Numerical Evaluation of D-Finite Functions

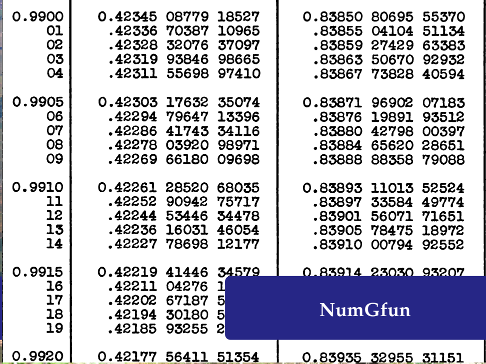
NumGfun and Beyond

Marc Mezzarobba

RISC, JKU Linz

Sage Days 49, Orsay
2013-06-20

D-Finite Functions



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02	.42328 32076 37097	.83859 27429 63383
03	.42319 93846 98665	.83863 50670 92932
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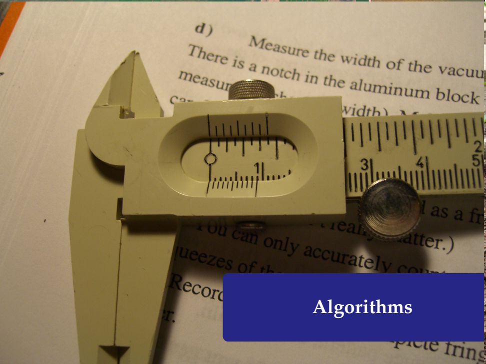
NumGfun

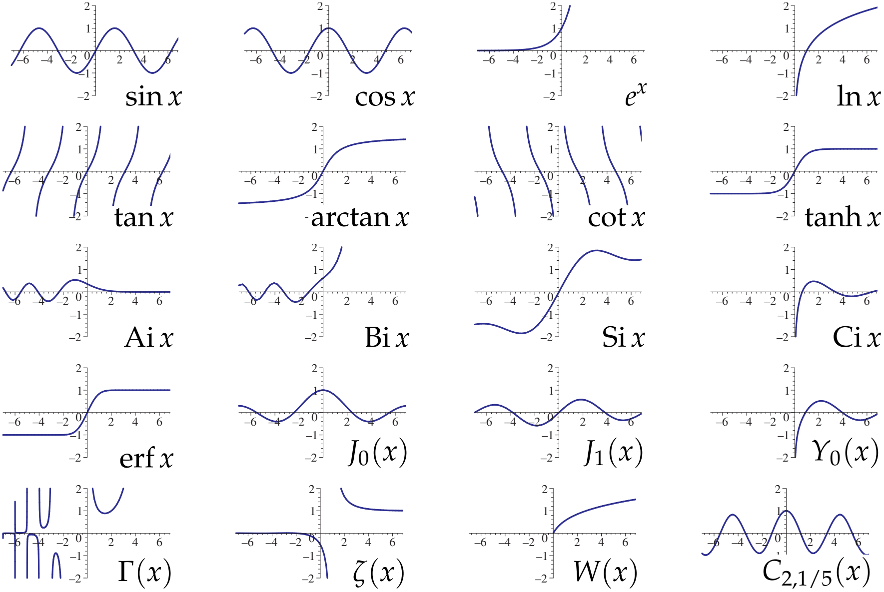


Algorithms

Outlook

D-Finite Functions

Elementary and Special Functions



D-Finite Functions

An analytic function $y(z) : \mathbb{C} \to \mathbb{C}$ is said to be D-finite (holonomic) iff it satisfies a linear (homogeneous) ODE with polynomial coefficients:

$$a_r(z)\, y^{(r)}(z) + \cdots + a_1(z)\, y'(z) + a_0(z)\, y(z) = 0, \quad a_j \in \mathbb{K}[z].$$

- The sequence of Taylor coefficients of a D-finite functions obeys a linear *recurrence relation* with polynomial coefficients.

Example: $y(z) = \sin z$

$$y''(z) + y(z) = 0 \qquad y(0) = 0, \quad y'(0) = 1$$

D-Finite Functions

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- The sequence of Taylor coefficients of a D-finite functions obeys a linear *recurrence relation* with polynomial coefficients.

Example: $y(z) = K_0(z)$ (modified Bessel function)

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

D-Finite Power Series

[Stanley...]

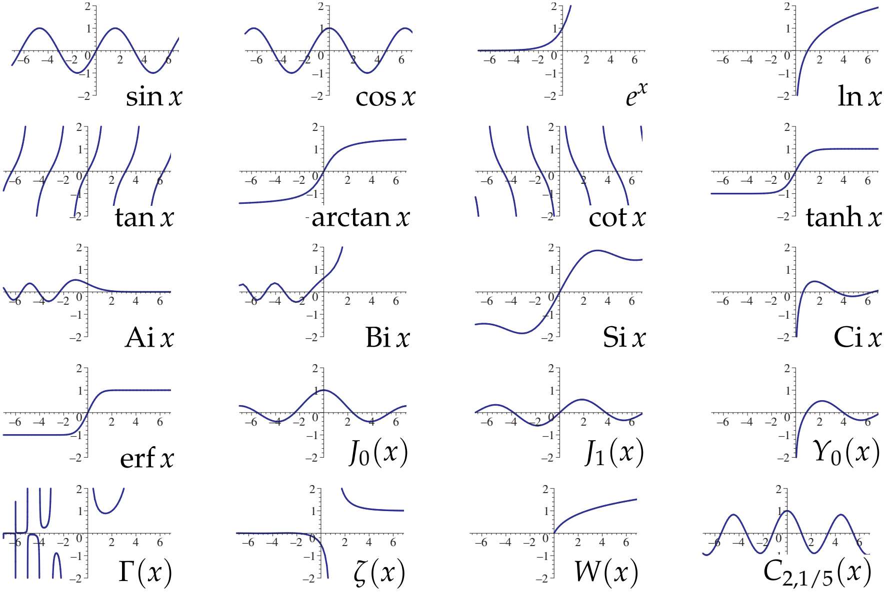
A formal power series $y(z) \in \mathbb{K}[[z]]$ is said to be D-finite (holonomic) iff it satisfies a linear (homogeneous) ODE with polynomial coefficients:

$$a_r(z)\, y^{(r)}(z) + \cdots + a_1(z)\, y'(z) + a_0(z)\, y(z) = 0, \quad a_j \in \mathbb{K}[z].$$

