Approximation Theory and Proof Assistants: Certified Computations

Nicolas Brisebarre and Damien Pous

Master 2 Informatique Fondamentale
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3.2. Interval functions

Definition

(Interval extension.) Let $X \in \mathbb{IR}$*, and let* $f : X \to \mathbb{R}$*. A function* $\tilde{f} : X \cap \mathbb{IR} \to \mathbb{IR}$ *is called an interval extension of* f *over* X *if:*

- *for all* $x \in X$, $R(f, \{x\}) = \tilde{f}([x, x])$*,*
- *for all* $Y \subset \mathbb{IR}$ *with* $Y \subset X$*, we have*

$$R(f, Y) \subset \tilde{f}(Y).$$

Several interval extensions are possible for the same function over the same X. Interval extensions of $\exp$ over $[-1, 1]$ include

- the function $[\underline{x}, \bar{x}] \mapsto [e^{\underline{x}}, e^{\bar{x}}]$.
- but also?

3.2. Interval functions

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If $f(x)$ is a rational *expression*, one means to get an interval extension of the function it denotes is to replace each occurrence of the variable x by the interval X, and "overload" all arithmetic operations with interval operations. The resulting extension is called *the natural interval extension*.

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Theorem

Given a rational expression denoting a real-valued function f, and its natural interval extension F, which we assume to be well-defined over some interval $X \in \mathbb{IR}$, then

1. $Z \subset Z' \subset X$ *implies* $F(Z) \subset F(Z')$ *(inclusion isotonicity);*
2. $R(f, X) \subset F(X)$ *(range enclosure).*

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We now would like to extend this notion of natural interval extension to a larger class of functions.

Definition

We call basic (or standard) functions the elements of

$$\mathfrak{S} = \Big\{ \sin, \cos, \exp, \tan, \log, x^{p/q}, \ldots \Big\}$$

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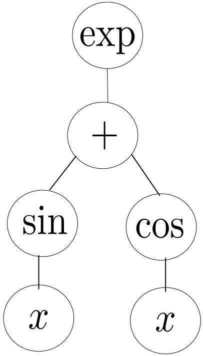
Definition

We call elementary function a symbolic expression built from constants and basic functions using arithmetic operations and composition. The class of elementary functions will be denoted $\mathcal{E}$. A function $f \in \mathcal{E}$ is given by an expression tree (or dag, for directed acyclic graph).

Elementary function: example of a dag

Example: $f_{\text{comp}}(x) = \exp(\sin(x) + \cos(x))$ over $[a, b]$.



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An interval valued function $F : X \cap \mathbb{IR} \to \mathbb{IR}$ *is inclusion isotonic over* $X \in \mathbb{IR}$ *if* $Z \subset Z' \subset X$ *implies* $F(Z) \subset F(Z')$.

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Theorem

Given an elementary function f *and an interval* X *over which the natural interval extension* F *of* f *is well-defined:*

1. F *is inclusion isotonic over* X;
2. $R(f, X) \subset F(X)$.

3.2. Interval functions

Example

Consider

$$f(x) = \left(\cos x - x^3 + x\right)(\tan x + 1/2)$$

over $[0, \pi/4]$. *To show that* f *has no zero in this range, we compute the natural interval extension*

$$f([0, \pi/4]) = \left[\frac{\sqrt{2}}{2} - \frac{\pi^3}{64}, 1 + \frac{\pi}{4}\right]\left[\frac{1}{2}, \frac{3}{2}\right] \subset [0.11, 2.68]\,.$$

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Exercise

Show that $f(x) = x - \sin x + 2/5$ *has no zero over* $[0, \pi/4]$*.*

3.2. Interval functions

Theorem

Let $X \in \mathbb{IR}$*. Let* f *be an elementary function such that any subexpression of* f *is Lipschitz continuous. Let* F *be an inclusion isotonic interval extension such that* $F(X)$ *is well-defined. Then, there exists* $\kappa > 0$*, depending on* F *and* X*, such that, if* $X = \bigcup_{i=1}^{k} X_i$*, with* $X_i \in \mathbb{IR}$ *for all* i*,then*

$$R(f, X) \subset \bigcup_{i=1}^{k} F(X_i) \subset F(X)$$

and

$$\operatorname{rad}\left(\bigcup_{i=1}^{k} F(X_i)\right) \leqslant \operatorname{rad}(R(f, X)) + \kappa \max_{i=1,\ldots,k} \operatorname{rad} X_i.$$

However, the number of subdivisions needed may be very large.

