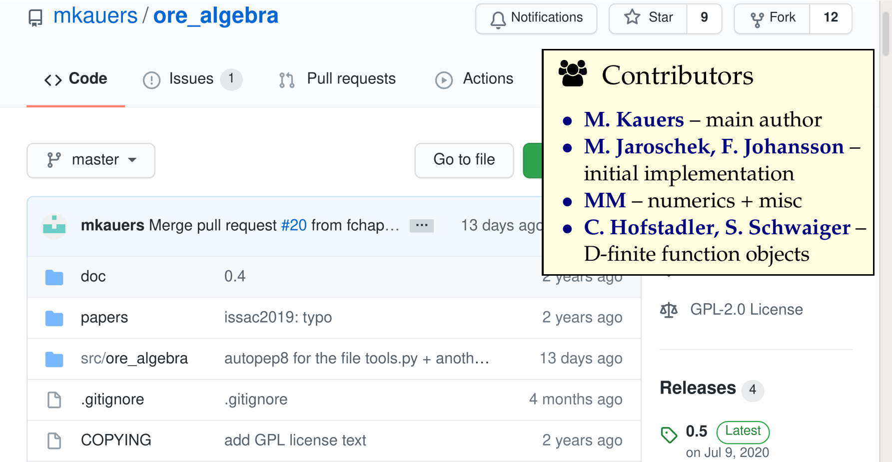
- The **"slice volume"** function satisfies a Picard-Fuchs eqn
- Except at critical values of the projection, it is analytic

➙ Compute initial values by recursive calls, integrate the equation

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

```
···· slice #2: ρ = 10866099/4849664
····· slice length = [3.95699242690042041342397892533404623584614411033674866606926914003 +/- 5.52e-66]
···· integrating PF equation over [1.010906176264399?, 2.989093823735602?]...
···· ...piece volume = [8.10844587166147220133178843300791539013253760904431939702317 34 +/- 8.50e-62]
··· slice volume = [24.8586391228704386869664696158225494398137813407163130742322 0 +/- 5.78e-60]
·· integrating PF equation over [-1, 1]...
·· ...piece volume = [39.4784176043574344753379639995046045412547976289631625 06 +/- 6.38e-55]
[39.478417604357434475337963999504604541254797628963162506 +/- 6.38e-55]
```

ore_algebra



