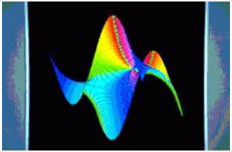
Rigorous Uniform Approximation of D-finite Functions

Alexandre Benoit (INRIA),
Joint work with
Mioara Joldeș (ENS Lyon, INRIA) and Marc Mezzarobba (INRIA)

March 16, 2011

MICROSOFT RESEARCH INRIA JOINT CENTRE

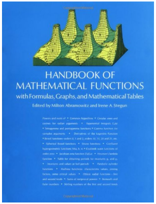


I Introduction

Approximation of D-finite Functions

Definition

A function is D-finite if it is solution of a linear differential equation with polynomial coefficients.



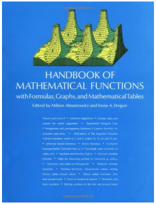
Examples

About 60% of Abramowitz & Stegun
cos, arccos, Airy functions, Bessel functions, ...

Approximation of D-finite Functions

Definition

A function is D-finite if it is solution of a linear differential equation with polynomial coefficients.



Examples

About 60% of Abramowitz & Stegun
cos, arccos, Airy functions, Bessel functions, ...

How can we approximate a D-finite function f?
Polynomial approximation:

$$f(x) \approx \sum_{i=0}^{n} f_i x^i$$

Uniform Approximation of D-finite Functions

Problem

Given an integer d, and a D-finite function f specified by a differential equation with polynomial coefficients and suitable boundary conditions, find the coefficients of a polynomial $p(x)$ of degree d and a "small" bound B such that $|p(x) - f(x)| < B$ for all x in $[-1, 1]$.

Uniform Approximation of D-finite Functions

Problem

Given an integer d, and a D-finite function f specified by a differential equation with polynomial coefficients and suitable boundary conditions, find the coefficients of a polynomial $p(x)$ of degree d and a “small” bound B such that $|p(x) - f(x)| < B$ for all x in $[-1, 1]$.

Applications: Repeated evaluation on a line segment

- Plot
- Numerical integration
- Computation of minimax approximation polynomials using the Remez algorithm

Rigorous Uniform Approximation of D-finite Functions

- Why?
  - Get the correct answer, not an “almost” correct one
  - Bridge the gap between scientific computing and pure mathematics - speed and reliability

Rigorous Uniform Approximation of D-finite Functions

- Why?
  - Get the correct answer, not an “almost” correct one
  - Bridge the gap between scientific computing and pure mathematics - speed and reliability
- How?
  - Use Floating-Point as support for fast computations
  - Bound roundoff, discretization, truncation errors in numerical algorithms
  - Compute enclosures instead of approximations

Rigorous Uniform Approximation of D-finite Functions

- Why?
  - Get the correct answer, not an "almost" correct one
  - Bridge the gap between scientific computing and pure mathematics - speed and reliability
- How?
  - Use Floating-Point as support for fast computations
  - Bound roundoff, discretization, truncation errors in numerical algorithms
  - Compute enclosures instead of approximations
- What?
  - Interval arithmetic

Chebyshev Series vs Taylor Series I

Two approximations of f:

- by Taylor series

$$f = \sum_{n=0}^{+\infty} c_n x^n, \ \ c_n = \frac{f^{(n)}(0)}{n!},$$

- or by Chebyshev series

$$f = \sum_{n=-\infty}^{+\infty} t_n T_n(x),$$

$$t_n = \frac{1}{\pi} \int_{-1}^{1} T_n(t) \frac{f(t)}{\sqrt{1-t^2}} dt.$$

Basic properties of Chebyshev polynomials

$$T_n(cos(\theta)) = \cos(n\theta)$$

$$\int_{-1}^{1} \frac{T_n(x) T_m(x)}{\sqrt{1-x^2}} dx = \begin{cases} 0 & \text{if } m \neq n \\ \pi & \text{if } m = 0 \\ \frac{\pi}{2} & \text{otherwise} \end{cases}$$

$$T_{n+1} = 2xT_n - T_{n-1}$$

$$T_0(x) = 1$$

$$T_1(x) = x$$

$$T_2(x) = 2x^2 - 1$$

$$T_3(x) = 4x^3 - 3x$$

Chebyshev Series vs Taylor Series I

Two approximations of f:

