

# Regular Singularities & Rigorous Numerics

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CNRS, École polytechnique

Periods workgroup, May 19, 2021



**Try it online!**

<http://marc.mezzarobba.net/oademo-periodswg>

# ODE Solving from a Computer Algebra Perspective

## Problem

Starting from a linear differential equation

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

with polynomial coefficients  $p_0, \dots, p_r$  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

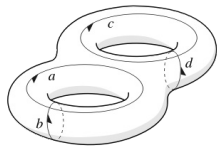
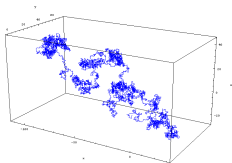
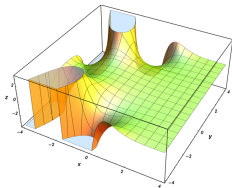
via **Picard-Fuchs equations**

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, ...]



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

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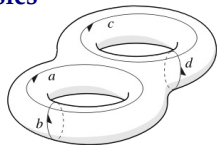
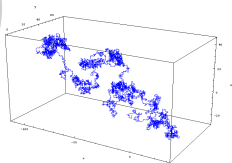
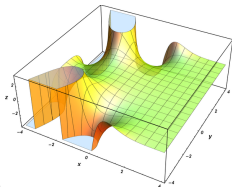
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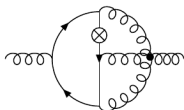


**Math. physics**

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

# Iterated Integrals

[Ablinger, Blümlein, Raab, Schneider, 2014]

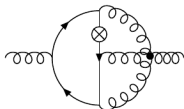


$$\int_0^1 \frac{x_5 dx_5}{x_5 - 1} \int_{x_5}^1 \frac{dx_4}{x_4 \sqrt{x_4 - \frac{1}{4}}} \int_{x_4}^1 \frac{dx_3}{x_3 \sqrt{x_3 - \frac{1}{4}}} \int_{x_3}^1 \frac{dx_2}{1 - x_2} \int_{x_2}^1 \frac{dx_1}{1 - x_1} = ?$$

(with suitable branch choices)

# Iterated Integrals

[Ablinger, Blümlein, Raab, Schneider, 2014]



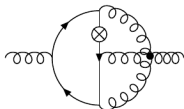
$$I(x) = \int_x^1 \frac{x_5 dx_5}{x_5 - 1} \int_{x_5}^1 \frac{dx_4}{x_4 \sqrt{x_4 - \frac{1}{4}}} \int_{x_4}^1 \frac{dx_3}{x_3 \sqrt{x_3 - \frac{1}{4}}} \int_{x_3}^1 \frac{dx_2}{1 - x_2} \int_{x_2}^1 \frac{dx_1}{1 - x_1} = ?$$

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

# Iterated Integrals

[Ablinger, Blümlein, Raab, Schneider, 2014]



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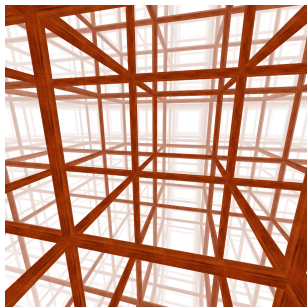
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sage: iint\_value(dop, myini, 1e-500)

[0.9708046956249312405 ... 59027603834204946 +/- 9.05e-501]



# Pólya Walks



For a random walk on  $\mathbb{Z}^d$  ( $d \geq 3$ ) 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

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

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

[thanks to B. Salvy]

First return after  $n$  steps:

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

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

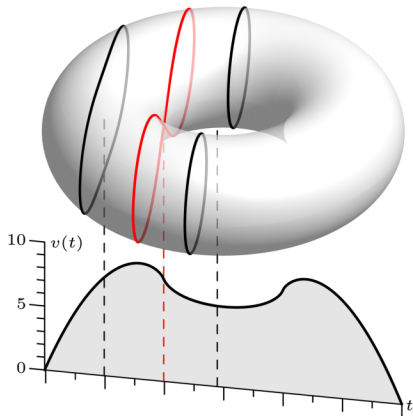
$$w(z) = 1 + f(z)w(z)$$

**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 =  $\tilde{O}(p)$**

```
.... slice #2:  $\rho = 10866099/4849664$ 
..... slice length = [3.95699242690042041342397892533404623584614411033674866606926914003 +/- 5.52e-66]
.... integrating PF equation over [1.0109061762643997, 2.989093823735602?]...
.... ...piece volume = [8.1084458716614722013317884330079153901325376090443193970231734 +/- 8.50e-62]
... slice volume = [24.85863912287043868696646961582254943981378134071631307423220 +/- 5.78e-60]
.. integrating PF equation over [-1, 1]...
.. ...piece volume = [39.478417604357434475337963999504604541254797628963162506 +/- 6.38e-55]
[39.478417604357434475337963999504604541254797628963162506 +/- 6.38e-55]
```