Example

Let $f(x) = e^{1/\cos x}$*, and let* p *be a degree-10 minimax approximation of* f *over* $[0,1]$*. Let*

$$\varepsilon(x) = f(x) - p(x).$$

Using the natural interval extension of ε*, we get* $\|\varepsilon\| \leqslant 298$*. But one can show that obtaining the actual value* $\|\varepsilon\| \approx 3.8325 \cdot 10^{-5}$ *by subdivision would require about* 10^7 *subintervals.*

Newton method

Theorem

Let $X \in \mathbb{R}$, let $f \in \mathcal{C}^2(X)$, s.t. $f'(x) \neq 0$ for all $x \in X$ and f has a unique, simple zero x^* in X. Then if x_0 is chosen sufficiently close to x^*, the sequence $(x_k)_{k \in \mathbb{N}}$ defined by

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} \quad \textit{for } k = 0, 1, 2, \ldots$$

converges quadratically fast toward x^*: there exists a constant C such that

$$\lim_{k \to +\infty} x_k = x^* \text{ and } |x_{k+1} - x^*| \leqslant C |x_k - x^*|^2.$$

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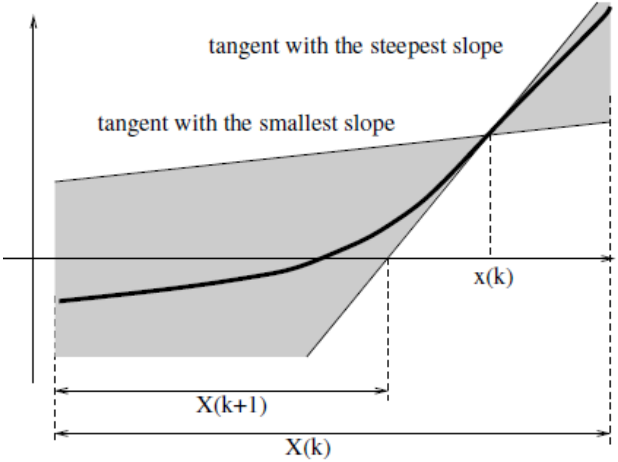
Let $x_k \in X_k$.

Let

$$X_{k+1} = \left(x_k - \frac{f(x_k)}{\widetilde{f'}(X_k)} \right) \cap X_k.$$

Interval Newton method



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$$X_{k+1} = \left(m_k - \frac{f(m_k)}{\widetilde{f'}(X_k)} \right) \cap X_k.$$

Interval Newton method

We first define the interval Newton operator

$$N(X) = m - \frac{f(m)}{\widetilde{f}'(X)}, \text{ with } m = \mathsf{mid}\,(X).$$

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Let m_k denote the middle of X_k and

$$X_{k+1} = N(X_k) \cap X_k, k = 0, 1, 2, \ldots.$$

Theorem

Assume that $N(X)$ is well defined. If X contains a unique, simple zero x^*, then so do all iterates $X_k, k \in \mathbb{N}$. Moreover, the intervals X_k form a nested sequence converging to $[x^*]$.

Interval Newton method

Theorem

Brouwer (1910)
Every continuous function f from a convex compact subset K of a Euclidean space to K itself has a fixed point.