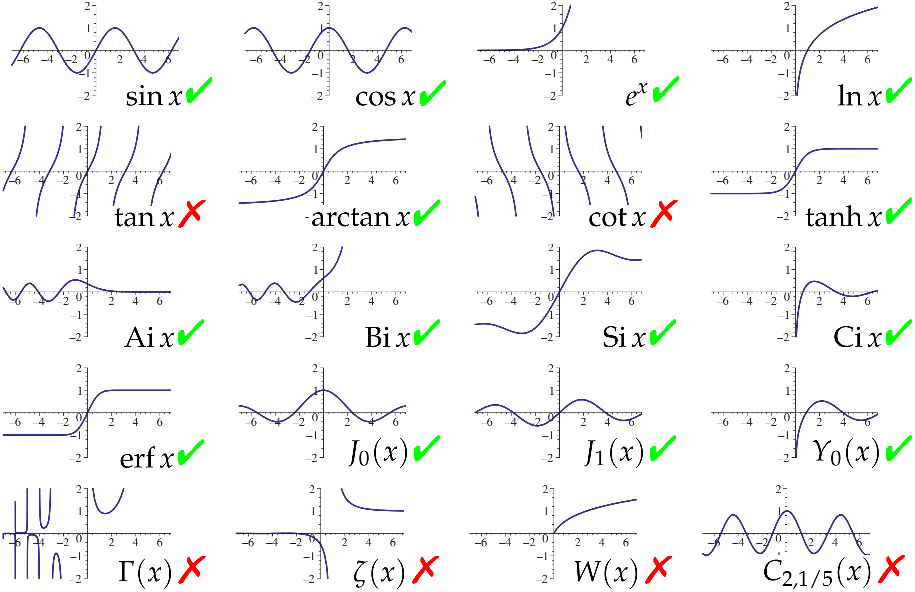
- A formal power series is D-finite iff its coefficients obey a linear recurrence relation with polynomial coefficients.
- Symbolic specifications [Joyal, Flajolet...] translate into algebraic / differential equations

Example: $$y(z) = \sum_{n=0}^{\infty} n! z^n$$
$$z^2\, y''(z) + (3z-1)\, y'(z) + y(z) = 0$$