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
```

Try It Yourself

In your browser

http://marc.mezzarobba.net/oaademo-periodswg

…Or locally

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Note:

- Code intended both for end users and as a personal playground
- Some experimental/undocumented features
- Talk to me if it does not *quite* do what you need!

An Implementation of Ore Polynomials

Ore polynomials
≈ skew polynomials that model
functional operators

$$\mathsf{K}(z)\langle\mathrm{D}\rangle = \{\text{polynomials in D over } \mathsf{K}(z) \text{ subject to } \mathrm{D}\,z = z\,\mathrm{D} + 1\}$$

$$\cong \{\textbf{differential operators}\}$$

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

```
sage: from ore_algebra import OreAlgebra
sage: Pol.<z> = PolynomialRing(QQ)
sage: Dop.<Dz> = OreAlgebra(Pol)
sage: Dz*z  # a differential operator
z*Dz + 1
```

Features

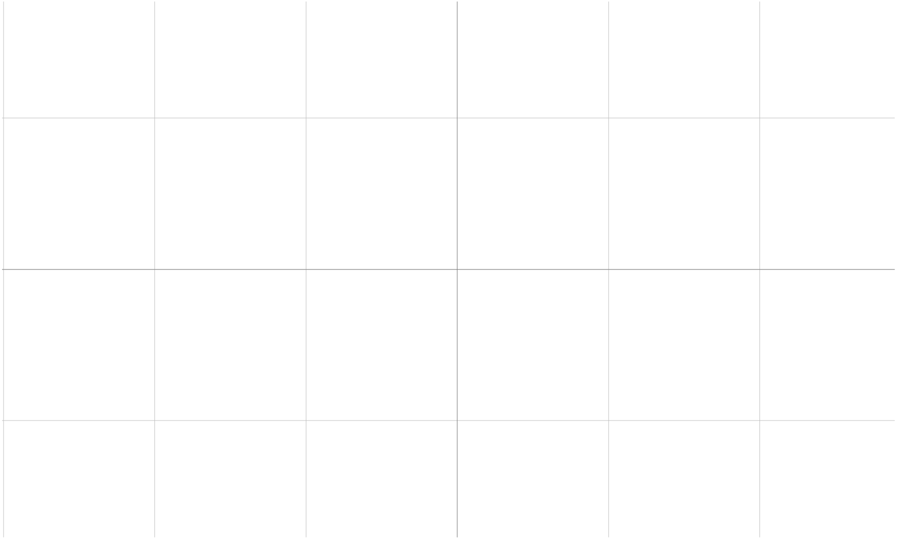