Interval Newton method

Theorem

Let $X \in \mathbb{IR}$, $f \in \mathcal{C}^1(X)$. Let $\widetilde{f'}$ an interval extension of f'. We assume $0 \notin \widetilde{f'}(X)$.
Let $I \in \mathbb{IR}$, $x \in I \subset X$, $N(I,x) := x - \widetilde{f'}(I)^{-1} f(x)$
If $N(I)$ is well defined, then the following statements hold:

(1) if I contains a zero x^* of f, then so does $N(I,x) \cap I$;

(2) if $N(I,x) \cap I = \emptyset$, then I contains no zero of f;

(3) if $N(I,x) \subseteq I$, then I contains a unique zero of f.

Interval Newton method

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Proof.

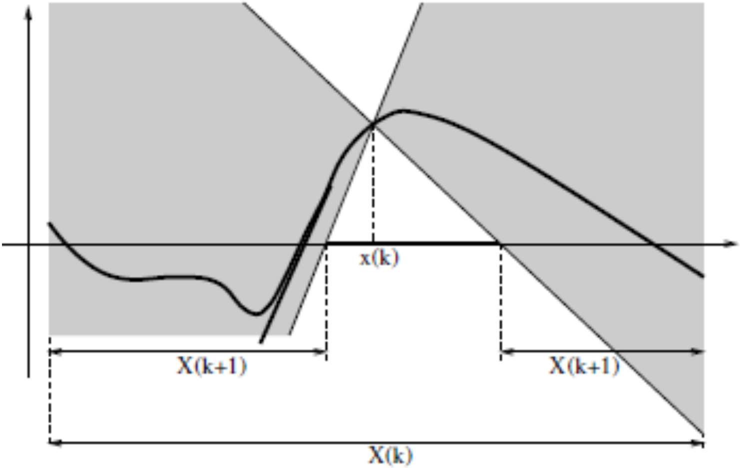
(1) Follows from Mean Value Theorem;

(2) Contra-positive of (1);

(3) Existence from Brouwer's fixed point theorem; uniqueness from non-vanishing $\widetilde{f}'$.

□

Interval Newton method



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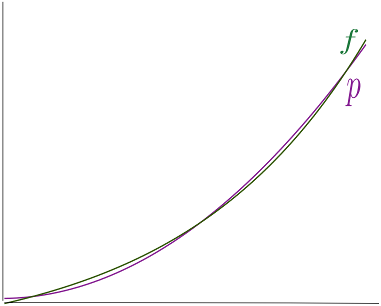
Chapter 4. Rigorous Polynomial Approximations

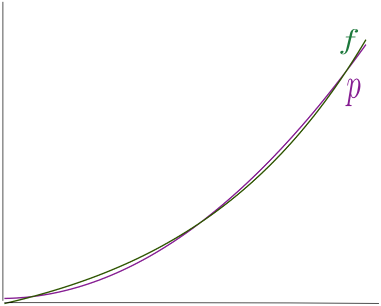
When Interval Arithmetic does not suffice: Computing supremum norms of approximation errors

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



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

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



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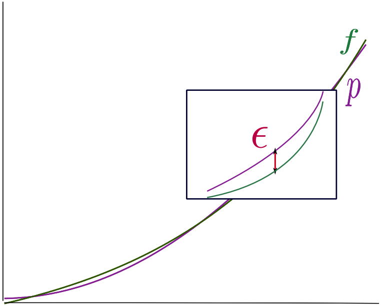
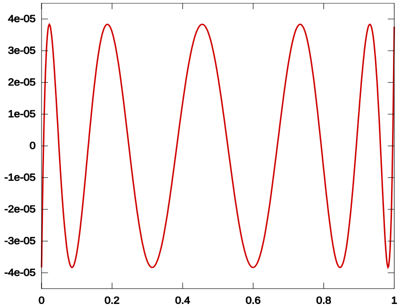
$f(x) = e^{1/\cos(x)}$, $x \in [0, 1]$, $p(x) = \sum_{i=0}^{10} c_i x^i$, $\varepsilon(x) = f(x) - p(x)$ s.t. $\|\varepsilon\|_\infty = \sup_{x \in [a,\, b]}\{|\varepsilon(x)|\}$ is as small as possible (Remez algorithm)





