Enclosing the Range of Factorable Functions

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The Class of Factorable Functions

Factorable Function: Defined by a finite recursive composition of

- binary sums
- binary products
- a given library of univariate functions

$$f(x) = \frac{x\exp(x)}{(x+5)^2} \xrightarrow[\text{form}]{\text{factored}} \begin{cases} v_1(x) = x \\ v_2(x) = \exp(v_1(x)) \\ v_3(x) = v_1(x)v_2(x) \\ v_4(x) = v_1(x) + 5 \\ v_5(x) = v_4(x)^2 \\ v_6(x) = \dfrac{1}{v_5(x)} \\ f(x) = v_3(x)v_5(x) \end{cases}$$

- Extremely inclusive class of functions
- Nearly every function that can be represented finitely on a computer

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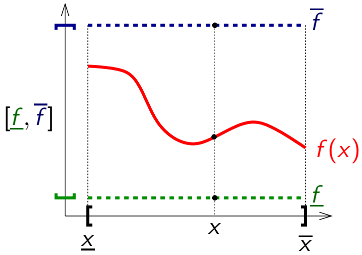

- Enclosing the set of solutions to computational problems
  - E.g., range of functions; enclosure of integral value; enclosure of ODE solutions; enclosure of LE/NLE solutions; etc.
- Cheap, but inherently conservative! (over-approximation)
- Requires new arithmetic for intervals of real numbers, $[\underline{x}, \overline{x}] := \{x \mid \underline{x} \leq x \leq \overline{x}\}$
  - Combine set operations on intervals with interval function evaluations
- Available Interval Packages: INTLAB (MATLAB), Profil/Bias (C++), FILIB++ (C++), etc.
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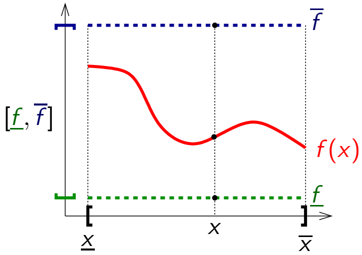

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Interval Analysis: Usual Binary Operations

$$X \odot Y := \{x \odot y : x \in X, y \in Y\}, \quad \odot \in \{+, -, \times, \div\}$$

- Let $X := [\underline{x}, \overline{x}]$, $Y := [\underline{y}, \overline{y}]$
- Addition:

$$X + Y = [\underline{x} + \underline{y}, \overline{x} + \overline{y}]$$

- Subtraction:

$$X - Y = [\underline{x} - \overline{y}, \overline{x} - \underline{y}]$$

  - We have $X - X = [\underline{x} - \overline{x}, \overline{x} - \underline{x}] \subseteq 0$ in general!

- Multiplication:

$$X \times Y = [\min M, \max M], \quad M := \{\underline{x}\underline{y}, \underline{x}\overline{y}, \overline{x}\underline{y}, \overline{x}\overline{y}\}$$

  - We have $X(Y + Z) \subseteq XY + XZ$, with equality <u>only</u> if $YZ \geq 0$ (subdistributivity)

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$$X/Y = X \times (1/Y), \quad 1/Y = [1/\overline{y}, 1/\underline{y}], \text{ if } 0 \notin Y$$

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$$f(X) := \{f(x) : x \in X\}$$

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- $x \mapsto \sqrt{x}$:
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- $x \mapsto x^{2k+1}$:
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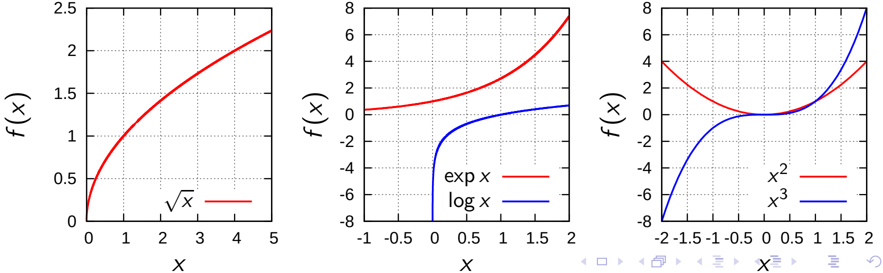