- Basic arithmetic (diff, shift, qdiff, qshift, custom)
- Gcrd, lclm, D-finite closure (incl. multivariate)
- Creative telescoping
- Polynomial, rational, asympt. series solutions
- Desingularization
- Guessing
- …

This talk:

- Numerical connection (differential case)

Analytic Continuation

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



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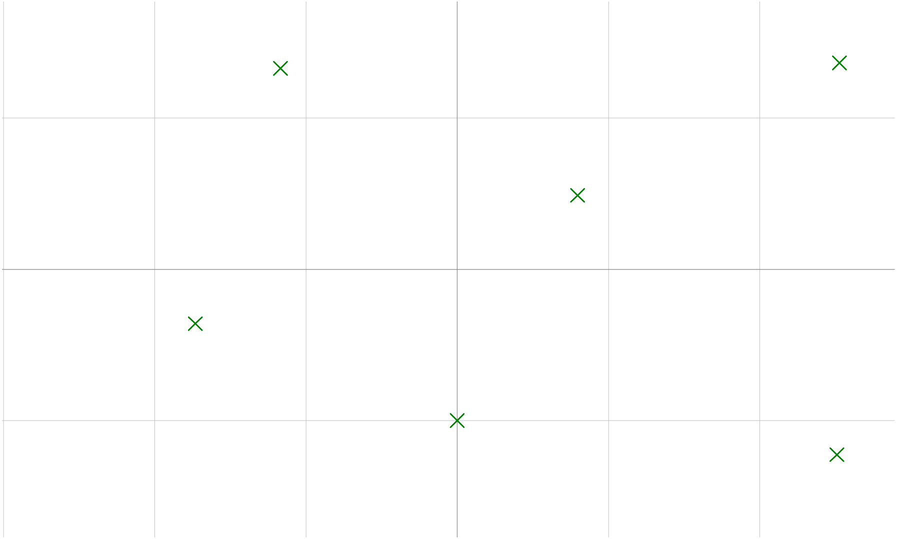

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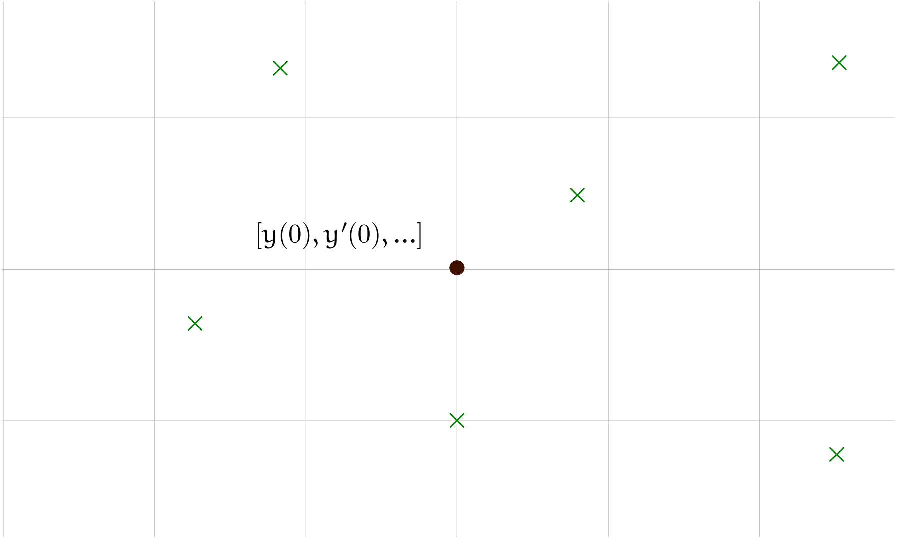

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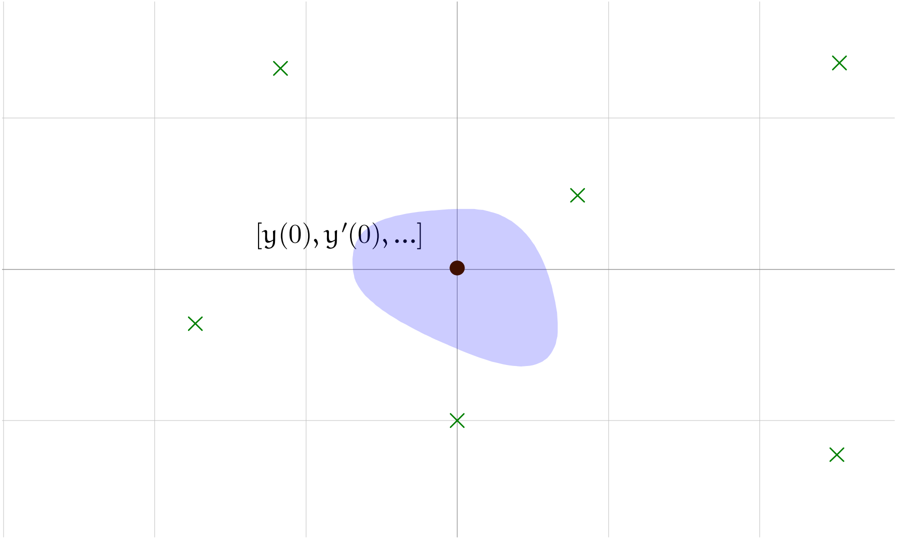

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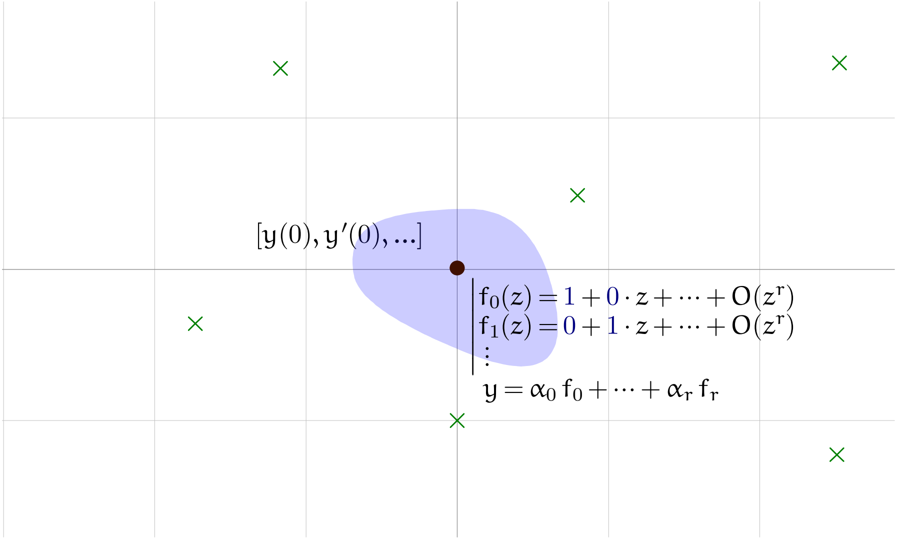

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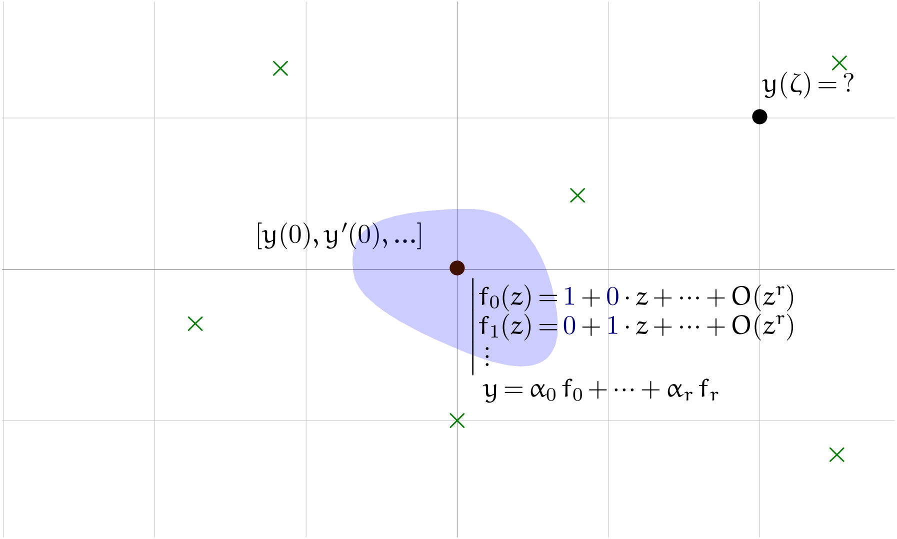

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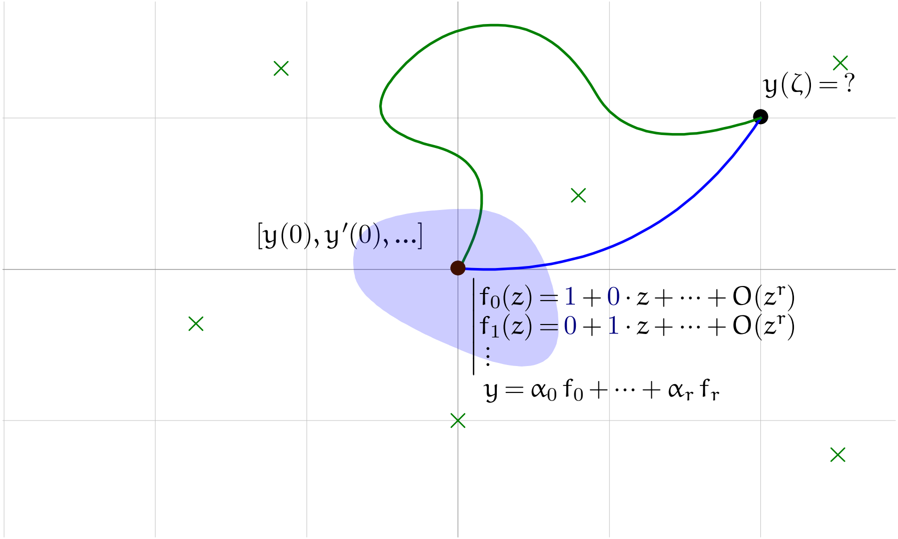
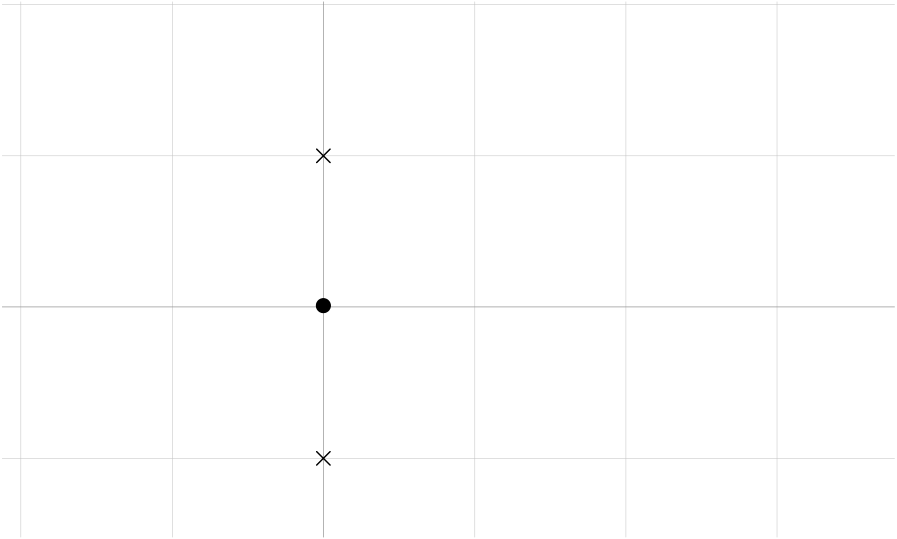


Transition Matrices