# ore\_algebra

mkauers / ore\_algebra

Notifications Star 9 Fork 12

<> Code Issues 1 Pull requests Actions

master

Go to file

mkauers Merge pull request #20 from fchap... 13 days ago

doc	0.4	2 years ago
papers	issac2019: typo	2 years ago
src/ore_algebra	autopep8 for the file tools.py + anothe...	13 days ago
.gitignore	.gitignore	4 months ago
COPYING	add GPL license text	2 years ago

GPL-2.0 License

Releases 4

0.5 Latest  
on Jul 9, 2020

### 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

$$K(z)\langle D \rangle = \left\{ \begin{array}{l} \text{polynomials in } D \text{ over } K(z) \\ \text{subject to } D z = z D + 1 \end{array} \right\}$$
$$\cong \{ \text{differential operators} \}$$

$$[z f(z)]' = z f'(z) + f(z)$$


```
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, lcm, D-finite closure (incl. multivariate)
- Creative telescoping
- Polynomial, rational, asympt. series solutions
- Desingularization
- Guessing
- ...

### This talk:

- Numerical connection (differential case)

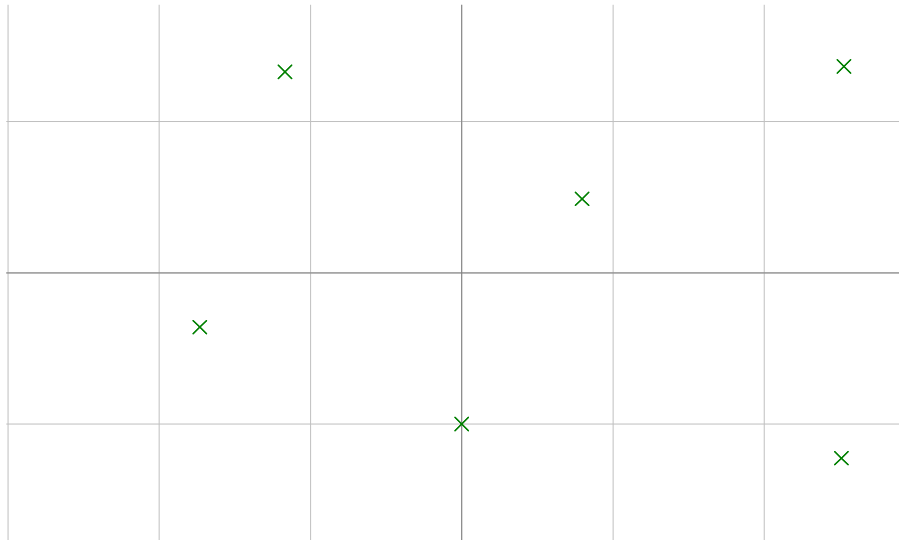
# Analytic Continuation

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



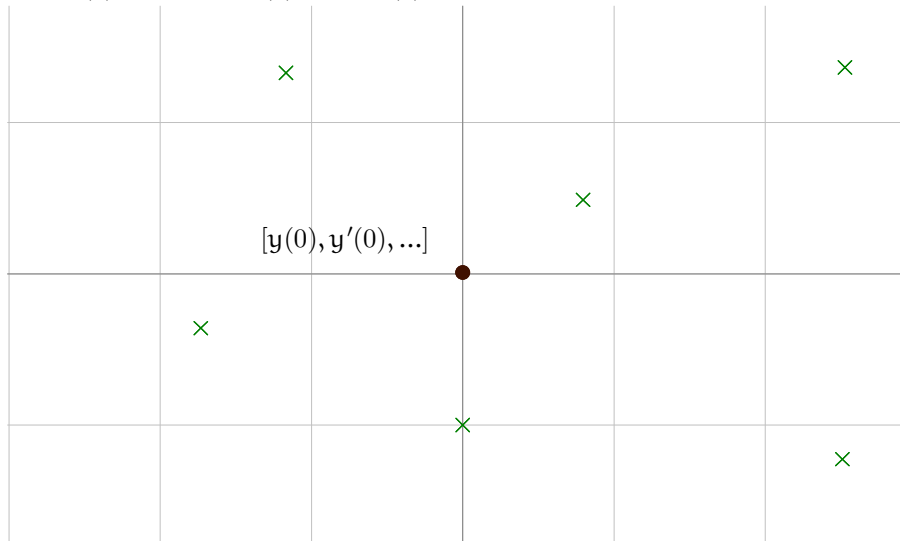