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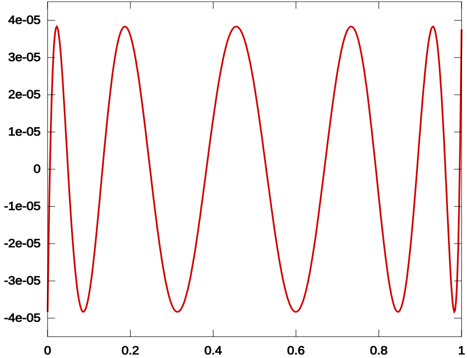

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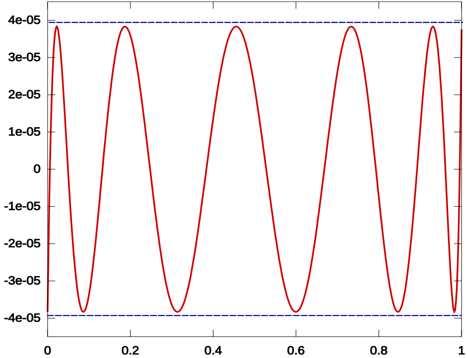

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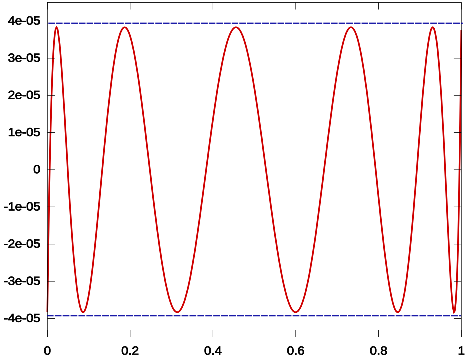
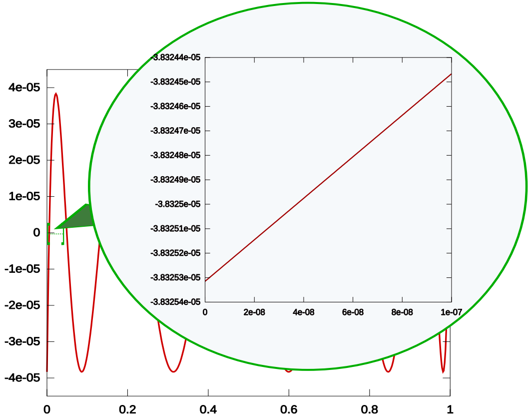


Using IA, $\varepsilon(x) \in [-233, 298]$, but $\|\varepsilon(x)\|_\infty \simeq 3.8325 \cdot 10^{-5}$

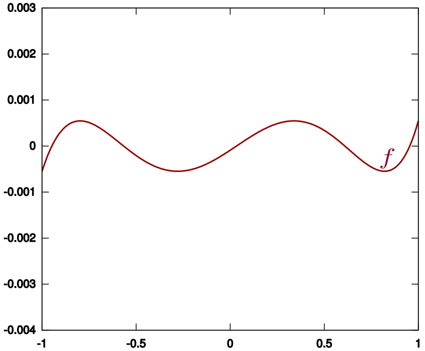
Why IA does not suffice: Overestimation

Overestimation can be reduced by using intervals of smaller width.



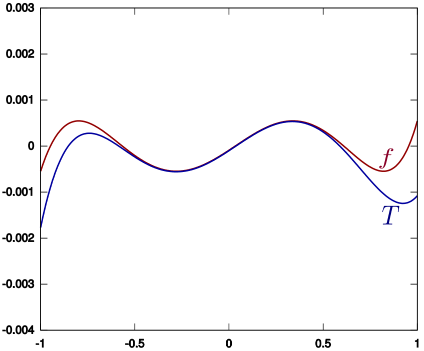
In this case, over $[0,1]$ we need 10^7 intervals!