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



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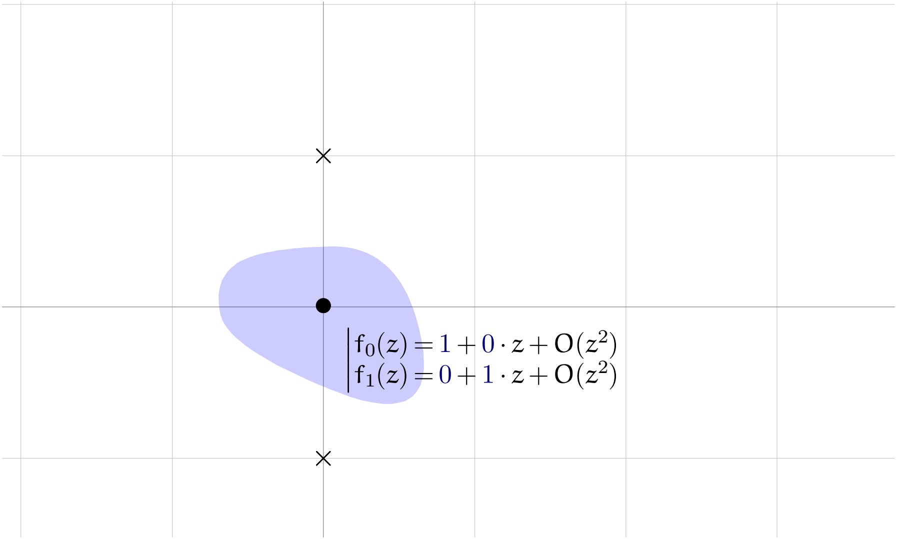

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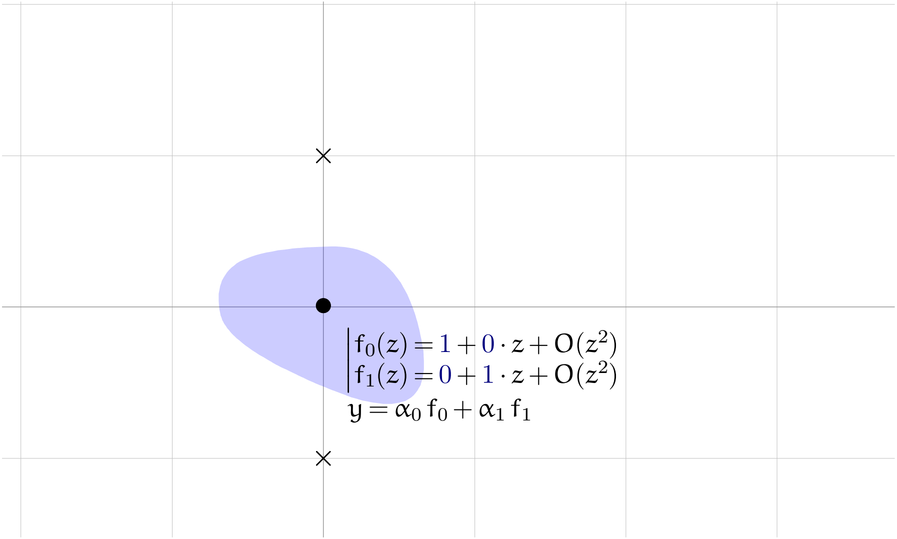

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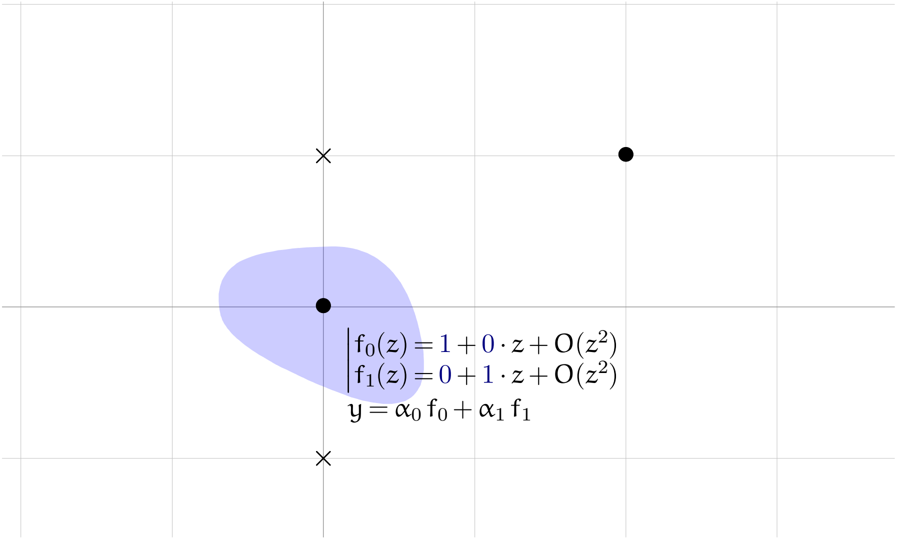

$$\left|\begin{array}{l} f_0(z) = 1 + 0\cdot z + O(z^2) \\ f_1(z) = 0 + 1\cdot z + O(z^2) \end{array}\right.$$

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

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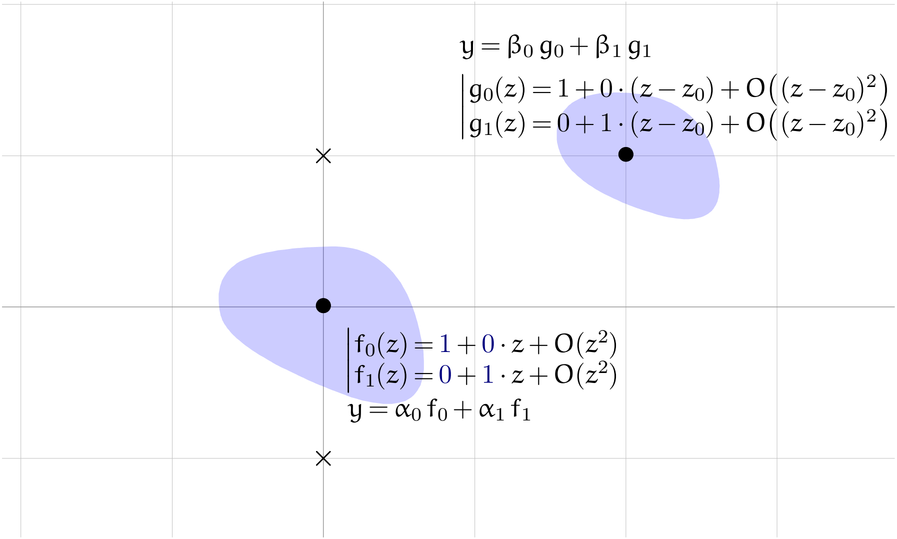

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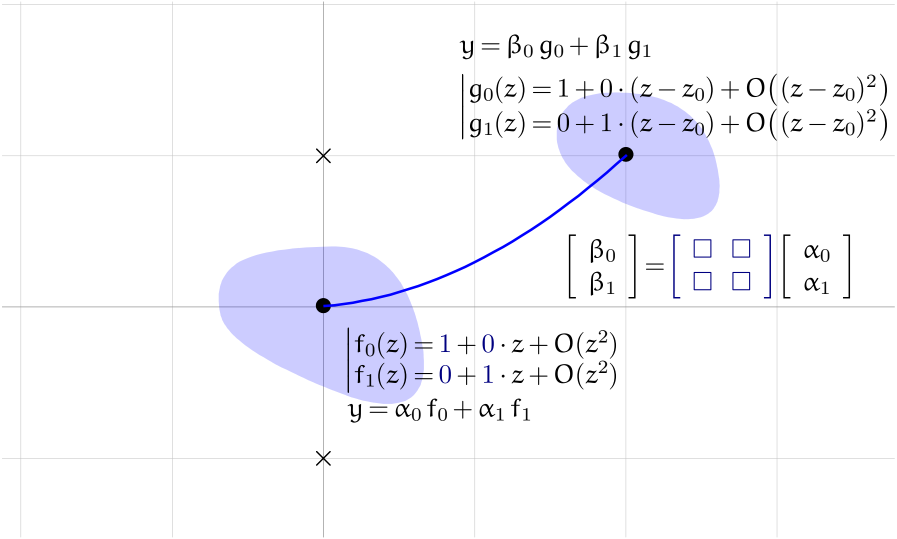

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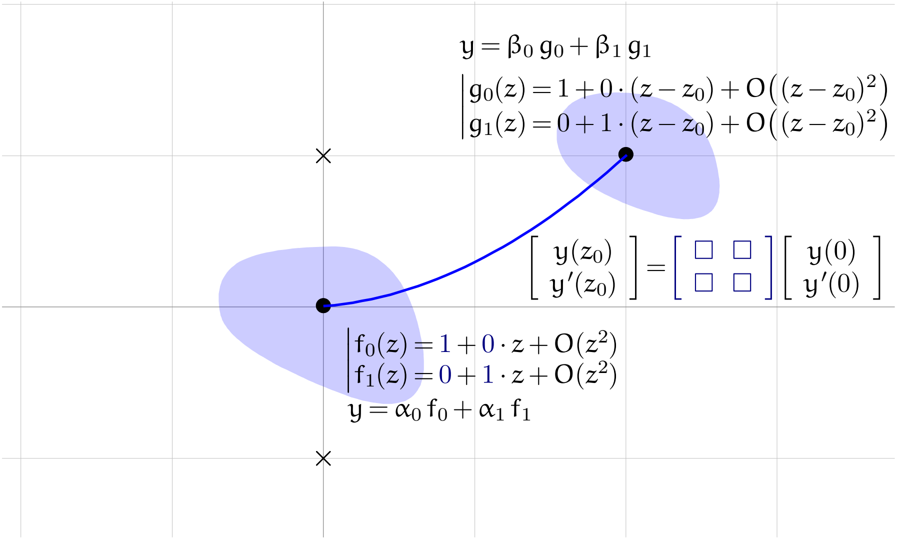

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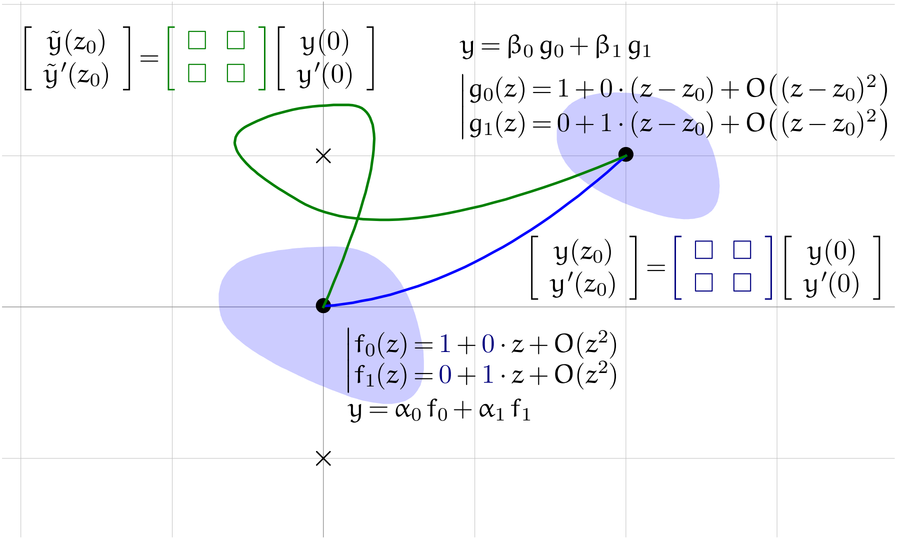


Regular Singular Points

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

