Rigorous Uniform Approximation of D-finite Functions

Mioara Joldes*

Joint work with
Alexandre Benoit**, Marc Mezzarobba**

* École Normale Supérieure de Lyon, Arénaire Team, Laboratoire de l'Informatique du Parallélisme
** INRIA Roquencourt, Algorithms Team

D-finite Functions

Definition

A function $y : \mathbb{R} \to \mathbb{R}$ is D-finite if it is solution of a (homogeneous) linear differential equation with polynomial coefficients:

$$L \cdot y = a_r y^{(r)} + a_{r-1} y^{(r-1)} + \cdots + a_0 y = 0, \quad a_i \in \mathbb{Q}[x]. \qquad (1)$$

D-finite Functions

Definition

A function $y : \mathbb{R} \to \mathbb{R}$ is D-finite if it is solution of a (homogeneous) linear differential equation with polynomial coefficients:

$$L \cdot y = a_r y^{(r)} + a_{r-1} y^{(r-1)} + \cdots + a_0 y = 0, \quad a_i \in \mathbb{Q}[x]. \tag{1}$$

Examples

$$f(x) = \exp(x) \quad \leftrightarrow \quad \{f' - f = 0,\ f(0) = 1\}.$$

D-finite Functions

Definition

A function $y : \mathbb{R} \to \mathbb{R}$ is D-finite if it is solution of a (homogeneous) linear differential equation with polynomial coefficients:

$$L \cdot y = a_r y^{(r)} + a_{r-1} y^{(r-1)} + \cdots + a_0 y = 0, \quad a_i \in \mathbb{Q}[x]. \qquad (1)$$

Examples

$f(x) = \exp(x) \quad \leftrightarrow \quad \{f' - f = 0,\ f(0) = 1\}.$
$\cos$, $\arccos$, Airy functions, Bessel functions, ...

D-finite Functions

Definition

A function $y : \mathbb{R} \to \mathbb{R}$ is D-finite if it is solution of a (homogeneous) linear differential equation with polynomial coefficients:

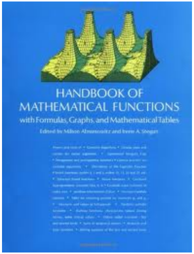
$$L \cdot y = a_r y^{(r)} + a_{r-1} y^{(r-1)} + \cdots + a_0 y = 0, \quad a_i \in \mathbb{Q}[x]. \qquad (1)$$

Examples

$f(x) = \exp(x) \quad \leftrightarrow \quad \{f' - f = 0,\ f(0) = 1\}.$

$\cos$, $\arccos$, Airy functions, Bessel functions, ...

About 60% of Abramowitz & Stegun



D-finite Functions

Definition

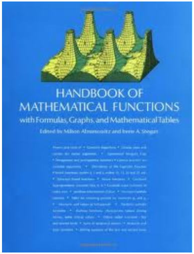
A function $y : \mathbb{R} \to \mathbb{R}$ is D-finite if it is solution of a (homogeneous) linear differential equation with polynomial coefficients:

$$L \cdot y = a_r y^{(r)} + a_{r-1} y^{(r-1)} + \cdots + a_0 y = 0, \quad a_i \in \mathbb{Q}[x]. \qquad (1)$$

Differential equation + initial conditions = Data Structure

Examples

$f(x) = \exp(x) \quad \leftrightarrow \quad \{f' - f = 0,\ f(0) = 1\}.$
$\cos$, $\arccos$, Airy functions, Bessel functions, ...
About 60% of Abramowitz & Stegun



D-finite Functions

Definition

A function $y : \mathbb{R} \to \mathbb{R}$ is D-finite if it is solution of a (homogeneous) linear differential equation with polynomial coefficients:

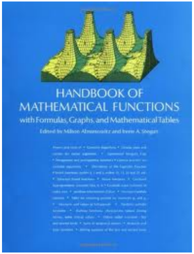
$$L \cdot y = a_r y^{(r)} + a_{r-1} y^{(r-1)} + \cdots + a_0 y = 0, \quad a_i \in \mathbb{Q}[x]. \qquad (1)$$