Elementary and Special Functions

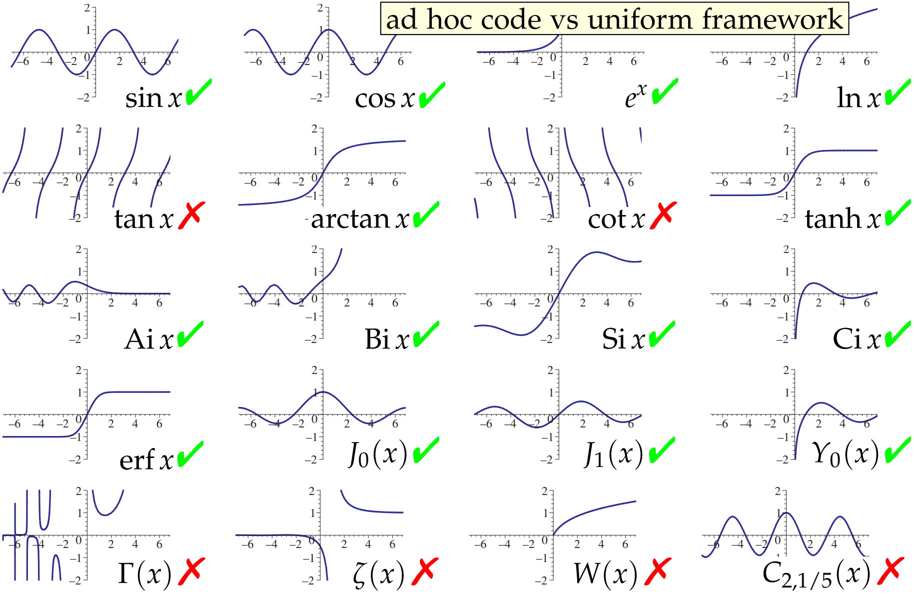


Elementary and Special Functions

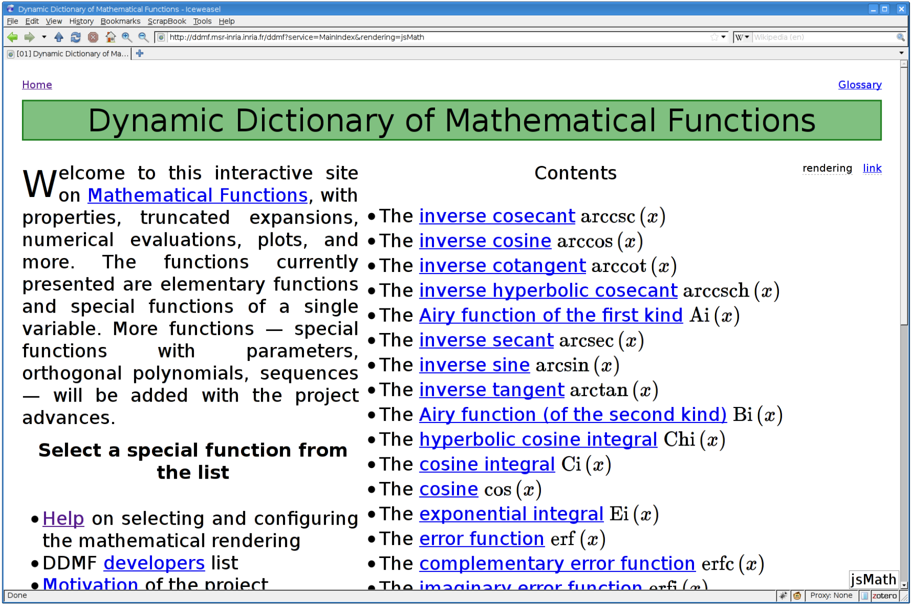


Elementary and Special Functions

ad hoc code vs uniform framework



A Dictionary of D-Finite Functions



A Dictionary of D-Finite Functions

http://ddmf.msr-inria.inria.fr

Home | Glossary

Dynamic Dictionary of Mathematical Functions

Welcome to this interactive site on Mathematical Functions, with properties, truncated expansions, numerical evaluations, plots, and more. The functions currently presented are elementary functions and special functions of a single variable. More functions — special functions with parameters, orthogonal polynomials, sequences — will be added with the project advances.

Benoit, Chyzak, Darrasse, Gerhold, M. & Salvy (2010)
+ Grégoire, Henriot, Koutschan

- DDMF developers list
- Motivation of the project

Contents

rendering link

- The inverse cosecant $\operatorname{arccsc}(x)$
- The inverse cosine $\arccos(x)$
- The inverse cotangent $\operatorname{arccot}(x)$
- The inverse hyperbolic cosecant $\operatorname{arccsch}(x)$
- The Airy function of the first kind $\operatorname{Ai}(x)$
- The inverse secant $\operatorname{arcsec}(x)$
- The inverse sine $\arcsin(x)$
- The inverse tangent $\arctan(x)$
- The Airy function (of the second kind) $\operatorname{Bi}(x)$
- The hyperbolic cosine integral $\operatorname{Chi}(x)$
- The cosine integral $\operatorname{Ci}(x)$
- The cosine $\cos(x)$
- The exponential integral $\operatorname{Ei}(x)$
- The error function $\operatorname{erf}(x)$
- The complementary error function $\operatorname{erfc}(x)$
- The imaginary error function $\operatorname{erfi}(x)$

jsMath

A Dictionary of D-Finite Functions

The Special Function Ai(x) - Iceweasel

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Home Glossary

The Special Function $\mathrm{Ai}(x)$

1. Differential equation

rendering link

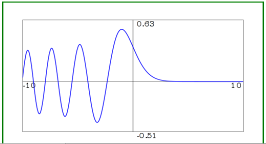
The function $\mathrm{Ai}(x)$ satisfies

$$\frac{d^2}{dx^2} y(x) - x y(x) = 0$$

with initial values $y(0) = 1/3\,\frac{\sqrt[3]{3}}{\Gamma(2/3)}$, $(y')(0) = -1/2\,\frac{\sqrt[6]{3}\,\Gamma(2/3)}{\pi}$.

metadata

2. Plot of $\mathrm{Ai}(x)$



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The Special Function Ai(x) - Iceweasel

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Home

Glossary

The Special

Our data structure:
LODE with polynomial coefficients
+ initial values
(D-finite function)

1. Differential equation

nk

The function $\mathrm{Ai}\,(x)$ satisfies

$$\frac{d^2}{dx^2} y\,(x) - x y\,(x) = 0$$

with initial values $y\,(0) = 1/3\,\frac{\sqrt[3]{3}}{\Gamma(2/3)}$, $(y')\,(0) = -1/2\,\frac{\sqrt[6]{3}\Gamma(2/3)}{\pi}$.

metadata

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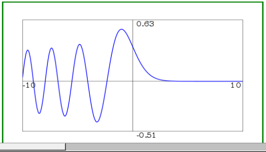

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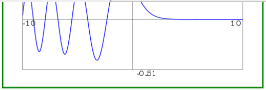
A Dictionary of D-Finite Functions



The Special Function Ai(x) - Iceweasel

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min = -10 max = 10 Submit Query

3. Numerical Evaluation

$$\mathrm{Ai}\,(1/4 + 1/4\,i) \approx 0.28881085 - 0.06285935\,i.$$

metadata

(Below, path may be either a point z or a broken-line path $[z_1, z_2, \ldots, z_n]$ along which to perform analytic continuation of the solution of the defining differential equation. Each z_k should be of the form `x + y*i`.)

path = 1/4+1/4*i precision = 8 Submit Query

4. Taylor expansion of $\mathrm{Ai}\,(x)$ at 0

- Expansion of AiryAi at 0:

$$\mathrm{Ai}\,(x) = \sum_{n=0}^{\infty} 1/3\,\frac{\sqrt[3]{3}x^{3\,n}}{9^n\Gamma\,(n+2/3)\,n!} - 1/9\,\frac{3^{2/3}x^{3\,n+1}}{9^n\Gamma\,(n+4/3)\,n!}.$$