“Definition”. Singular points ($a_r(\zeta) = 0$) where all solutions are “tame”:

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

Local solutions at reg. sing. $\zeta = 0$ [Fuchs, 1866]

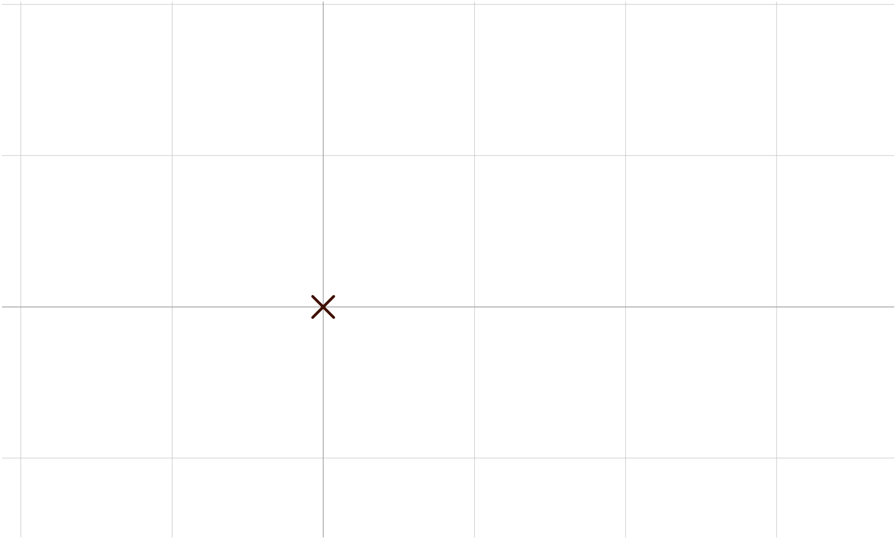
On some slit neighborhood $D \backslash \mathbb{R}_{\leqslant 0}$,
$\mathcal{L} \cdot y = 0$ has a full basis of solutions of the form

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

- **General form:** $\displaystyle y(z) = \sum_{\nu \in \Lambda} \sum_{k=0}^{t} y_{\nu,k}\, z^\nu \frac{\log^k z}{k!}$ $\qquad \displaystyle \Lambda = \bigcup_i (\lambda_i + \mathbb{N}) \subset \mathbb{C}$
- **“Canonical” basis**: dual of $\left\{ y \mapsto y_{\nu,k} \;\middle|\; \begin{array}{l} \nu \text{ root of } \textbf{indicial polynomial}, \\ k < \operatorname{mult}(\nu) \end{array} \right\}$
  - Natural generalization of $x^i + O(x^r)$ at ordinary points
  - *Not* the usual Frobenius basis!