Differential equation + initial conditions = Data Structure

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:

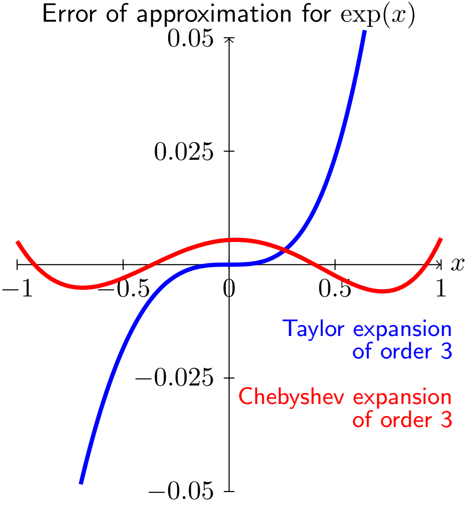
- by Taylor series

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

- or by Chebyshev series

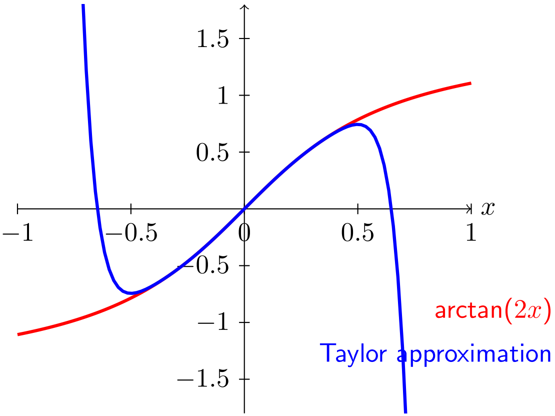
$$f = \sum_{n=-\infty}^{+\infty} t_n T_n(x),$$

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



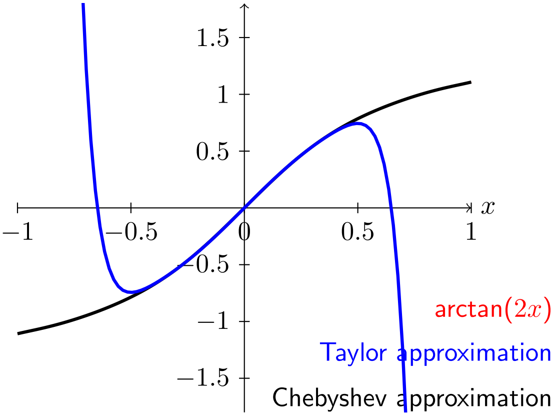
Chebyshev Series vs Taylor Series II

Bad approximation outside its circle of convergence



Chebyshev Series vs Taylor Series II

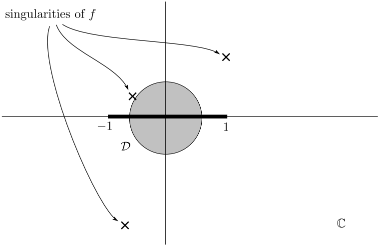
Approximation of arctan$(2x)$ by Chebyshev expansion of degree 11



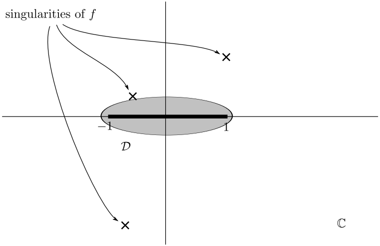
Chebyshev Series vs Taylor Series III

Convergence Domains :

For Taylor series:
disc centered at $x_0 = 0$ which avoids all the singularities of f



For Chebyshev series:
elliptic disc with foci at ± 1 which avoids all the singularities of f

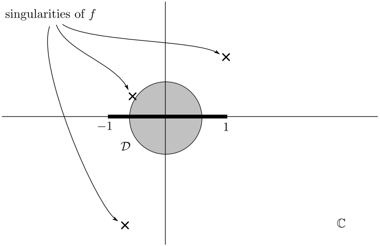


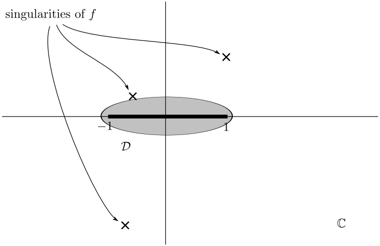
Chebyshev Series vs Taylor Series III

Convergence Domains :

