Chebyshev Interpolation Polynomial-based Tools for Rigorous Computing

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April 9, 2010

Motivation

Problem:

- Global optimization
- Quadrature
- ODE solving
- etc.

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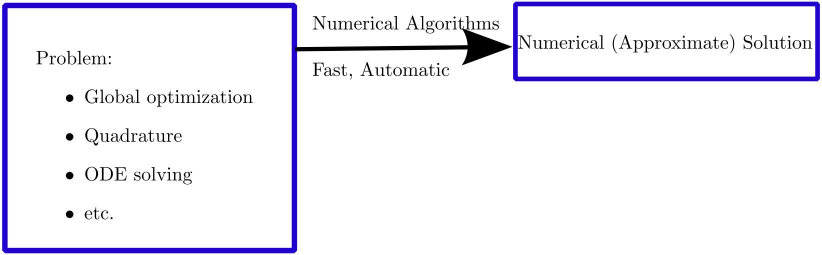
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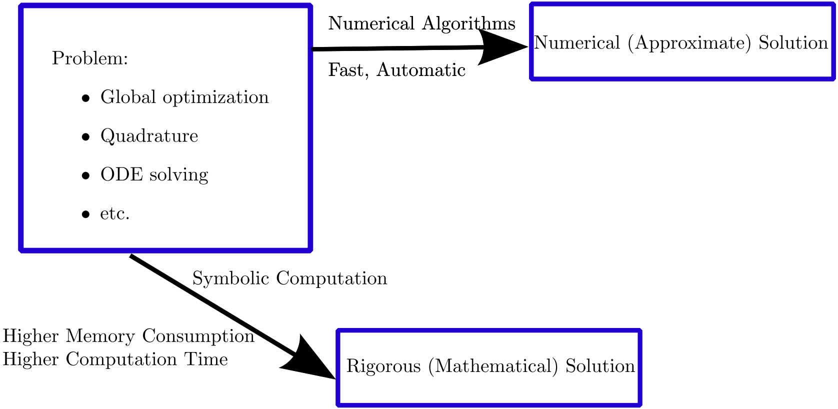
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Higher Computation Time
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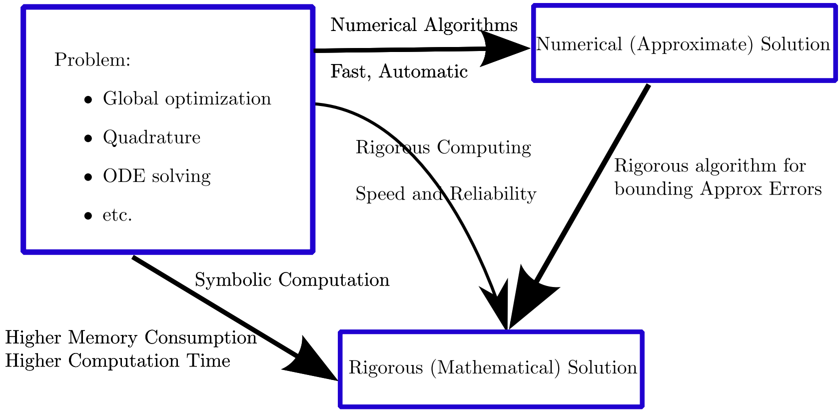

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Numerical Algorithms
Fast, Automatic
Numerical (Approximate) Solution
Rigorous Computing
Speed and Reliability
Rigorous algorithm for
bounding Approx Errors
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  2. Taylor models (TM)

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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. $x \in [-1,2], f(x) = x^2 + x + 1$
  $F(X) = X^2 + X + 1$
  $F([-1,2]) = [-1,2]^2 + [-1,2] + [1,1]$
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  $F([-1, 2]) = [0, 4] + [-1, 2] + [1, 1]$
  $F([-1, 2]) = [0, 7]$
  $x \in [-1, 2], f(x) \in [0, 7]$, but $\mathtt{Im}(f) = [3/4, 7]$

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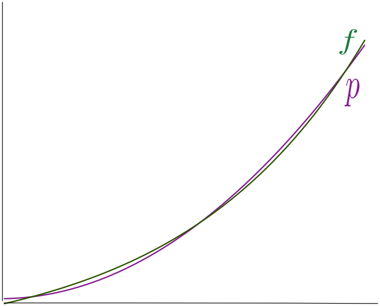
Computing supremum norms of approximation errors

$$f(x) = e^x,\ x \in [0,1],\ \ p(x) = \sum_{i=0}^{5} c_i x^i,\ \ \varepsilon(x) = f(x) - p(x)$$



