Rigorous Uniform Approximation of D-finite Functions

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Joint work with
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D-finite Functions

**Definition**

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

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

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\]  (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 \([-1, 1]\). 

**Applications:**
- Repeated evaluation on a line segment
- Plot
- Numerical integration
- Computation of minimax approximation polynomials using the Remez algorithm
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Why?

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

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
  \[ f = \sum_{n=-\infty}^{+\infty} t_n T_n(x), \]
  \[ t_n = \frac{1}{\pi} \int_{-1}^{1} T_n(t) \frac{f(t)}{\sqrt{1 - t^2}} dt. \]

Basic properties of Chebyshev polynomials

\[ T_n(\cos(\theta)) = \cos(n\theta) \]

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

\[ T_{n+1} = 2xT_n - T_{n-1} \]
\[ T_0(x) = 1 \]
\[ T_1(x) = x \]
\[ T_2(x) = 2x^2 - 1 \]
\[ T_3(x) = 4x^3 - 3x \]
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Bad approximation outside its circle of convergence

\[
\text{arctan}(2x)
\]

Taylor approximation
Approximation of $\arctan(2x)$ by Chebyshev expansion of degree 11.
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 $\pm 1$ 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 $f$
- Taylor series cannot converge over entire $[-1, 1]$ unless all singularities lie outside the unit circle.

For Chebyshev series:
- elliptic disc with foci at $\pm 1$ which avoids all the singularities of $f$
- Chebyshev series converge over entire $[-1, 1]$ as soon as there are no real singularities in $[-1, 1]$. 
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Chebyshev Series vs Taylor Series IV

Truncation Error:

**Taylor series, Lagrange formula:**

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

\[ f(x) - T(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)^{n+1}. \]
Truncation Error:

### Taylor series, Lagrange formula:
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### Chebyshev series, Bernstein-like formula:
\[
\forall x \in [-1, 1], \exists \xi \in [-1, 1] \text{ s.t. } f(x) - P(x) = \frac{f^{(n+1)}(\xi)}{2^n(n+1)!}.
\]
Truncation Error:

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

**Chebyshev series, Bernstein-like formula:**

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

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

...we lose at most 2 bits $\Lambda_{10} = 2^{2.2}$...

...we lose at most 3 bits $\Lambda_{30} = 2^{3.05}$...

...we lose at most 3 bits $\Lambda_{500} = 2^{3.78}$...
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].

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$$\|f - p\|_{\infty} = \sup_{-1 \leq x \leq 1} |f(x) - p(x)|.$$

Then

$$\|f - \pi_d(f)\|_{\infty} \leq \left(\frac{4}{\pi^2} \log d + O(1)\right) \|f - p^*_d\|_{\infty} \overset{\Lambda_d}{\leq}$$

(2)
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$$\|f - \pi_d(f)\|_{\infty} \leq \left( \frac{4}{\pi^2} \log d + O(1) \right) \left\| f - p^*_d \|_{\infty} \right\|_{\infty} \Lambda_d$$ (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:

- Monomial basis: Verified integration of Taylor Models (Makino & Berz, 1998)
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.
Theorem (60's, BenoitJoldesMezzarobba11)

\[ \sum u_n T_n(x) \text{ is solution of a linear differential equation with polynomial coefficients iff the sequence } u_n \text{ is cancelled by a linear recurrence with polynomial coefficients.} \]
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Recurrence relation + good initial conditions \(\Rightarrow\) Fast numerical computation of the coefficients

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

Rec: \( u(n + 1) = \frac{u(n)}{n+1} \)

\[
\begin{align*}
  u(0) &= 1 & 1/0! &= 1 \\
  u(1) &= 1 & 1/1! &= 1 \\
  u(2) &= 0,5 & 1/2! &= 0,5 \\
  \vdots & & \vdots \\
  u(50) &\approx 3,28.10^{-65} & 1/50! &\approx 3,28.10^{-65}
\end{align*}
\]
Chebyshev Series of D-finite Functions

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<td><strong>Rec</strong>: ( u(n + 1) = \frac{u(n)}{n+1} )</td>
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<td>0</td>
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<td>50</td>
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<td>(\approx 2, 934.10^{-80})</td>
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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 $I_n(1) \sim (2n)!$ 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
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Newton polygon of a Chebyshev recurrence
Algorithm for Computing the Coefficients

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
    \[
    \left( u^{[i]}(N + 2s), \ldots, u^{[i]}(N + i), \ldots, u^{[i]}(N + 1) \right) = (0, \ldots, 1, \ldots, 0)
    \]
- combine the \( s \) sequences \( u^{[i]} \) according to the \( r \) boundary conditions and the \( s - r \) symmetry relations
Example: Back to exp

\[ u(52) = 0 \]
\[ u(51) = 1 \]
\[ u(50) = -102 \]

\[ \vdots \]
\[ u(2) \approx -4.72 \times 10^{80} \]
\[ u(1) \approx 1.96 \times 10^{81} \]
\[ u(0) \approx -4.4 \times 10^{81} \]

\[ I_{52}(1) \approx 2.77 \times 10^{-84} \]
\[ I_{51}(1) \approx 2.88 \times 10^{-82} \]
\[ I_{50}(1) \approx 2.93 \times 10^{-80} \]

\[ \vdots \]
\[ I_{2}(1) \approx 0.14 \]
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  C &= \sum_{n=-50}^{50} u(n)T_n(0) \approx -3,48.10^{81} \\
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Example: Back to exp

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\frac{u(52)}{C} = 0 \quad \quad I_{52}(1) \approx 2,77.10^{-84}
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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.
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 $\tau$ defined by

$$\tau(y)(t) = y_0 + \int_0^t a(x)y(x)dx.$$
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For all rational functions $a(x)$, if $\frac{||a||_\infty^j}{j!} < 1$ then $\forall i \geq j$, $\tau^i$ 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 \( P, B \)
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: \(0.58 \cdot 10^{-14}\).