Rigorous Polynomial Approximations and Applications

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Predictions for Scientific Computing Fifty Years From Now*

– 12 predictions

*L.N. Trefethen, "Numerical Analysis and Computers - 50 Years of Progress", June 17, 1998

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> *"In truth, however, no amount of computer power will change the fact that most numerical problems cannot be solved symbolically. You have to make approximations, and floating-point arithmetic is the best general-purpose approximation idea ever devised."*

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> *"We will tell the machine what we want, and the machine, an intelligent control system sitting atop an encyclopedia of numerical methods, will juggle computational possibilities at incomprehensible speed until it has solved the problem to the accuracy required. Then it will give us the answer; and if we insist, it may even tell us something of how it got there."*

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Floating point (FP) Arithmetic I

A real number is approximated in machine by a rational x:

$$x = (-1)^s \times m \times \beta^e$$

- β is the radix (usually $\beta = 2$)
- s is a sign bit
- m is the mantissa, a rational number of n_m digits in radix β:

$$m = d_0, d_1 d_2 ... d_{n_m - 1}$$

- e is the exponent, a signed integer on n_e bits

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- Arénaire team develops the Correctly Rounded Libm (CRLibm*).

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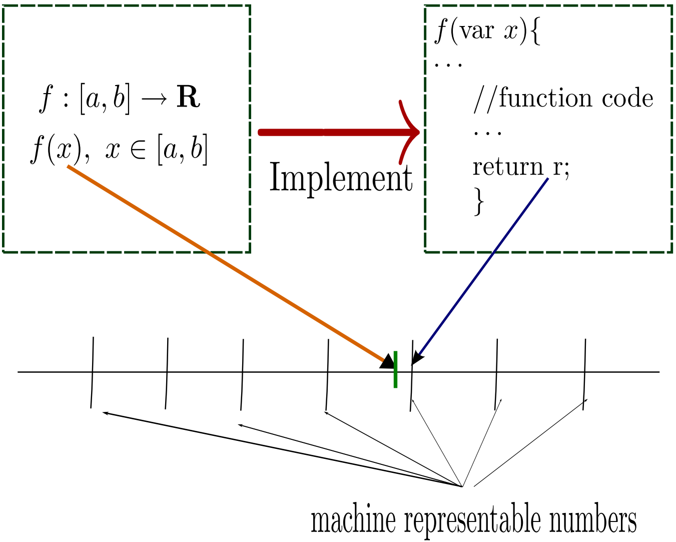
Correctly rounded functions



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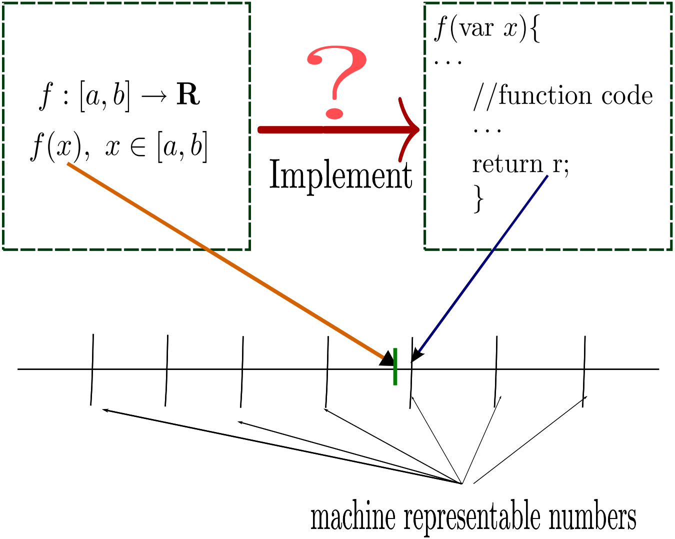

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$\exp, \ln, \cos, \sin, \arctan, \sqrt{\ }, \ldots$

Goal: evaluation of φ to a given accuracy η.

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- Step 0. Computation of hardest-to-round cases: V. Lefèvre and J.-M. Muller, TaMaDi project.
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- Mathematica and Chebfun fail to answer;

The Mathematica Book: "the only information it has about your integrand is a sequence of numerical values for it. If you give a sufficiently pathological integrand, Mathematica may simply give you the wrong answer for the integral."

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What is the correct answer, then ?

