Tools for Rigorous Computing using Chebyshev Series Approximations

Nicolas Brisebarre   Mioara Joldes

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  2. Taylor models (TM)
- Where? Beam Physics (M. Berz, K. Makino), Lorentz attractor (W. Tucker), Flyspeck project (R. Zumkeller)

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  2. Taylor models (TM)
  3. Chebyshev models (CM)
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Practical Examples:

- Computing supremum norms of approximation error functions:

$$\sup_{x \in [a,b]} \{|f(x) - g(x)|\},$$

  where g is a very good approximation of f.

- Rigorous quadrature:

$$\pi = \int_0^1 \frac{4}{1+x^2} \mathrm{d}x$$

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- Range bounding for functions
  Eg. $x \in [-1, 2], f(x) = x^2 - x + 1$
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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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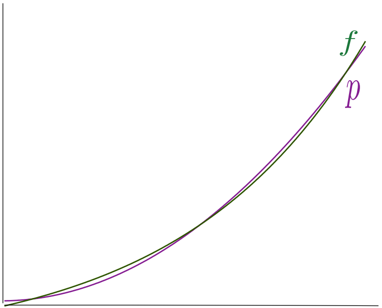
When Interval Arithmetic does not suffice: Computing supremum norms of approximation errors

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



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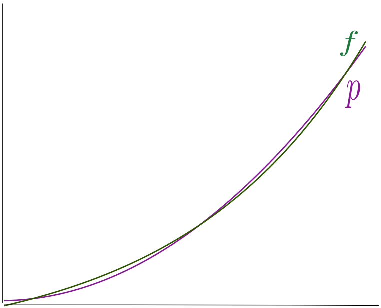

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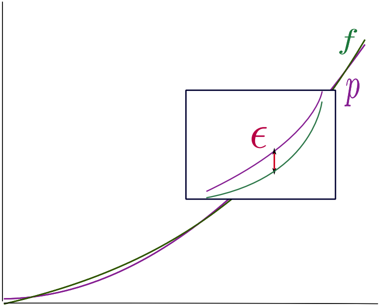

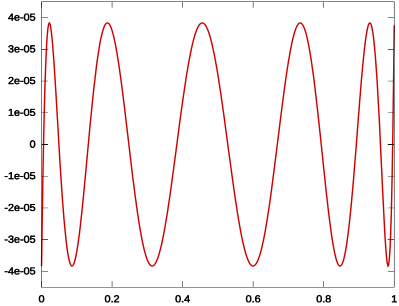

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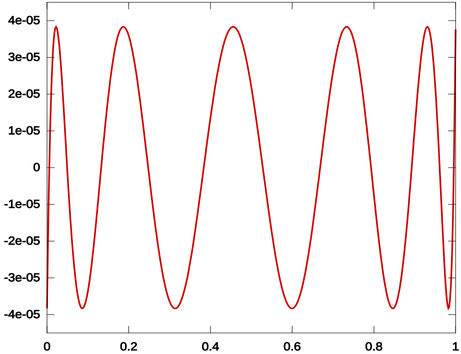

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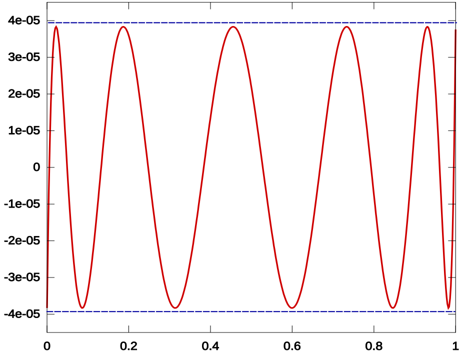

