

BOUND ERRORS!  **TCS**
EDITION

SUPNORM

FOR

NEWBIES

**RIGOROUS,
AUTOMATIC,
GUARANTEED
A PRORI
QUALITY,
FORMALLY
CERTIFIED**

**AVAILABLE IN
SOLLYA**



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Mioara Joldes

Journées TAMADI,
27-28 Oct. 2010

Supremum Norms and Rigorous Polynomial Approximations

Based on:

- S. Chevillard, J. Harrison, M.J., Ch. Lauter, *Efficient and accurate computation of upper bounds of approximation errors*, accepted for TCS.
- N. Brisebarre, M.J., *Chebyshev interpolation polynomial-based tools for rigorous computing*, ISSAC 2010.

Supremum Norms and Rigorous Polynomial Approximations

Outline

- Origin and Motivation of Supremum Norms Computations
 \rightsquigarrow Previous techniques

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- Origin and Motivation of Supremum Norms Computations
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- Chebyshev Models
- Comparison, Experimental Results

Origins

- Development of `libms`.
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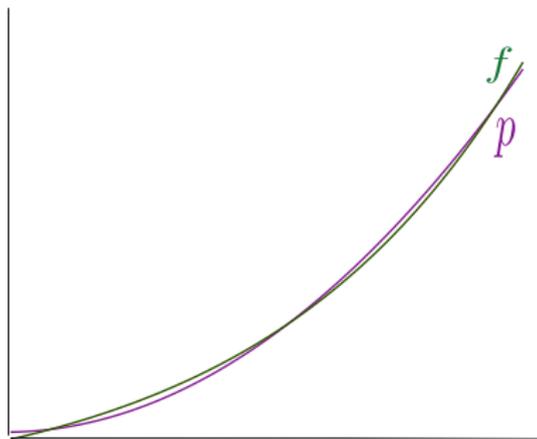
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 - Bound the error between p and f : compute

$$\|\varepsilon\|_{\infty} = \sup_{x \in [a, b]} \{|\varepsilon(x)|\}$$

where $\varepsilon(x) = f(x) - p(x)$ or $\varepsilon(x) = p(x)/f(x) - 1$.