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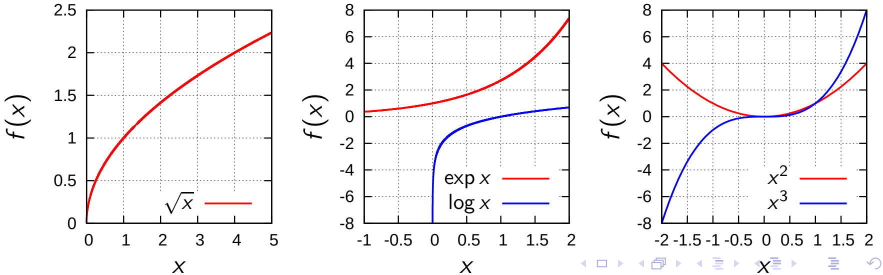

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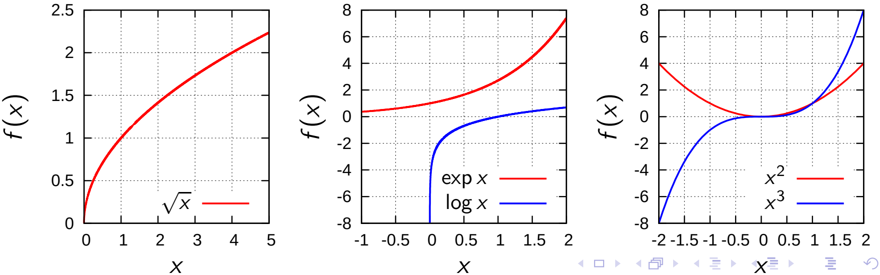

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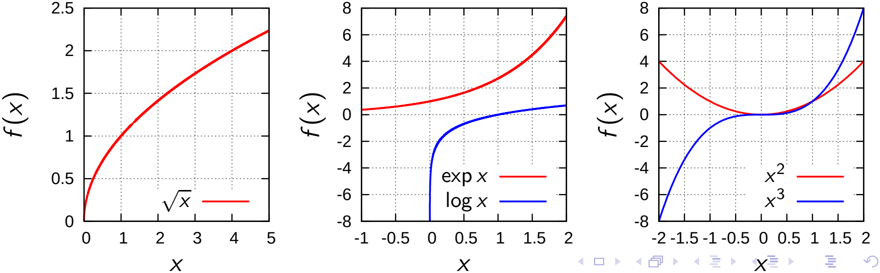

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$$f(x) = \frac{x\exp(x)}{(x+5)^2}$$

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v_6(x) &= \frac{1}{v_5(x)} & V_6^X &= \left[\frac{1}{36}, \frac{1}{16}\right] = [0.027, 0.063] \\
f(x) &= v_3(x)v_6(x) & F^X &= [-2.719, 2.719][0.027, 0.063] = [-0.171, 0.172]
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Convergence of Interval Estimators

- **Hausdorff Metric:** $q(X, Y) := \max\{|\underline{x} - \underline{y}|, |\overline{x} - \overline{y}|\}$
- **Hausdorff Convergence Order, β:**

$$q(T_h(Y), \bar{h}(Y)) \leq \tau\, \mathrm{w}(Y)^{\beta},\ \forall Y \subseteq Z$$

Classical Results: Hausdorff convergence order of natural interval extensions is (no less than) 1; of centered forms (no less than) 2

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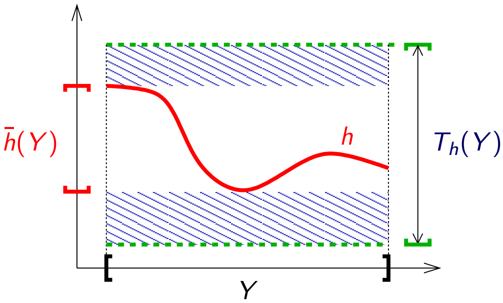

