Rigorous Polynomial Approximation
Using Taylor Models in Coq

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Outline

1. Introduction and Motivations
2. Presentation of Taylor Models
3. Formalization of Taylor Models in Coq
4. Benchmarks and Timings
5. Conclusion and Future Work
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Introduction and Motivations

Context and Motivations

- **Polynomial approximation**
  - A common way to represent real functions on machines
  - Only solution for platforms where only $+, -, \times$ are available
  - Used by most computer algebra systems

- **Bounds for approximation errors**
  - Not always available or guaranteed to be accurate in numerical software
  - Yet they may be crucial to ensure the reliability of systems
  - A key part of the TaMaDi project formalization effort for computing the “worst-case accuracy” for all elementary functions
Rigorous Polynomial Approximation

In the setting of rigorous polynomial approximation (RPA):
Approximate the function while fully controlling the error

- May use floating-point arithmetic as support for efficient computation
- Systematically compute interval enclosures instead of mere approximations
Goal

Implement rigorous polynomial approximation in a formal setting, implying:

- Use techniques from *symbolic/numeric computation*: amenable to formal methods
- **Genericity**: implementation extensible and applicable to a large class of problems
- **Efficiency**: evaluate the computational capabilities of the formal proof assistant before starting proving anything
- **Formal verification**: ensure the provided error bound is (tight and) not underestimated
Floating-Point (FP) Arithmetic

Reals numbers can be approximated in machines by floating-point numbers, which are rational numbers of the form

\[ x = M \times 2^{e-p+1} \quad \text{with} \quad 2^{p-1} \leq |M| < 2^p \]

- the integer \( p \geq 1 \) is the precision of the considered FP format
- the integer \( M \) is the integral significand of \( x \)
- the integer \( e \) is the exponent of \( x \)
Interval Arithmetic (IA)

- Interval = pair of floating-point (FP) numbers
- E.g., \( \pi \in [3.1415, 3.1416] \)
- Operations on intervals (satisfying enclosure property), e.g.:
  \([2, 4] - [0, 1] = [1, 4]\) (we have \( \forall x \in [2, 4], \forall y \in [0, 1], x - y \in [1, 4] \))
- Tool for bounding the range of functions
- A naive use of IA cannot be successful
- Dependency problem: for \( F(x) := x - x \) and \( X = [1, 5] \), the IA evaluation gives \( F(X) = [-4, 4] \) while the image of \( X \) by \( F \) is \([0, 0]\)
- Moreover, IA is not directly applicable to bound the approximation error \( e := p - f \) given that the values of \( f \) and \( p \) will be very near
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Taylor Models

Definition

An order-$n$ Taylor Model (TM) for a function $f : D \subset \mathbb{R} \rightarrow \mathbb{R}$ over $I$ is a pair $(T, \Delta)$ where $T$ is a degree-$n$ polynomial and $\Delta$ is an interval, such that $\forall x \in I, f(x) - T(x) \in \Delta$.

The polynomial $T$ is typically a Taylor expansion of $f$ at $x_0 \in I$ and the interval remainder $\Delta$ provides an enclosure of the approximation error.

Our Approach

As regards $T$: small interval coefficients with floating-point bounds $\Rightarrow$ rounding errors are directly handled by the interval arithmetic $\Rightarrow$ the true coefficients of the Taylor expansion lie inside these intervals.
Taylor-Lagrange Remainder

**Theorem (Taylor-Lagrange)**

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

\[
f(x) = \left( \sum_{i=0}^{n} \frac{f^{(i)}(x_0)}{i!} (x - x_0)^i \right) + \frac{f^{(n+1)}(\xi)}{(n+1)!} (x - x_0)^{n+1}.
\]

- **Taylor expansion**
- \( \Delta(x, \xi) \)

**Outline**

For \( T \): Compute interval enclosures of \( \frac{f^{(i)}(x_0)}{i!}, \ i = 0, \ldots, n \).

For \( \Delta \): Compute enclosure of \( \Delta(x, \xi) \):

Compute enclosure of \( \frac{f^{(n+1)}(\xi)}{(n+1)!} \) and deduce \( \Delta := \frac{f^{(n+1)}(I)}{(n+1)!} (I - x_0)^{n+1} \).
Taylor-Lagrange Remainder

**Theorem (Taylor-Lagrange)**

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

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

Taylor expansion + $\Delta(x, \xi)$

**Outline**

For $T$: Compute interval enclosures of $\frac{f^{(i)}(x_0)}{i!}$, $i = 0, \ldots, n$.

For $\Delta$: Compute enclosure of $\Delta(x, \xi)$:

Compute enclosure of $\frac{f^{(n+1)}(\xi)}{(n + 1)!}$ and deduce $\Delta := \frac{f^{(n+1)}(I)}{(n + 1)!} (I - x_0)^{n+1}$.