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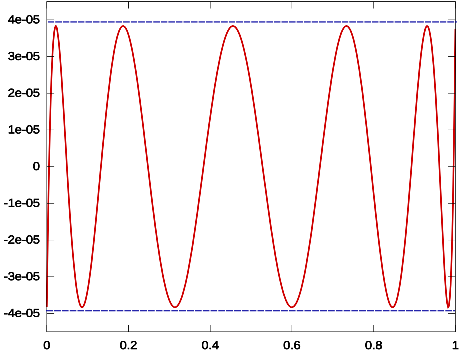
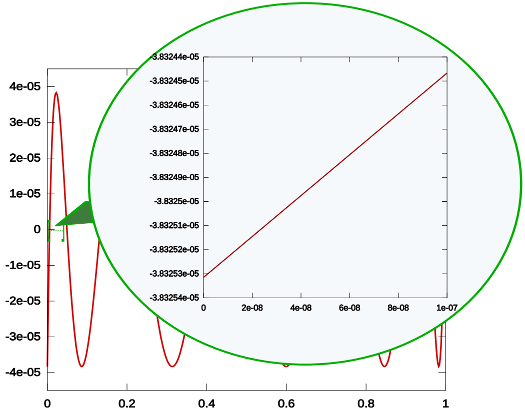


Using IA, $\varepsilon(x) \in [-233, 298]$, but $\|\varepsilon(x)\|_\infty \simeq 3.8325 \cdot 10^{-5}$

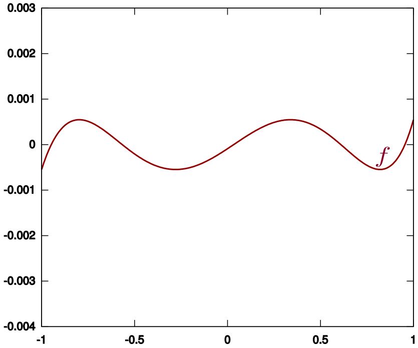
Why IA does not suffice: Overestimation

Overestimation can be reduced by using intervals of smaller width.



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

Rigorous polynomial approximations



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f replaced with
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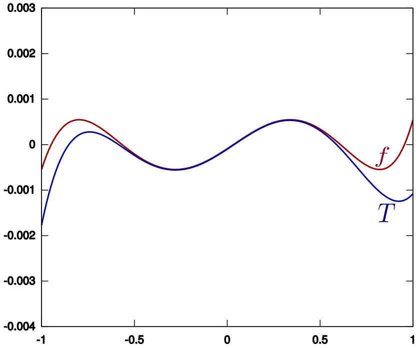

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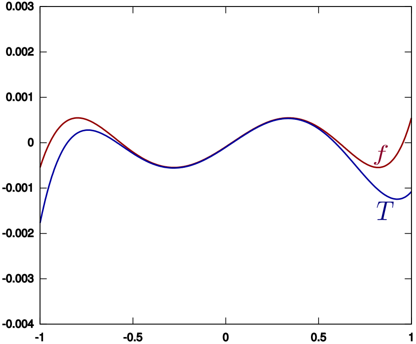

Rigorous polynomial approximations

f replaced with a rigorous polynomial approximation : $(T, \boldsymbol{\Delta})$
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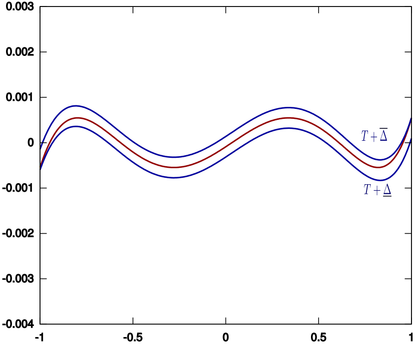

Main point of this talk: How to compute $(T, \boldsymbol{\Delta})$?

Taylor Models

Idea: Consider Taylor approximations

Taylor Models - How do we obtain them?