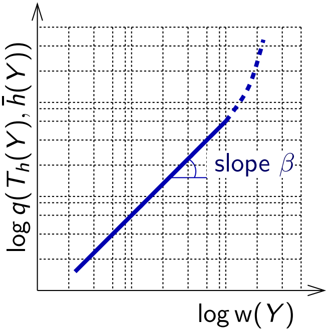

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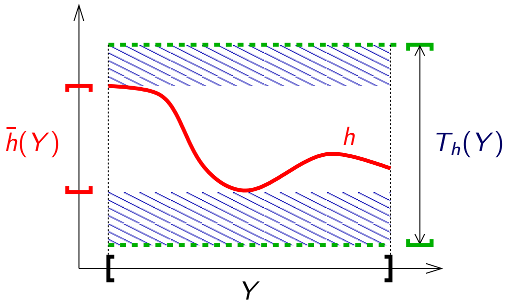
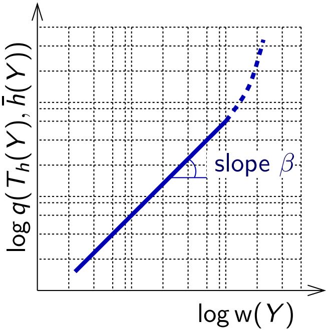
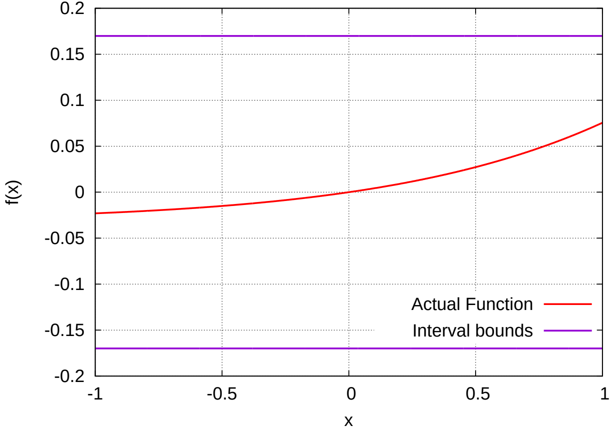




Classical Results: Hausdorff convergence order of natural interval extensions is (no less than) 1; of centered forms (no less than) 2

IA - Issues


0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
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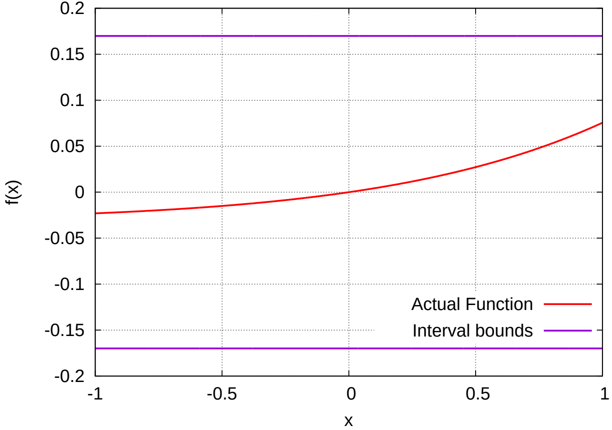
f(x)
-1
-0.5
0
0.5
1
x
Actual Function
Interval bounds

IA - Issues



We calculated $F^X = [-0.171, 0.172]$, however we can see from the graph that the tightest possible interval would have been $F^X = [f(-1), f(1)] = [-0.023, 0.076]$

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We lose all dependency information with interval analysis.

We will now move on to a method which does keep some dependency information in order to provide tighter bounds.

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Addition is trivial once again, for $\mathcal{T}_A^q(x) = \mathcal{T}_B^q(x) + \mathcal{T}_C^q(x)$

We get $\mathcal{T}_A^q(x) = \sum_{n=0}^{q}(a_{(B,n)} + a_{(C,n)})x^n + \mathcal{R}_B^q + \mathcal{R}_C^q$

TM - Multiplication I

Lets consider $\mathcal{T}_A^q(x) = \mathcal{P}_A^q(x) + \mathcal{R}_A^q = \mathcal{T}_B^q(x)\mathcal{T}_C^q(x)$

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If we examine the first term we have:

$$\mathcal{P}_B^q(x)\mathcal{P}_C^q(x) = \sum_{n=0}^{q} a_{(B,n)} \left(\sum_{m=0}^{q} a_{(C,m)} x^{n+m} \right)$$

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We want to keep all the terms where $n + m \leq q$, so we have

$$\mathcal{P}_A^q(x) = \sum_{n=0}^{q} a_{(B,n)} \left(\sum_{m=0}^{q-n} a_{(C,m)} x^{n+m} \right)$$