Composite functions $\Rightarrow$ enclosure for $\Delta$ can be **largely overestimated**
Methodology of Taylor Models

Define arithmetic operations on Taylor Models:

- $\text{TM}_{\text{add}}, \text{TM}_{\text{mul}}, \text{TM}_{\text{comp}}, \text{and } \text{TM}_{\text{div}}$
- E.g., $\text{TM}_{\text{add}} : \left( (P_1, \Delta_1), (P_2, \Delta_2) \right) \mapsto (P_1 + P_2, \Delta_1 + \Delta_2)$.

A two-fold approach:

- **Apply these operations recursively** on the structure of the function
- **Use Taylor-Lagrange remainder for atoms** (i.e., for base functions)
Methodology of Taylor Models

Define arithmetic operations on Taylor Models:

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A two-fold approach:

- Apply these operations recursively on the structure of the function
- Use Taylor-Lagrange remainder for atoms (i.e., for base functions)

$\Rightarrow$ Need to consider a relevant class for base functions, so that:

- We can easily compute their successive derivatives
- The interval remainder computed for these atoms is thin enough
**Definition**

A $D$-finite function is a solution of a homogeneous linear ordinary differential equation with polynomial coefficients:

$$a_r(x)y^{(r)}(x) + \cdots + a_1(x)y'(x) + a_0(x)y(x) = 0, \quad \text{for } a_k \in \mathbb{K}[X]$$

**Example (exp)**

The function $y = \exp$ is fully determined by $\{y' - y = 0, \ y(0) = 1\}$

Most common functions are $D$-finite ($\sin, \cos, \arcsin, \arccos, \sinh, \cosh, \arcsinh, \arccosh, Si, Ci, Shi, Chi, \arctan, \exp, \ln, Ei, \text{erf}, Ai, Bi, \ldots$). $\tan$ is not.
Taylor Series of $D$-finite Functions

**Theorem**

A function represented by a Taylor series $f(x) = \sum_{n=0}^{\infty} u_n (x - x_0)^n$ is $D$-finite if and only if the sequence $(u_n)$ of its Taylor coefficients satisfies a linear recurrence with polynomial coefficients.

\[ \text{recurrence relation} \quad \Rightarrow \quad \text{fast numerical computation} \quad \text{of Taylor coefficients} \]

**Example** ($\exp$)

Taylor series: $\exp(x) = \sum_{n=0}^{\infty} \frac{\exp(x_0)}{n!} (x - x_0)^n$

Recurrence: $\forall n \in \mathbb{N}, \ u_{n+1} = \frac{u_n}{n+1}$ \quad Initial condition: $u_0 = \exp(x_0)$
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Tools and Libraries Involved in our Formalization

We are using:

- The Coq/SSReflect proof assistant: an interactive theorem prover combining a higher-order logic and a richly-typed functional programming language;
- The CoqInterval library for Multiple-Precision Floating-Point Interval Arithmetic in Coq, based on:
- The Flocq library for Multiple-Precision Floating-Point Arithmetic, itself based on:
- The Reals library from the Coq Standard Library, which consists of a classical axiomatization of the real numbers
Focus on Genericity

- Aim: being as **generic** as possible in our Coq formalization
- TM: instance of Rigorous Polynomial Approximation (RPA)
- RPA: \((P, \Delta)\) where \(P\) is not necessarily a Taylor polynomial
- Genericity for the type of \(P\), the implementation of such polynomials, as well as the type of \(\Delta\)
Choice of a Modularization Mechanism

- \text{Coq} provides three mechanisms for modularization:
  - Type Classes
  - Structures
  - Modules

- Like the CoqInterval library, our formalization uses Modules,
  - less flexible than Type Classes or Structures (first-class), but with a
  - better computational behavior: Modules instantiations are performed
    statically $\Rightarrow$ the executed code is more compact
  - ability to switch implementations
A Generic Implementation of TMs: Modular Hierarchy

BaseOps

PolyOps

RigPolyApprox

TaylorModel

FullOps

IntervalOps

TaylorRec

PolyOps

TaylorPoly
Example of Use

**Definition (TM for \textit{exp})**

Definition \texttt{exp\_rec} (n : nat) (u : T) := tdiv u (tnat n). (*\in\textit{TaylorRec}*).

Definition \texttt{T\_exp} n u := trec1 \texttt{exp\_rec} (texp u) n. (*\in\textit{TaylorPoly}*).

Definition \texttt{TM\_exp} n X X0 := RPA (T\_exp n X0)\texttt{(Trem T\_exp n X X0)}. (*\in\textit{TaylorModel}*).

**Example (TM for \textit{exp} on \([1/2, 1]\))**

(* Library/modules preliminary invocations & global precision setting omitted *)

Let \texttt{a} := \texttt{Float 1 (-1)}. (* = \frac{1}{2} *)

Let \texttt{b} := \texttt{Float 2 (-1)}. (* = 1 *)

Let \texttt{X} := \texttt{Ibnd a b}.

Let \texttt{c} := \texttt{I\_midpoint (Ibnd a b)}. (* = \frac{a+b}{2} *)

Let \texttt{X0} := \texttt{Ibnd c c}.

Let \texttt{deg} := 10\%nat.

Let \texttt{tm} := \texttt{TM\_exp deg X X0}.