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

- $f(x) = \underbrace{\sum_{i=0}^{n} \frac{f^{(i)}(x_0)(x-x_0)^i}{i!}}_{T(x)} + \underbrace{\Delta_n(x, \xi)}_{\text{remainder}}$
- $\Delta_n(x, \xi) = \frac{f^{(n+1)}(\xi)(x-x_0)^{n+1}}{(n+1)!}$, $x \in [a, b]$, ξ lies strictly between x and x_0

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- How to compute the coefficients $\dfrac{f^{(i)}(x_0)}{i!}$ of $T(x)$?
- How to compute an interval enclosure $\boldsymbol{\Delta}$ for $\Delta_n(x,\xi)$?

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$f(x) \to [u_0 \, v_0, u_0 \, v_1 + u_1 \, v_0, \ldots, [0, 13.5]]$ But $f^{(4)}([0,1]) = [0, 8]$

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Taylor Models Philosophy

For bounding the remainders:

- For “basic functions” use Lagrange formula.
- For “composite functions”use a two-step procedure:
  - compute models (T, I) for all basic functions;
  - apply algebraic rules with these models, instead of operations with the corresponding functions.

Taylor Models Issues

Example:

$f(x) = \arctan(x)$ over $[-0.9, 0.9]$
$p(x)$ - minimax, degree 15
$\varepsilon(x) = p(x) - f(x)$

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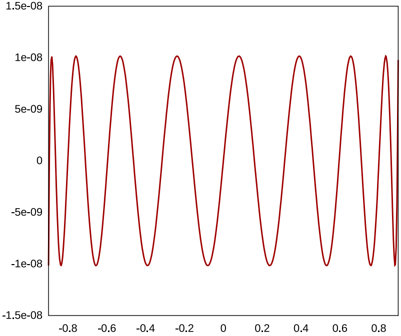

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In this case Taylor approximations are not good, we need theoretically a TM of degree 120.

Practically, the computed interval remainder can not be made sufficiently small due to overestimation

Consequence: Remainder bounds are unsatisfactory in our case.

Our Approach - Chebyshev Models

Basic idea:

- Use a polynomial approximation better than Taylor:

  - Chebyshev interpolation polynomial[3].
  - Chebyshev truncated series.

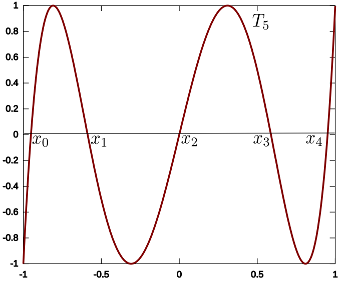
- Use the two step approach as Taylor Models:

  - compute models (P, I) for basic functions;
  - apply algebraic rules with these models, instead of operations with the corresponding functions.

[3] N. Brisebarre, M. Joldes, Chebyshev interpolation polynomial-based tools for rigorous computing. In Proceedings of the 2010 international Symposium on Symbolic and Algebraic Computation (Munich, Germany, July 25 - 28, 2010). ACM, New York, NY, 147-154

Quick Reminder: Chebyshev Polynomials

Over $[-1, 1]$, $T_n(x) = \cos(n \arccos x)\,, n \geq 0$.



"Chebyshev nodes": n distinct real roots in $[-1, 1]$ of T_n:
$x_i = \cos\left(\frac{(i+1/2)\,\pi}{n}\right), i = 0, \ldots, n-1$.

Chebyshev Models: using interpolation polynomial

$P(x) = \sum_{i=0}^{n} p_i T_i(x)$ interpolates f at $x_k \in [-1, 1]$, Chebyshev nodes of order $n+1$.

Chebyshev Models: using interpolation polynomial

$P(x) = \sum_{i=0}^{n} p_i T_i(x)$ interpolates f at $x_k \in [-1, 1]$, Chebyshev nodes of order $n + 1$.

Computation of the coefficients

$p_i = \sum_{k=0}^{n} \frac{2}{n+1} f(x_k) T_i(x_k), \ i = 0, \dots, n$

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Computation of the coefficients

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Remark: Currently, this step is more costly than in the case of TMs. We can use truncated Chebyshev series instead.