Computer Assisted Proofs

Formal proof of Kepler's conjecture

Prove the inequality:
$2\pi - 2x \arcsin((\cos 0.797) \sin(\pi/x)) > 2.097 - 0.0331x$,
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Mathematica book: "It is therefore worthwhile to go as far as you can symbolically, and then resort to numerical methods only at the very end."

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Tools:

$\rightsquigarrow$ Interval arithmetic (IA)

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  $F([-1, 2]) = [-1, 6]$
  $x \in [-1, 2], f(x) \in [-1, 6]$, but $\mathtt{Im}(f) = [3/4, 3]$

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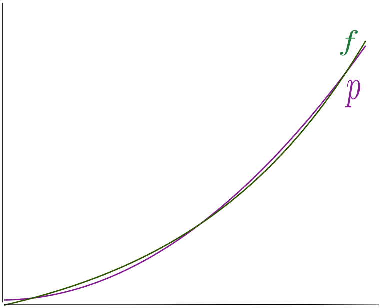
When Interval Arithmetic does not suffice: Computing supremum norms of approximation errors

$f(x) = e^{1/\cos(x)},\ x \in [0,1],\ p(x) = \sum_{i=0}^{10} c_i x^i,$



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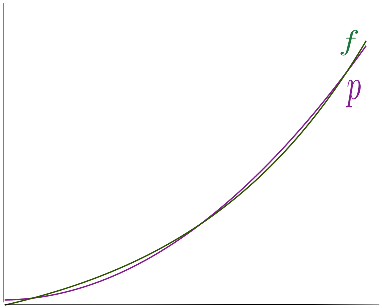

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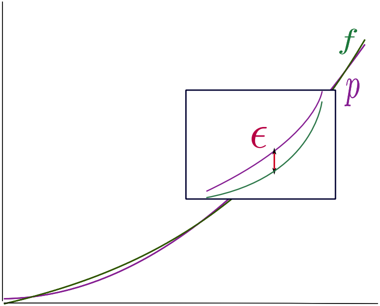
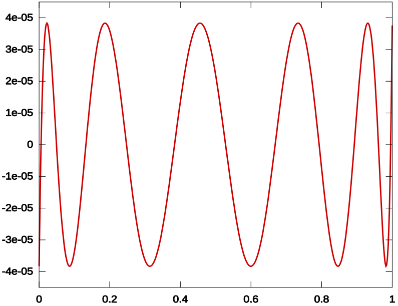
$f(x) = e^{1/\cos(x)}$, $x \in [0, 1]$, $p(x) = \sum_{i=0}^{10} c_i x^i$, $\varepsilon(x) = f(x) - p(x)$ s.t. $\|\varepsilon\|_\infty = \sup_{x \in [a,\, b]}\{|\varepsilon(x)|\}$ is as small as possible (Remez algorithm)





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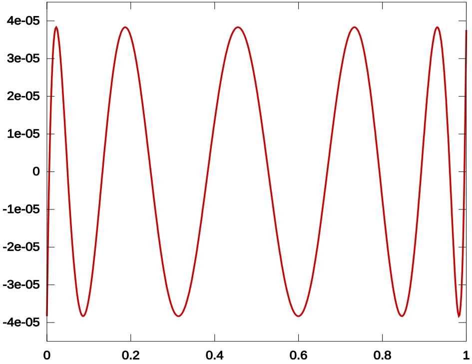

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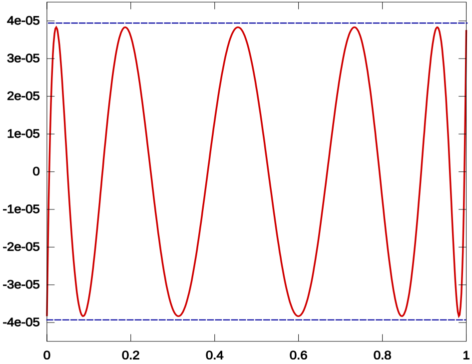