For Taylor series:
disc centered at $x_0 = 0$ which avoids all the singularities of f

For Chebyshev series:
elliptic disc with foci at ± 1 which avoids all the singularities of f



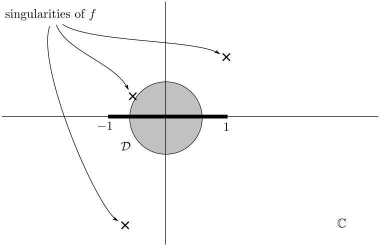


- Taylor series can not converge over entire $[-1, 1]$ unless all singularities lie outside the unit circle.

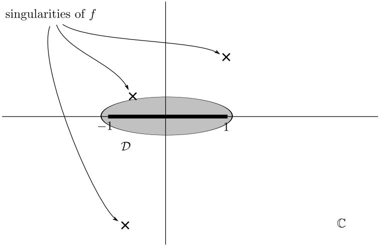
Chebyshev Series vs Taylor Series III

Convergence Domains :

For Taylor series:
disc centered at $x_0 = 0$ which avoids all the singularities of f



For Chebyshev series:
elliptic disc with foci at ± 1 which avoids all the singularities of f



- Taylor series can not converge over entire $[-1, 1]$ unless all singularities lie outside the unit circle.
- ✓ Chebyshev series converge over entire $[-1, 1]$ as soon as there are no real singularities in $[-1, 1]$.

Chebyshev Series vs Taylor Series IV

Truncation Error :

Taylor series, Lagrange formula:

$\forall x \in [-1, 1],\ \exists \xi \in [-1, 1]$ s.t.

$$f(x) - T(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)^{n+1}.$$

Chebyshev Series vs Taylor Series IV

Truncation Error :

Taylor series, Lagrange formula:

$$\forall x \in [-1,1],\ \exists \xi \in [-1,1] \ \text{ s.t.}$$
$$f(x) - T(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)^{n+1}.$$

Chebyshev series, Bernstein-like formula:

$$\forall x \in [-1,1],\ \exists \xi \in [-1,1] \ \text{ s.t.}$$
$$f(x) - P(x) = \frac{f^{(n+1)}(\xi)}{2^n (n+1)!}.$$

Chebyshev Series vs Taylor Series IV

Truncation Error :

Taylor series, Lagrange formula:

$\forall x \in [-1,1],\ \exists \xi \in [-1,1]\ \ \text{s.t.}$

$$f(x) - T(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)^{n+1}.$$

Chebyshev series, Bernstein-like formula:

$\forall x \in [-1,1],\ \exists \xi \in [-1,1]\ \ \text{s.t.}$

$$f(x) - P(x) = \frac{f^{(n+1)}(\xi)}{2^n(n+1)!}.$$

[✓] We should have an improvement of 2^n in the width of the Chebyshev truncation error.

Quality of approximation of truncated Chebyshev series compared to best polynomial approximation

It is well-known that truncated Chebyshev series $\pi_d(f)$ are *near-best* uniform approximations [Chap 5.5, Mason & Handscomb 2003].

Quality of approximation of truncated Chebyshev series compared to best polynomial approximation

It is well-known that truncated Chebyshev series $\pi_d(f)$ are *near-best* uniform approximations [Chap 5.5, Mason & Handscomb 2003].

Let p_d^* is the polynomial of degree at most d that minimizes $\|f - p\|_\infty = \sup_{-1 \leq x \leq 1} |f(x) - p(x)|$.

Quality of approximation of truncated Chebyshev series compared to best polynomial approximation

It is well-known that truncated Chebyshev series $\pi_d(f)$ are *near-best* uniform approximations [Chap 5.5, Mason & Handscomb 2003].