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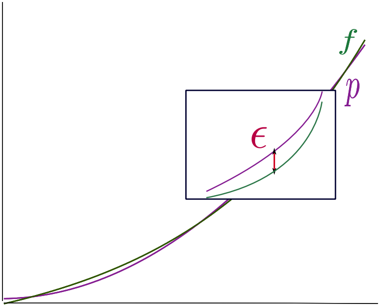

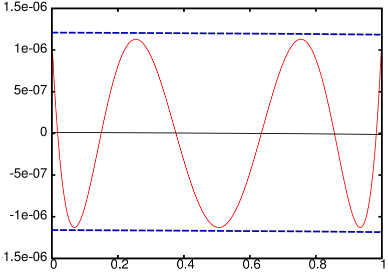

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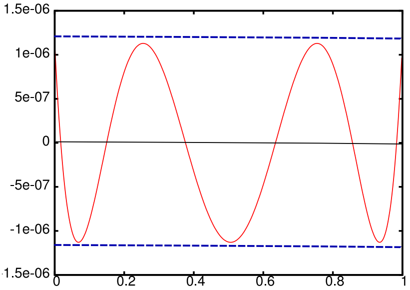

Why IA does not suffice: Overestimation

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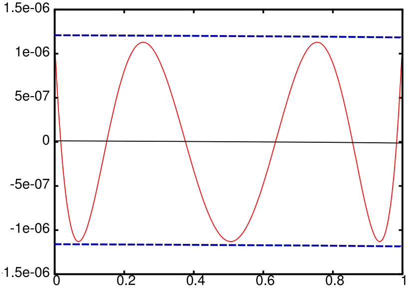
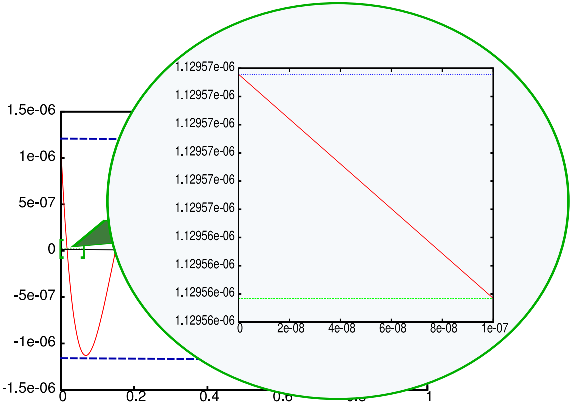


Using IA, $\varepsilon(x) \in [-0.4, 0.4]$, but $\|\varepsilon(x)\|_\infty \simeq 1.1295 \cdot 10^{-6}$:

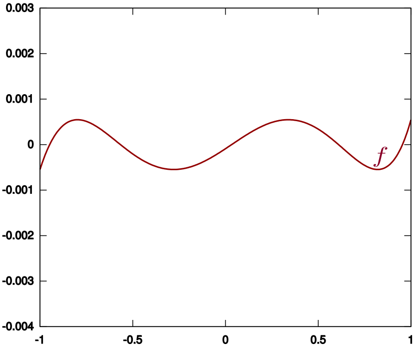
Why IA does not suffice: Overestimation

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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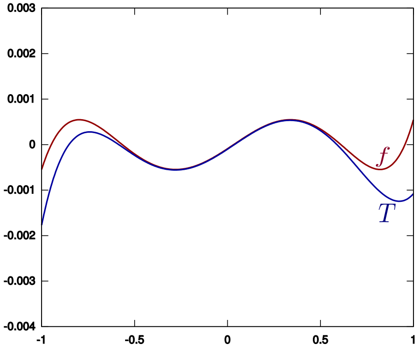

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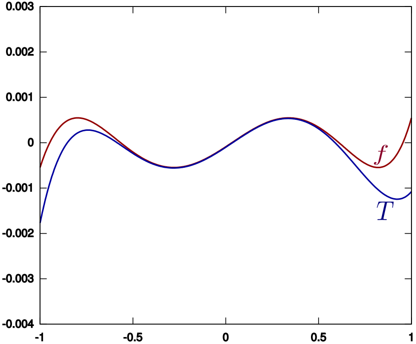

Rigorous polynomial approximations

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

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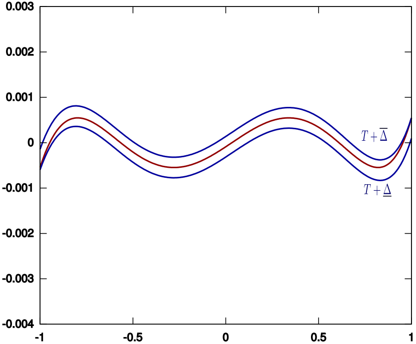

Main point of this talk: How to compute $(T, \boldsymbol{\Delta})$?

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 $\Delta_n(x, \xi)$?