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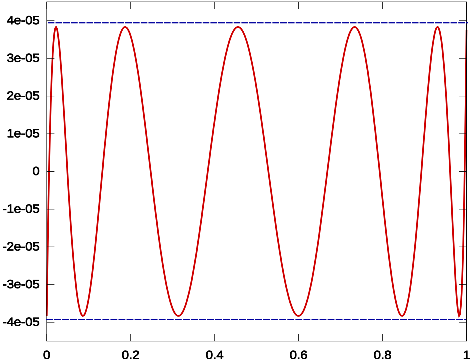
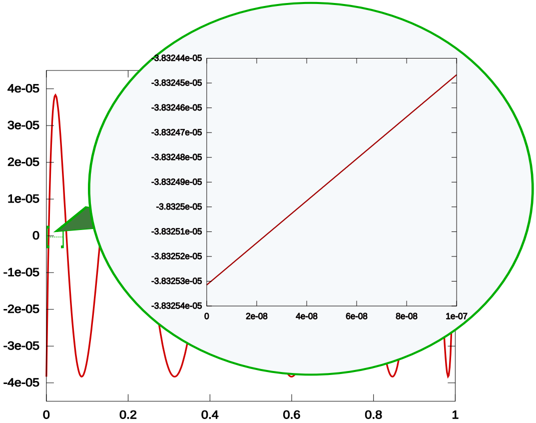


Using IA, $\varepsilon(x) \in [-233, 298]$, but $\|\varepsilon(x)\|_\infty \simeq 3.8325 \cdot 10^{-5}$

Why IA does not suffice: Overestimation

Overestimation can be reduced by using intervals of smaller width.

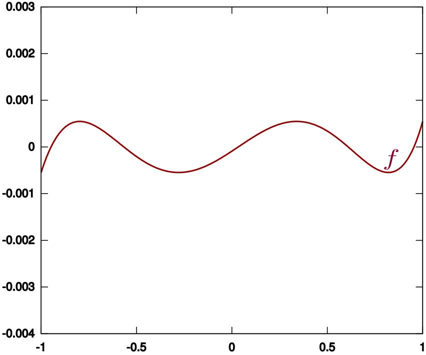


In this case, over $[0, 1]$ we need 10^7 intervals!

Why IA does not suffice: Overestimation

Use the appropriate tools!

Rigorous polynomial approximations (RPAs)



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f replaced with
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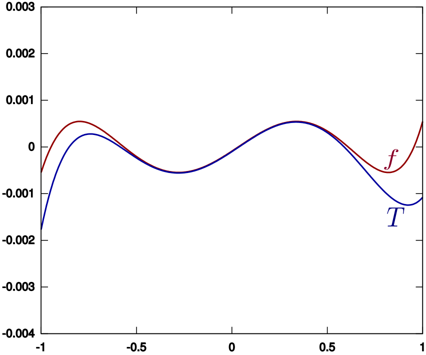

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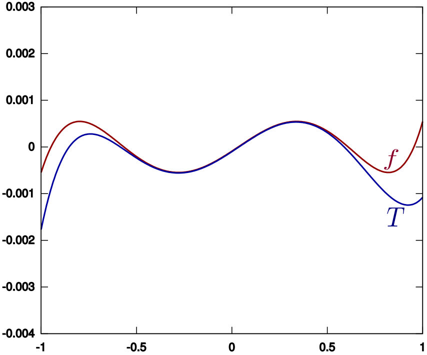

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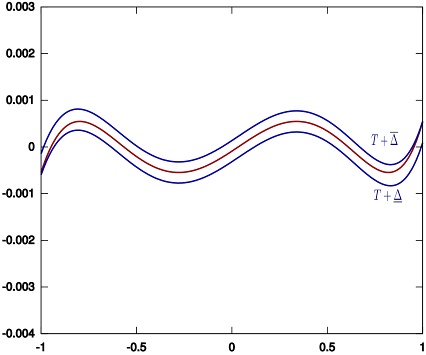

Main point of this talk: How to compute $(T, \mathbf{\Delta})$?

Rigorous polynomial approximations (RPAs) Contributions of this thesis:

– f replaced with a rigorous polynomial approximation : $(T, \mathbf{\Delta})$
– Currently we deal with "sufficiently smooth" univariate functions f over $[a, b]$.

(1). Analyse and refine existing RPAs based on Taylor series $\rightsquigarrow$ Taylor Models (TMs).

(2). Certify RPAs based on best polynomial approximations: use intermediary RPAs obtained in (1), (3).

(3). Bring forth near-best RPAs: based on Chebyshev Series $\rightsquigarrow$ Chebyshev Models (CMs).

- f is an elementary function, e.g. $\exp(1/\cos(x))$;
- f is a D-finite function, i.e. solution of an ordinary differential equation with polynomial coefficients, e.g. $\exp$, Airy, Bessel.