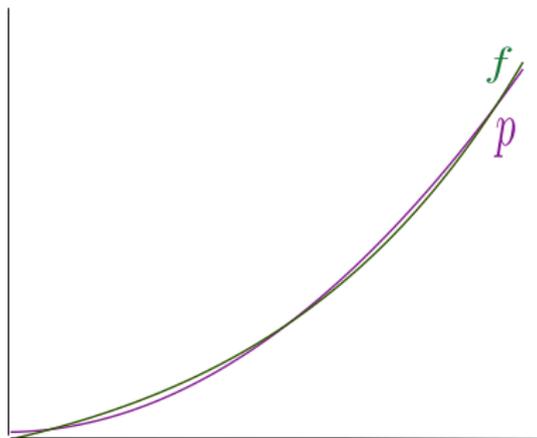
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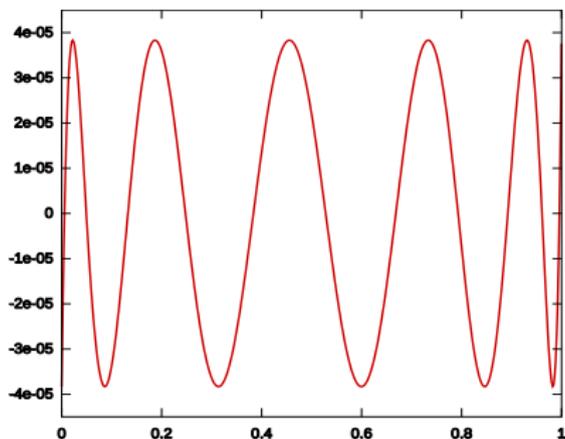
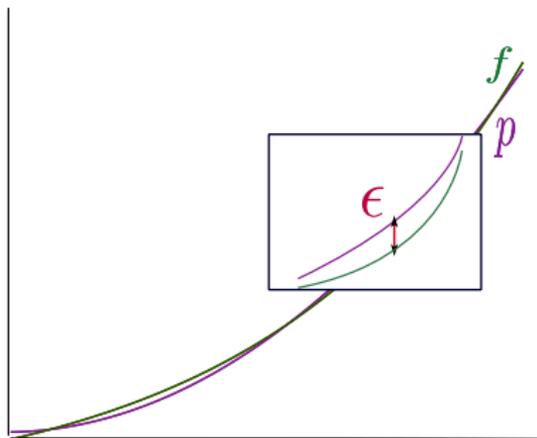
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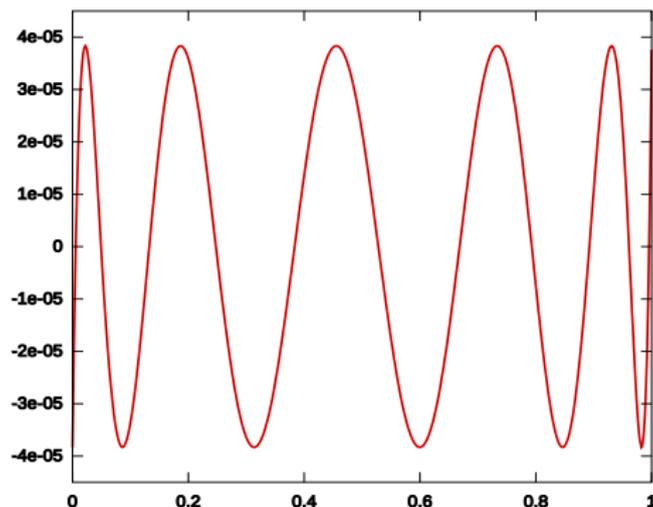
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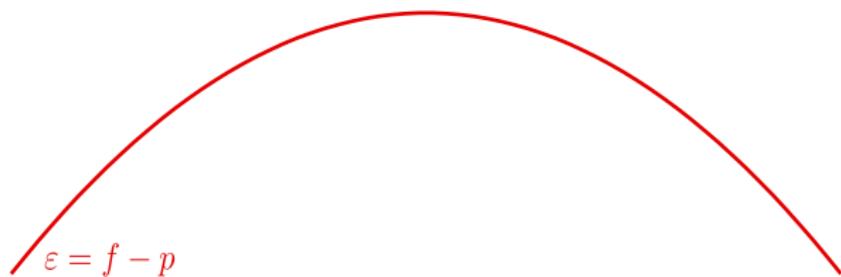


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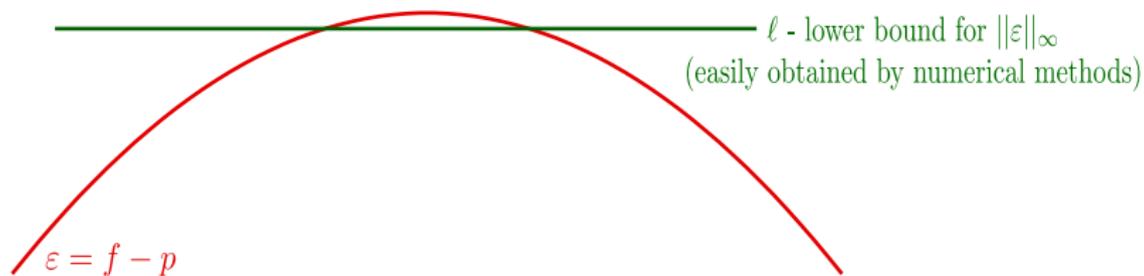
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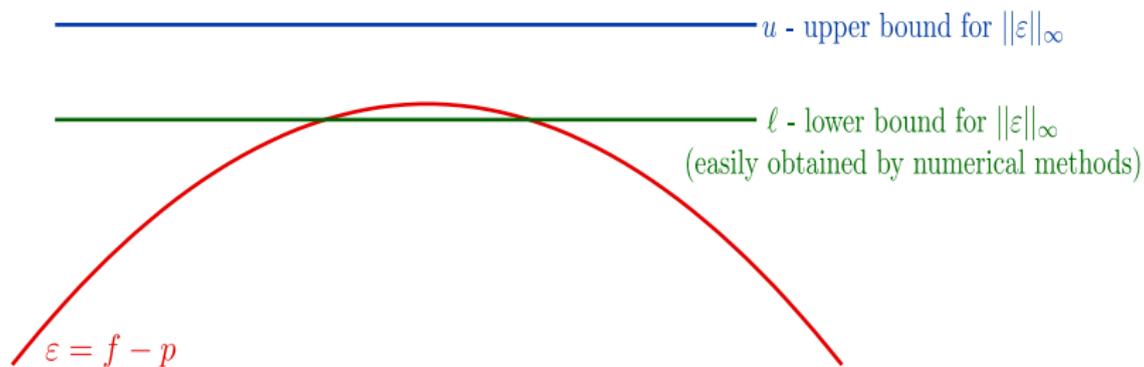
Our problem - How to find l and u such that $\|\varepsilon\|_\infty \in [l, u]$?