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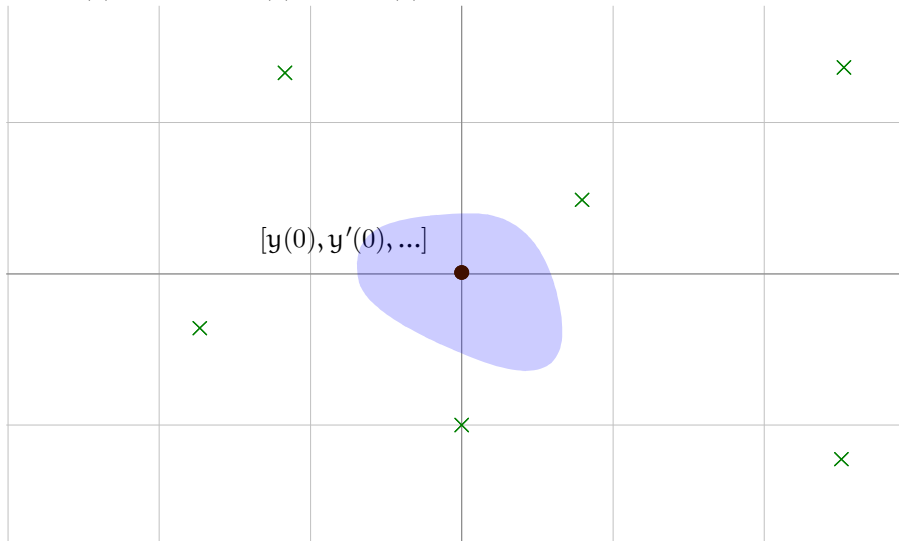
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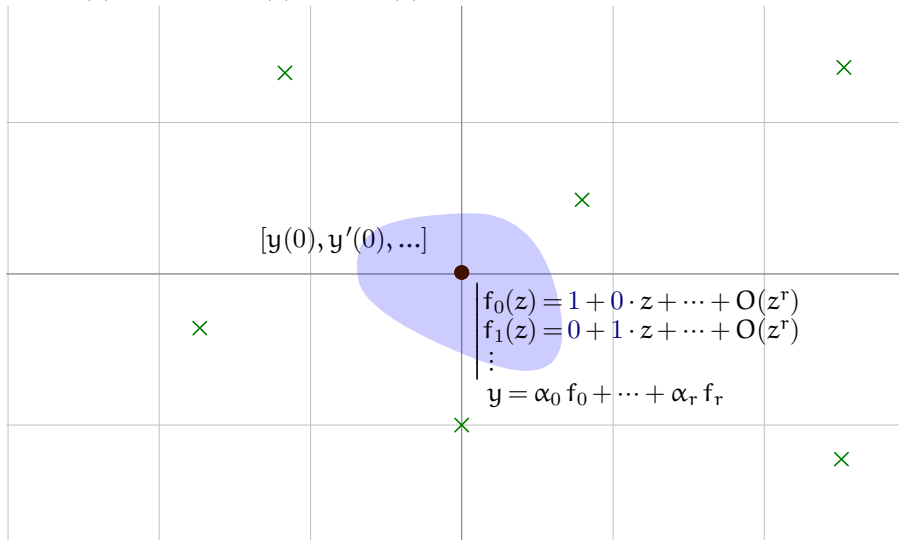
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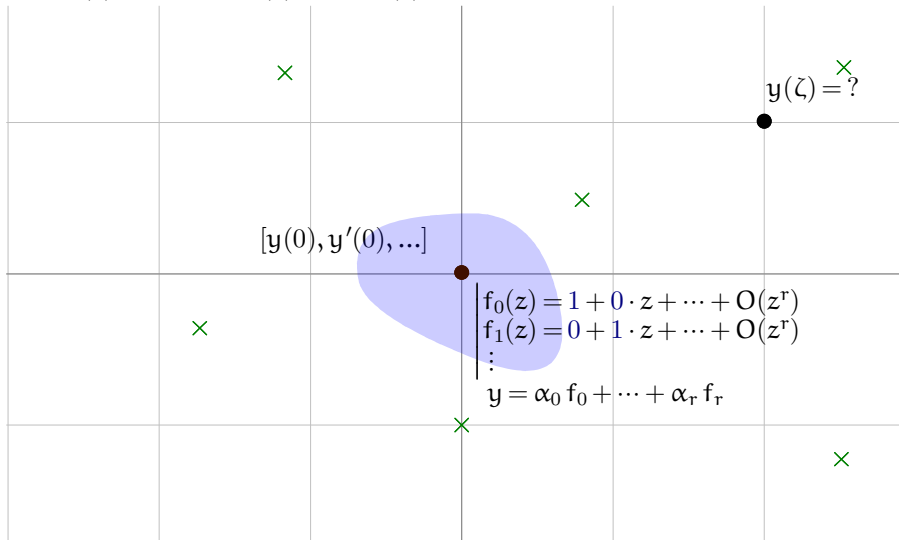
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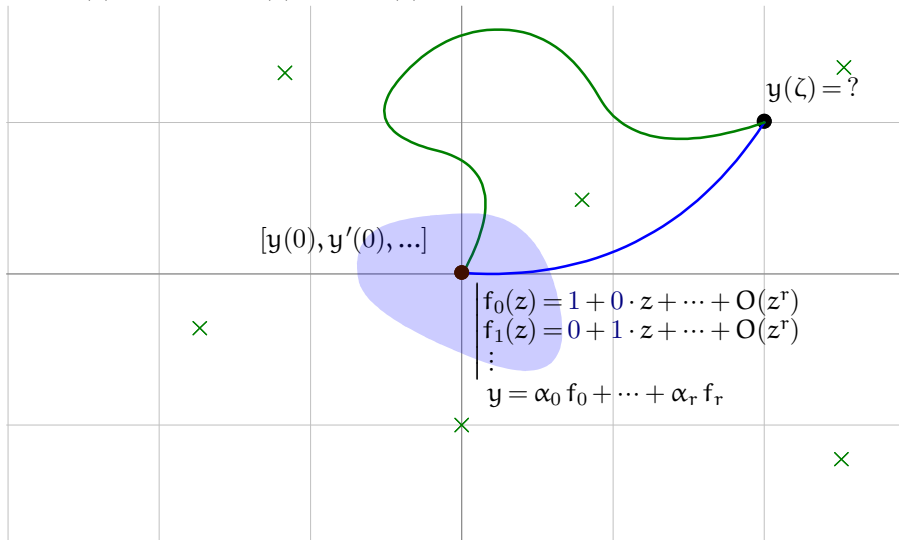
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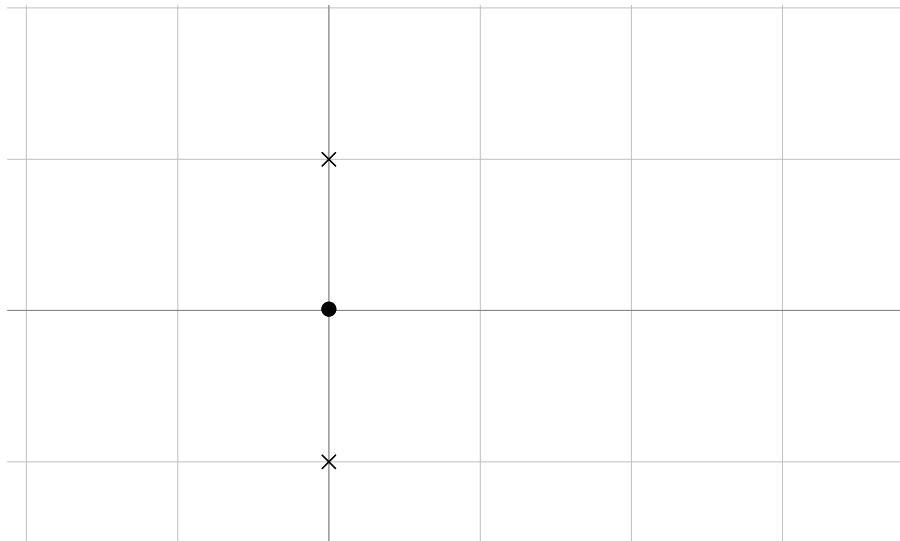
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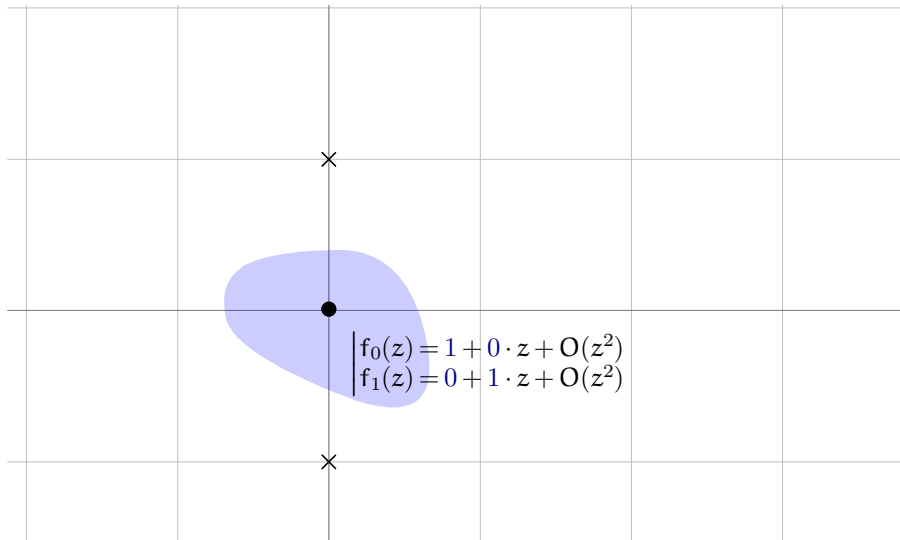
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x

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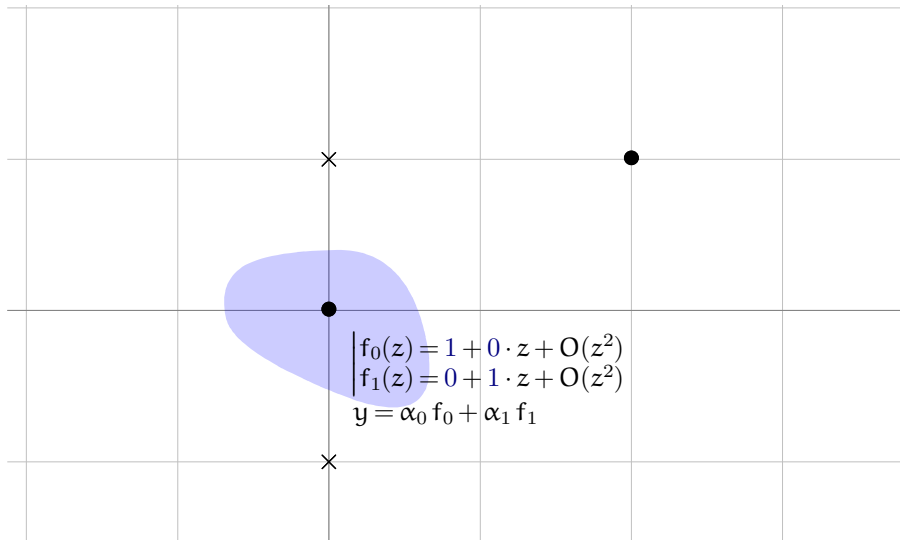
x

$$\begin{cases} f_0(z) = 1 + 0 \cdot z + O(z^2) \\ f_1(z) = 0 + 1 \cdot z + O(z^2) \end{cases}$$

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

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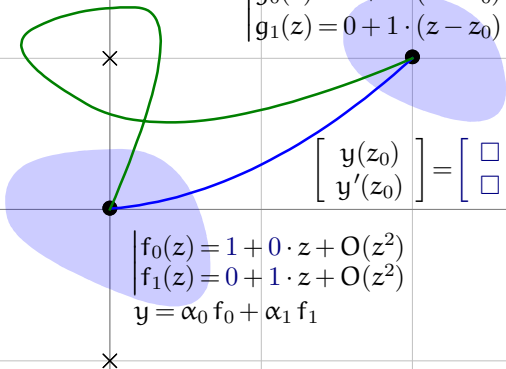
$$\begin{bmatrix} \tilde{y}(z_0) \\ \tilde{y}'(z_0) \end{bmatrix} = \begin{bmatrix} \square & \square \\ \square & \square \end{bmatrix} \begin{bmatrix} y(0) \\ y'(0) \end{bmatrix}$$