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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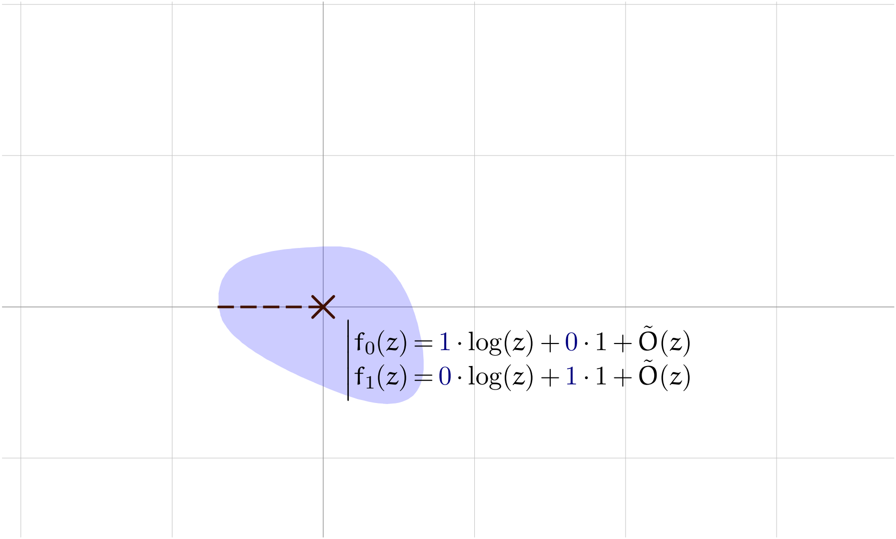

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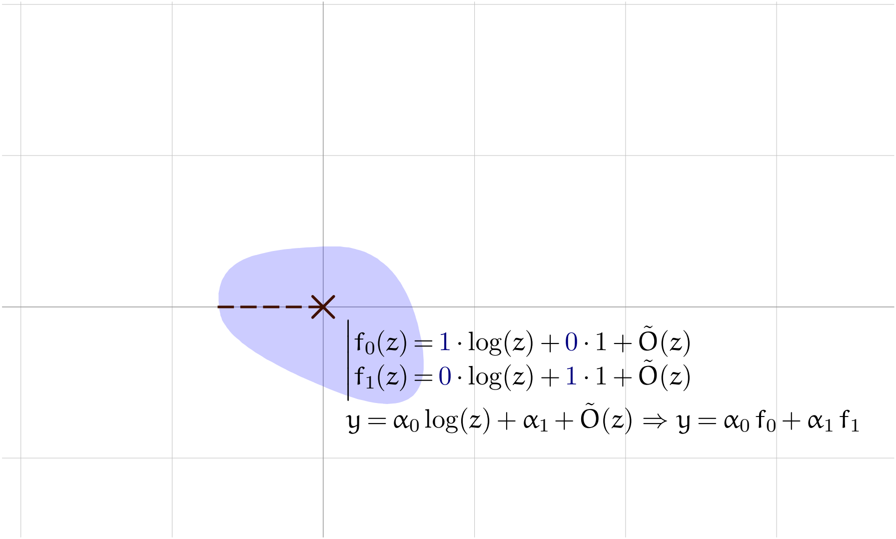

$$\left| \begin{array}{l} f_0(z) = 1 \cdot \log(z) + 0 \cdot 1 + \tilde{\mathrm{O}}(z) \\ f_1(z) = 0 \cdot \log(z) + 1 \cdot 1 + \tilde{\mathrm{O}}(z) \end{array} \right.$$

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

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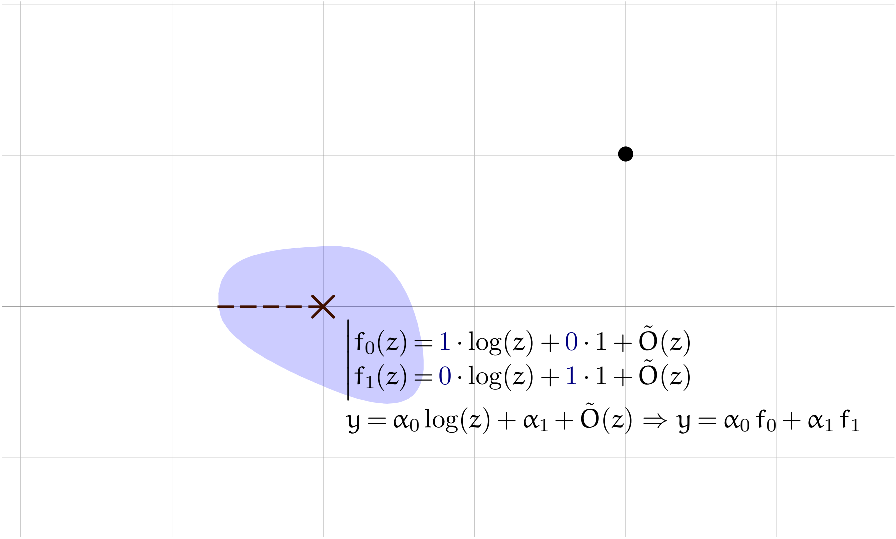

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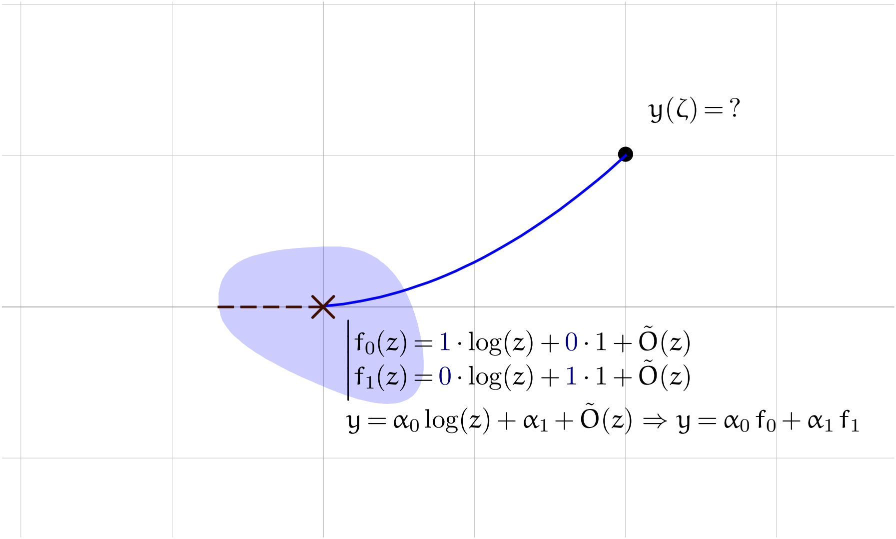
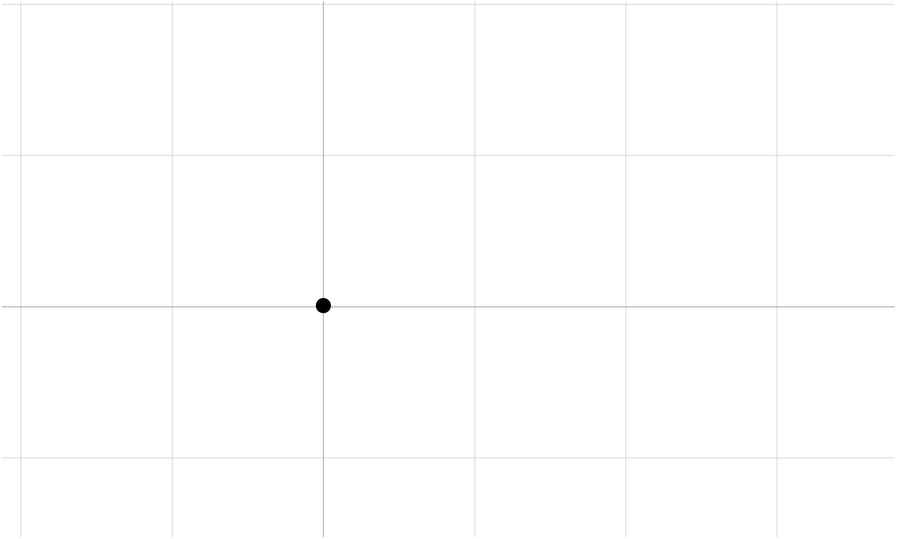
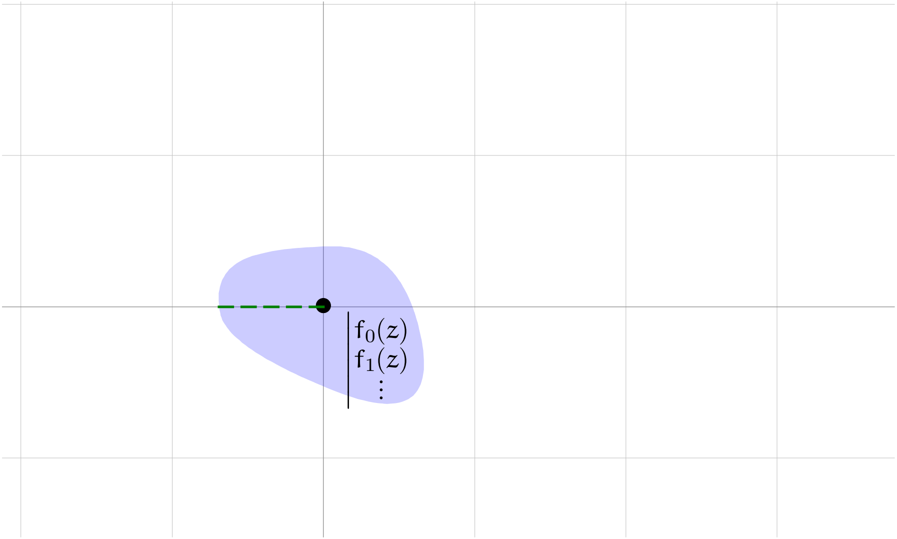


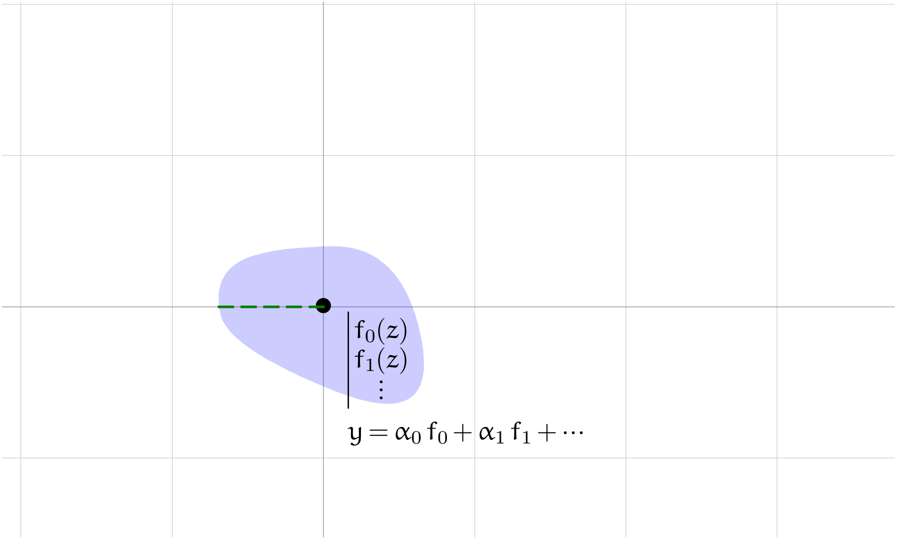
Regular Singular Transition Matrices



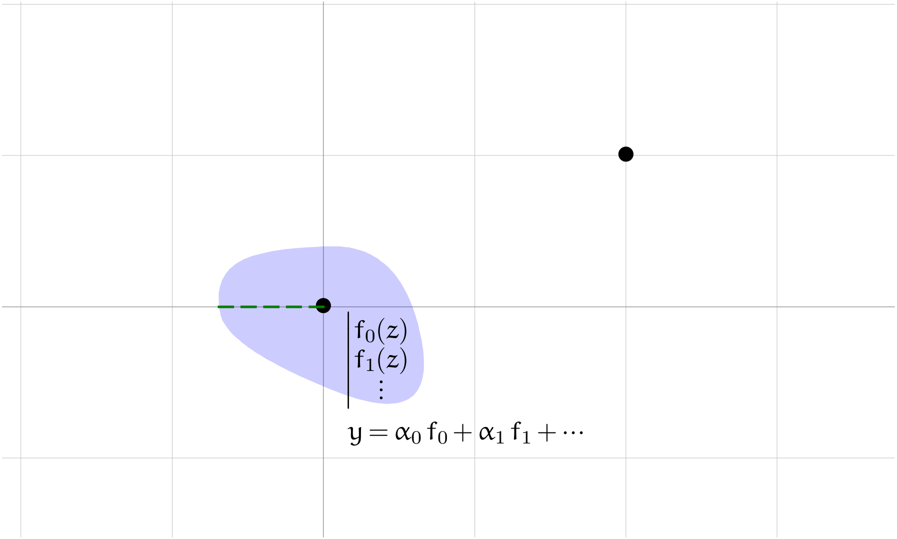
Regular Singular Transition Matrices



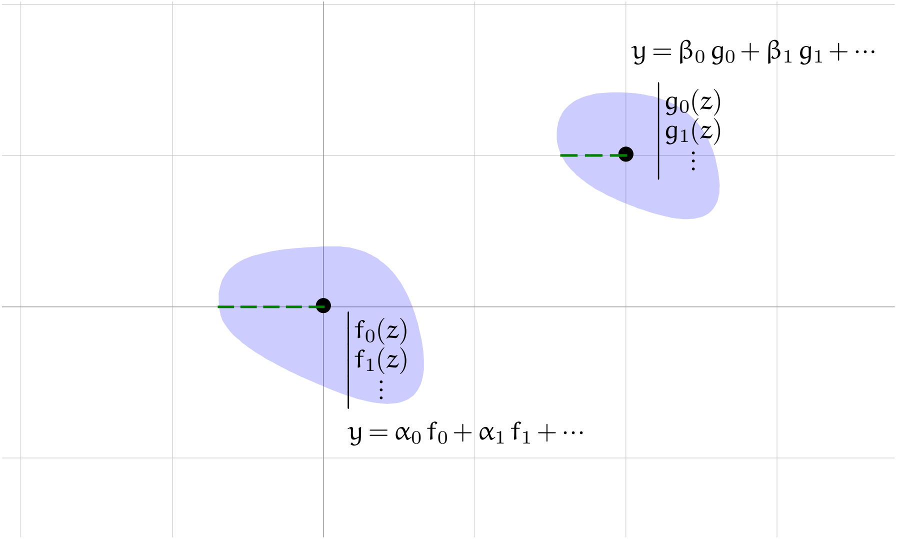
Regular Singular Transition Matrices



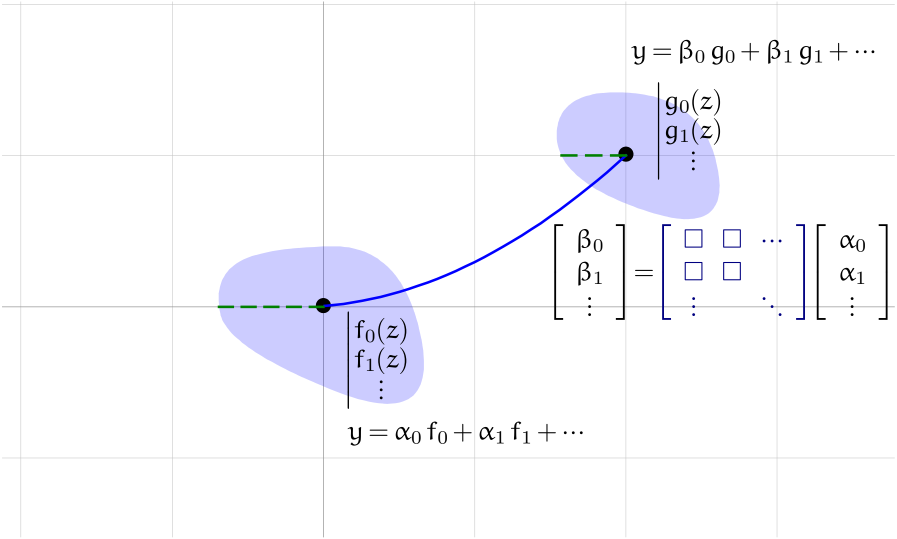
Regular Singular Transition Matrices



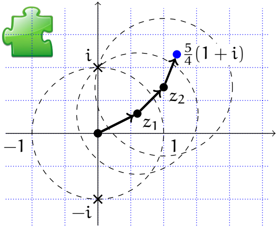
Regular Singular Transition Matrices



Regular Singular Transition Matrices



Under the Hood