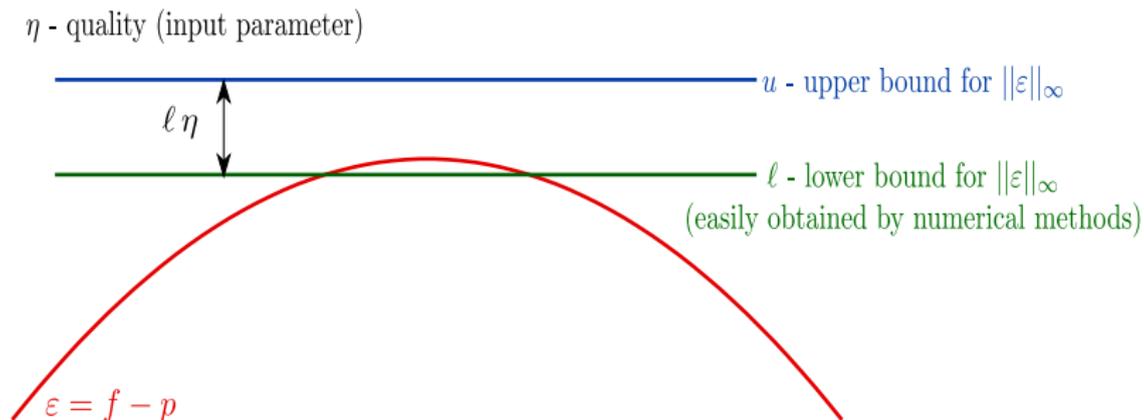
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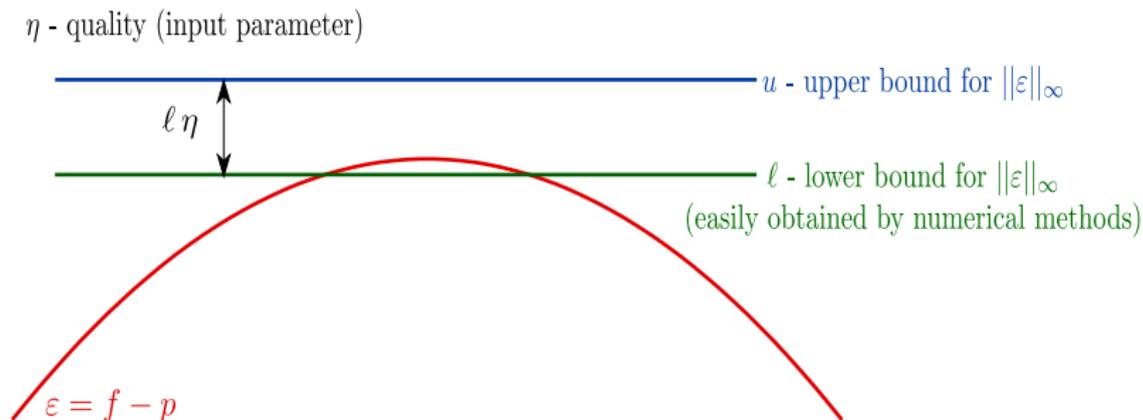
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Actual difficulty: **certified** upper bound u

