Numerical Evaluation of D-Finite Functions in SageMath

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> ICMS 2016, Berlin July 11th, 2016

arxiv:1607.01967 [cs.SC]

A Non-Scientific Aside

Rigorous Multiple-Precision Evaluation of D-Finite Functions in SageMath

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Abstract. We present a new open source implementation in the Sage-Math computer algebra system of algorithms for the numerical solution of linear ODEs with polynomial coefficients. Our code supports regular singular connection problems and provides rigorous error bounds.

1 Introduction

Many special functions satisfy differential equations

$$p_r(x)f^{(r)}(x) + \cdots + p_1(x)f'(x) + p_0(x)f(x) = 0$$
 (1)

whose coefficients p_i depend polynomially on the variable x. In virtually all cases, such special functions can be defined by complementing (1) either with simple initial values f(0), f'(0),... or with constraints on the asymptotic behavior of f(x) as x approaches a singular point. For example, the error function satisfies

$$\operatorname{erf}''(x) + 2x \operatorname{erf}'(x) = 0$$
, $\operatorname{erf}(0) = 0$, $\operatorname{erf}'(0) = \frac{2}{\sqrt{\pi}}$,

while the modified Bessel function K_0 is the solution of

 $xK_0''(x) + K_0'(x) - xy(x) = 0$ s.t. $K_0(x) = -\log(x/2) - \gamma + O_{x\to 0}(x)$. (3)

This observation has led to the idea of developing algorithms that deal with these functions in a uniform way, using the ODE (1) as a data structure [11.2]. In this context, solutions of linear ODEs with polynomial coefficients are called *Definite* (or holonomic) functions. These names originate from combinatories, where D-finite power series arise naturally as generating functions [17.4]. While classical saccial functions trucingly satisfy ODEs of order 2 to 4 with simple

* Supported in part by ANR grant ANR-14-CE25-0018-01 (FastRelax).

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Extended abstract for a talk given at the 5th International Congress on Mathematical Software (ICMS 2016), Accepted for publication in the proceedings, but withdrawn due to a disarreement with Sortinger about the above public domain notice. "This article is in the public domain. In jurisdictions where this is not possible, any entity is granted the perpetual right to use this work for any purpose, without any condition other that those required by law."

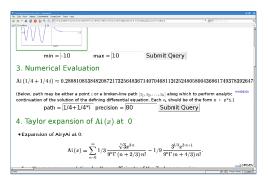
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What it Is: A Successor for NumGfun



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

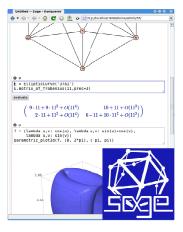
[Benoit, Chyzak, Darrasse, Gerhold, Grégoire, Koutschan, M., Salvy 2010–]

NumGfun

[M. 2010]

- General D-Finite functions
- Arbitrary precision
- Rigorous error bounds
- Maple
- Oriented towards special functions

What it Is: A SageMath Implementation



- Python library
- "A viable alternative to Magma, Maple, Mathematica and Matlab"

sage: Pols.<z> = PolynomialRing(QQ)

sage: Pols

Univariate Polynomial Ring in z

sage:
$$(z + 1)*(z-1)$$

 $z^2 - 1$



http://sagemath.org/

GNU GPL v2+

What it Is: Based on ore_algebra

[Kauers, Jaroschek, Johansson, 2013-]

sage: from ore_algebra import OreAlgebra

sage: DiffOps.<Dz> = OreAlgebra(Pols)

sage: DiffOps

Univariate Ore algebra in Dz over Univariate Polynomial Ring

in z over Rational Field

sage: Dz*z

z*Dz + 1

Features: Euclidean arithmetic, closure properties, formal solutions, desingularization, first-order factors, guessing...



http://www.risc.jku.at/research/combinat/software/ore_algebra/

What it Is: The -analytic Branch

- Symbolic-numeric extensions for ore_algebra
- Real & complex arithmetic based on Arb ({Real,Complex}BallField in Sage)

[Johansson 2012-]

- Both for "end users" and for prototyping algorithms
- Development branch, not (yet) integrated into any release of ore_algebra



http://marc.mezzarobba.net/code/ore_algebra-analytic
GNU GPL v2+

What it Does: Special Functions

```
sage: diffop = Dz^2 - z
sage: diffop.numerical_solution(
        [1/(gamma(2/3)*3^(2/3)), -1/(gamma(1/3)*3^(1/3))],
        [0, i], 1e-40)
   [0.3314933054321411889845293326171343458866 +/- 5.51e-41] +
   [-0.31744985896844377347764292790925852645896 +/- 7.23e-42]*I
sage: ComplexBallField(138)(i).airy_ai()
   [0.33149330543214118898452933261713434588655 +/- 5.25e-42] +
```