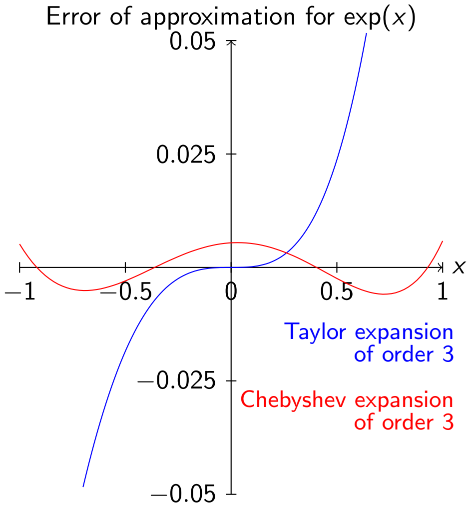
- by Taylor series

$$f = \sum_{n=0}^{+\infty} c_n x^n, \quad c_n = \frac{f^{(n)}(0)}{n!},$$

- or by Chebyshev series

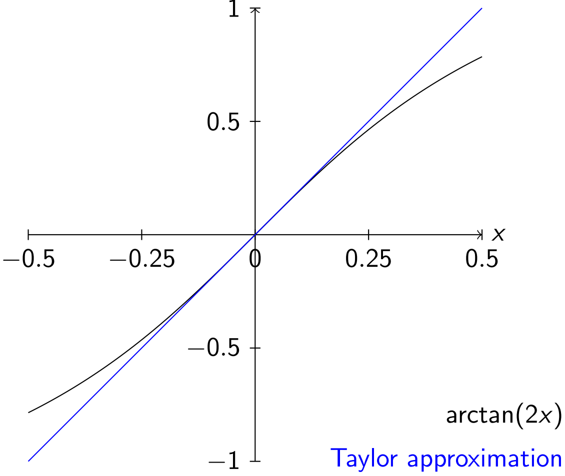
$$f = \sum_{n=-\infty}^{+\infty} t_n T_n(x),$$

$$t_n = \frac{1}{\pi} \int_{-1}^{1} T_n(t) \frac{f(t)}{\sqrt{1-t^2}} dt.$$



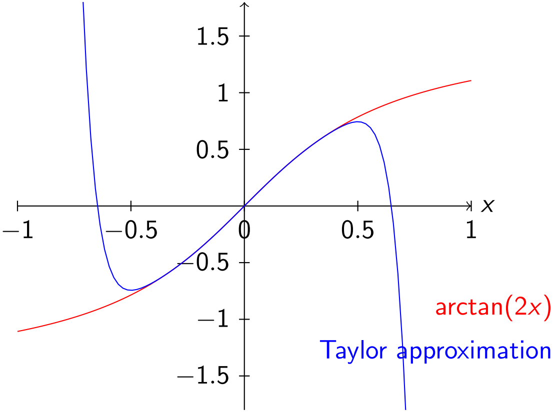
Chebyshev Series vs Taylor Series II

Approximation of $\arctan(2x)$ by Taylor expansion of degree 1



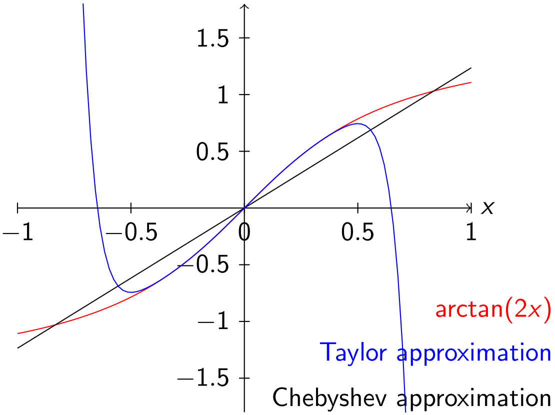
Chebyshev Series vs Taylor Series II

Bad approximation outside its circle of convergence



Chebyshev Series vs Taylor Series II

Aspproximation of arctan($2x$) by Chebyshev expansion of degree 1



Previous Work

Computation of the Chebyshev coefficients for D-finite functions

- Using a relation between coefficients Clenshaw (1957)
- Using the recurrence relation between the coefficients Fox-Parker (1968)
- The tau method of Lanczos (1938), Ortiz (1969-1993)

Validation:

- Kaucher-Miranker (1984)

Our Work

Given a linear differential equation with polynomial coefficients, boundary conditions and an integer d

- Compute a polynomial approximation p on $[-1, 1]$ of degree d of the solution f in the Chebyshev basis in $O(d)$ arithmetic operations.
- Compute a sharp bound B such that $|f(x) - p(x)| < B,\ x \in [-1, 1]$ in $O(d)$ arithmetic operations.