Rigorous polynomial approximations



Rigorous polynomial approximations

f replaced with
- polynomial approximation T of degree n



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f replaced with
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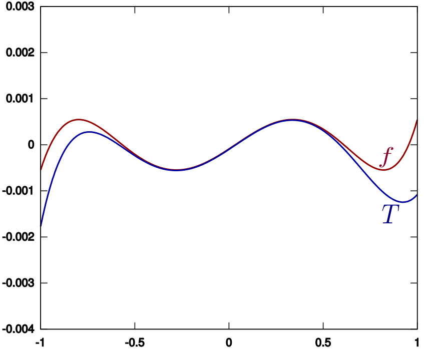
- interval $\mathbf{\Delta}$ s. t. $f(x) - T(x) \in \mathbf{\Delta}, \forall x \in [a, b]$



Rigorous polynomial approximations

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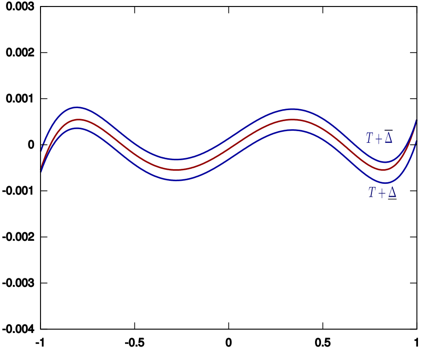

How to compute $(T, \boldsymbol{\Delta})$?

Chebyshev Models

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Let $I = [a,b]$, we define Chebyshev polynomials over I as

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$T_{n+1}^{[a,b]}$ has $n+1$ distinct extrema in $[a,b]$ (Chebyshev nodes of the first kind):

$$\nu_k^{[a,b]} = \frac{a+b}{2} + \frac{b-a}{2}\cos\left(\frac{k\pi}{n}\right),\ k = 0,\ldots,n.$$

Chebyshev Models

We recall

Lemma 1

Let $W_{\overline{\nu}}(x) = \prod_{k=0}^{n} (x - \nu_k^{[a,b]})$. *We have*

$$W_{\overline{\mu}}(x) = \frac{(b-a)^{n+1}}{2^{2n}}(1-x^2)U_{n-1}^{[a,b]}(x)$$

and

$$\max_{x \in [a,b]} |W_{\overline{\mu}}(x)| = \frac{(b-a)^{n+1}}{2^{2n}}.$$

Chebyshev Models

Lemma 2

(Taylor-Lagrange-like formula.) Let $n \in \mathbb{N}$*, and let* $f \in \mathcal{C}^{n+1}([a,b])$*. Let* $P \in \mathbb{R}_n[X]$ *be the interpolation polynomial of* f *at the Chebyshev nodes* $\left(\mu_k^{[a,b]}\right)_{0 \leqslant k \leqslant n}$*. For all* $x \in [a,b]$*, there exists* $\xi_x \in (a,b)$ *such that*

$$f(x) = P(x) + \frac{(b-a)^{n+1} f^{(n+1)}(\xi_x)}{2^{2n}(n+1)!}(1-x^2)U_{n-1}^{[a,b]}(x) .$$

Chebyshev Models - How do we obtain them?

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- $$f(x) = \underbrace{\sum_{k=0}^{n} p_k T_k^{[a,b]}(x)}_{T(x)} + \underbrace{\Delta_n(x, \xi_x)}_{\text{remainder}}$$
- $\Delta_n(x, \xi_x) = \frac{(b-a)^{n+1} f^{(n+1)}(\xi_x)}{2^{2n}(n+1)!}(1-x^2)U_{n-1}^{[a,b]}(x)$, $x \in [a,b]$, ξ lies strictly between a and b

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- How to compute the coefficients p_i of $T(x)$?
- How to compute an interval enclosure $\boldsymbol{\Delta}$ for $\Delta_n(x,\xi_x)$?