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e.g. $f(x) = \sin(x)$, $p(x) = x q(x)$ and $\varepsilon(x) = p(x)/f(x) - 1$.
- Could generate a complete formal proof without much effort.

State of the art

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 \rightsquigarrow **Not rigorous**: we might miss some of the zeros.
- General-purpose rigorous global optimization algorithms¹
 - use Interval Arithmetic (IA)
 - Branch and bound: bisection, Interval Newton's algorithm.

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Interval Arithmetic (IA)

- Each interval = pair of floating-point numbers
(multiple precision IA libraries exist, e.g. MPFI²)

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Eg. $x \in [-1, 2], f(x) = x^2 - x + 1$
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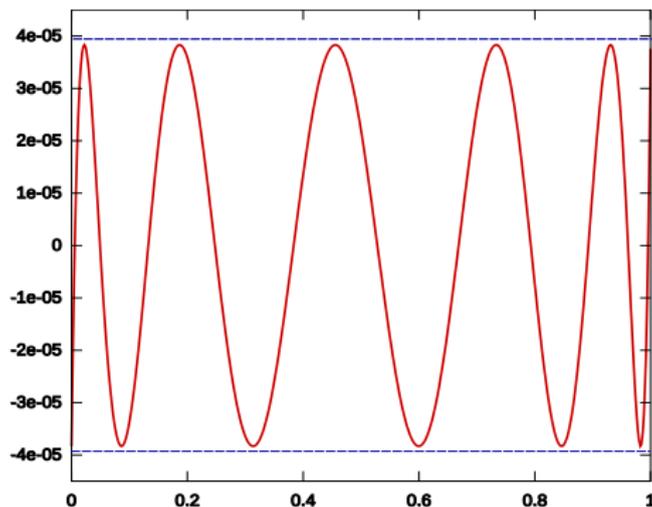
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 $F([-1, 2]) = [-1, 6]$
 $x \in [-1, 2], f(x) \in [-1, 6],$ but $\text{Im}(f) = [3/4, 3]$

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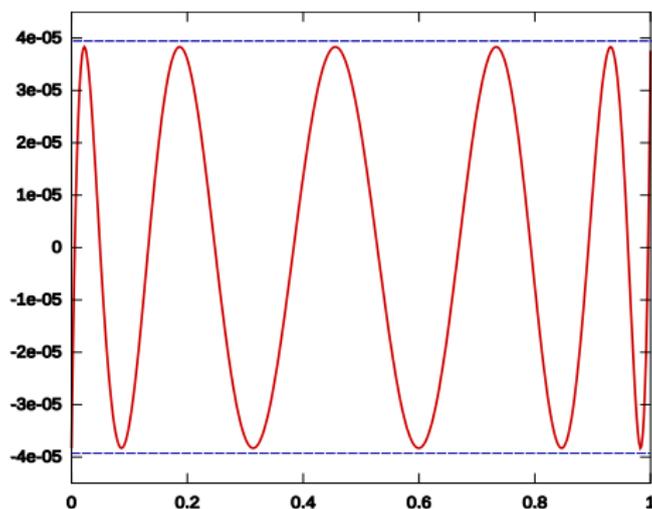
Example (IA -Dependency phenomenon):