Automatic Differentiation - Point intervals

Compute $f^{(i)}(x_0)$ - f represented as an expression tree

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

What happens when f is a composite function?

$$\color{blue}{f(x)} = \underbrace{\sum_{i=0}^{n} \frac{f^{(i)}(x_0)(x - x_0)^i}{i!}}_{\color{blue}{T(x)}} + \underbrace{\Delta_n(x, \xi)}_{\color{blue}{\text{remainder}}}$$

The interval bound $\mathbf{\Delta}$ for $\Delta_n(x, \xi) = \dfrac{f^{(n+1)}(\xi)(x - x_0)^{n+1}}{(n+1)!}$,

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Example: $f(x) = e^{1/\cos x}$, over $[0,1]$, $n = 13$, $x_0 = 0.5$.

Using AD: $\boldsymbol{\Delta} = [-1.93 \cdot 10^2,\ 1.35 \cdot 10^3]$

In fact, $f(x) - T(x) \in [0, 4.56 \cdot 10^{-3}]$

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Q: What does influence the width of the interval bound for the remainder?

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Q: What does influence the width of the interval bound for the remainder?

- The way we compute an interval enclosure for the remainder using simply this formula for any function

Taylor Models Philosophy

For bounding the remainders:

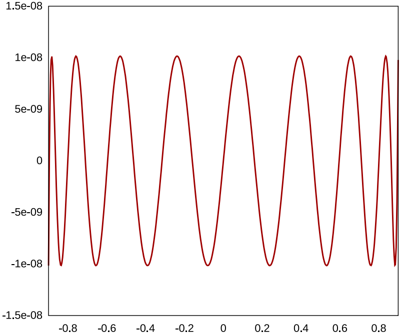
- For “basic functions” use AD.
- For “composite functions”use a two-step procedure:
  - compute models (T, I) for all basic functions;
  - apply algebraic rules with these models, instead of operations with the corresponding functions.

Taylor Models Issues

Example:

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

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



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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

Consequence: Remainder bounds are unsatisfactory in our case.

Our Approach - Chebyshev Models

Basic idea:

- Use a polynomial approximation better than Taylor: Chebyshev interpolation polynomial.
- Use the two step approach as Taylor Models:

- compute models (P, I) for basic functions;
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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.

Our Approach - Chebyshev Models

Compute models (P, I) for basic functions f, where P is the Chebyshev interpolation polynomial

- How to compute the coefficients of P?
- How to bound the remainder?
- What basis for representing P?
- What are the algebraic rules with these models ?

Chebyshev Models - Choice of Basis Polynomials

We used:

- Newton Basis
- Chebyshev Basis - discussed in what follows

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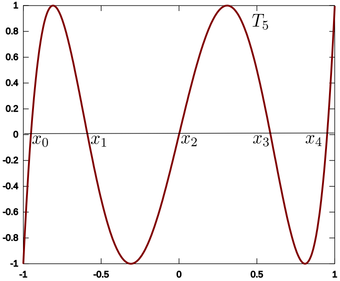
Note: choice of other bases is not detailed in this talk
"Moral principle: Unless you're really, really sure that another set of basis functions is better, use Chebyshev polynomials.",J. P. Boyd[1]

[1] University of Michigan, http://www-personal.umich.edu/~jpboyd/

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:
$x_i = \cos\left(\frac{(i+1/2)\,\pi}{n}\right), i = 0, \ldots, n-1$.

Interpolation polynomials - "Basic" Functions Step

Let $\{y_i, i = 0, \ldots, n\}$ be $n+1$ points in $[-1, 1]$. There exists a unique polynomial P of degree $\leq n$ s.t.
$P(y_i) = f(y_i), \forall i = 0, \ldots, n$, or if y_i is repeated k times,
$P^{(j)}(y_i) = f^{(j)}(y_i), \forall j = 0, \ldots, k-1.$

- all y_i equal, P is the Taylor polynomial of f
- all y_i distinct: Lagrange interpolation

Interpolation polynomials - "Basic" Functions Step

Let $\{y_i, i = 0, \ldots, n\}$ be $n+1$ points in $[-1, 1]$. There exists a unique polynomial P of degree $\leq n$ s.t.
$P(y_i) = f(y_i), \forall i = 0, \ldots, n$, or if y_i is repeated k times,
$P^{(j)}(y_i) = f^{(j)}(y_i), \forall j = 0, \ldots, k-1$.

- all y_i equal, P is the Taylor polynomial of f
- Lagrange remainder:
  $\forall x \in [-1, 1],\ \exists \xi \in [-1, 1]\ \text{ s.t.}$
  $$f(x) - P(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - y_i)^{n+1}.$$

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Interpolation Error - "Basic" Function Step

Lagrange remainder:

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

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Note:

- Optimal choice of interpolation points is the Chebyshev nodes, $W_{\overline{x}}(x) = \frac{1}{2^n} T_{n+1}(x)$.