Chebyshev Models: computations of the coefficients

$$P(x) = \sum_{i=0}^{n} p_i T_i^{[a,b]}(x), \text{ with } p_i = \sum_{k=0}^{n} \frac{2}{n} f\left(\nu_k^{[a,b]}\right) T_i^{[a,b]}\left(\nu_k^{[a,b]}\right) = \sum_{k=0}^{n} \frac{2}{n} f\left(\nu_k^{[a,b]}\right) T_i(\nu_k) = \sum_{k=0}^{n} \frac{2}{n} f\left(\nu_k^{[a,b]}\right) T_k(\nu_i).$$

Reminder: Clenshaw's method for evaluating Chebyshev sums

Algorithm

Input Chebyshev coefficients $c_0, \ldots, c_N$, a point t

Output $\sum_{k=0}^{N} c_k T_k(t)$

1. $b_{N+1} \leftarrow 0$, $b_N \leftarrow c_N$
2. for $k = N-1, N-2, \ldots, 1$
   1. $b_k \leftarrow 2tb_{k+1} - b_{k+2} + c_k$
3. return $c_0 + tb_1 - b_2$

This algorithm runs in $O(N)$ arithmetic operations.

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This algorithm runs in $O(N)$ arithmetic operations.

It works also if t and the c_k's are intervals!

Chebyshev Models: computations of the coefficients

$$P(x) = \sum_{i=0}^{n} p_i T_i^{[a,b]}(x), \text{ with } p_i = \sum_{k=0}^{n} \frac{2}{n} f\left(\nu_k^{[a,b]}\right) T_k(\nu_i).$$

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We replace the ν_k's and the $f(\nu_k)$'s with interval enclosures, and then perform an interval evaluation with Clenshaw's method: the coefficients p_i are intervals.

Chebyshev Models: bounding the remainder

$\Delta_n(x,\xi_x) = \frac{(b-a)^{n+1} f^{(n+1)}(\xi_x)}{2^{2n}(n+1)!}(1-x)^2 U_{n-1}^{[a,b]}(x)$, $x \in [a,b]$, ξ lies strictly between a and b.

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$|\Delta_n(x, \xi_x)|$ is bounded by $\frac{(b-a)^{n+1} \left| f^{(n+1)}([a,b]) \right|}{2^{2n}(n+1)!}$.

Chebyshev Models: bounding the remainder

$\Delta_n(x,\xi_x) = \frac{(b-a)^{n+1} f^{(n+1)}(\xi_x)}{2^{2n}(n+1)!}(1-x)^2 U_{n-1}^{[a,b]}(x)$, $x \in [a,b]$, ξ lies strictly between a and b.

$|\Delta_n(x,\xi_x)|$ is bounded by $\frac{(b-a)^{n+1}\left|f^{(n+1)}([a,b])\right|}{2^{2n}(n+1)!}$.

If f satisfies a differential equation with polynomial coefficients: fairly easy to retrieve an upper bound for $\left|f^{(n+1)}([a,b])\right|$.

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Otherwise?

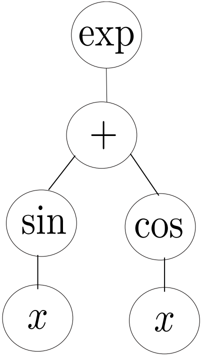
Chebyshev Models "Philosophy"

For bounding the remainders:

- For "basic functions" use Taylor-Lagrange-like statement.
- For "composite functions" use a two-step procedure:
  - compute models $(T, \mathbf{\Delta})$ for all basic functions;
  - apply algebraic rules with these models, instead of operations with the corresponding functions.

Chebyshev Models - Two-step procedure

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



Chebyshev Models - Two-step procedure

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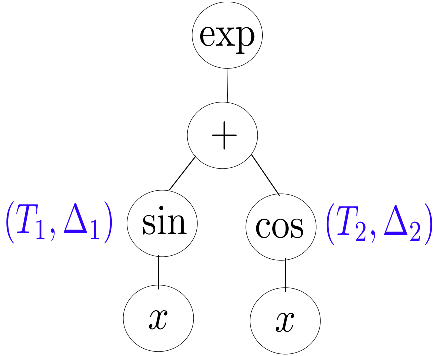