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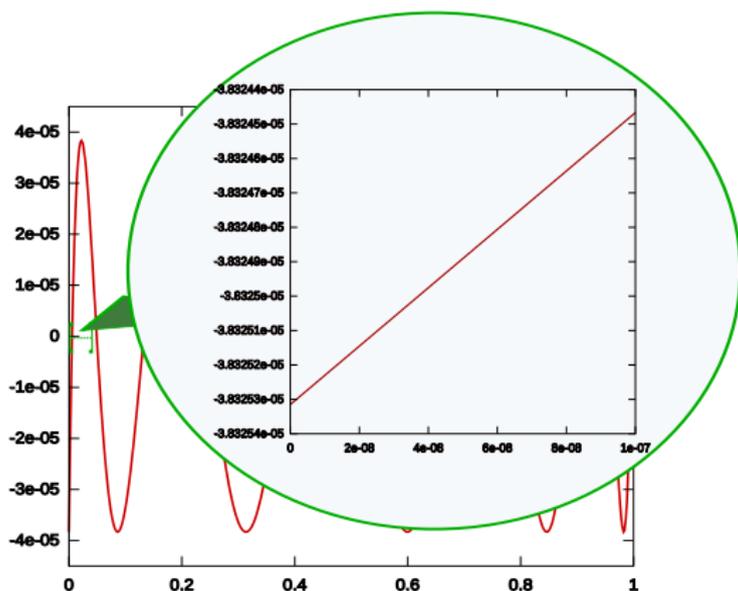
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Using IA, $\varepsilon(x) \in [-233, 298]$, but $\|\varepsilon(x)\|_\infty \simeq 3.8325 \cdot 10^{-5}$

Example (IA - Dependency phenomenon):

Overestimation can be reduced by using intervals of smaller width.



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

Ad-hoc techniques

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 - polynomial approximation T
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- None of these techniques correctly handles removable discontinuities.

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Ingredients of our algorithm

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- $\|f - p\|_\infty \leq \|f - T\|_\infty + \|T - p\|_\infty \rightsquigarrow$ Relative error case
slightly more technical

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Taylor Models

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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 .

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

- $$\Delta_n(x, \xi) = \frac{f^{(n+1)}(\xi)(x - x_0)^{n+1}}{(n + 1)!}, \quad x \in [a, b], \quad \xi \text{ lies strictly between } x \text{ and } x_0$$

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• How to compute the coefficients $\frac{f^{(i)}(x_0)}{i!}$ of $T(x)$?

• How to compute an interval enclosure Δ for $\Delta_n(x, \xi)$?

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

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- Automatic differentiation and Lagrange formula:
 $\Delta = [-1.93 \cdot 10^2, 1.35 \cdot 10^3]$

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Example :

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

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

- Automatic differentiation and Lagrange formula:

$$\Delta = [-1.93 \cdot 10^2, 1.35 \cdot 10^3]$$

- Cauchy's Estimate

$$\Delta = [-9.17 \cdot 10^{-2}, 9.17 \cdot 10^{-2}]$$

What happens when f is a composite function?

The interval bound Δ for $\Delta_n(x, \xi)$ can be largely overestimated.

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- Taylor Models

$$\Delta = [-9.04 \cdot 10^{-3}, 9.06 \cdot 10^{-3}]$$

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 - Operations: Addition

Given two Taylor Models for f_1 and f_2 , over $[a, b]$, degree n :
 $f_1(x) - P_1(x) \in \Delta_1$ and $f_2(x) - P_2(x) \in \Delta_2, \forall x \in [a, b]$.

Addition

$$(P_1, \Delta_1) + (P_2, \Delta_2) = (P_1 + P_2, \Delta_1 + \Delta_2).$$

Taylor Models - Operations: Multiplication

Given two Taylor Models for f_1 and f_2 , over $[a, b]$, degree n :
 $f_1(x) - P_1(x) \in \Delta_1$ and $f_2(x) - P_2(x) \in \Delta_2$, $\forall x \in [a, b]$.

