Bilan de la partie CoqApprox

Debriefing of the CoqApprox formalisation

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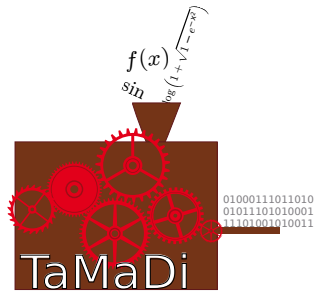
Joint works with Nicolas Brisebarre, Mioara Joldeș, Micaela Mayero, Jean-Michel Muller, Ioana Pașca, Laurence Rideau, Laurent Théry

Final meeting of the TaMaDi project
Monday 7th October 2013
ENS de Lyon



Outline

Context and Motivations

What? Compute polynomial approximations of univariate functions with certified error bounds: for a given function f over an interval[1] $\boldsymbol{I}$, compute P, ϵ and formally prove that $\forall x \in \boldsymbol{I},\ |f(x) - P(x)| \leqslant \epsilon$

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How? Rely on Taylor models and interval arithmetic

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Overview of Taylor Models (TMs)

The function f is replaced with $(P, \boldsymbol{\Delta})$, where $P(x) = \sum_{i=0}^{n} P_i \cdot (x - x_0)^i$ and $\boldsymbol{\Delta}$ is an interval.

A Taylor Model $(P, \boldsymbol{\Delta})$ over $\boldsymbol{I}$ approximates a whole set of functions:

$$[\![(P, \boldsymbol{\Delta})]\!]_{\boldsymbol{I}} = \{f : \boldsymbol{I} \to \mathbb{R} \mid \forall x \in \boldsymbol{I},\ f(x) - P(x) \in \boldsymbol{\Delta}\}\,.$$

Taylor-Lagrange formula and interval-based Taylor models

Theorem (Taylor-Lagrange formula)

If f is $n+1$ times derivable on $\boldsymbol{I}$, then $\forall x \in \boldsymbol{I}$, $\exists \xi$ between x_0 and x s.t.:

$$f(x) = \underbrace{\left(\sum_{i=0}^{n} \frac{f^{(i)}(x_0)}{i!} (x - x_0)^i \right)}_{P(x)} + \underbrace{\frac{f^{(n+1)}(\xi)}{(n+1)!} (x - x_0)^{n+1}}_{\Delta_n(x_0, x, \xi)}.$$

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Naive algorithm to compute an interval-based Taylor model

- Input: function f, intervals $\boldsymbol{I}$ and $\boldsymbol{x_0}$ (containing x_0), integer $n \geqslant 0$
- Output: $(\boldsymbol{P}, \boldsymbol{\Delta})$, where polynomial $\boldsymbol{P}$ has interval coefficients $\frac{f^{(i)}(\boldsymbol{x_0})}{i!}$ and $\boldsymbol{\Delta}$ is an enclosure of $\Delta_n(x_0, x, \xi)$ for $x, \xi \in \boldsymbol{I}$ and $x_0 \in \boldsymbol{x_0}$

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$\rightarrow$ Rounding errors are easily handled by interval arithmetic

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$\rightarrow$ Rounding errors are easily handled by interval arithmetic

$\rightarrow$ Uniform computation of $(\boldsymbol{P}, \boldsymbol{\Delta})$

Methodology of Taylor models

Define arithmetic operations on Taylor models $\mathtt{TM}_{\mathtt{add}}, \mathtt{TM}_{\mathtt{mul}}, \mathtt{TM}_{\mathtt{comp}}, \mathtt{TM}_{\mathtt{div}}$:

- Addition: $(\boldsymbol{P}_1, \boldsymbol{\Delta}_1) \oplus (\boldsymbol{P}_2, \boldsymbol{\Delta}_2) = (\boldsymbol{P}_1 + \boldsymbol{P}_2, \boldsymbol{\Delta}_1 + \boldsymbol{\Delta}_2)$
- Similar rule for multiplication, composition, and division

A two-step strategy:

1. Apply these operations recursively on the structure of the function
2. For basic functions: compute $\boldsymbol{\Delta}$ using the Taylor-Lagrange formula

Why using this 2-step strategy for composite functions?

Interval enclosures $\boldsymbol{\Delta}$ for $\Delta_n(x_0, x, \xi)$ can be **largely overestimated**.

Example

$f(x) = e^{1/\cos x}$ over $\boldsymbol{I} = [0, 1]$ around $x_0 = \frac{1}{2}$, with $n = 13$.