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Let $n \in \mathbb{N}$, $n+1$ times differentiable function f over $[a,b]$ around x_0.

$$f(x) = \underbrace{\sum_{i=0}^{n} \frac{f^{(i)}(x_0)(x-x_0)^i}{i!}}_{T(x)} + \underbrace{\Delta_n(x)}_{\boldsymbol{\Delta}}$$

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- For obtaining $\boldsymbol{\Delta}$:

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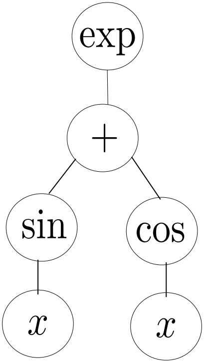
Taylor Models $\rightsquigarrow$ Algebra of RPAs

Example: $f_{\mathrm{comp}}(x) = \exp(\sin(x) + \cos(x))$



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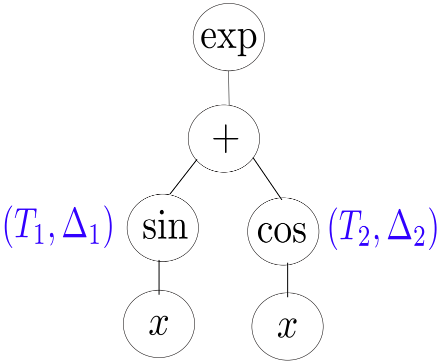

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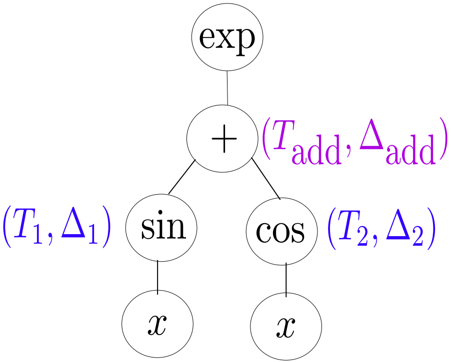

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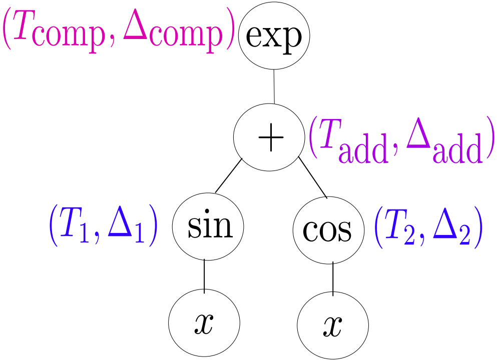

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Supremum norm example

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$f(x) = \arctan(x)$ over $[-0.9, 0.9]$
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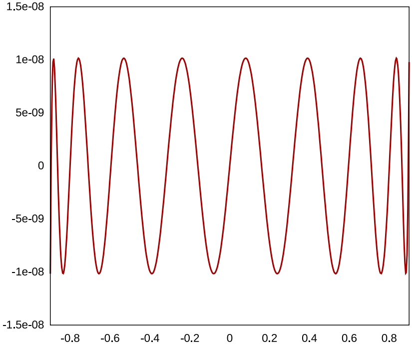

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    - closed truncation error formula

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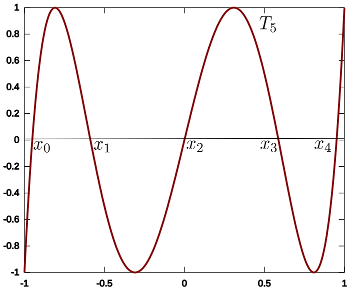

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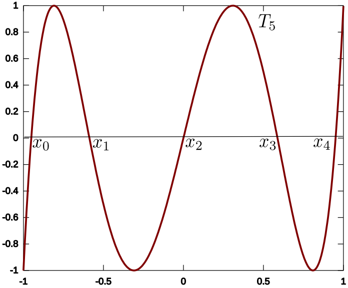

Chebyshev nodes: n distinct real roots in $[-1, 1]$ of T_n

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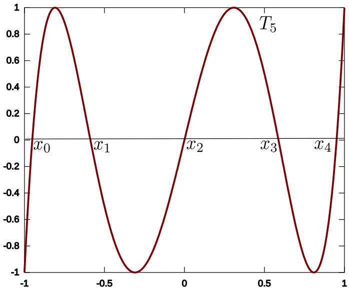