[-0.31744985896844377347764292790925852645896 +/- 1.59e-42]*I

What it Does: Polynomial Approximations

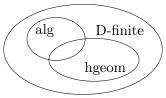
```
sage: diffop
   Dz^2 - z
sage: from ore_algebra.analytic import
      polynomial_approximation as polapprox
sage: polapprox.on_interval(diffop,
        [1/(gamma(2/3)*3^(2/3)), -1/(gamma(1/3)*3^(1/3))],
        [[-1,1]], 1e-10)
   [-0.0005136124318 +/- 3.11e-14]*z^7 + [0.001972375574 +/-
   5.11e-13*z^6 + [2.373692757e-8 +/- 1.52e-18]*z^5 + [-
   0.021568281826 +/- 7.76e-13*z^4 + [0.05917133936 +/- 2.27e-
   12|*z^3 + [-3.780865636e-10 +/- 3.16e-20|*z^2 + [-3.780865636e]
   0.2588194037 + / - 2.12e-11 *z + [0.3550280539 + / - 2.94e-11]
```

What it Does: D-Finite Functions

[Stanley, Zeilberger... 1980-]

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

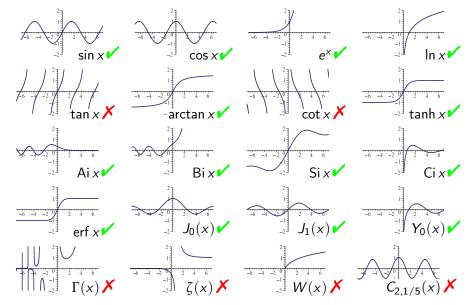
$$a_r(z) y^{(r)}(z) + \cdots + a_1(z) y'(z) + a_0(z) y(z) = 0, \qquad a_j \in \mathbb{K}[z]$$



Philosophy:

Provide **general algorithms** for D-finite functions, using { ODE + initial values } as a data structure.

What it Does: D-Finite Functions



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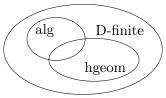
Numerical Evaluation of D-Finite Functions in Sage

What it Does: D-Finite Functions

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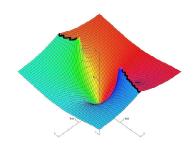
$$a_r(z) y^{(r)}(z) + \cdots + a_1(z) y'(z) + a_0(z) y(z) = 0, \qquad a_j \in \mathbb{K}[z]$$



Philosophy:

Provide **general algorithms** for D-finite functions, using { ODE + initial values } as a data structure.

What is Does: Analytic Continuation



$$y(z) = \arctan(z)$$

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

```
sage: dop = (z^2+1)*Dz^2 + 2*z*Dz
sage: dop.numerical_solution(
        ini=[0,1], path=[0,1])
   [0.78539816339744831 +/- 1.08e-18]
sage: dop.numerical_solution(
        ini=[0,1],
        path=[0,i+1,2*i,i-1,0,1])
   13.9269908169872415
        +/- 4.81e-171
  + [+/- 4.63e-21]*I
```

What it Does: Transition Matrices

$$f(z) = 1 \qquad = 1 + 0 \cdot z + O(z^2)$$

$$g(z) = \arctan(z) \qquad = 0 + 1 \cdot z + O(z^2)$$

$$\left[\begin{array}{c} \square & \square \\ \square & \square \end{array} \right] = \left[\begin{array}{c} f(1) & g(1) \\ f'(1) & g'(1) \end{array} \right]$$

What it Does: Regular Singular Points

The previous examples only involved **ordinary** (= non-singular) points.

$$z^2 y''(z) + z y'(z) + (z^2 - \nu^2) y(z) = 0$$

0 singular point; regular in this case

Theorem [Fuchs, 1866]

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

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

Examples: $z^{\sqrt{2}}$, $z^{-3/2} \log z$

What it Does: Regular Singular Connection Problems

$$\begin{bmatrix} y(1) \\ y'(1) \end{bmatrix} = \begin{bmatrix} \Box & \Box \\ \Box & \Box \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} \quad \text{where } y(z) = a \log z + b + O(z)$$

Applications: special functions, analytic combinatorics, resummation...