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Interpolation Error: Lagrange remainder

$$\forall x \in [-1,1],\ \exists \xi \in [-1,1] \ \text{ s.t.}$$
$$f(x) - P(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n}(x - x_i).$$

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- ✓ We should have an improvement of 2^n in the width of the remainder, compared to Taylor remainder.

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Computation of the coefficients (for "basic" functions)

Interpolation Error: Lagrange remainder (for "basic" functions)

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Computation of the coefficients (for "basic" functions)

Interpolation Error: Lagrange remainder (for "basic" functions)

- For composite functions,use algebraic rules (addition, multiplication, composition) with models

- Note: Chebfun - "Computing Numerically with Functions Instead of Numbers" (N. Trefethen et al.): Chebyshev interpolation polynomials are already used, but the approach is not rigorous

Chebyshev Models: using truncated Chebyshev series

$$P(x) = {\sum_{k=0}^{n}}' a_k T_k(x), \text{ where } a_k = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x) T_k(x)}{\sqrt{1-x^2}} \mathrm{d}x.$$

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Computation of the coefficients (for “basic” D-finite functions)

- recurrence formulae for computing a_k

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Computation of the coefficients (for “basic” D-finite functions)

- recurrence formulae for computing a_k Remark: As fast as TMs.

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Computation of the coefficients (for "basic" D-finite functions)

Truncation Error: Bernstein-like formula (for "basic" D-finite functions)

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

Chebyshev Models: using truncated Chebyshev series

$$P(x) = {\sum_{k=0}^{n}}' a_k T_k(x), \text{ where } a_k = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x) T_k(x)}{\sqrt{1-x^2}} \mathrm{d}x.$$

Computation of the coefficients (for “basic” D-finite functions)

Truncation Error: Bernstein-like formula (for “basic” D-finite functions)

- For composite functions,use algebraic rules (addition, multiplication, composition) with models

Chebyshev Models - Operations: Addition

Given two Chebyshev Models for f_1 and f_2, over $[a, b]$, degree n:
$f_1(x) - P_1(x) \in \mathbf{\Delta}_1$ and $f_2(x) - P_2(x) \in \mathbf{\Delta}_2$, $\forall x \in [a, b]$.

Addition
$(P_1, \mathbf{\Delta}_1) + (P_2, \mathbf{\Delta}_2) = (P_1 + P_2, \mathbf{\Delta}_1 + \mathbf{\Delta}_2)$.

Chebyshev Models - Operations: Multiplication

Given two Chebyshev Models for f_1 and f_2, over $[a, b]$, degree n:
$f_1(x) - P_1(x) \in \mathbf{\Delta}_1$ and $f_2(x) - P_2(x) \in \mathbf{\Delta}_2$, $\forall x \in [a, b]$.

Multiplication
We need algebraic rule for: $(P_1, \mathbf{\Delta}_1) \cdot (P_2, \mathbf{\Delta}_2) = (P, \mathbf{\Delta})$ s.t.
$f_1(x) \cdot f_2(x) - P(x) \in \mathbf{\Delta}$, $\forall x \in [a, b]$

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$$f_1(x) \cdot f_2(x) \in \underbrace{P_1 \cdot P_2}_{} + \underbrace{\boldsymbol{P_2} \cdot \mathbf{\Delta}_1 + \boldsymbol{P_1} \cdot \mathbf{\Delta}_2 + \mathbf{\Delta}_1 \cdot \mathbf{\Delta}_2}_{\boldsymbol{I_2}}.$$

$$\underbrace{(P_1 \cdot P_2)_{0 \ldots n}}_{P} + \underbrace{(P_1 \cdot P_2)_{n+1 \ldots 2n}}_{\boldsymbol{I_1}}$$

$$\mathbf{\Delta} = \boldsymbol{I_1} + \boldsymbol{I_2}$$

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$$\boldsymbol{\Delta} = \boldsymbol{I_1} + \boldsymbol{I_2}$$

In our case, for bounding "$\boldsymbol{P}$s": $\boldsymbol{P} = p_0 + \sum_{i=1}^{n} p_i \cdot [-1, 1]$.