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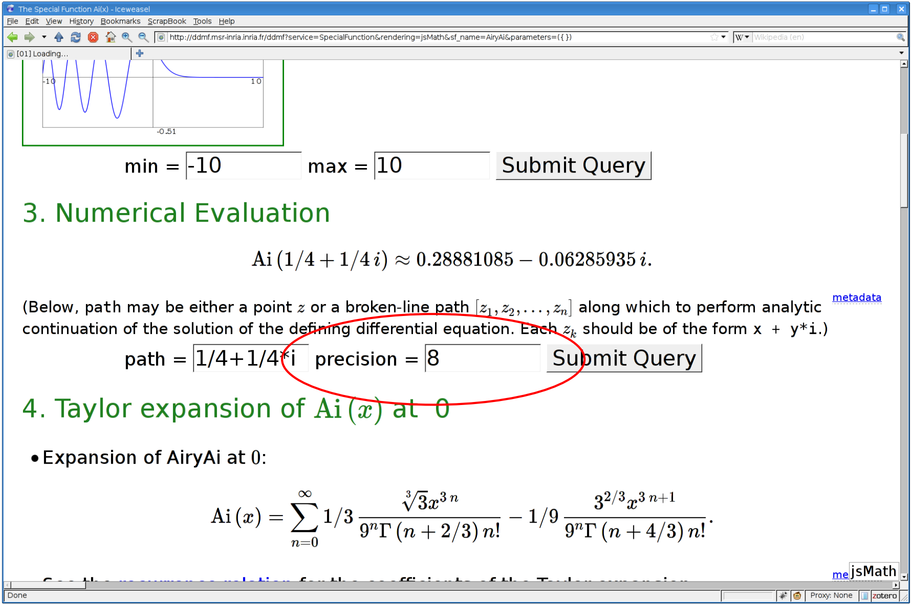
A Dictionary of D-Finite Functions



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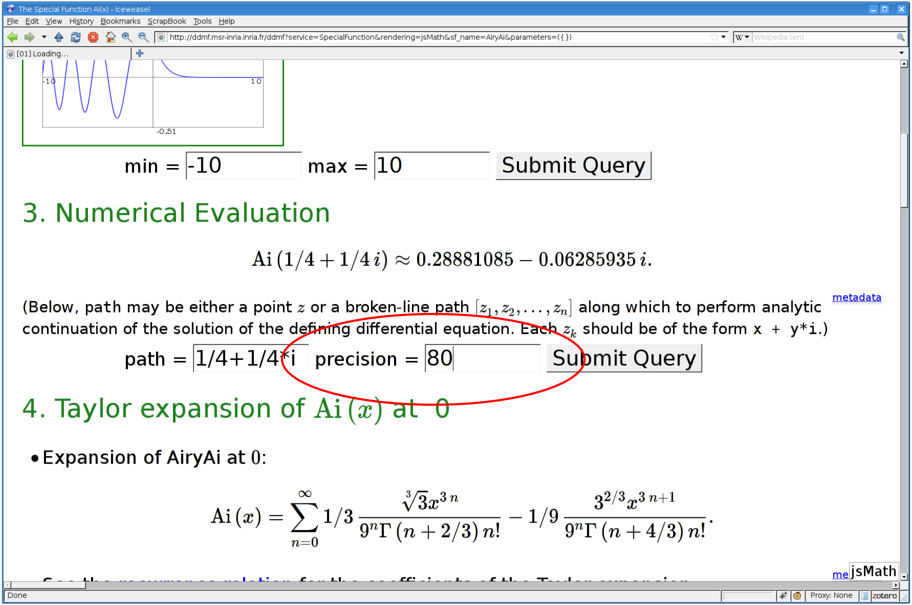

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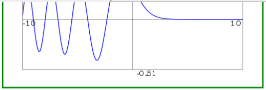

min = -10 max = 10 Submit Query

3. Numerical Evaluation

$$\mathrm{Ai}\,(1/4 + 1/4\,i) \approx 0.28881085384820872173256483671407046811262524805800436861749378392647$$

(Below, path may be either a point z or a broken-line path $[z_1, z_2, \ldots, z_n]$ along which to perform analytic continuation of the solution of the defining differential equation. Each z_k should be of the form x + y*i.) metadata

path = 1/4+1/4*i precision = 80 Submit Query

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- Expansion of AiryAi at 0:

$$\mathrm{Ai}\,(x) = \sum_{n=0}^{\infty} 1/3\, \frac{\sqrt[3]{3}x^{3\,n}}{9^n \Gamma\,(n+2/3)\, n!} - 1/9\, \frac{3^{2/3}x^{3\,n+1}}{9^n \Gamma\,(n+4/3)\, n!}.$$

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The Special Function Ai(x) - Iceweasel
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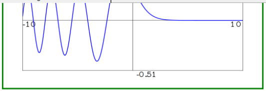

- computed from the ODE
- rigorous error bounds
- arbitrary precision

min = -10 max = 10

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$\mathrm{Ai}\,(1/4+1/4\,i) \approx 0.2888108538482087217325648367140704681126252480580043686174937839264 7$

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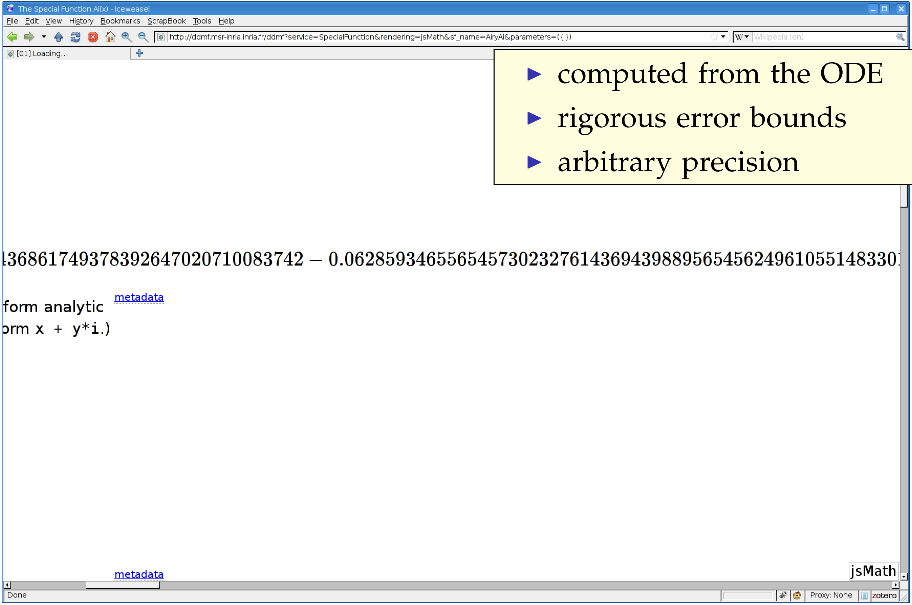