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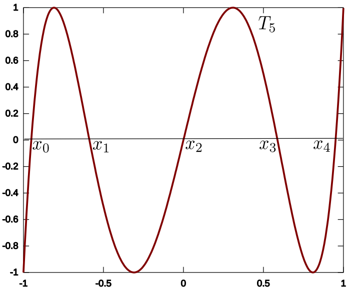

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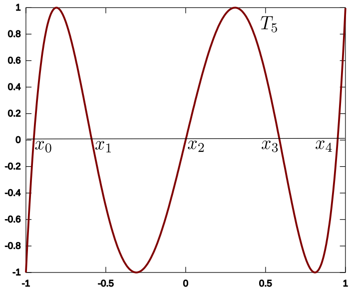

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Chebyshev Series vs Taylor Series I

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

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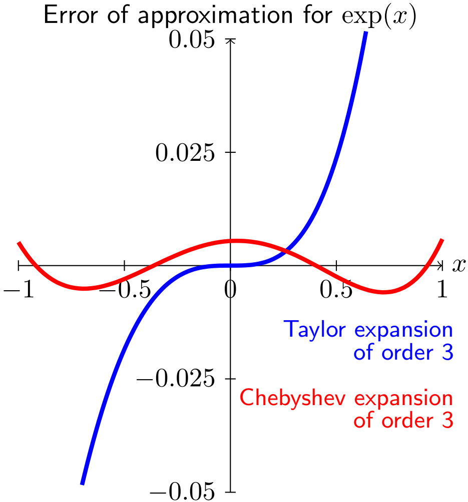
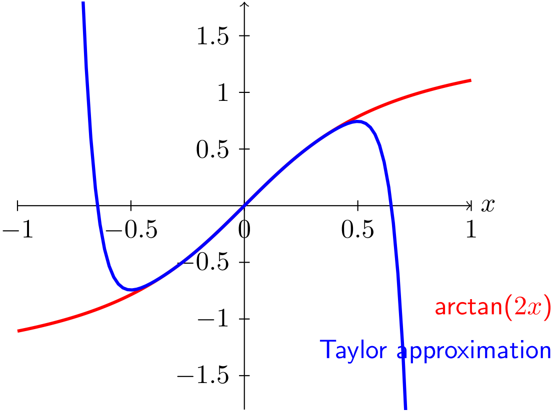


Chebyshev Series vs Taylor Series II

Bad approximation outside its circle of convergence



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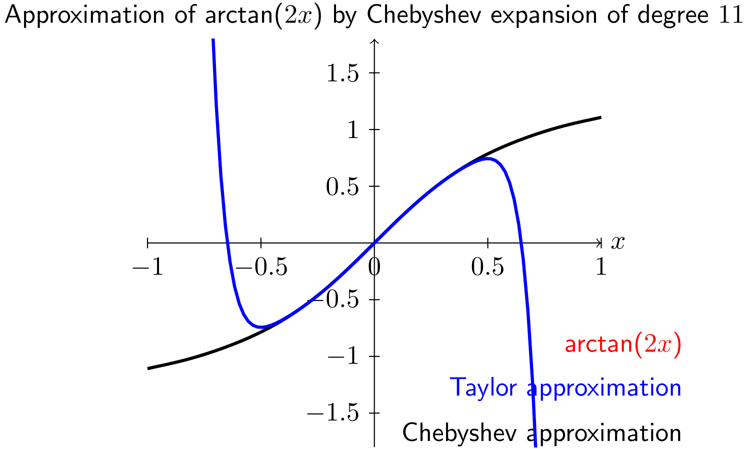

Chebyshev Series vs Taylor Series III

Convergence Domains :

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

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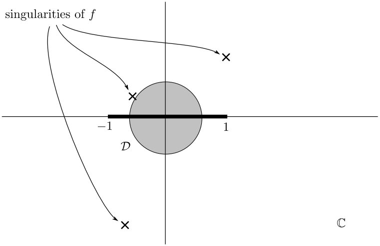
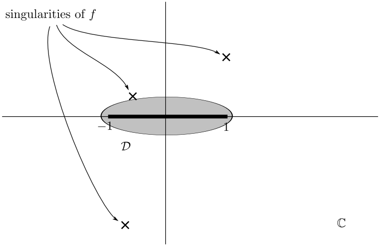
elliptic disc with foci at ± 1 which avoids all the singularities of f