Chebyshev Models - Operations: Composition

Given CMs for f_1 over $[c, d]$, for f_2 over $[a, b]$, degree n:
$f_1(y) - P_1(y) \in \mathbf{\Delta}_1$, $\forall y \in [c, d]$ and $f_2(x) - P_2(x) \in \mathbf{\Delta}_2$, $\forall x \in [a, b]$.

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Remark: $(f_1 \circ f_2)(x)$ is f_1 evaluated at $y = f_2(x)$.
We need: $f_2([a,b]) \subseteq [c,d]$, checked by $\boldsymbol{P_2} + \mathbf{\Delta}_2 \subseteq [c,d]$

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$f_1(f_2(x)) \in P_1(f_2(x)) + \mathbf{\Delta}_1$

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$f_1(f_2(x)) \in P_1(P_2(x) + \boldsymbol{\Delta}_2) + \boldsymbol{\Delta}_1$

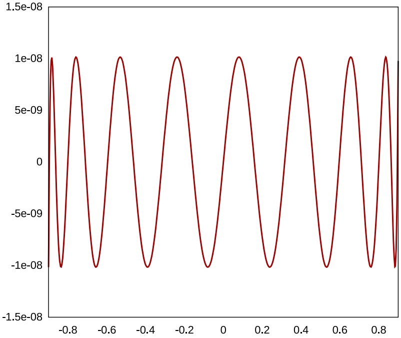
Extract polynomial and remainder: P_1 can be evaluated using only additions and multiplications: Clenshaw's algorithm

Chebyshev Models - Supremum norm example

Example:

$f(x) = \arctan(x)$ over $[-0.9, 0.9]$
$p(x)$ - minimax, degree 15
$\varepsilon(x) = p(x) - f(x)$

$\|\varepsilon\|_\infty \simeq 10^{-8}$



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In this case Taylor approximations are not good, we need theoretically a TM of degree 120.
Practically, the computed interval remainder can not be made sufficiently small due to overestimation.

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In this case Taylor approximations are not good, we need theoretically a TM of degree 120.
Practically, the computed interval remainder can not be made sufficiently small due to overestimation.

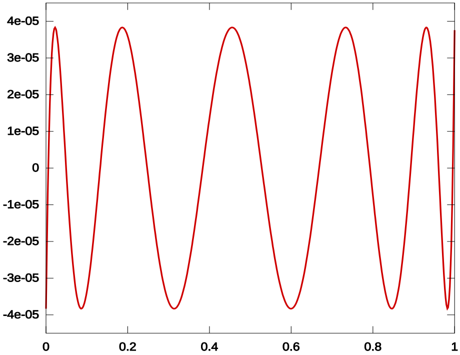
A CM of degree 60 works.

Chebyshev Models - Supremum norm example

Example: $\varepsilon(x) = f(x) - p(x)$

$f(x) = e^{1/\cos x}$, over $[0,1]$, $p(x)$ - minimax, degree 10

$\|\varepsilon(x)\|_\infty \simeq 3.8325 \cdot 10^{-5}$



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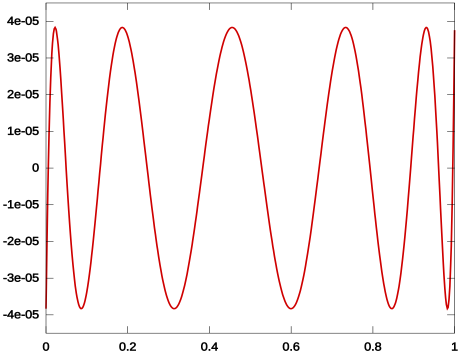
$\|\varepsilon(x)\|_\infty \simeq 3.8325 \cdot 10^{-5}$

Need: TM of degree 30.