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The Special Function Ai(x) - Iceweasel

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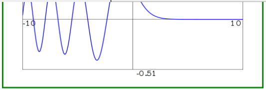

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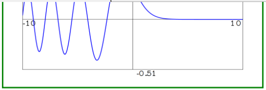

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A Dictionary of D-Finite Functions

The Special Function Ai(x) - Iceweasel

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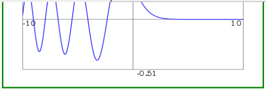

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path = -5 precision = 80 Submit Query

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The Special Function Ai(x) - Iceweasel

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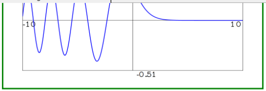

min = -10 max = 10

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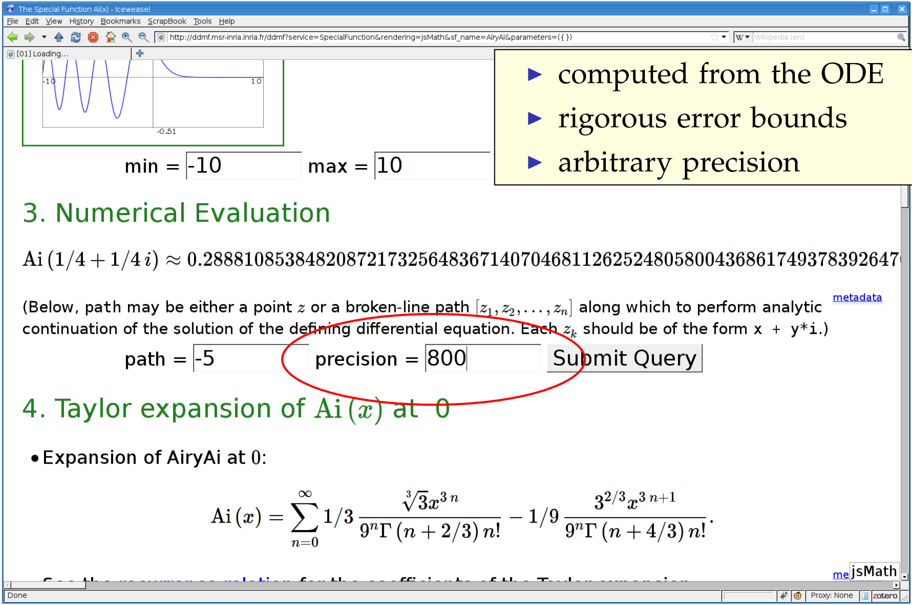

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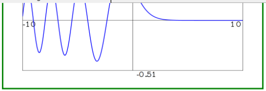

min = -10 max = 10

- computed from the ODE
- rigorous error bounds
- arbitrary precision

3. Numerical Evaluation

$$\mathrm{Ai}\,(-5) \approx 0.350761009024114319788016327696742221484443250893087208211128178049911192682$$

metadata

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path = -5 precision = 800 Submit Query

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NumGfun

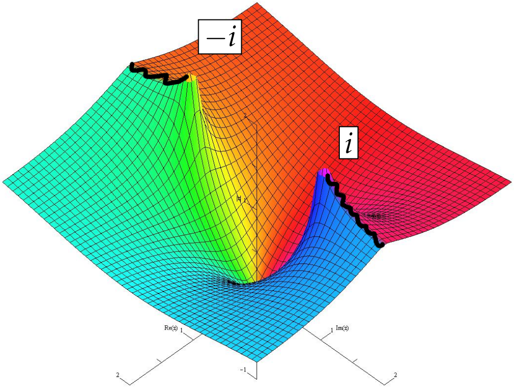
NumGfun

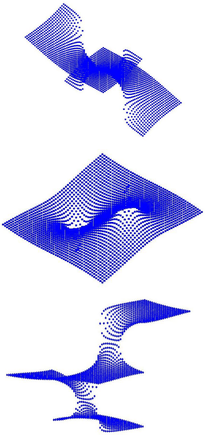
http://algo.inria.fr/libraries/ (GNU LGPL)

http://algo.inria.fr/libraries/papers/gfun.html

- B. Salvy and P. Zimmermann. Gfun: a Maple package for the manipulation of generating and holonomic functions in one variable. ACM TOMS, 1994.
- M. Mezzarobba. NumGfun: a Package for Numerical and Analytic Computation with D-finite functions. ISSAC 2010.
- M. Mezzarobba. Autour de l'évaluation numérique des fonctions D-finies. PhD thesis, École polytechnique, 2011.

arctan z





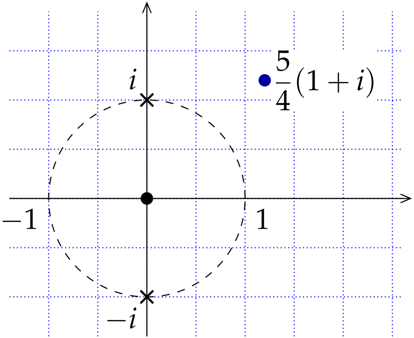
(Re)