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# Regular Singular Points

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

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

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

## Local solutions at reg. sing. $\zeta = 0$

[Fuchs, 1866]

On some slit neighborhood  $D \setminus \mathbb{R}_{\leq 0}$ ,

$\mathcal{L} \cdot y = 0$  has a full basis of solutions of the form

$$z^\lambda (y_0(z) + y_1(z) \log z + \dots + y_t(z) \log^t z), \quad \lambda \in \bar{\mathbb{Q}}, \quad y_i \text{ analytic on } D.$$

► **General form:** 
$$y(z) = \sum_{\nu \in \Lambda} \sum_{k=0}^t y_{\nu,k} z^\nu \frac{\log^k z}{k!} \quad \Lambda = \bigcup_i (\lambda_i + \mathbb{N}) \subset \mathbb{C}$$

► “**Canonical**” basis: dual of  $\left\{ y \mapsto y_{\nu,k} \mid \begin{array}{l} \nu \text{ root of } \mathbf{indicial \ polynomial}, \\ k < \text{mult}(\nu) \end{array} \right\}$

- Natural generalization of  $x^i + O(x^r)$  at ordinary points
- *Not* the usual Frobenius basis!

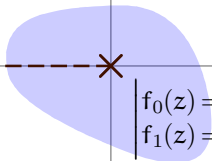
# Initial Conditions at Regular Singular Points

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