Chebyshev Models - Supremum norm example

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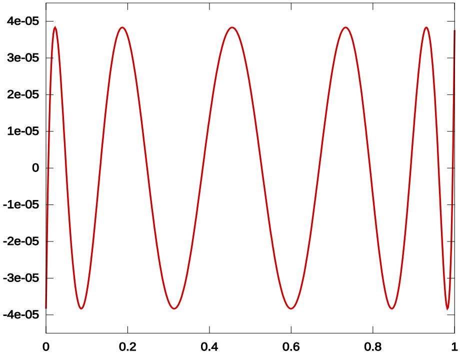
$f(x) = e^{1/\cos x}$, over $[0, 1]$, $p(x)$ - minimax, degree 10

$\|\varepsilon(x)\|_\infty \simeq 3.8325 \cdot 10^{-5}$

Need: TM of degree 30.
CM of degree 13.



CMs vs. TMs

Comparison between remainder bounds for several functions:

$f(x)$, I, n	CM	Exact bound	TM	Exact bound
$\sin(x)$, $[3, 4]$, 10	$1.19 \cdot 10^{-14}$	$1.13 \cdot 10^{-14}$	$1.22 \cdot 10^{-11}$	$1.16 \cdot 10^{-11}$
$\arctan(x)$, $[-0.25, 0.25]$, 15	$7.89 \cdot 10^{-15}$	$7.95 \cdot 10^{-17}$	$2.58 \cdot 10^{-10}$	$3.24 \cdot 10^{-12}$
$\arctan(x)$, $[-0.9, 0.9]$, 15	$5.10 \cdot 10^{-3}$	$1.76 \cdot 10^{-8}$	$1.67 \cdot 10^{2}$	$5.70 \cdot 10^{-3}$
$\exp(1/\cos(x))$, $[0, 1]$, 14	$5.22 \cdot 10^{-7}$	$4.95 \cdot 10^{-7}$	$9.06 \cdot 10^{-3}$	$2.59 \cdot 10^{-3}$
$\frac{\exp(x)}{\log(2+x)\ \cos(x)}$, $[0, 1]$, 15	$9.11 \cdot 10^{-9}$	$2.21 \cdot 10^{-9}$	$1.18 \cdot 10^{-3}$	$3.38 \cdot 10^{-5}$
$\sin(\exp(x))$,$[-1, 1]$, 10	$9.47 \cdot 10^{-5}$	$3.72 \cdot 10^{-6}$	$2.96 \cdot 10^{-2}$	$1.55 \cdot 10^{-3}$

CMs vs. TMs

Operations complexity:

- ✓ Addition ($O(n)$), Multiplication($O(n^2)$) and Composition ($O(n^3)$) have similar complexity.
- ✓ Initial computation of coefficients for all "basic" D-finite functions is similar ($O(n)$).

Comparison between remainder bounds for several functions:

$f(x)$, I, n	CM	Exact bound	TM	Exact bound
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What about other polynomial approximations?

- Remez (minimax):
  - X More costly to obtain (more complex numerical algorithm);
  - X Existent close formula for remainder has the same quality as the one we use.

Quality of approximation compared to minimax

Remark: It is known [Ehlich & Zeller, 1966] that Chebyshev interpolants are "near-best":

$$\|\varepsilon\|_\infty \leq \underbrace{\left(2 + (2/\pi)\log(n)\right)}_{\Lambda_n} \|\varepsilon_{\text{minimax}}\|_\infty$$

- $\Lambda_{15} = 3.72... \rightarrow$ we lose at most 2 bits
- $\Lambda_{30} = 4.16... \rightarrow$ we lose at most 3 bits
- $\Lambda_{100} = 4.93... \rightarrow$ we lose at most 3 bits
- $\Lambda_{100000} = 9.32... \rightarrow$ we lose at most 4 bits