(Im)

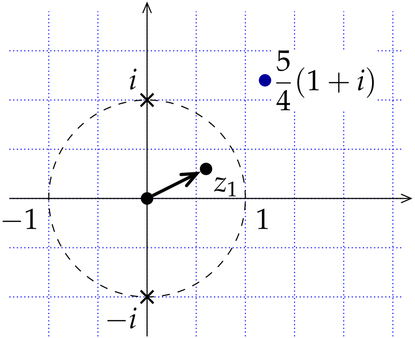
(arg)

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

Numerical Analytic Continuation



Numerical Analytic Continuation



$$\begin{bmatrix} y(z_1) \\ y'(z_1) \end{bmatrix} = \begin{bmatrix} 1 & 0{,}5705170238\cdots + 0{,}2200896807\ldots i \\ 0 & 0{,}7288378766\cdots - 0{,}2065997130\ldots i \end{bmatrix} \begin{bmatrix} y(0) \\ y'(0) \end{bmatrix}$$

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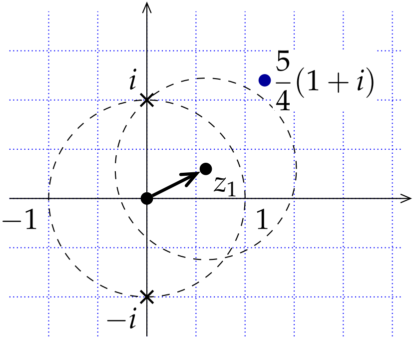

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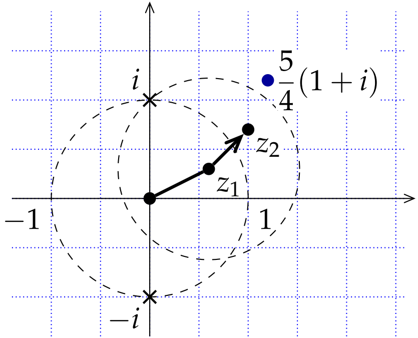

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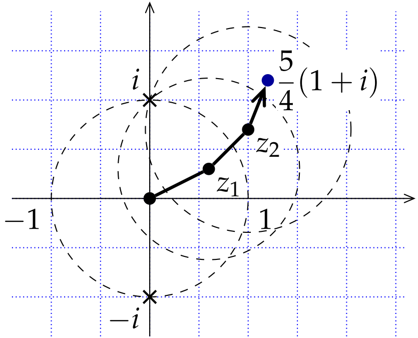
$$\begin{bmatrix} y(z_2) \\ y'(z_2) \end{bmatrix} = \begin{bmatrix} 1 & 0{,}3656231471 \cdots + 0{,}3290407483 \ldots i \\ 0 & 0{,}7515011402 \cdots - 0{,}0792619810 \ldots i \end{bmatrix} \begin{bmatrix} y(z_1) \\ y'(z_1) \end{bmatrix}$$

Numerical Analytic Continuation



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Regular Singular Points

$$z^2\, y''(z) + z\, y'(z) + (z^2 - \nu^2)\, y(z)$$

0 singular point

regular singular

irregular singular

for any solution y,
$\exists N$ s.t. $y(z) \;=\; O(1/|z|^N)$
as $z \;\to\; 0$

Ex.: $y(z) \;=\; z^{\sqrt{2}},\, y(z) \;=\; \dfrac{\log z}{z}$

non-poly. growth
(w.r.t. $1/|z|$) possible
as $z \;\to\; 0$

Ex.: $y(z) \;=\; e^{1/z}$

Solutions at Regular Singular Points

Theorem [Fuchs, 1866]

Assume 0 is a regular singular point of an ODE with meromorphic coefficients.
Then, on some neighborhood D of 0, there exists a basis of solutions of the form

$$z^{\lambda}\left(y_0(z) + y_1(z)\log z + \cdots + y_t(z)\log^t z\right), \quad z \in D \setminus \{0\}$$

where $\lambda \in \bar{\mathbb{Q}}$ and the y_i are analytic on D.

Asympotics of Linear Recurrence Sequences

This is AsyRec, A Maple package accompanying Doron Zeilberger's article:

It finds the asymptotics of solutions of (homog.) linear recurrence equations with polynomial coefficients, using the Birkhoff-Trjitzinsky method .

```
> recop := (n+2)^2*N^2-(7*n^2+21*n+16)*N-8*(n+1)^2;
```

$$recop := (n+2)^2 N^2 - (7n^2 + 21n + 16) N - 8 (n+1)^2$$

```
> AsyC(recop, n, N, 5, [2, 10], 1000);
```

0.36755259694786136634,

$$\frac{8^n \left(1 - \frac{1}{3n} + \frac{1}{27n^2} + \frac{1}{81n^3} + \frac{1}{243n^4} + \frac{11}{2187n^5}\right)}{n}$$

[Wimp & Zeilberger 1985, Zeilberger 2008-2009]

Singularity Analysis

[Flajolet, Odlyzko]

Principle

asymptotic behaviour of $y(z) = \sum_n y_n z^n$ at its singularities

$$\Big\downarrow \text{ mechanical transfer}$$

asymptotic behaviour of (y_n) at infinity

- Constants by singularity analysis
  + numerical analytic continuation
  [Flajolet & Puech 1986]

Outlook

D-Finite Functions in Sage

What is there

- ~~Nothing right now~~
- Arithmetic of diff. operators via Plural's G-algebras

Main goals

Modern versions of the main features of

- gfun
- Mgfun
- NumGfun
- (part of) DEtools
- ...