TM - Multiplication II

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We know that everything remaining has to end up in $\mathcal{R}_A^q$, so we can overestimate what is left by substituting X for x,

$$\mathcal{R}_A^q = \sum_{n=1}^{q} a_{(B,n)} \left(\sum_{m=q+1-n}^{q} a_{(C,m)} X^{n+m} \right) + \mathcal{P}_B^q(X)\mathcal{R}_C^q + \mathcal{P}_C^q(X)\mathcal{R}_B^q + \mathcal{R}_B^q\mathcal{R}_C^q$$

TM - Remainder

It is possible to show that the remainder of a Taylor expansion is:

$$f(x) - \mathcal{P}_f^q(x) = \frac{f^{(q+1)}(c)}{(q+1)!}x^{q+1}$$

where c is between 0 and x, one way of getting $\mathcal{R}_f^q$ is to overestimate this as follows:

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More recently we have shown for definite functions that are monotonically increasing or decreasing that the maximum error of a Taylor function occurs at an endpoint of the approximation range.

So a valid interval for $\mathcal{R}_f^q$ can be calculated by examining the endpoints of $f(x) - \mathcal{P}_f^q(x)$.

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We wish to be able to evaluate $\mathcal{T}_o^q(\mathcal{T}_i^q(x))$, in order to evaluate all of the operations in our factorable function.

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First we can see that $\mathcal{T}_o^q(\mathcal{T}_i^q(x)) = \mathcal{P}_o^q(\mathcal{T}_i^q(x)) + \mathcal{R}_o^q$. The linear combination of monomials can be evaluated using the Horner scheme. Where

$$\begin{aligned} b_q &= a_{o,q} \\ b_{q-1} &= a_{o,q-1} + x b_q \\ &\vdots \\ b_0 &= a_{o,0} + x b_1 \\ \mathcal{P}_o^q(x) &= b_0 \end{aligned}$$

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We replace x with $\mathcal{T}_i^q(x)$ in the scheme and compute the recursion using addition and multiplication of TMs.

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The naive way to bound this is to simply evaluate $\mathcal{T}_i^q(X)$

We are also able to use some smarter methods where we can get better bounds for the lower order terms.

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Let us use the same example as before:

$$f(x) = \frac{x\exp(x)}{(x+5)^2}$$

$$v_1(x) = x \qquad \mathcal{T}^3_{v_1} = x$$

$$v_2(x) = \exp(v_1(x)) \qquad \mathcal{T}^3_{v_2} = 1 + x + 0.5x^2 + 0.167x^3 + [0, 0.0114]$$

$$v_3(x) = v_1(x)v_2(x) \qquad \mathcal{T}^3_{v_3} = x + x^2 + 0.5x^3 + [-0.280, 0.280]$$

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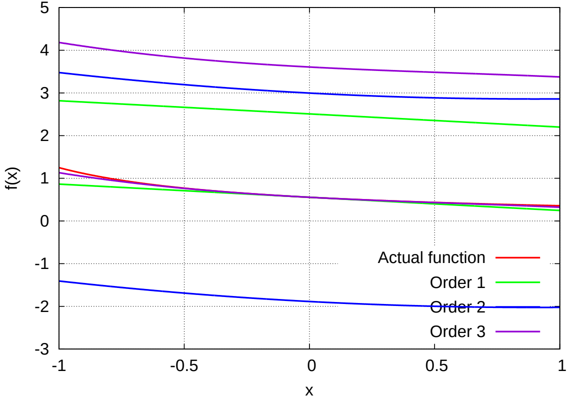
This can end up badly for as in the example of $g(x) = \frac{1}{x+1.8}$



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$$a_n = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x) T_n(x)}{\sqrt{1 - x^2}} dx$$

Chebyshev polynomials

Chebyshev polynomials are a different basis to monomials used in Taylor expansions. We can approximate a function, $f(x)$, where $x \in [-1, 1]$.