Multiplication

We need algebraic rule for: $(P_1, \Delta_1) \cdot (P_2, \Delta_2) = (P, \Delta)$ s.t.
 $f_1(x) \cdot f_2(x) - P(x) \in \Delta$, $\forall x \in [a, b]$

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$$f_1(x) \cdot f_2(x) \in \underbrace{P_1 \cdot P_2}_{P} + \underbrace{P_2 \cdot \Delta_1 + P_1 \cdot \Delta_2 + \Delta_1 \cdot \Delta_2}_{I_2}.$$

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

$$\Delta = I_1 + I_2$$

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$$\Delta = I_1 + I_2$$

In our case, for bounding “ P s”: IA evaluation.

Taylor Models - Operations: Composition

Given TMs for f_1 over $[c, d]$, for f_2 over $[a, b]$, degree n :

$$f_1(y) - P_1(y) \in \Delta_1, \forall y \in [c, d] \text{ and } f_2(x) - P_2(x) \in \Delta_2, \forall x \in [a, b].$$

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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 $P_2 + \Delta_2 \subseteq [c, d]$

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$$f_1(f_2(x)) \in P_1(f_2(x)) + \Delta_1$$

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We need: $f_2([a, b]) \subseteq [c, d]$, checked by $P_2 + \Delta_2 \subseteq [c, d]$

$$f_1(f_2(x)) \in P_1(P_2(x) + \Delta_2) + \Delta_1$$

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

TMs for functions with removable discontinuities

Example: $F(x) = \frac{\sin(x)}{\log(1+x)}$ over $[-\frac{1}{2}, \frac{1}{2}]$.

Taylor expansion exists, but using classical tm arithmetic:
we need a tm for $\frac{1}{y}$ over $[\log(\frac{1}{2}), \log(\frac{3}{2})] \ni 0$ which cannot be
computed.

TMs for functions with removable discontinuities

Keep remainders in "relative" way:

TM for $f(x) = \sin(x)$ in 0, order $n + 1$, over $[-\frac{1}{2}, \frac{1}{2}]$.

TM for $g(x) = \log(1 + x)$ in 0, order $n + 1$, over $[-\frac{1}{2}, \frac{1}{2}]$.

$$\frac{f}{g} = \frac{x \times (T_f(x) + r_f x^n)}{x \times (T_g(x) + r_g x^n)}$$

Example:

$$\frac{f}{g} = \frac{x \times (1 - \frac{1}{6}x^2 + r_f x^3)}{x \times (1 - \frac{1}{2}x + \frac{1}{3}x^2 + r_g x^3)}$$

TMs for functions with removable discontinuities

Need: tm of order n for $F = \frac{f}{g}$ over I , knowing that $x_0 \in I$ root of order $k > 0$ of f and g .

Idea: Keep remainders in "relative" way: $\mathbf{r} = \Delta \times (x - x_0)^{n+k}$

- Compute tms of order $n + k$ for f and g in x_0 .
- Formally simplify $\frac{f}{g}$ by $(x - x_0)^k$, then compute using regular tm arithmetic
- All operations can be easily extended to work with "relative remainders"

So far, some key points in our supnorm algorithm...

- f replaced with a rigorous polynomial approximation: (T, Δ)
- use **modified Taylor Models** for computing (T, Δ) .
- $\|f - p\|_\infty \leq \|f - T\|_\infty + \|T - p\|_\infty$

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- use **modified Taylor Models** for computing (T, Δ) .
- $\|f - p\|_\infty \leq \|f - T\|_\infty + \|T - p\|_\infty$

Note: Our algorithm can fail if Δ can not be made small enough.
Solution: Cut the interval into sub-intervals or use ChebModels⁴

⁴N. 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

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Computing $\|T - p\|_\infty$ not discussed in this talk.