A more ambitious goal

D-Finite functions as "first-class citizens"

Use them to implement special functions

(Cf. DDMF)

Developments Planned or in Progress (that I know of)

- Fredrik Johansson, Manuel Kauers, Maximilian Jaroschek
  `ore_algebra` 0.1 released two days ago!
  Ore operators, closure properties, guessing…
- ANR Magnum
  tools for analytic combinatorics project(?)
- Matthieu Dien, Marguerite Zamansky
  multivariate lazy power series prototype
- Eviatar Bach (mentored by Burcin Erocal and Flavia Stan)
  special functions, in part via D-finiteness GSOC project

Beyond NumGfun

Why Maple?

Historical reasons...
It was a pain.

Current plans

- C/C++ library
- basic analytic continuation code in `arb`
  (with Fredrik Johansson)
- Sage interface?

Wishlist

	Maple	Sage
a compiled language	✗	limited
a type system	✗	✗
sane semantics	✗	✓
differential operators, D-finite funs	✓	soon?
floating-point, interval arithmetic	minimal	✓
algebraic numbers	limited	✓ (?)
symbolic special functions, branch cuts...	✓	minimal
asymptotics	✓	✗
ability to fix/extend the system!	✗	✓

Making Numerics Reliable

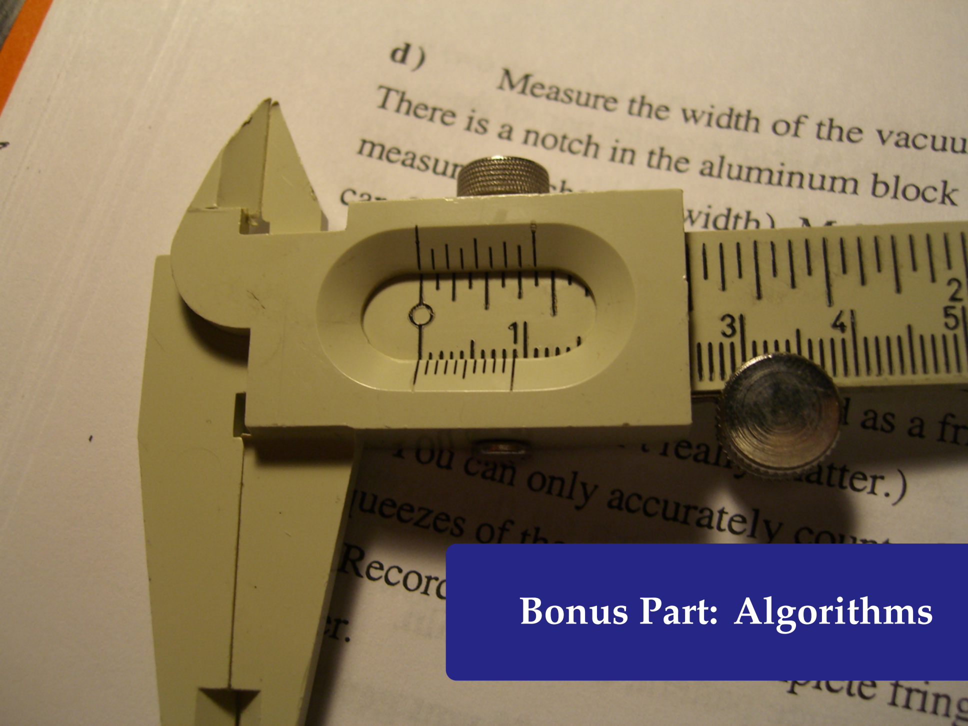
Real/complex mid-rad interval arithmetic, aka ball arithmetic

$$(3.1415926535897932384626433832 8, \quad 2\cdot 10^{-30})$$

multiple-precision floating-point number

machine precision (rel?) error bound

- Make balls the default for `RR`, `CC`?
- ...in a backward-compatible way?
- Functions that do not provide guaranteed results would still be allowed to return (accurate-in-practice result, ∞)



Bonus Part: Algorithms

Evaluation Algorithm

[Chudnovsky & Chudnovsky 1988]

Main Ideas

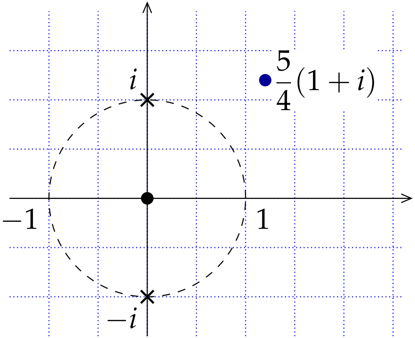
0 fast integer multiplication

1 binary splitting

2 analytic continuation

3 *bit burst*

2. Taylor series method for ODEs



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

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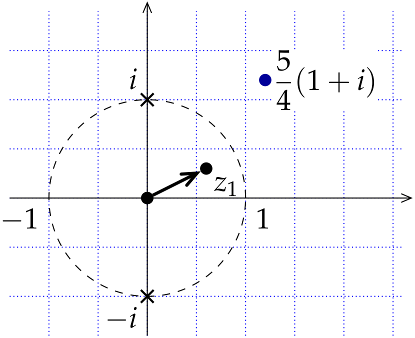

$$\arctan\left(\frac{5}{4}(1+i)\right) = ?$$

$$\begin{bmatrix} y(z_1) \\ y'(z_1) \end{bmatrix} = \begin{bmatrix} 1 & 0{,}570\ldots+0{,}220\ldots i \\ 0 & 0{,}728\ldots-0{,}206\ldots i \end{bmatrix} \begin{bmatrix} y(0) \\ y'(0) \end{bmatrix}$$