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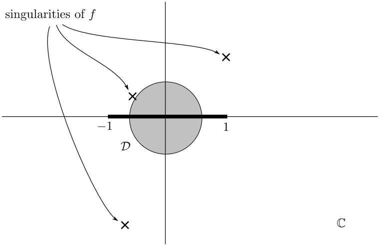

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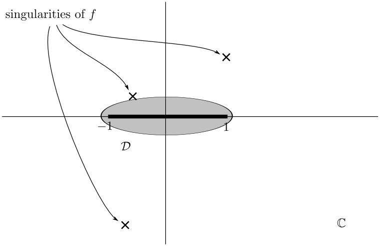

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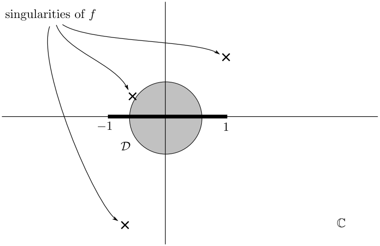

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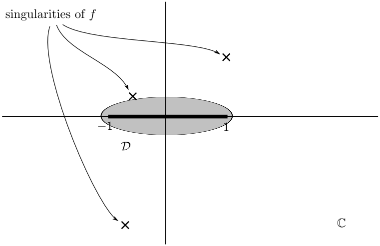

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✓ Chebyshev series converge over entire $[-1, 1]$ as soon as there are no real singularities in $[-1, 1]$.

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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- $\Lambda_{10} = 2.22... \rightarrow$ 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

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Truncation Error :

Taylor series, Lagrange formula:

$$\forall x \in [-1,1],\ \exists \xi \in [-1,1] \ \text{ s.t.}$$
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[✓] We should have an improvement of 2^n in the width of the Chebyshev truncation error.

Computing the coefficients

Chebyshev series of $f = \sum_{i=-\infty}^{+\infty} t_i T_i(x)$:

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$\rightsquigarrow$ Chebyshev Interpolant (CI)

Chebyshev Models with CI: Supremum norm example

Example:

$f(x) = \arctan(x)$ over $[-0.9, 0.9]$
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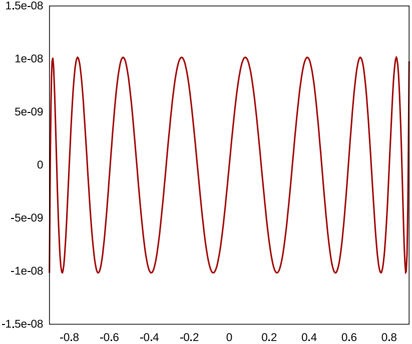

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A CM of degree 60 works.

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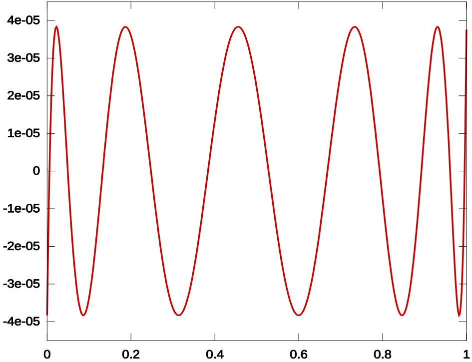

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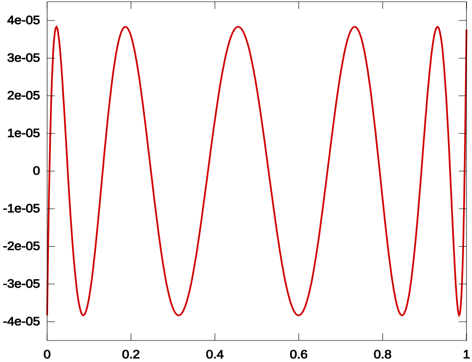

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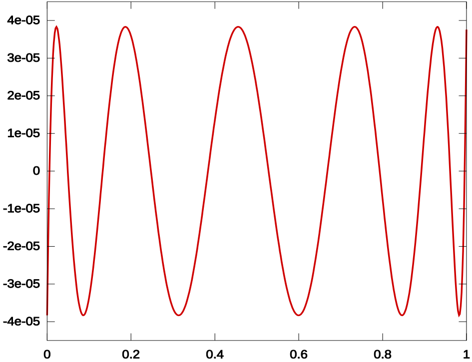

Example:

Compute:

$$\int_0^3 \sin\left(\frac{1}{(10^{-3}+(1-x)^2)^{3/2}}\right) \mathrm{d}x.$$

- Maple15: 0.7499743685;
- Pari/GP: $0.7927730971479080755500978354$;
- Mathematica and Chebfun fail to answer;
- Chen, '06: 0.7578918118.