- Automatic differentiation and Taylor-Lagrange formula:
  $\boldsymbol{\Delta} = [-1.94 \cdot 10^2,\ 1.35 \cdot 10^3]$

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- Automatic differentiation and Taylor-Lagrange formula:
  $\boldsymbol{\Delta} = [-1.94 \cdot 10^2,\ 1.35 \cdot 10^3]$
- Taylor models:
  $\boldsymbol{\Delta} = [-8.74 \cdot 10^{-4}, 4.63 \cdot 10^{-3}]$

Generic computation of sharp remainders for basic functions

Algorithm (Zumkeller's technique)

Input: $\boldsymbol{F}$: interval evaluator for function f; $\boldsymbol{x_0} \subset \boldsymbol{I}$ and $n \in \mathbb{N}$
Input: $\boldsymbol{T}(\boldsymbol{y_0}, n)$: order-$n$ Taylor polynomial of f around $\boldsymbol{y_0}$
Output: $(\boldsymbol{P}, \boldsymbol{\Delta})$

1: $\boldsymbol{P} \leftarrow \boldsymbol{T}(\boldsymbol{x_0}, n)$
2: $\boldsymbol{\Gamma} \leftarrow [X^{n+1}]\, \boldsymbol{T}(\boldsymbol{I}, n+1)$
3: **if** $(\sup \boldsymbol{\Gamma} \leqslant 0$ **or** $\inf \boldsymbol{\Gamma} \geqslant 0)$ **and** $\boldsymbol{I}$ is bounded **then**
4: $\quad \boldsymbol{a} \leftarrow [\inf \boldsymbol{I}]$
5: $\quad \boldsymbol{b} \leftarrow [\sup \boldsymbol{I}]$
6: $\quad \boldsymbol{\Delta_a} \leftarrow \boldsymbol{F}(\boldsymbol{a}) - \boldsymbol{P}\,(\boldsymbol{a} - \boldsymbol{x_0})$
7: $\quad \boldsymbol{\Delta_b} \leftarrow \boldsymbol{F}(\boldsymbol{b}) - \boldsymbol{P}\,(\boldsymbol{b} - \boldsymbol{x_0})$
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9: $\quad \boldsymbol{\Delta} \leftarrow \boldsymbol{\Delta_a} \vee \boldsymbol{\Delta_b} \vee \boldsymbol{\Delta_{x_0}}$
10: **else**
11: $\quad \boldsymbol{\Delta} \leftarrow \boldsymbol{\Gamma} \times (\boldsymbol{I} - \boldsymbol{x_0})^{n+1}$
12: **end if**

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2: $\boldsymbol{\Gamma} \leftarrow [X^{n+1}]\ \boldsymbol{T}(\boldsymbol{I}, n+1)$ — Compute an enclosure of $f^{(n+1)}(\xi)/(n+1)!,\ \xi \in \boldsymbol{I}$
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Evaluate the Taylor-Lagrange remainder of f at three point-intervals of $\boldsymbol{I}$

9: $\quad \boldsymbol{\Delta} \leftarrow \boldsymbol{\Delta_a} \vee \boldsymbol{\Delta_b} \vee \boldsymbol{\Delta_{x_0}}$
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Generic computation of sharp remainders for basic functions

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D-finite functions (a.k.a. holonomic functions)

Definition

A D-finite function is a solution of a homogeneous linear ordinary differential equation (LODE) with polynomial coefficients:
$a_r(x)y^{(r)}(x) + \cdots + a_1(x)y'(x) + a_0(x)y(x) = 0$, for given $a_k \in \mathbb{K}[X]$.

Property

The Taylor coefficients of these functions satisfy a *linear recurrence with polynomial coefficients* $\rightarrow$ fast numerical computation of the coefficients

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Example (the exponential function)

The Taylor coefficients of $\exp$ at x_0 satisfy the recurrence
$\forall n \geqslant 1,\ u_n = u_{n-1}/n$, with $u_0 = \exp(x_0)$ as an initial condition.

$\ln$, $\sin$, $\arcsin$, $\sinh$, $\operatorname{arcsinh}$, $\arctan$, $\operatorname{arctanh}$... are D-finite; $\tan$ isn't

The Coq formal proof assistant

We use Coq for

- programming
  - richly typed functional language
  - specify algorithms and theorems
- proving
  - use higher-order logic
  - build proofs interactively
  - develop automatic tactics
  - check proofs

The Coq formal proof assistant

We use Coq for

- programming
  - richly typed functional language
  - specify algorithms and theorems
  - **perform computations**
- proving
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Focus on efficiency before completing the proofs

We followed a "prototype and prove" strategy:

1. Code the algorithms in Coq to evaluate its computational capabilities
2. Formally prove the CoqApprox library

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2. Formally prove the CoqApprox library

	# Lines of code		# Proved lemmas
	Specs	Proofs	
CoqApprox v1	794	570	47
CoqApprox v2	2707	4564	452

Focus on a formalisation that is modular and extensible

When formalising Taylor models $(\boldsymbol{P}, \boldsymbol{\Delta})$, focus on being generic w.r.t.