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Experimental results - Supnorm Algorithm with TMs

f	$[a, b]$	$\deg(p)$	$\deg(T)$	mode	quality $-\log_2 \eta$	time NR	time R
$\exp(x) - 1$	$[-0.25, 0.25]$	5	13	rel.	37.6	14	42
$\log_2(1 + x)$	$[-2^{-9}, 2^{-9}]$	7	17	rel.	83.3	41	103
$\arcsin(x + m)$	$[a_3, b_3]$	22	32	rel.	15.9	270	364
$\cos(x)$	$[-0.5, 0.25]$	15	22	rel.	19.5	93	139
$\exp(x)$	$[-0.125, 0.125]$	25	34	rel.	42.3	337	443
$\sin(x)$	$[-0.5, 0.5]$	9	17	abs.	21.5	13	39
$\exp(\cos^2 x + 1)$	$[1, 2]$	15	44	rel.	25.5	180	747
$\tan(x)$	$[0.25, 0.5]$	10	22	rel.	26.0	47	94
$x^{2.5}$	$[1, 2]$	7	20	rel.	15.5	27	73
$\sin(x)/(\exp(x) - 1)$	$[-2^{-3}, 2^{-3}]$	15	27	abs.	15.5	43	168

Values for example #3:

$$m = \frac{770422123864867}{2^{50}}, \quad a_3 = \frac{-205674681606191}{2^{53}}, \quad b_3 = \frac{205674681606835}{2^{53}}.$$

In the last columns, “NR” stands for “not rigorous” and “R” stands for “rigorous”.

Timings are given in milliseconds on a Core i7-975.

Taylor Models Issues

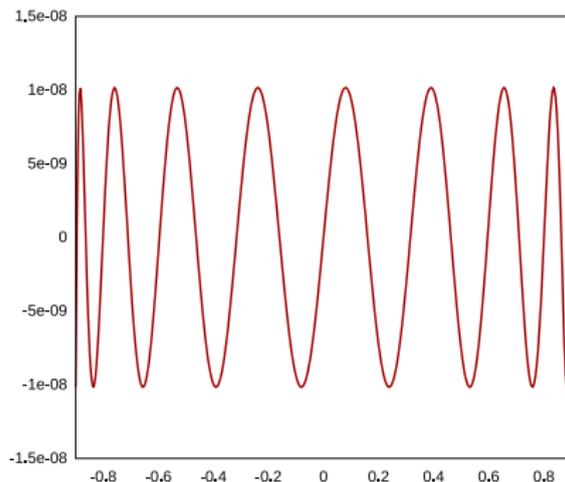
Example:

$f(x) = \arctan(x)$ 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

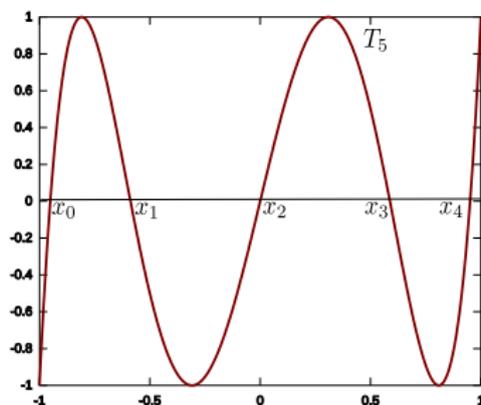
Chebyshev Models

Basic idea:

- Use a polynomial approximation better than Taylor:
 - Chebyshev interpolation polynomial.
 - 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 (work in Chebyshev basis).

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 :

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

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 $n + 1$.

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Computation of the coefficients

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

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

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

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Computation of the coefficients

Interpolation Error: Lagrange remainder

$\forall x \in [-1, 1], \exists \xi \in [-1, 1]$ 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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- ✗ For composite functions, overestimation of $f^{(n+1)}$

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Computation of the coefficients (for “basic” functions)

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

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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

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

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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.