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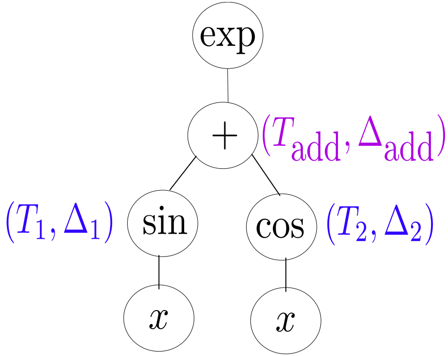

Chebyshev Models - Two-step procedure

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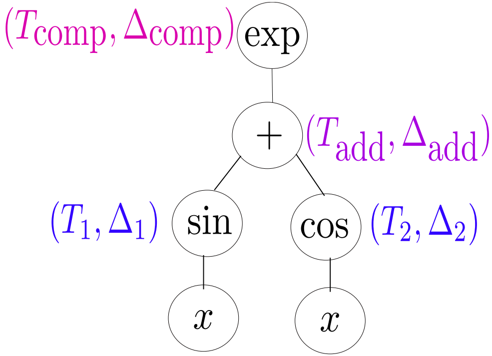

Chebyshev Models - Operations: Addition

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

For multiplication, we have: $T_m^{[a,b]}(x) \cdot T_n^{[a,b]}(x) = \dfrac{T_{m+n}^{[a,b]} + T_{|m-n|}^{[a,b]}}{2}$.

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Consider $P(x) = \sum_{i=0}^{n} p_i T_i^{[a,b]}(x)$ and $Q(x) = \sum_{i=0}^{n} q_i T_i^{[a,b]}(x)$.

We have $P(x) \cdot Q(x) = \sum_{k=0}^{2n} c_k T_k^{[a,b]}(x)$, where

$$c_k = \left(\sum_{|i-j|=k} p_i q_j + \sum_{i+j=k} p_i q_j \right) /2.$$

The cost is $O(n^2)$ operations.

Chebyshev Models - Operations: Multiplication

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

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

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In our case, for bounding "$\boldsymbol{P}$s": Interval Arithmetic evaluation.

Ranges of polynomials

Observe that we heavily used enclosures of ranges of polynomials. This raises (at least) two questions:

Ranges of polynomials

Observe that we heavily used enclosures of ranges of polynomials. This raises (at least) two questions:

- How do we compute these enclosures?
- why would this process yield tight enclosures?

Ranges of polynomials - How do we compute these enclosures?

- A first option: let $p(x) = a_0 + a_1 T_1^{[a,b]}(x) + \cdots + a_n T_n^{[a,b]}(x)$, as, $p(I)$ is bounded by $p(x) = |a_0| + |a_1| + \cdots + |a_n|$.

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- Another possibility is to use Bernstein's basis: indeed, one can show that if

  $$p(x) = \sum_{k=0}^{n} p_k B_{n,k}(x),$$

  then for all $x \in [0,1]$, we have

  $$\min_{[0,1]} p \geqslant \min_k p_k \qquad \text{and} \qquad \max_{[0,1]} p \leqslant \max_k p_k.$$

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- Tighter methods based on Descartes' rule of signs, Sturm's theorem, sums of squares (Hilbert's 17th problem), companion matrices, etc.

Ranges of polynomials

Second, why would this process yield tight enclosures? Our basic functions are analytic, and hence the coefficients of Chebyshev interpolants (quickly) converge to 0.

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: using truncated Chebyshev series

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

[1] solutions of Linear Differential Equations with polynomial coefficients

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Computation of the coefficients (for "basic" D-finite functions[1])

- recurrence formulae[2] for computing a_k

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[2] A. Benoit and B. Salvy, Chebyshev Expansions for Solutions of Linear Differential Equations, ISSAC '09: Proceedings of the twenty-second international symposium on Symbolic and algebraic computation, 23-30, ISSAC '09. ACM, New York, NY, 23-30

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

$$\exists \xi \in [-1,1] \text{ s.t. } \|f-P\|_\infty = \frac{\left|f^{(n+1)}(\xi)\right|}{2^n(n+1)!}.$$

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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

[1] solutions of Linear Differential Equations with polynomial coefficients