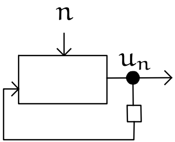


Taylor method

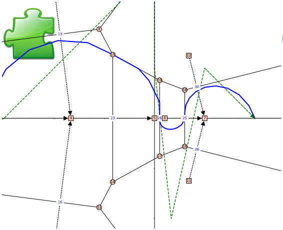
$$\sum_{\nu\in\lambda+\mathbb{Z}}\ \sum_{k=0}^{K} y_{\nu,k}\, z^{\nu}\, \frac{\log(z)^k}{k!}$$

$$L(S_n^{-1}, n+S_k)\cdot(y_{n,k})=0$$

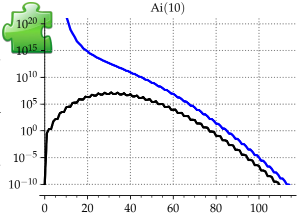
Logarithmic series



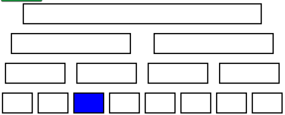
Recurrences



Path optimization



Error bounds



Binary splitting

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

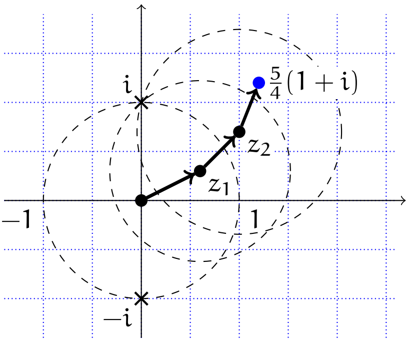
`https://github.com/mkauers/ore_algebra/`

Perspectives

- Irregular singular case
- p-adic points
- Performance improvements

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** (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.)

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.)

Proof.

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

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:

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

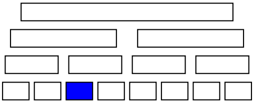
(And conversely, for D-finite formal power series.)

- Easy to generate
- 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 $\displaystyle\sum_{\nu\in\lambda+\mathbb{Z}}\sum_{k=0}^{K} y_{\nu,k}\, z^{\nu}\,\frac{\log(z)^k}{k!}$
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
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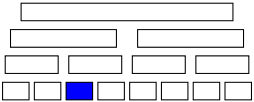


[Schroeppel 1972; Brent 1976; Chudnovsky & Chudnovsky 1988; van der Hoeven 1999, 2001; M. 2010, 2012]

Error Bounds

Rounding Errors

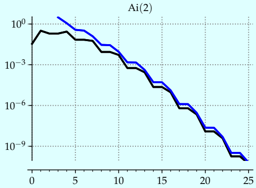
Real & complex arithmetic based on **Arb** [Johansson 2012–]

({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]

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**:

$$L(z, {}^{d}/_{dz}) \cdot u = 0 \qquad \underset{\text{“bounded by”}}{\ll} \qquad \underset{\text{for us: always 1st order}}{\hat{u}'(z) - \hat{a}(z)\,\hat{u}(z) = 0}$$

- 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

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

residual ($\approx$ 1st negl. term)

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

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**

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

- **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**

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

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