Chebyshev Models: using truncated Chebyshev series

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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

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

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

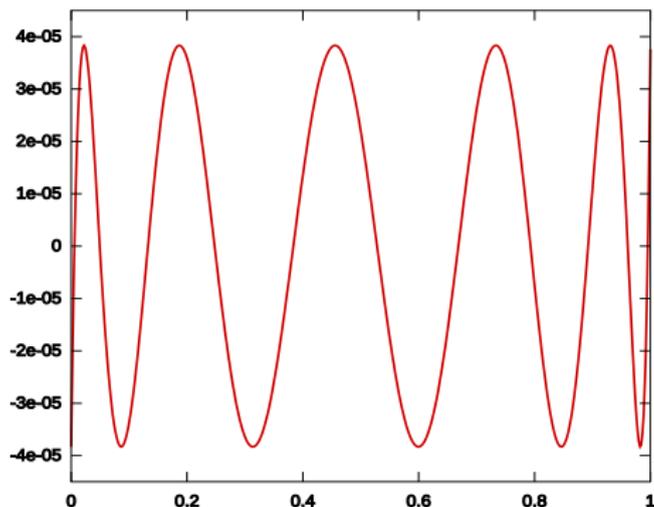
- For composite functions, use algebraic rules (addition, multiplication, composition) with models

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

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



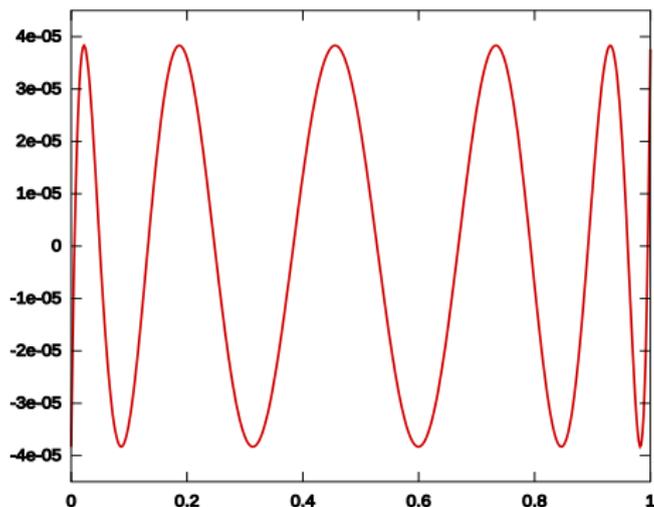
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Need: TM of degree 30.



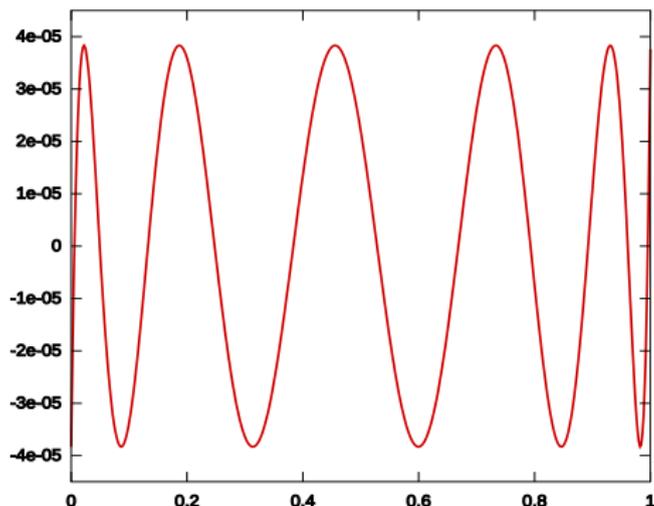
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Need: TM of degree 30.
CM of degree 13.



Comparison between remainder bounds for several functions:

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

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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Quality of approximation compared to minimax

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

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

- $\Lambda_{15} = 3.72\dots \rightarrow$ we lose at most 2 bits
- $\Lambda_{30} = 4.16\dots \rightarrow$ we lose at most 3 bits
- $\Lambda_{100} = 4.93\dots \rightarrow$ we lose at most 3 bits
- $\Lambda_{100000} = 9.32\dots \rightarrow$ 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	$\sin(\exp(x)), [-1, 1], 10$	$9.47 \cdot 10^{-5}$	$3.72 \cdot 10^{-6}$	$1.78 \cdot 10^{-6}$

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