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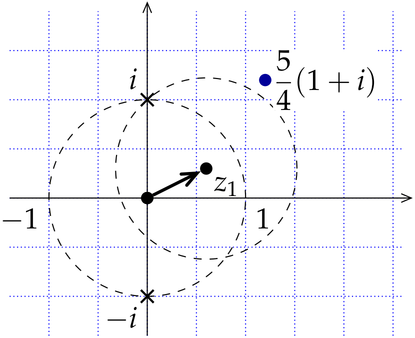

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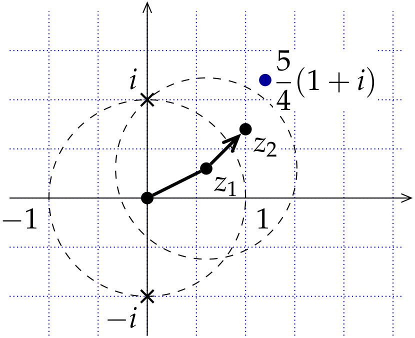

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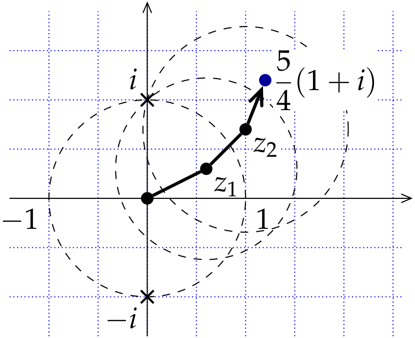

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$\dots$

Evaluation Algorithm

[Chudnovsky & Chudnovsky 1988]

Main Ideas

0 fast integer multiplication
1 binary splitting
2 analytic continuation
3 *bit burst*

0. One can multiply two integers of $\leqslant n$ bits in $M(n) = O(n \log n \, 2^{O(\log^* n)})$ bit ops [Fürer 2007].

Evaluation Algorithm

[Chudnovsky & Chudnovsky 1988]

Main Ideas

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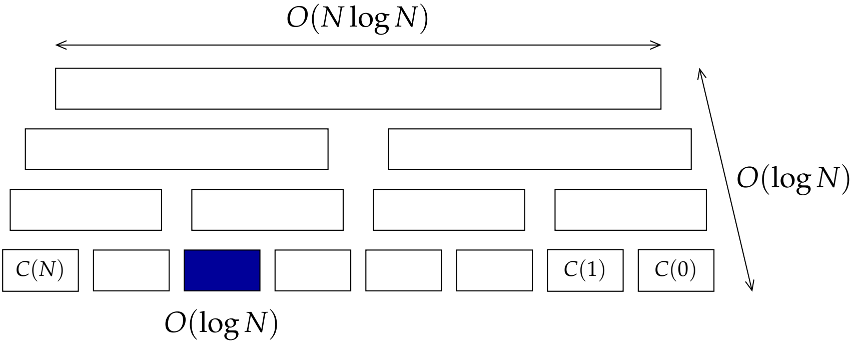
1. Within the disk of convergence of a Taylor expansion: fast series summation algorithm based on the recurrence



Evaluation Algorithm

[Chudnovsky & Chudnovsky 1988]

Main Ideas

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3 *bit burst*

3. High-precision inputs:
   use analytic continuation even if the series converges!

$$\begin{aligned} z_0 = 10_2 &\to z_1 = 10{,}1_2 \\ &\to z_2 = 10{,}101_2 \\ &\to z_3 = 10{,}1011011_2 \\ &\to z_4 = 10{,}101101110010100_2 \\ &\to \ldots \\ &\to z \ = 10.10110111001010011000 \ldots\ldots_2 \simeq e \end{aligned}$$

$\sin(e) = \sin(2{,}718...) = ?$

Evaluation Algorithm

[Chudnovsky & Chudnovsky 1988]

Main Ideas

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3 *bit burst*

Theorem

[(Chudnovsky^2, van der Hoeven, M.)]

The evaluation point z being fixed, one may compute $y(z)$ with error bounded by 2^{-n} in

$$O\Big(M(n \cdot (\log n)^2)\Big)$$

bit operations using $O(n)$ bits of memory.

Error Bounds

$$\sum_{n=0}^{\infty} y_n z^n = \sum_{n=0}^{N-1} y_n z^n + \underbrace{\sum_{n=N}^{\infty} y_n z^n}_{?}$$

Compute suitable truncation orders (and other bounds)?

A priori bounds tend to be easier to use in fast algorithms.

Bounds

[van der Hoeven, M. & Salvy]

Idea: Replace y, by a simpler function that “dominates” it.

Differential equation / Recurrence

Bound Parameters

$\kappa, \alpha, \ldots \in \mathbb{Q}$ or $\bar{\mathbb{Q}}$ s.t.

$$|y_n| \leqslant n!^{\kappa} \cdot \alpha^n \cdot \varphi(n)$$

Main Tools:
Cauchy majorants
Saddle-point method

Symbolic Bounds

- Human-Readable (as far as possible!)
- Asymptotically tight

Numeric Bounds

- Conservative approx. of parameters
- Faster (no algebraic numbers)

Credits

The following images were used in this document:

- *Tables of the error function and its derivative*. US National Bureau of Standards, 1954 (public domain)
- `http://commons.wikimedia.org/wiki/File:2011-06-14_10-25-33_Austria_Niederösterreich_Mannsdorf_an_der_Donau.jpg` (by Hansueli Krapf, Creative Commons Attribution-Share Alike 3.0 Unported)
- `http://commons.wikimedia.org/wiki/File:Calipers_in_physics_lab.jpg` (by User:Falcorian, Creative Commons Attribution-Share Alike)