II Computation of the coefficients

Chebyshev Series of D-finite Functions

Theorem (60's, BenoitJoldesMezzarobba11)

$\sum u_n T_n(x)$ is solution of a linear differential equation with polynomial coefficients iff the sequence u_n is cancelled by a linear recurrence with polynomial coefficients.

Chebyshev Series of D-finite Functions

Theorem (60's, BenoitJoldesMezzarobba11)

$\sum u_n T_n(x)$ is solution of a linear differential equation with polynomial coefficients iff the sequence u_n is cancelled by a linear recurrence with polynomial coefficients.

Recurrence relation + good initial conditions ⇒ Fast numerical computation of the coefficients

Taylor: $exp = \sum \frac{1}{n!} x^n$
Rec: $u(n+1) = \frac{u(n)}{n+1}$

$u(0) = 1$	$1/0! = 1$
$u(1) = 1$	$1/1! = 1$
$u(2) = 0,5$	$1/2! = 0,5$
$\vdots$	$\vdots$
$u(50) \approx 3,28.10^{-65}$	$1/50! \approx 3,28.10^{-65}$

Chebyshev Series of D-finite Functions

Theorem (60's, BenoitJoldesMezzarobba11)

$\sum u_n T_n(x)$ is solution of a linear differential equation with polynomial coefficients iff the sequence u_n is cancelled by a linear recurrence with polynomial coefficients.

Recurrence relation + good initial conditions ⇒ Fast numerical computation of the coefficients

Taylor: $exp = \sum \frac{1}{n!} x^n$
Rec: $u(n+1) = \frac{u(n)}{n+1}$

$u(0) = 1$	$1/0! = 1$
$u(1) = 1$	$1/1! = 1$
$u(2) = 0,5$	$1/2! = 0,5$
$\vdots$	$\vdots$
$u(50) \approx 3,28.10^{-65}$	$1/50! \approx 3,28.10^{-65}$

Chebyshev: $exp = \sum I_n(1) T_n(x)$
Rec: $u(n+1) = -2nu(n) + u(n-1)$

$u(0) = 1,266$	$I_0(1) \approx 1,266$
$u(1) = 0,565$	$I_1(1) \approx 0,565$
$u(2) \approx 0,136$	$I_2(1) \approx 0,136$
$\vdots$	$\vdots$

Chebyshev Series of D-finite Functions

Theorem (60's, BenoitJoldesMezzarobba11)

$\sum u_n T_n(x)$ is solution of a linear differential equation with polynomial coefficients iff the sequence u_n is cancelled by a linear recurrence with polynomial coefficients.

Recurrence relation + good initial conditions $\Rightarrow$ Fast numerical computation of the coefficients

Taylor: $exp = \sum \frac{1}{n!} x^n$
Rec: $u(n+1) = \frac{u(n)}{n+1}$

$u(0) = 1$	$1/0! = 1$
$u(1) = 1$	$1/1! = 1$
$u(2) = 0,5$	$1/2! = 0,5$
$\vdots$	$\vdots$
$u(50) \approx 3,28.10^{-65}$	$1/50! \approx 3,28.10^{-65}$

Chebyshev: $exp = \sum I_n(1) T_n(x)$
Rec: $u(n+1) = -2nu(n) + u(n-1)$

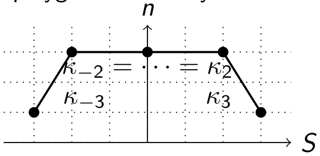
$u(0) = 1,266$	$I_0(1) \approx 1,266$
$u(1) = 0,565$	$I_1(1) \approx 0,565$
$u(2) \approx 0,136$	$I_2(1) \approx 0,136$
$\vdots$	$\vdots$
$u(50) \approx 4,450.10^{67}$	$I_{50}(1) \approx 2,934.10^{-80}$

Convergent and Divergent Solutions of the Recurrence

Study of the Chebyshev recurrence

If $u(n)$ is solution, then there exists another solution $v(n) \sim \frac{1}{u(n)}$

Newton polygon of a Chebyshev recurrence

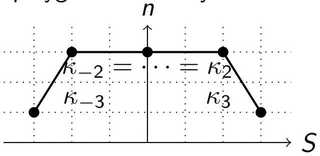


Convergent and Divergent Solutions of the Recurrence

Study of the Chebyshev recurrence

If $u(n)$ is solution, then there exists another solution $v(n) \sim \frac{1}{u(n)}$