- the datatype chosen for $\boldsymbol{\Delta}$
- the datatype chosen for the coefficients of $\boldsymbol{P}$
- the implementation of polynomial operations (in a given basis)

$\rightarrow$ Rely on the module system of Coq

- and generic w.r.t. the correctness proofs (to easily add new functions)

$\rightarrow$ Implement and prove generic algorithms

Coq libraries involved in the formalisation

- SSReflect/MathComponents
  - tactic facilities
  - libraries on arithmetic, lists, and big operators such as $\sum$ and $\prod$
- Coq.Interval
  - Abstract interface for intervals (`IntervalOps`)
  - Instantiation to intervals with floating-point bounds
  - Formal verification with respect to the Reals standard library:

    for $x, y : \mathbb{R}$

    and $\boldsymbol{X}, \boldsymbol{Y} : \mathbb{IR}$

    $$x \in \boldsymbol{X} \ \wedge \ y \in \boldsymbol{Y} \implies x + y \in \boldsymbol{X} + \boldsymbol{Y}$$

    $$x \in \boldsymbol{X} \implies \exp(x) \in \mathbf{exp}(\boldsymbol{X})$$

Summary of available functions and operations

Fun/Op	Reals	Coq.Interval	CoqApprox v2
cst	☒	☒	☒
id	☒	☒	☒
inv	☒	☒	☒
$\sqrt{\cdot}$	☒	☒	☒
$\frac{1}{\sqrt{\cdot}}$	☒	☒	☒
exp	☒	☒	☒
sin	☒	☒	☒
cos	☒	☒	☒
tan	☒	☒	☐
arctan	☒	☒	☐
ln	☒	☐	☐
arcsin	☐	☐	☐
arccos	☐	☐	☐
$+$			☒
$\times$			☒
$\circ$			☒
$\div$			☒

Comparison with a dedicated tool implemented in C

Sollya [S.Chevillard, M.Joldeș, C.Lauter]

- written in C
- based on the C libraries GMP, MPFR and MPFI
- contains an implementation of univariate Taylor models
- in an imperative programming framework
- polynomials as arrays of coefficients
- not formally proved

CoqApprox

- formalised in Coq
- based on the internals of the library Coq.Interval
- implements Taylor models using a similar algorithm
- in a purely-functional programming framework
- polynomials as lists of coefficients (linear access time)
- formally proved in Coq

Some benchmarks for basic functions

	Execution time			Approximation error		
	Coq	Sollya	Coq/Sollya	naive Coq	Coq	Sollya
$f(x) = 1/x$ $\boldsymbol{I} = [1, 3]$ deg=100 prec=125	**0.022s**	0.165s	7.6x faster	$1 \cdot 2^{0}$	$\mathbf{1 \cdot 2^{-101}}$	
$f(x) = \sqrt{x}$ $\boldsymbol{I} = [1, 3]$ deg=100 prec=125	**0.037s**	0.169s	4.5x faster	$1.98 \cdot 2^{-12}$	$\mathbf{1.60 \cdot 2^{-112}}$	
$f(x) = \sin x$ $\boldsymbol{I} = [-1, 1]$ deg=80 prec=500	0.146s	**0.092s**	1.6x slower	$1.79 \cdot 2^{-402}$		

Column "naive Coq" $\rightsquigarrow$ naive use of the Taylor-Lagrange formula
Column "Coq" $\rightsquigarrow$ rely on Zumkeller's technique

Some benchmarks for composite functions

	Execution time			Approximation error		
	Coq	Sollya	Coq/Sollya	naive Coq	Coq	Sollya
$f(x) = e^x \sin x$ $\boldsymbol{I} = [-\frac{3}{2}, \frac{3}{2}]$ deg=100 prec=500	1.010s	**0.306s**	3.3x slower	$1.63 \cdot 2^{-423}$		
$f(x) = e^{1/\cos x}$ $\boldsymbol{I} = [0, 1]$ deg=100 prec=100	52.92s	**0.653**	81x slower	$1.97 \cdot 2^{-49}$	$\mathbf{1.99 \cdot 2^{-89}}$	$\mathbf{1.98 \cdot 2^{-89}}$
$f(x) = \frac{\sin x}{\cos x}$ $\boldsymbol{I} = [-1, 1]$ deg=100 prec=100	11.15s	**0.570s**	20x slower	$1.45 \cdot 2^{26}$	$1.12 \cdot 2^{-64}$	$\mathbf{1.82 \cdot 2^{-96}}$