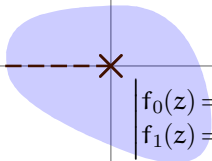
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$$f_0(z) = 1 \cdot \log(z) + 0 \cdot 1 + \tilde{O}(z)$$

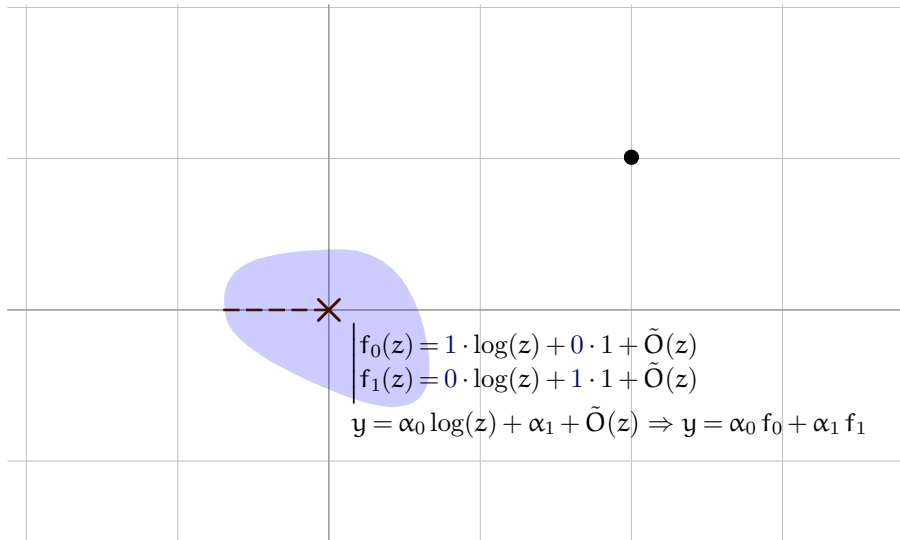
$$f_1(z) = 0 \cdot \log(z) + 1 \cdot 1 + \tilde{O}(z)$$

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



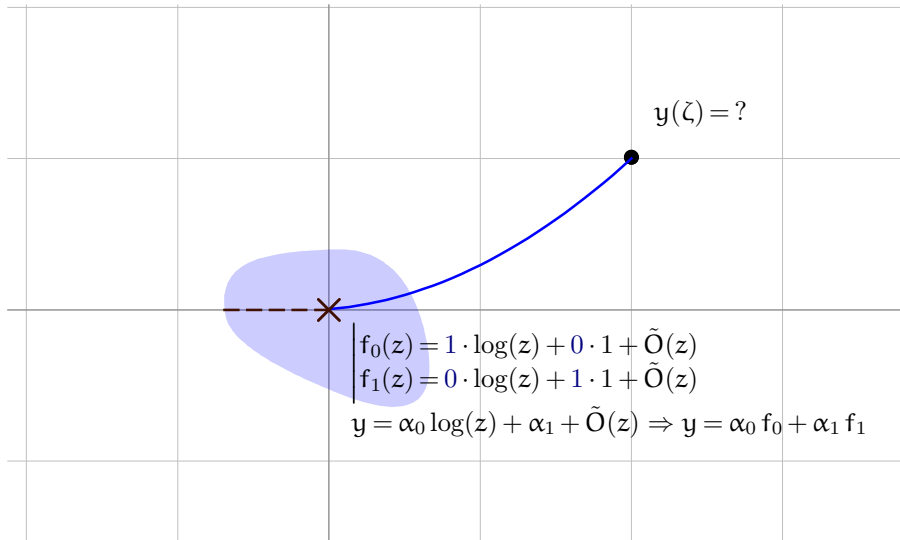
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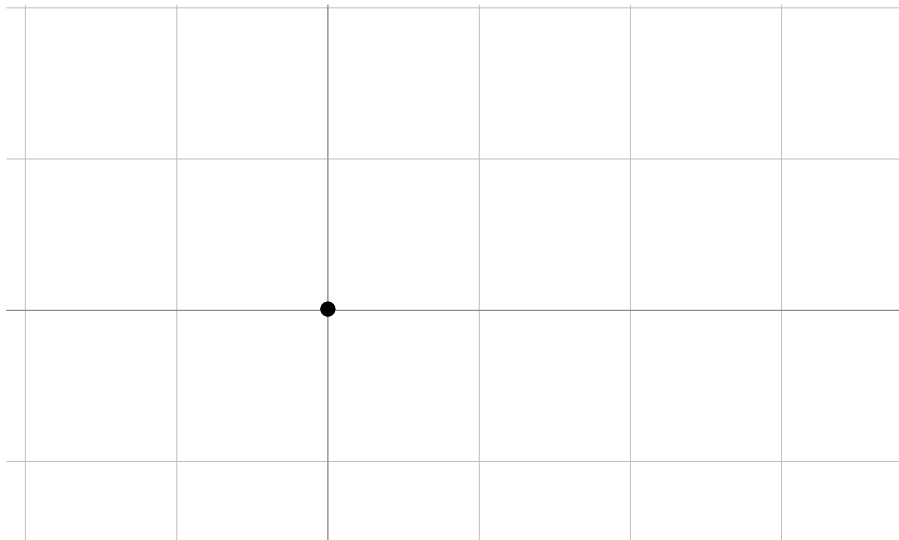


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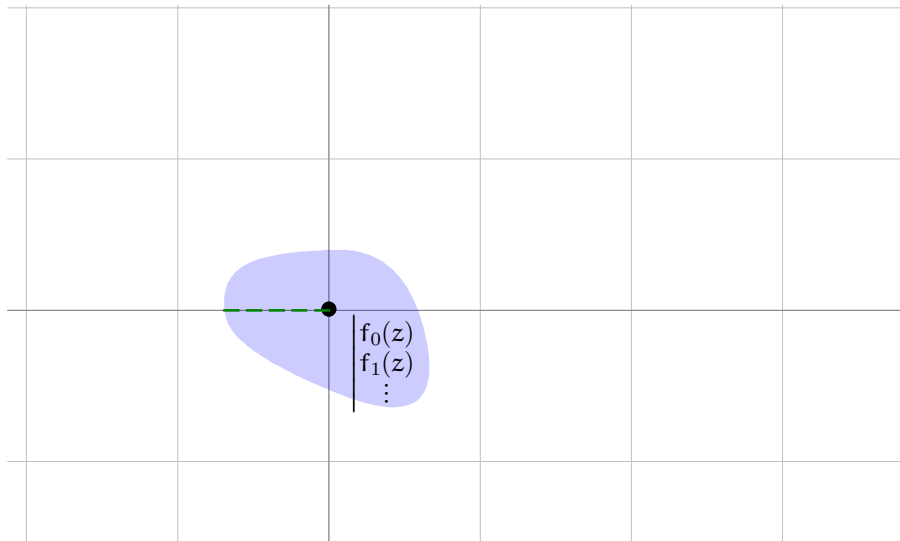
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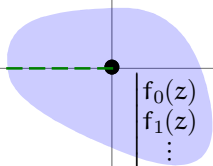
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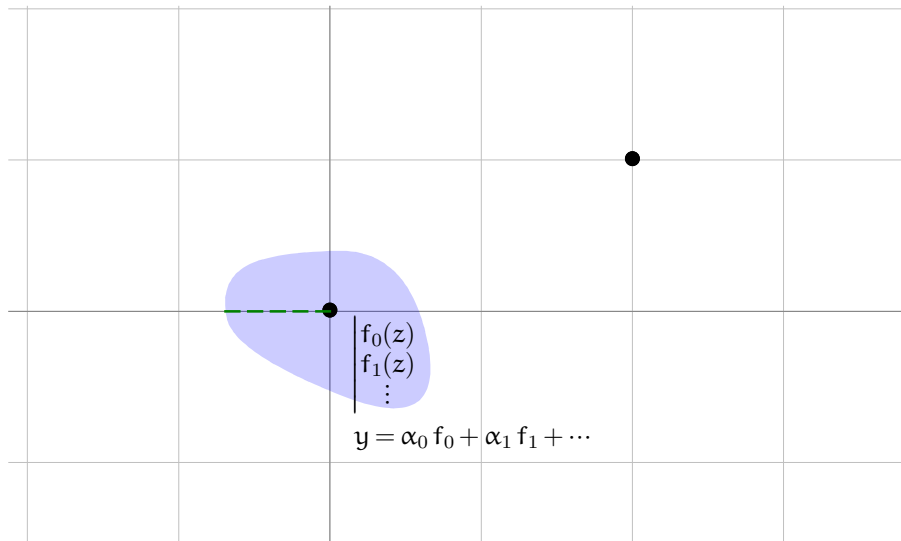


# Regular Singular Transition Matrices

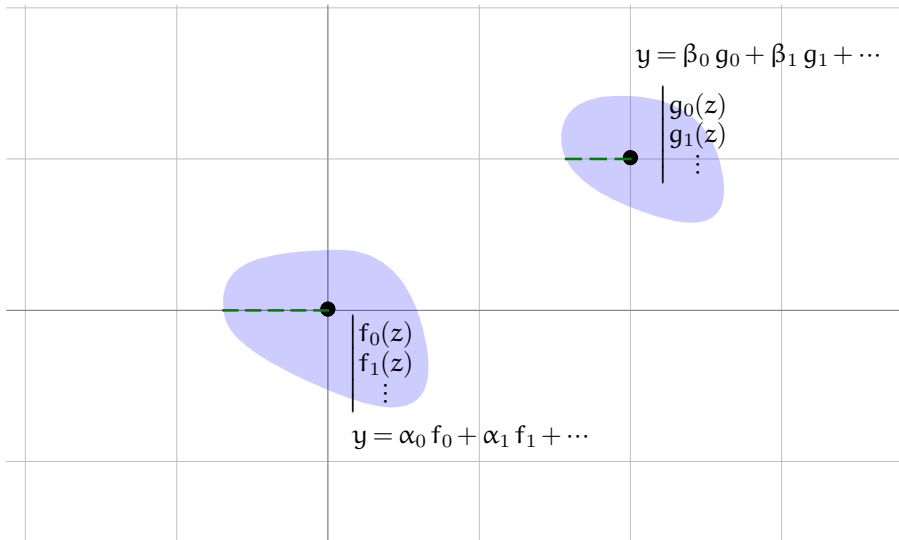


$$y = \alpha_0 f_0 + \alpha_1 f_1 + \dots$$

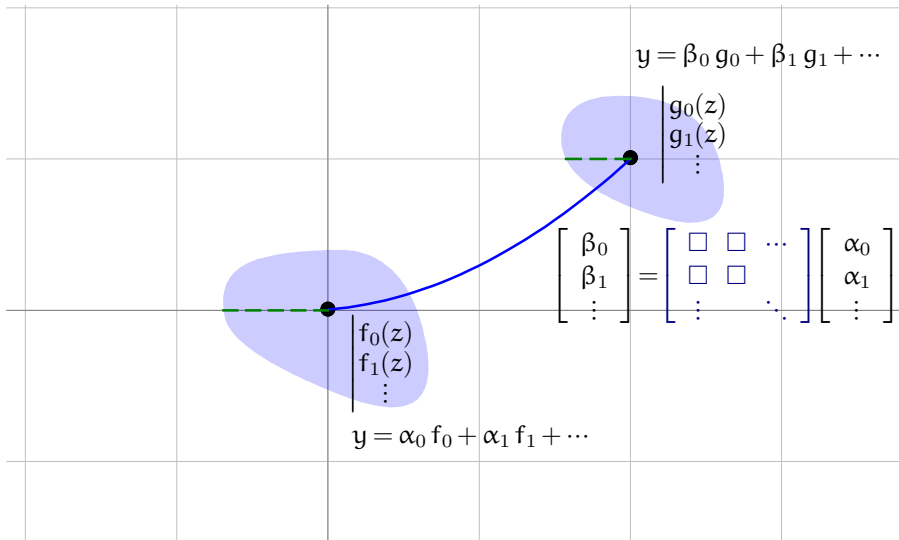
# Regular Singular Transition Matrices



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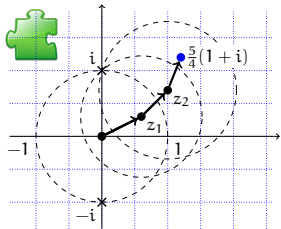


# Regular Singular Transition Matrices






# Under the Hood



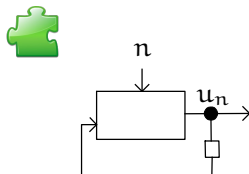
Taylor method