What is the correct answer, then ?
Using CMs: $0.749974368527[1,3]$.

CMs vs. TMs

Comparison between remainder bounds for several functions:

$f(x)$, I, n	CM	Timing (ms)	TM	Timing (ms)
$\sin(x)$, $[3,\ 4]$, 10	$1.19 \cdot 10^{-14}$	4	$1.22 \cdot 10^{-11}$	2
$\arctan(x)$, $[-0.25,\ 0.25]$, 15	$7.89 \cdot 10^{-15}$	10	$2.58 \cdot 10^{-10}$	4
$\arctan(x)$, $[-0.9,\ 0.9]$, 15	$5.10 \cdot 10^{-3}$	14	$1.67 \cdot 10^{2}$	7
$\exp(1/\cos(x))$, $[0,\ 1]$, 14	$5.22 \cdot 10^{-7}$	31	$9.06 \cdot 10^{-3}$	14
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Computing the coefficients

Chebyshev series of $f = \sum_{i=-\infty}^{+\infty} t_i T_i(x)$:

– Orthogonality $\rightsquigarrow t_i = \dfrac{1}{\pi}\displaystyle\int_{-1}^{1} T_i(t)\frac{f(t)}{\sqrt{1-t^2}}dt$

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Remark: Currently, this step is more costly than in the case of TMs. Use Truncated Chebyshev Series (TCS) instead: for D-finite functions.

D-finite Functions

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

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

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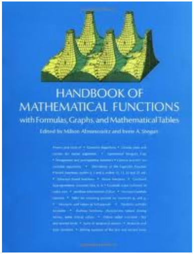

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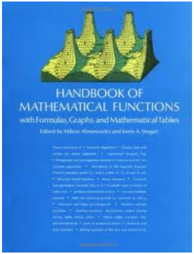

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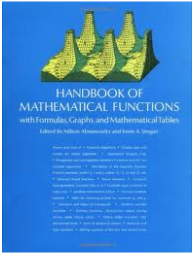
How to obtain a near-minimax RPA of degree d for a D-finite function in $O(d)$?



Chebyshev Series of D-finite Functions

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

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

$u(0) = 1$	$1/0! = 1$
$u(1) = 1$	$1/1! = 1$
$u(2) = 0.5$	$1/2! = 0.5$
$\vdots$	$\vdots$
$u(50) \approx 3.28 \cdot 10^{-65}$	$1/50! \approx 3.28 \cdot 10^{-65}$

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

$u(0) = 1.266$	$I_0(1) \approx 1.266$
$u(1) = 0.565$	$I_1(1) \approx 0.565$
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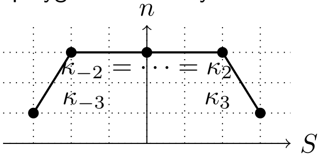
Convergent and Divergent Solutions of the Recurrence

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



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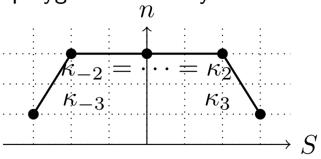

For the recurrence $u(n+1) + 2nu(n) - u(n-1)$

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

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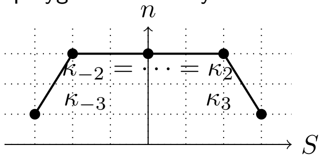

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Miller's algorithm

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

Example: Back to $\exp$

$$\begin{aligned} u(52) &= 0 \\ u(51) &= 1 \\ u(50) &= -102 \\ &\vdots \\ u(2) &\approx -4.72 \cdot 10^{80} \\ u(1) &\approx 1.96 \cdot 10^{81} \\ u(0) &\approx -4.4 \cdot 10^{81} \end{aligned}$$

$$\begin{aligned} I_{52}(1) &\approx 2.77 \cdot 10^{-84} \\ I_{51}(1) &\approx 2.88 \cdot 10^{-82} \\ I_{50}(1) &\approx 2.93 \cdot 10^{-80} \\ &\vdots \\ I_2(1) &\approx 0.14 \\ I_1(1) &\approx -0.57 \\ I_0(1) &\approx 1.27 \end{aligned}$$