\texttt{Eval native\_compute in (approx tm)}. \texttt{Eval native\_compute in (error tm)}. 
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# Quick Presentation of the Sollya Tool

<table>
<thead>
<tr>
<th><strong>Sollya</strong></th>
<th><strong>CoqApprox</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Written in C</td>
<td>Formalized in Coq</td>
</tr>
<tr>
<td>Based on the MPFI library (Multiple-Precision FP IA)</td>
<td>Based on the CoqInterval library</td>
</tr>
<tr>
<td>Contains an implementation of Taylor Models</td>
<td>Implements Taylor Models using a similar algorithm</td>
</tr>
<tr>
<td>In an imperative-programming framework</td>
<td>In a functional-programming framework</td>
</tr>
<tr>
<td>Polynomials as arrays of coefficients</td>
<td>Polynomials as lists of coefficients (linear access time)</td>
</tr>
<tr>
<td>Not formally proved</td>
<td>Formal verification in progress</td>
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</tbody>
</table>
Some Benchmarks for Base Functions

<table>
<thead>
<tr>
<th></th>
<th>Timing</th>
<th></th>
<th>Approximation error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>CoQ</td>
<td>SOLLYA</td>
</tr>
<tr>
<td>arctan</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>prec=120, deg=8</td>
<td></td>
<td>11.45s</td>
<td>1.03s</td>
</tr>
<tr>
<td>$I=[1, 2]$</td>
<td></td>
<td>7.43×10^{-29}</td>
<td>2.93×10^{-29}</td>
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<tr>
<td>split in 256</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>exp</td>
<td></td>
<td>38.10s</td>
<td>16.39s</td>
</tr>
<tr>
<td>prec=600, deg=40</td>
<td></td>
<td>6.23×10^{-182}</td>
<td>6.22×10^{-182}</td>
</tr>
<tr>
<td>$I=[\ln 2, 1]$</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>split in 256</td>
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</table>

When the interval $I$ has been split into sub-intervals (of equal length), the timings are for the total duration of the computations while the approximation error is for the last subinterval.
### Some Benchmarks for Composite Functions

<table>
<thead>
<tr>
<th></th>
<th>Timing</th>
<th>Approximation error</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>COQ</td>
<td>SOLLYA</td>
</tr>
<tr>
<td>(\exp \times \sin)</td>
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<td></td>
</tr>
<tr>
<td>(\text{prec}=200, \text{deg}=10)</td>
<td>1m22s</td>
<td>12.05s</td>
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<tr>
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<tr>
<td>split in 2048</td>
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<td></td>
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<tr>
<td>(\exp \circ \sin)</td>
<td>3m24s</td>
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<tr>
<td>(I=[1/2, 1])</td>
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<td></td>
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<tr>
<td>split in 2048</td>
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- When the interval \(I\) has been split into sub-intervals (of equal length), the timings are for the total duration of the computations while the approximation error is for the last subinterval.
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Towards Fully Formally Verified Polynomial Approximation

We can formalize the predicate saying that a TM is valid (i.e., whose error is not underestimated) using the following definition:

**Definition**

Let $f : I \rightarrow \mathbb{R}$ be a function, $x_0$ be a small interval around an expansion point $x_0$. Let $T$ be a polynomial with interval coefficients $a_0, \ldots, a_n$ and $\Delta$ an interval. We say that $(T, \Delta)$ is a Taylor model of $f$ at $x_0$ on $I$ when

$$
\begin{align*}
& x_0 \subseteq I, \\
& 0 \in \Delta, \\
& \forall \xi_0 \in x_0, \exists \alpha_0 \in a_0, \ldots, \alpha_n \in a_n, \forall x \in I, \quad f(x) - \sum_{i=0}^{n} \alpha_i (x - \xi_0)^i \in \Delta.
\end{align*}
$$
Proofs are in Progress

<table>
<thead>
<tr>
<th>Fun/Op</th>
<th>Available in CoqInterval</th>
<th>Implemented in CoqApprox</th>
<th>Proved in CoqApprox</th>
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<tr>
<td>$\text{TM}_{\text{div}}$</td>
<td>✓</td>
<td></td>
<td>□</td>
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</tbody>
</table>
Conclusion

- An implementation of Taylor Models inside the Coq proof assistant taking advantage of the CoqInterval library for Interval Arithmetic
- **Symbolic/numeric approach** based on $D$-finite recurrences
- **Genericity** achieved thanks to a heavy use of Coq modules
- **Efficiency**: timings in Coq are just one order of magnitude slower than a conventional implementation in C
- Implementation carried on in a framework suitable for formal proof
Future Work

- Add more functions
- Finish the proofs
- Use persistent arrays instead of lists?
- Optimize the multiplication algorithm for composite functions
- Consider “Chebyshev Models” which should provide tighter remainders

Aim: Use our CoqApprox library in a full verification chain for TaMaDi
Thank you for your attention!

The TaMaDi project homepage: https://tamadiwiki.ens-lyon.fr/
http://tamadi.gforge.inria.fr/CoqApprox/