Quality of approximation compared to minimax

No	$f(x)$, I, n	CM	Exact bound	Minimax
1	$\sin(x)$, $[3,\ 4]$, 10	$1.19 \cdot 10^{-14}$	$1.13 \cdot 10^{-14}$	$1.12 \cdot 10^{-14}$
2	$\arctan(x)$, $[-0.25,\ 0.25]$, 15	$7.89 \cdot 10^{-15}$	$7.95 \cdot 10^{-17}$	$4.03 \cdot 10^{-17}$
3	$\arctan(x)$, $[-0.9,\ 0.9]$, 15	$5.10 \cdot 10^{-3}$	$1.76 \cdot 10^{-8}$	$1.01 \cdot 10^{-8}$
4	$\exp(1/\cos(x))$, $[0,\ 1]$, 14	$5.22 \cdot 10^{-7}$	$4.95 \cdot 10^{-7}$	$3.57 \cdot 10^{-7}$
5	$\frac{\exp(x)}{\log(2+x)\ \cos(x)}$, $[0,\ 1]$, 15	$9.11 \cdot 10^{-9}$	$2.21 \cdot 10^{-9}$	$1.72 \cdot 10^{-9}$
6	$\sin(\exp(x))$,$[-1,\ 1]$, 10	$9.47 \cdot 10^{-5}$	$3.72 \cdot 10^{-6}$	$1.78 \cdot 10^{-6}$

Rigorous quadrature

Example:

$$\pi = \int_0^1 \frac{4}{1+x^2} dx$$

- Compute a TM/CM $(P, \boldsymbol{I})$ for $f(x) = \dfrac{4}{1+x^2}$.

Rigorous quadrature

Example:

$$\pi = \int_0^1 \frac{4}{1+x^2} dx$$

- Compute a TM/CM $(P, \boldsymbol{I})$ for $f(x) = \dfrac{4}{1+x^2}$.

  $P(x) + \underline{\boldsymbol{I}} \leq f(x) \leq P(x) + \overline{\boldsymbol{I}}$

Rigorous quadrature

Example:

$$\pi = \int_0^1 \frac{4}{1+x^2} dx$$

- Compute a TM/CM $(P, \boldsymbol{I})$ for $f(x) = \dfrac{4}{1+x^2}$.

$$\int_a^b (P(x) + \underline{\boldsymbol{I}})\mathrm{d}x \leq \int_a^b f(x)\mathrm{d}x \leq \int_a^b (P(x) + \overline{\boldsymbol{I}})\mathrm{d}x$$

Rigorous quadrature

Example:

$$\pi = \int_0^1 \frac{4}{1+x^2} \mathrm{d}x$$

Order	Subdiv.	Bound TM[4]	Bound CM
5	1	[3.0231893333333, 8.5807786666666]	[3.0986941190195, 3.1859962140742]
	4	[3.1415363229415, 3.1416629536292]	[3.1415907717769, 3.1415943610772]
	16	[3.1415926101614, 3.1415926980786]	[3.1415926531269, 3.1415926539131]
10	1	[-2.1984010266006, 3.2113963175267]	[3.1411981994969, 3.1419909934525]
	4	[3.1415926519535, 3.1415926546870]	[3.1415926535805, 3.1415926535990]
	16	[3.1415926535897, 3.1415926535897]	[3.1415926535897932, 3.1415926535897932]

[4] Results taken from M. Berz, K. Makino, "New Methods for High-Dimensional Verified Quadrature", Reliable Computing 5:13-22, 1999

Conclusion

- CMs are potentially useful in various rigorous computing applications: smaller remainders than TMs, similar computing times.
- Current implementation: in Maple `www.ens-lyon.fr/LIP/Arenaire/Ware/ChebModels/`.
- Work in progress: use Chebyshev truncated series instead of Chebyshev interpolation polynomials.
- Future work: extend to multivariate functions