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

X We inherit all issues related to overestimation of $f^{(n+1)}$

Chebyshev interpolation polynomial - "Basic" Function Step

$P(x) = \sum_{i=0}^{n} p_i T_i(x)$ 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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Remark: Currently, this step is more costly than in the case of TMs.

Chebyshev Models - Operations

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 $f_2(x) - P_2(x) \in \mathbf{\Delta}_2$, $\forall x \in [a, b]$.

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

Where $\divideontimes$ is:

- Addition
- Multiplication
- Composition

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Where $\divideontimes$ is:

- Addition
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- Composition

This is the "hidden difficult part" in designing such models: $\mathbf{\Delta}$ has to be kept tight, while $(P, \mathbf{\Delta})$ has to be computed fast.

Chebyshev Models - Operations: Addition

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

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Multiplication
We need algebraic rule for: $(P_1, \mathbf{\Delta}_1) \cdot (P_2, \mathbf{\Delta}_2) = (P, \mathbf{\Delta})$ s.t.
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$$f_1(x) \cdot f_2(x) \in \underbrace{P_1 \cdot P_2} + \underbrace{\boldsymbol{P_2} \cdot \mathbf{\Delta}_1 + \boldsymbol{P_1} \cdot \mathbf{\Delta}_2 + \mathbf{\Delta}_1 \cdot \mathbf{\Delta}_2}_{\boldsymbol{I_2}}.$$

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

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

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

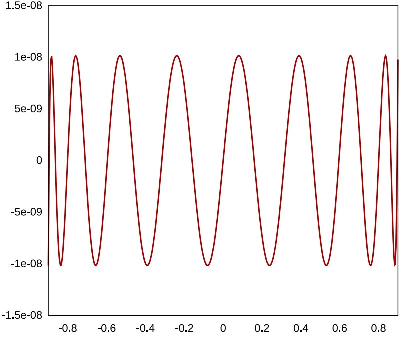
Extract polynomial and remainder: P_1 can be evaluated using only additions and multiplications: Clenshaw's algorithm

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

A CM of degree 60 works.

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.
- X Initial computation of coefficients for "basic functions" is slower with CMs ($O(n^2)$) vs. TMs ($O(n)$)

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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	$9.47 \cdot 10^{-5}$	$3.72 \cdot 10^{-6}$	$1.78 \cdot 10^{-6}$

What about other polynomial approximations?

What about other polynomial approximations?

- Truncated Chebyshev series:

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

✓ possible speed-up: recurrence formulae for computing polynomial coefficients for "basic functions"

?? Possible loss in the quality of remainder.

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[2]	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]

[2] 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, but require more computing time.
- Current implementation: partially Sollya and Maple.
- Work in progress: use Chebyshev truncated series instead of Chebyshev interpolation polynomials.
- Future work: extend to multivariate functions

How to reduce the width of the remainder?

Monotonic properties of the remainder can be infered for "basic" functions [3]:

[3] Corollary in R. Zumkeller, "Global Optimization in Type Theory", PhD thesis, page 84

How to reduce the width of the remainder?

Monotonic properties of the remainder can be infered for "basic" functions [3]:

If $f^{(n+1)}([a,b]) \geq 0$, and T is Taylor polynomial of degree n for f , $\dfrac{f-T}{(x-x_0)^{n+1}}$ is monotonic over $[a,b]$: the remainder can be exactly bounded using two evaluations of $f-T$ in the end points of $[a,b]$.

[3] Corollary in R. Zumkeller, "Global Optimization in Type Theory", PhD

How to reduce the width of the remainder?

Monotonic properties of the remainder can be infered for "basic" functions [3]:

Example: $f(x) = \log(x)$, over $[0.001, 1.001]$, $n = 13$, $x_0 = 0.5$.

$$\Delta_n(x,\xi) = \frac{-1}{\xi^{14}} \cdot \frac{(x-0.5)^{14}}{14!}$$

$$\boldsymbol{\Delta} \subseteq [-2.66 \cdot 10^{31}, 2.63 \cdot 10^{-10}]$$

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With Z's remark, $f(x) - T(x) \in [-3.06, 7.89 \cdot 10^{-31}]$

[3] Corollary in R. Zumkeller, "Global Optimization in Type Theory", PhD thesis, page 84

Interpolation Error - "Basic" Function Step

We can prove (a generalization of Zumkeller's remark):

if $f^{(n+1)}$ is monotonic over I, then $\frac{f(x)-P(x)}{W_{\overline{y}}(x)}$ is monotonic over I.
The remainder can be exactly bounded using two evaluations in the end points of I