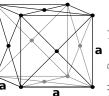
```
sage: dop4 = ((-1 + z)*z^3*(2 + z)*(3 + z)*(6 + z)*(8 + z)*(6 + z)*(8 + z)*(9 + z)*(
                                                           z)*(4 + 3*z)^2*Dz^4 + 2*z^2*(4 + 3*z)*(-3456 - 2304*z + 3*z)*(-3
                                                           3676*z^2 + 4920*z^3 + 2079*z^4 + 356*z^5 + 21*z^6)*Dz^3
                                                            + 6*z*(-5376 - 5248*z + 11080*z^2 + 25286*z^3 +
                                                            19898*z^4 + 7432*z^5 + 1286*z^6 + 81*z^7)*Dz^2 + 12*(-
                                                           384 + 224*z + 3716*z^2 + 7633*z^3 + 6734*z^4 + 2939*z^5
                                                            + 604*z^6 + 45*z^7)*Dz + 12*z*(256 + 632*z + 702*z^2 +
                                                           382*z^3 + 98*z^4 + 9*z^5)
sage: dop4.local_basis_monomials(0)
```

 $[1/6*log(z)^3, 1/2*log(z)^2, log(z), 1]$

sage: dop4.local_basis_monomials(1)

$$[1, (z - 1)*log(z - 1), z - 1, (z - 1)^2]$$





 $dop6 = 410085196915322880 z^{35} + 112905266474211563520 z^{34} + 1171669263761496$ $1489920z^{33} + 690817401287078917363200z^{32} + 27204862643846611522761600z^{31} +$ $778811406918247228618497600 z^{30} + 17044384124115240781429792800 z^{29} + 294245234$ $066850000428339092800 z^{28} + 4083424587805117060272476125800 z^{27} + 459730295491197962$ $35386142827300 z^{26} + 419695598890898253203455876749930 z^{25} + 30642971761740916717179$ $85958725620 z^{24} + 17169584489259696388755804636033570 z^{23} + 645817719616848100772794$ $3401088177035093275526304300 z^{16} - 3528341032098896995323439017117956856150 z^{15} 7964369518593778029521056070442794466900 z^{14} - 1428050072616278625471284116387500$ $19522403983976171775697600000 z^9 + 21137039158366320685856256980012112000000 z^8 +$ $226826935539348046904466472955088000000000 z^7 + 149381834281462611905463546716160 \lor$ $2452480000000000 z^4 - 110432794077974589015077314560000000000 z^3 - 353898708207580$

 $(3964156903514787840 z^{36} + 1104718489963413534720 z^{35} + 117871088739930352834560 z^{34} +$ 7183287516644479615795200 $z^{33} + 293105835218942903781855360 z^{32} + 870657237873$ $3851120z^{29} + 51457898672013865098111291247320z^{28} + 60652283497953184068452162523$ $7020z^{27} + 5835366836846027182876920856348950z^{26} + 4545520250182635897460621998197$ $4015 z^{25} + 279153404467502062948531557838260750 z^{24} + 125227539937283713406150704262$ $216920199750 z^{21} - 169948182933507479161257565568616530700 z^{20} - 1154969594776277160$ $649077785983820553870 z^{19} - 5548694490781020038019823355124585193590 z^{18} 20745229517577451272377158241970915439245\,z^{17} - 62232963928794638659423069651761 \backslash$ $3578764537043031861206473715269343000 z^{12} - 31297658464933476345181066385800419642$ $948027345434850305279520000000 z^7 + 18060134934884299834847099345568000000000 z^6 100213400891192102370293326036992000000000z^5 - 83859064515985136495903099458560$ 03372544000000000000000) Dz +

 $(8133356405487237120z^{37} + 2294131782043664317440z^{36} + 251295328534762193633280z^{35} +$ $15795453015240816970091520 z^{34} + 666093618246765502077439680 z^{33} + 2046937571$ 7991216960 $z^{30} + 134696914854304536722281866954300$ $z^{29} + 165183365498487607982012588$ $46813455 z^{26} + 895865319327471447638111289873238710 z^{25} + 44897110742643849065299259$ $174648133542750 z^{22} - 386265894549826881229123104470731096440 z^{21} - 3163259131060568$ $584546113343781987561220 z^{20} - 16636182069413821170544684047556220568150 z^{19} 66246740089393676080981537130378090658525\,z^{18} - 2090802458728506315663121374496195\backslash$ $61543730 z^{17} - 529097465740104776391772834675033946593335 z^{16} - 10650386207573139293$ 91639361032363453750930 z^{15} - 1653651644685620142167009422124022555221700 z^{14} - 1829\ $383474513975929874027770563298831967800 z^{13} - 108870989683690580666028414927762156$ $0000 z^7 - 1334658535726482371536908049179648000000000 z^6 - 941977534006524837182879$ $892148234640584704000000000000000z^3 - 37458505751548575098585088000000000000000000z^2 +$ 0000) $Dz^2 +$