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Conclusion and Perspectives

CoqApprox: a Coq library of Rigorous Polynomial Approximation

- Efficient computation of Taylor models with sharp remainders
- Machine-checked proofs of correctness based on generic data-types

$\rightarrow$ we can thus formally prove that $|f(x) - TM_f(x)| \leqslant \epsilon_1$ for $x \in \boldsymbol{I}$.

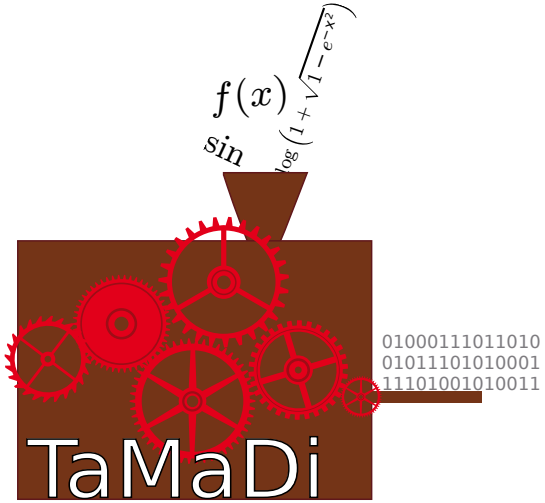
To do: combine CoqApprox with a polynomial global optimisation method

- E.g., rely on Bernstein polynomials or Sums of Squares in Coq
- Devise a tactic to formally prove $|TM_f(x) - P(x)| < \epsilon_2$ for $x \in \boldsymbol{I}$.

$\rightarrow$ will be able to automatically prove $|f(x) - P(x)| < \epsilon$ for $x \in \boldsymbol{I}$.

See Nicolas' talk on tomorrow for more perspectives.

End of the talk



Thank you for your attention!

The CoqApprox homepage:
http://tamadi.gforge.inria.fr/CoqApprox/

Taylor-Lagrange remainder and validity predicate

Theorem (Taylor-Lagrange)

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$$f(x) = \underbrace{\left(\sum_{i=0}^{n} \frac{f^{(i)}(x_0)}{i!} (x - x_0)^i \right)}_{\textit{Taylor expansion}} + \underbrace{\frac{f^{(n+1)}(\xi)}{(n+1)!} (x - x_0)^{n+1}}_{\Delta_n(x_0, x, \xi)}.$$

Definition (`i_validTM`)

$(\boldsymbol{P}, \boldsymbol{\Delta})$ is a valid Taylor Model for f over $\boldsymbol{I}$ around $\boldsymbol{x_0}$ if $\boldsymbol{x_0} \subset \boldsymbol{I}$, $0 \in \boldsymbol{\Delta}$, and

$$\forall x_0 \in \boldsymbol{x_0},\ \exists \alpha_0 \in \boldsymbol{P}_0, \ldots, \alpha_n \in \boldsymbol{P}_n,\ \forall x \in \boldsymbol{I},\ \ f(x) - \sum_{i=0}^{n} \alpha_i \cdot (x - x_0)^i \in \boldsymbol{\Delta}.$$

Validity predicate for floating-point Taylor models

From any pair $(\boldsymbol{P}, \boldsymbol{\Delta})$ that satisfies `i_validTM`, we can easily produce a pair $(P, \boldsymbol{\Delta'})$ where P is polynomial with floating-point coefficients s.t.:

Definition (`f_validTM`)

$(P, \boldsymbol{\Delta'})$ is a valid TM for f over $\boldsymbol{I}$ around $\boldsymbol{x_0}$ if we have $\boldsymbol{x_0} \subset \boldsymbol{I}$, $0 \in \boldsymbol{\Delta'}$, and

$$\forall x_0 \in \boldsymbol{x_0}, \quad \forall x \in \boldsymbol{I}, \quad f(x) - \sum\nolimits_i P_i \cdot (x - x_0)^i \in \boldsymbol{\Delta'}.$$

In the code, the function `i2f_tm` transforms $(\boldsymbol{P}, \boldsymbol{\Delta})$ into $(P, \boldsymbol{\Delta'})$.