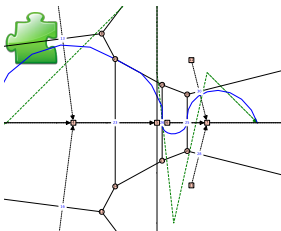
$$\sum_{v \in \lambda + \mathbb{Z}} \sum_{k=0}^K \mathbf{y}_{v,k} z^v \frac{\log(z)^k}{k!}$$

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

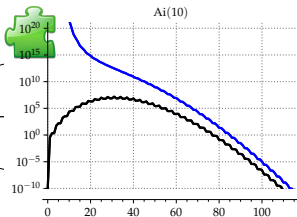
Logarithmic series



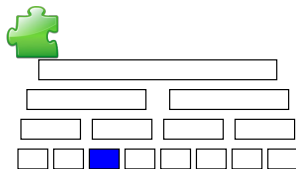
Recurrences



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/](https://github.com/mkauers/ore_algebra/)

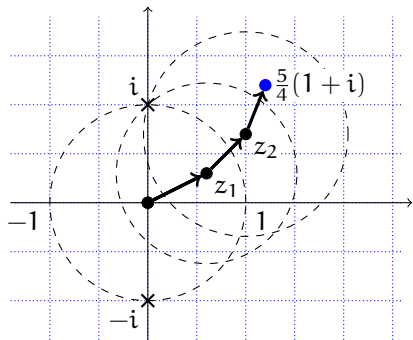


### Perspectives

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

**Bug reports, feature requests, examples welcome!**

# A Taylor Series Method



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

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

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

...

- ▶ 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:

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

**Proof.**

$$y = \sum_{n=-\infty}^{\infty} y_n z^n \quad \leftrightarrow \quad Y = (y_n)_{n \in \mathbb{Z}}$$

$$\mathbf{D} \cdot y = \sum_{n=-\infty}^{\infty} (n+1) y_{n+1} z^n \quad \leftrightarrow \quad (\mathbf{S}n) \cdot Y$$

$$\mathbf{z} \cdot y = \sum_{n=-\infty}^{\infty} y_{n-1} z^n \quad \leftrightarrow \quad \mathbf{S}^{-1} \cdot Y$$