 $(6219625486549063680 z^{38} + 1775531336308022522880 z^{37} + 199409996635132589752320 z^{36} +$ $12904862497592448920163840 z^{35} + 561222248755128125708191680 z^{34} + 17798695421$ $6897880 z^{27} + 1015534278806669843159745327151252620 z^{26} + 54963382760530760750687544$ $63346793150591937974700130 z^{21} - 17566486109105161467894504789161406270600 z^{20} 73673650638461574538679743097050051115220z^{19} - 24040743896755739891331729697533$ $3795990859905959226579320 z^{16} - 1835553795134837646262350779261931882894750 z^{15} 98684069708388548285600000\,z^{11} + 3777365646243762653104795884206143332000000\,z^{10} +$ $4908954989144320000000000 z^6 - 893959103422093803323305262745600000000000 z^5 - 1000 \setminus 1000 + 100$ $83705719332806676962561024000000000000 z^4 + 2564203084567737476418017280000000000$ 00000000000000z) Dz³ +

 $(2192816677949990400 z^{39} + 633490213477308768000 z^{38} + 72864986011484455353600 z^{37} +$ $4847486869795537260532800 z^{36} + 217014017048761645614816000 z^{35} + 708801699580$ $8676620z^{32} + 56201587732740449959670675451690z^{31} + 73584775932673052902450424098$ $4110 z^{28} + 508882813920850610699235633677324220 z^{27} + 291338677229064650128281265554$ $8475524386210 z^{24} - 84400724272601405065271773264397209530 z^{23} - 1309329548085768562$ $973129072537724164955 z^{22} - 8229269199062442444264260234977847805360 z^{21} 35948740918844475140318574840001115213670 z^{20} - 1192466813203331345939144884033$ $0697311126386896036767490 z^{17} - 707778167790136602728038144967670916837350 z^{16} 95068892397133773199630362250506960000000 z^{10} - 322447694713681036240924354097202$ $159256944109024208981780480000000000000 z^5 + 11283852768448237101798156288000000000$ $00000000000000 z^2) Dz^4 +$

 $(390720062616543744 z^{40} + 114216661424360307456 z^{39} + 13440822351615963069696 z^{38} +$ $917965180366474611870720 z^{37} + 42237673932263775988570560 z^{36} + 14182188393104$ $2720z^{33} + 12205694666919011642462560650930z^{32} + 16425102239444377898676373653$ $4191 z^{29} + 124533460849620200009711445328730256 z^{28} + 743593796442908540070532245488$ $4390547047\ z^{25} - 9198824722943404205447421299404277112\ z^{24} - 27944986880240251417567 \setminus 10^{-2}$ 7041789492570017 z^{23} - 1907863427661939885576723126598906643790 z^{22} - 85740836464757\ $10050757565542672979674555 z^{21} - 28405587296847231070183606856583770811720 z^{20} 69574258175312955514440713973653616428745z^{19} - 11499143689248771166993784982491$ $2517430330 z^{18} - 70378017201579863364495432167182725333675 z^{17} + 2616419665010891478$

 $(35882454730090752 z^{41} + 10612604051614486656 z^{40} + 1276532600942212775168 z^{39} +$ $89393980129433032096320 z^{38} + 4221606838983473228197008 z^{37} + 145494567985766484$ $898923048 z^{36} + 3840828004490920060950969480 z^{35} + 80160062388267727172211985080 z^{34} +$ $15796834464054711973645322142 z^{31} + 1986708322085667572665525016037411 z^{30} + 1526308$ $2383031406770429022758762048 z^{29} + 94068732852089205756130773605094705 z^{28} + 4410553$ $26809673226795399591264079041112 z^{25} - 31072001737970299221405533198706303141 z^{24} 226886176666918560987240200768631693150z^{23} - 1033954017266382248984767586852072$ $344191 z^{22} - 3356732946224373601649087937349109785896 z^{21} - 757312621278500761889122 \setminus 344191 z^{22} - 3356732946224373601649087937349109785896 z^{21} - 757312621278500761889122 \setminus 344191 z^{22} - 34419 z^{22} - 344191 z^{22} - 34419 z^{22} - 34419 z^{22} - 34419$ $5542456994124245 z^{20} - 9076459539413303184641722134776573895810 z^{19} + 10278671248090$ $335377408918358815408788425 z^{18} + 85149274357043292385925033653294291853550 z^{17} +$ $6871562346484465378000000\,z^{13} - 119682652007548350954457856750250720000000\,z^{12} -$