Newton polygon of a Chebyshev recurrence



For the recurrence $u(n+1) + 2nu(n) - u(n-1)$

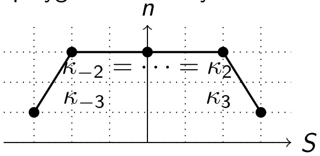
Two independent solutions are $I_n(1) \sim \frac{1}{(2n)!}$ and $K_n(1) \sim (2n)!$

Convergent and Divergent Solutions of the Recurrence

Study of the Chebyshev recurrence

If $u(n)$ is solution, then there exists another solution $v(n) \sim \frac{1}{u(n)}$

Newton polygon of a Chebyshev recurrence



For the recurrence $u(n+1) + 2nu(n) - u(n-1)$

Two independent solutions are $I_n(1) \sim \frac{1}{(2n)!}$ and $K_n(1) \sim (2n)!$

Miller's algorithm

To compute the first N coefficients of the most convergent solution of a recurrence relation of order 2

- Initialize $u(N) = 0$ and $u(N-1) = 1$ and compute the first coefficients using the recurrence backwards
- Normalize u with the initial condition of the recurrence

Algorithm for Computing the Coefficients

Algorithm

Input: *a differential equation of order r with boundary conditions*
Output: *a polynomial approximation of degree N of the solution*

- *compute the Chebyshev recurrence of order $2s \geq 2r$*
- *for i from 1 to s*
    - *using the recurrence relation backwards, compute the first N coefficients of the sequence $u^{[i]}$ starting with the initial conditions*

$$\left(u^{[i]}(N+2s), \cdots, u^{[i]}(N+i), \cdots, u^{[i]}(N+1)\right) = (0, \cdots, 1, \cdots, 0)$$

- *combine the s sequences $u^{[i]}$ according to the r boundary conditions and the $s-r$ symmetry relations*

Example: Back to exp

$$u(52) = 0 \qquad I_{52}(1) \approx 2,77.10^{-84}$$
$$u(51) = 1 \qquad I_{51}(1) \approx 2,88.10^{-82}$$
$$u(50) = -102 \qquad I_{50}(1) \approx 2,93.10^{-80}$$
$$\vdots \qquad \vdots$$
$$u(2) \approx -4,72.10^{80} \qquad I_2(1) \approx 0,14$$
$$u(1) \approx 1,96.10^{81} \qquad I_1(1) \approx -0,57$$
$$u(0) \approx -4,4.10^{81} \qquad I_0(1) \approx 1,27$$

Example: Back to exp

$$u(52) = 0 \qquad I_{52}(1) \approx 2,77.10^{-84}$$

$$u(51) = 1 \qquad I_{51}(1) \approx 2,88.10^{-82}$$

$$u(50) = -102 \qquad I_{50}(1) \approx 2,93.10^{-80}$$

$$\vdots \qquad \vdots$$

$$u(2) \approx -4,72.10^{80} \qquad I_{2}(1) \approx 0,14$$

$$u(1) \approx 1,96.10^{81} \qquad I_{1}(1) \approx -0,57$$

$$u(0) \approx -4,4.10^{81} \qquad I_{0}(1) \approx 1,27$$

$$C = \sum_{n=-50}^{50} u(n) T_n(0) \approx -3,48.10^{81}$$

Example: Back to exp

$$\frac{u(52)}{C} = 0 \qquad I_{52}(1) \approx 2,77.10^{-84}$$

$$\frac{u(51)}{C} \approx -2,88.10^{-82} \qquad I_{51}(1) \approx 2,88.10^{-82}$$

$$\frac{u(50)}{C} \approx 2,93.10^{-80} \qquad I_{50}(1) \approx 2,93.10^{-80}$$

$$\vdots \qquad \vdots$$

$$\frac{u(2)}{C} \approx 0,14 \qquad I_{2}(1) \approx 0,14$$

$$\frac{u(1)}{C} \approx -0,57 \qquad I_{1}(1) \approx -0,57$$

$$\frac{u(0)}{C} \approx 1.27 \qquad I_{0}(1) \approx 1,27$$

$$C = \sum_{n=-50}^{50} u(n)\, T_n(0) \approx -3,48.10^{81}$$

III Validation

Fixed Point Theorem Applied to a Differential Equation

f is solution of

$$y'(x) - a(x)y(x) = 0, \text{ with } y(0) = y_0,$$

if and only if f is a fixed point of τ defined by

$$\tau(y)(t) = y_0 + \int_0^t a(x)y(x)dx.$$

Fixed Point Theorem Applied to a Differential Equation

f is solution of

$$y'(x) - a(x)y(x) = 0, \text{ with } y(0) = y_0,$$

if and only if f is a fixed point of τ defined by

$$\tau(y)(t) = y_0 + \int_0^t a(x)y(x)dx.$$

For all rational functions $a(x)$, there exists i such that τ^i is a contraction map from the space of continuous functions to itself. We deduce:

$$\tau^i(B(p,R)) \subset B(p,R) \implies f \in B(p,R)$$

Fixed Point Theorem Applied to a Differential Equation

f is solution of

$$y'(x) - a(x)y(x) = 0, \text{ with } y(0) = y_0,$$

if and only if f is a fixed point of τ defined by

$$\tau(y)(t) = y_0 + \int_0^t a(x)y(x)dx.$$

For all rational functions $a(x)$, there exists i such that τ^i is a contraction map from the space of continuous functions to itself. We deduce:

$$\tau^i(B(p,R)) \subset B(p,R) \implies f \in B(p,R)$$

Goal: Computation of R

Given p, find i, p_i and R_i such that $\tau^i(B(p,R)) \subset B(p_i,R_i) \subset B(p,R)$

Algorithm for a Differential Equation of Order 1

Given p, find i, p_i and R_i such that $\tau^i(B(p,R)) \subset B(p_i,R_i) \subset B(p,R)$

Algorithm (Find R)

- $p_0 := p$
- *while* $i! < \|a\|_\infty^i$
  - *Compute* $p_i(t)$ *a "good" approximation of* $y_0 + \int_0^t a(x)p_{i-1}(x)dx$
  - $M_i = \|\tau(p_{i-1}) - p_i\|_\infty$
- *Return*

$$R = \frac{\|p_i - p\|_\infty + \sum_{j=1}^{i} M_j \frac{\|a\|_\infty^j}{j!}}{1 - \frac{\|a\|_\infty^i}{i!}}$$

Algorithm for a Differential Equation of Order 1

Given p, find i, p_i and R_i such that $\tau^i(B(p,R)) \subset B(p_i,R_i) \subset B(p,R)$

Algorithm (Find R)

- $p_0 := p$
- *while* $i! < \|a\|_\infty^i$
  - *Compute* $p_i(t)$ *a "good" approximation of* $y_0 + \int_0^t a(x)p_{i-1}(x)dx$
  - $M_i = \|\tau(p_{i-1}) - p_i\|_\infty$
- *Return*

$$R = \frac{\|p_i - p\|_\infty + \sum_{j=1}^{i} M_j \frac{\|a\|_\infty^j}{j!}}{1 - \frac{\|a\|_\infty^i}{i!}}$$

$f \in B(p,R) \implies f = \tau^i(f) \in B(p_i,R_i)$, with

$$R_i = \sum_{j=1}^{i} \frac{\|a\|_\infty^j M_j}{j!} + \|a\|_\infty^i R \frac{|t|^i}{i!}$$

Algorithm for a Differential Equation of Order 1

Given p, find i, p_i and R_i such that $\tau^i(B(p,R)) \subset B(p_i,R_i) \subset B(p,R)$

Algorithm (Find R)

- $p_0 := p$
- *while* $i! < \|a\|_\infty^i$
  - *Compute* $p_i(t)$ *a "good" approximation of* $y_0 + \int_0^t a(x)p_{i-1}(x)dx$
  - $M_i = \|\tau(p_{i-1}) - p_i\|_\infty$
- *Return*

$$R = \frac{\|p_i - p\|_\infty + \sum_{j=1}^i M_j \frac{\|a\|_\infty^j}{j!}}{1 - \frac{\|a\|_\infty^i}{i!}}$$

$f \in B(p,R) \implies f = \tau^i(f) \in B(p_i,R_i)$, with

$$R_i = \sum_{j=1}^{i} \frac{\|a\|_\infty^j M_j}{j!} + \|a\|_\infty^i R \frac{|t|^i}{i!}$$

$$\|f - p\|_\infty \leq \|f - p_i\|_\infty + \|p - p_i\|_\infty \leq R_i + \|p - p_i\|_\infty = R$$

IV Conclusion

Final Algorithm

Algorithm

INPUT: Differential equation with boundary conditions and a degree d
OUTPUT: a polynomial approximation of degree d and a bound

- *Compute an approximation P of degree d of the solution with the first algorithm*
- *Compute the bound B of the approximation with the second algorithm.*
- *return the pair P, B*