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$$
C = \sum_{n=-50}^{50} u(n) T_n(0) \approx -3.48 \cdot 10^{81}
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Example: Back to $\exp$

$$\frac{u(52)}{C} = 0 \qquad\qquad I_{52}(1) \approx 2.77 \cdot 10^{-84}$$

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$$\vdots \qquad\qquad \vdots$$

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Validation

Fixed Point Theorem Applied to a Differential Equation: f is solution of

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

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For all rational functions $a(x)$, if $\dfrac{\|a\|_\infty^j}{j!} < 1$ 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 $|f(x) - p(x)| < B,\ x \in [-1, 1]$.

Find B

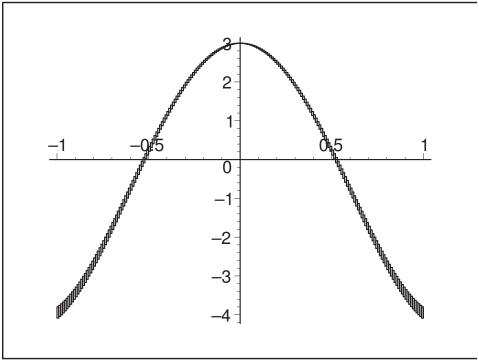
- $p_0 := p$
- while $i! < \|a\|_\infty^i$
  - Compute $p_i(t)$ a rigorous approximation of $\tau(p_{i-1}) = \int_0^t a(x) p_{i-1}(x) dx$ s.t. $\|\tau(p_{i-1}) - p_i\|_\infty < M$.
- Return

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

Certified Plots

Random Example:

$(60x^2 + 75 + 9x^4)y(x) + (-4x^3 - 12x)y'(x) + (x^4 + 6x^2 + 9)y''(x)$,
$y(0) = 3,\ y'(0) = 0.$
Compute coefficients of polynomial of degree 30.



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$\rightsquigarrow$ What about the 12 predictions and beyond?

No	$f(x)$, I, n	CM bound	TM bound
1	$\sin(x)$, $[3,\ 4]$, 10	$1.19 \cdot 10^{-14}$	$\mathbf{5.95 \cdot 10^{-15}}$
2	$\arctan(x)$, $[-0.25,\ 0.25]$, 15	$7.89 \cdot 10^{-15}$	$\mathbf{1.06 \cdot 10^{-15}}$
3	$\arctan(x)$, $[-0.9,\ 0.9]$, 15	$5.10 \cdot 10^{-3}$	$\mathbf{5.81 \cdot 10^{-4}}$
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5	$\frac{\exp(x)}{\log(2+x)\ \cos(x)}$, $[0,\ 1]$, 15	$\mathbf{4.86 \cdot 10^{-9}}$	$4.60 \cdot 10^{-8}$
6	$\sin(\exp(x))$,$[-1,\ 1]$, 10	$\mathbf{2.56 \cdot 10^{-5}}$	$1.01 \cdot 10^{-4}$
7	$\tanh(x + 0.5) - \tanh(x - 0.5)$, $[-1, 1]$, 10	$1.75 \cdot 10^{-3}$	$\mathbf{7.28 \cdot 10^{-4}}$
8	$\sqrt{x + 1.0001}$, $[-1, 0]$, 10	$\mathbf{3.64 \cdot 10^{-2}}$	0.11
9	$\sqrt{x + 1.0001} \cdot \sin(x)$, $[-1, 0]$, 10	$\mathbf{3.32 \cdot 10^{-2}}$	$7.06 \cdot 10^{-2}$
10	$\frac{1}{1+4x^2}$, $[-1, 1]$, 10	$\mathbf{1.13 \cdot 10^{-2}}$	$1.39 \cdot 10^{2}$
11	$\sin^2(x) + \cos^2(x)$, $[-1, 1]$, 10	$\mathbf{3.91 \cdot 10^{-9}}$	$2.23 \cdot 10^{-8}$

Table: Examples of bounds *1 CM vs. 2 TMs*.