$$f(x) = \mathcal{P}_f(x) = \sum_{n=0}^{\infty} a_n T_n(x)$$

where the Chebyshev polynomials, $T_n(x)$, are

$$T_n(x) = \cos(n \arccos(x))$$

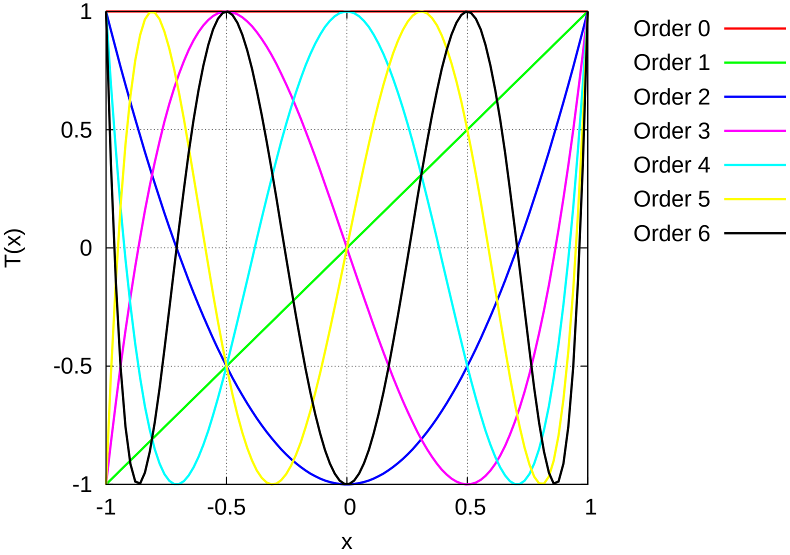
and the coefficients, a_n can be calculated via

$$a_n = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x) T_n(x)}{\sqrt{1 - x^2}} dx$$

We can convert exactly from the Chebyshev basis back to the monomial basis.

Chebyshev	Monomial
$T_0(x)$	1
$T_1(x)$	x
$T_2(x)$	$2x^2 - 1$
$T_3(x)$	$4x^3 - 3x$
$T_4(x)$	$8x^4 - 8x^2 + 1$
$T_5(x)$	$16x^5 - 20x^3 + 5x$

Chebyshev polynomials



Chebyshev Models

A Chebyshev model is created via the propagation of truncated Chebyshev expansions with a remainder term. The remainder term bounds the rest of the infinite sum.

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Addition is trivial once again, for $\mathcal{C}_A^q(x) = \mathcal{C}_B^q(x) + \mathcal{C}_C^q(x)$

We get $\mathcal{C}_A^q(x) = \sum_{n=0}^q (a_{(B,n)} + a_{(C,n)}) T_n(x) + \mathcal{R}_B^q + \mathcal{R}_C^q$

CM - Multiplication I

The multiplication of two Chebyshev basis functions is different to the monomial basis. $T_n(x)T_m(x) = \frac{1}{2}(T_{|n-m|}(x) + T_{n+m}(x))$

This is an advantage as with Taylor models when $n + m > q$ we had to bound the whole term, but with Chebyshev models only half the result has to be bound.

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However this is also a disadvantage, as before when you multiplied two terms together the result was only one term. With this basis you get at least twice as many terms.

For multivariate multiplication you get 2^{n_v} terms, where n_v is the number of variables.

CM - Multiplication II

Lets consider $\mathcal{C}_A^q(x) = \mathcal{P}_A^q(x) + \mathcal{R}_A^q = \mathcal{C}_B^q(x)\mathcal{C}_C^q(x)$

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If we do a simple multiplication we get:

$$\mathcal{C}^q_A(x) = \mathcal{P}^q_B(x)\mathcal{P}^q_C(x) + \mathcal{P}^q_B(x)\mathcal{R}^q_C + \mathcal{P}^q_C(x)\mathcal{R}^q_B + \mathcal{R}^q_B\mathcal{R}^q_C$$

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Following a similar procedure to Taylor models

$$\mathcal{P}_A^q(x) = \frac{1}{2}\sum_{n=0}^{q} a_{(B,n)}\left(\sum_{m=0}^{q-n} a_{(C,m)}\,T_{n+m}(x) + \sum_{m=0}^{q} a_{(C,m)}\,T_{|n-m|}(x)\right)$$

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$$\mathcal{P}_A^q(x) = \frac{1}{2}\sum_{n=0}^{q} a_{(B,n)}\left(\sum_{m=0}^{q-n} a_{(C,m)}T_{n+m}(x) + \sum_{m=0}^{q} a_{(C,m)}T_{|n-m|}(x)\right)$$

We bound what is left over by replacing x with X

$$\mathcal{R}_A^q = \frac{1}{2}\sum_{n=1}^{q} a_{(B,n)}\left(\sum_{m=q+1-n}^{q} a_{(C,m)}T_{n+m}(X)\right) + \mathcal{P}_B^q(X)\mathcal{R}_C^q + \mathcal{P}_C^q(X)\mathcal{R}_B^q + \mathcal{R}_B^q\mathcal{R}_C^q$$

CM - Coefficients

Unlike for the coefficients of Taylor expansion, calculating the coefficients of a Chebyshev expansion is a lot more difficult.