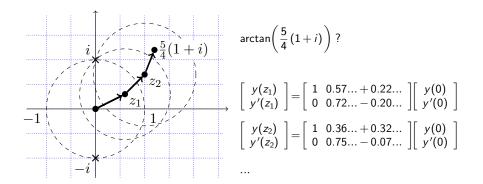
 $040421804170816 z^{39} + 204216444469816446653424 z^{38} + 7214118624119937529541160 z^{37} +$ $357395670676 z^{32} + 112862055818213392356279768225402 z^{31} + 8863404948364755698667411$ $4079724 z^{28} + 85059388463264142313662526542420618 z^{27} + 2481695683318164448040331315$ 2741167478185137320 $z^{22} - 367088786736715063908412462166156515566$ $z^{21} - 136331238303$ $988349001415414181532146340 z^{20} + 2052937632229799753666758504303681446150 z^{19} +$ $8942220864711302092023950168348534856300z^{18} + 22112779083456047399791690319673356$ $808000 z^{17} + 36662299830964853548300895468723502480000 z^{16} + 38663936209054739955701 \setminus$ $110778754739301057544560000000\,z^{13} - 45957581844555068108338692961807200000000\,z^{12} 0000000 z^{10} + 10970395301506611292814537164800000000000 z^9 + 9713112405197935942595$ $53382400000000000 z^8 + 42609787194207838925037772800000000000 z^7 + 7564670791225$

 $(27122036833024 z^{43} + 8208413201024064 z^{42} + 1028987679702510976 z^{41} + 75518451)$ $137118783792z^{40} + 3743195619381989907184z^{39} + 135369638077546936261428z^{38} + 374561$ $5314367420203992832 z^{37} + 81811619367860049045984675 z^{36} + 144046663724820391377433$ $4250z^{35} + 20724331113040275023719172850z^{34} + 245446627541652046097792768214z^{33} +$ $63963621496746370188659696702 z^{30} + 602621255648485924378700672331054 z^{29} + 19351926$ 818935455901289133872622 $z^{26} - 297645962803933196564873733670191774$ $z^{25} - 1329742929$ 5534019664017777438417359311914 $z^{22} + 7565280951156009750992823479550694170$ $z^{21} + 7565280951156009750992823479550694170$ $83328126336960183101771239549883786325z^{20} + 29785983697247118038201732716290595$ $4310017920000 z^{17} + 974982625144110654834660688990434600000 z^{16} + 809214817274247946$ $000000000000 z^8 + 2995053035474379315363840000000000000 z^7 + 227699120806114222080$ $0000000000000000 z^6) Dz^8$

order 8, degree 43, 43-digit coefficients

(Wall time: $\approx 10 \text{ min}$)

How it Works: A Taylor Series Method



At each step, compute the sum of the power series expansion of each entry of the transition matrix.

The idea extends to the regular singular case.

How it Works: 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.)

Leads to fast algorithms (not fully implemented yet)

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

Best complexity: time $O(M(n \log^2 n))$, space O(n)for fixed z and $\varepsilon = 2^{-n}$

How it Works: Error Bounds

Truncation Error

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

Majorants [Cauchy; ...; van der Hoeven 2001; M. & Salvy 2010; M. 2016 ?]

Bound the differential equation with a simple "model equation":

$$y'(z) = a(z) y(z)$$
 \ll $g'(z) = \frac{1}{(1-\alpha z)} g(z)$

Solve the model equation and study the solutions:

$$\left|\sum_{k=n}^{+\infty} y_n z^n\right| \leqslant \sum_{k=n}^{+\infty} g_n |z|^n \leqslant ?$$

• ... Using the **residuals** $L(y_0 + \cdots + y_{n-1}z^{n-1})$ to obtain tight bounds



Summary

What it is: an extension of ore_algebra written in/for SageMath What it does: numerical analytic continuation & singular connection, for arbitrary D-finite functions, with rigorous error bounds How it works: Taylor series, analytic continuation, recurrences, majorants, ball arithmetic...



Code available at

 $\verb|http://marc.mezzarobba.net/code/ore_algebra-analytic|$



Perspectives

Fast algorithms, lower-level code, evaluation on intervals, D-finite functions as objects, irregular singular connection problems [van der Hoeven 2006]...

Comments, bug reports, feature requests, examples welcome!

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