# Recurrences

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

(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  $\varepsilon = 2^{-p}$



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

# Recurrences

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

$$[b_s(\nu + S_k) \cdot S_{\nu}^s + \dots + b_1(\nu + S_k) S_{\nu} + b_0(\nu + S_k)] \cdot (\mathbf{y}_{\nu, k}) = 0.$$

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

Best **boolean** complexity:

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

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



[Schroepfel 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)

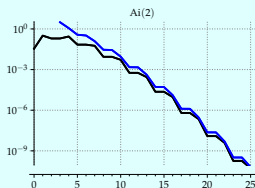
[Heuberger, M. & others]

- ▶ 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

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

- ▶ Majorant series
- ▶ "Adaptive" bounds using residuals



[M. 2019]



# The Method of Majorants

[Cauchy 1842]

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

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

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

$$L(z, d/dz) \cdot u = 0 \quad \ll \quad \hat{u}'(z) - \hat{a}(z) \hat{u}(z) = 0$$

"bounded by"                      for us: always 1st order

- ▶ Solve the model equation and study the solutions:

$$\hat{u}(z) = \exp \int^z \hat{a}(w) dw \quad \left| \sum_{n=N}^{+\infty} u_n z^n \right| \leq \sum_{n=N}^{+\infty} \hat{u}_n |z|^n \leq \dots$$

# 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

$$A x = b$$

$$A \in GL_n(\mathbb{C}), \quad \|A^{-1}\| \leq M$$

$$A \tilde{x} = \tilde{b}$$

← computed approx.

$$\|x - \tilde{x}\| \leq M \cdot \underbrace{\|b - \tilde{b}\|}_{\text{known}}$$

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

# 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**

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

► **Majorant property:**

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

► **Solving the model equation**

$$v(z) = h(z) \left( \underset{\substack{\nearrow \\ \text{choose } \text{cst} = 0}}{\text{cst}} + \int^z \frac{t^{-1} \hat{q}(t)}{h(t)} dt \right)$$

$= O(z^N)$

$$\text{where } h(z) = \exp \int^z t^{-1} \hat{a}(t) dt$$

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