Let p_d^* is the polynomial of degree at most d that minimizes $\|f - p\|_\infty = \sup_{-1 \leq x \leq 1} |f(x) - p(x)|$.

$$\|f - \pi_d(f)\|_\infty \leqslant \underbrace{\left(\frac{4}{\pi^2}\log d + O(1)\right)}_{\Lambda_d} \|f - p_d^*\|_\infty \qquad (2)$$

Quality of approximation of truncated Chebyshev series compared to best polynomial approximation

It is well-known that truncated Chebyshev series $\pi_d(f)$ are *near-best* uniform approximations [Chap 5.5, Mason & Handscomb 2003].

Let p_d^* is the polynomial of degree at most d that minimizes $\|f - p\|_\infty = \sup_{-1 \leq x \leq 1} |f(x) - p(x)|$.

$$\|f - \pi_d(f)\|_\infty \leqslant \underbrace{\left(\frac{4}{\pi^2} \log d + O(1)\right)}_{\Lambda_d} \|f - p_d^*\|_\infty \qquad (2)$$

- $\Lambda_{10} = 2.22... \rightarrow$ we lose at most 2 bits
- $\Lambda_{30} = 2.65... \rightarrow$ we lose at most 2 bits
- $\Lambda_{100} = 3.13... \rightarrow$ we lose at most 3 bits
- $\Lambda_{500} = 3.78... \rightarrow$ we lose at most 3 bits

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)
- Monomial basis: Verified integration of Taylor Models (Makino & Berz, 1998)

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.

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 ⇒ 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: $u(n+1) = -2nu(n) + u(n-1)$

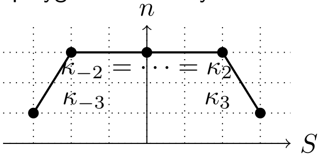
$u(0) = 1,266$	$I_0(1) \approx 1,266$
$u(1) = 0,565$	$I_1(1) \approx 0,565$
$u(2) \approx 0,136$	$I_2(1) \approx 0,136$
$\vdots$	$\vdots$
$u(50) \approx 4,450.10^{67}$	$I_{50}(1) \approx 2,934.10^{-80}$

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

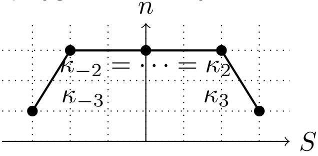


Convergent and Divergent Solutions of the Recurrence

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 $u(n+1) + 2nu(n) - u(n-1)$

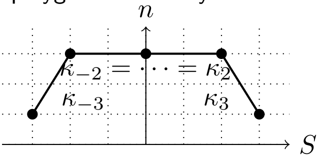
Two independent solutions are $I_n(1) \sim \frac{1}{(2n)!}$ and $K_n(1) \sim (2n)!$

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 $\exp$

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

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 $\exp$

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

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

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

$$\vdots \qquad \vdots$$

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

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

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

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

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.

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

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

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

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

For all rational functions $a(x)$, if $\frac{\|a\|_\infty^j}{j!} < 1$ then $\forall i \geqslant j$, τ^i is a contraction map.

Algorithm for a Differential Equation of Order 1

Given p, compute a sharp bound B such that
$|f(x) - p(x)| < B,\ x \in [-1, 1]$.

Algorithm (Find B)

- $p_0 := p$
- *while* $i! < \|a\|_\infty^i$
  - *Compute* $p_i(t)$ *a rigorous approximation of* $\tau(p_{i-1}) = \int_0^t a(x) p_{i-1}(x) dx$ *s.t.* $\|\tau(p_{i-1}) - p_i\|_\infty < M$.
- *Return*

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

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 $P,\ B$*

Random Example

Example

$(x+5)y^{(3)}(x)+(-x^3-5x^2+4x+5)y^{(2)}(x)+(6x^3+6+3x)y^{(1)}(x)+(-3x^3-x^2-2x+4)y(x)=0, \quad y(0)=-6, y^{(1)}(0)=1, y^{(2)}(0)=-2$

Compute coefficients of polynomial of degree 30.
Validated bound: $0.58 \cdot 10^{-14}$.