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Directly evaluating this integral can be impossible.

The options are numerical integration or interpolation.

CM - Remainder

We can evaluate the remainder of a Chebyshev expansion using the derivative, in a similar way to the Taylor expansion.

$$\mathcal{R}_f^q = \frac{f^{q+1}(X)}{2^q(q+1)!}$$

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More recently we have shown for convex or concave functions that are monotonically increasing or decreasing that the maximum error of a Taylor function occurs at an endpoint of the approximation range.

So a valid interval for $\mathcal{R}_f^q$ can be calculated by examining the endpoints of $f(x) - \mathcal{P}_f^q(x)$.

CM - Composition

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$$\mathcal{P}_o^q(x) = a_{o,0} + xb_1(x) - b_2(x)$$

where $b_1(x)$ and $b_2(x)$ can be calculated by knowing $\forall k > q,\ b_k(x) = 0$ and

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This method can be used to evaluate the composition $\mathcal{P}_o^q(\mathcal{C}_i^q(x))$, by replacing x in the relations above with $\mathcal{C}_i^q(x)$

Note that we could replace x with $\mathcal{T}_i^q(x)$ if we desire to keep the monomial basis.

CM - Bounding

For the composition of Chebyshev models we need to ensure that the range of $\mathcal{C}_i^q(x)$ is $[-1, 1]$. This is because the expansion only creates an approximation for this part of the outer function.

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If the range of the $\mathcal{C}_i^q(x)$ is $[\alpha,\beta]$ we can do a linear transformation on it. $\mathcal{C}_{i'}^q(x) = (\mathcal{C}_i^q(x) - \frac{\alpha+\beta}{2})\frac{\beta-\alpha}{2}$ as well as modifying the outer function $f_{o'}(x) = f_o\left(\frac{\beta-\alpha}{2}x + \frac{\alpha+\beta}{2}\right)$

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We can bound Chebyshev models in a similar way to Taylor models.

The naive way to bound this is to simply evaluate $\mathcal{C}_i^q(X)$

We are also able to use some smarter methods where we can get better bounds for the lower order terms.

CM - Example

Let us use the same example as before, $f(x) = \frac{x\exp(x)}{(x+5)^2}$

$$v_1(x) = x \qquad \mathcal{C}^3_{v_1} = x$$

$$v_2(x) = \exp(v_1(x)) \qquad \mathcal{C}^3_{v_2} = 1.267 + 1.130x + 0.272\,T_2(x) + 0.044\,T_3(x) + [-0.007, 0.007]$$

$$v_3(x) = v_1(x)v_2(x) \qquad \mathcal{C}^3_{v_3} = 0.565 + 1.402x + 0.587\,T_2(x) + 0.136\,T_3(x) + [-0.029, 0.029]$$

$$v_4(x) = v_1(x) + 5 \qquad \mathcal{C}^3_{v_4} = 5 + x$$

$$v_5(x) = v_4(x)^2 \qquad \mathcal{C}^3_{v_5} = 25.5 + 10x + 0.5\,T_2(x)$$

$$v_6(x) = \frac{1}{v_5(x)} \qquad \mathcal{C}^3_{v_6} = 0.043 - 0.017x + 0.003\,T_2(x) - 0.0003\,T_3(x) + [-0.0003, 0.0003]$$

$$f(x) = v_3(x)v_6(x) \qquad \mathcal{C}^3_{f} = 0.013 - 0.047x + 0.013\,T_2(x) - 0.002\,T_3(x) + [-0.005, 0.005]$$

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Example

Lets examine bounds for the function $f(x) = \frac{x\exp(x)}{(x+5)^2}$ with $x \in X = [-1, 1]$