Formal Global Optimisation with Taylor Models

TYPES
20 April 2006

Roland Zumkeller
LogiCal project, École Polytechnique, Paris

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Outline

- Global Optimisation
  - Problem: finding the minimum and maximum value of a given objective function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ on a certain domain $[a_1; b_1] \times \ldots \times [a_n; b_n]$
  - Traditional methods based on interval arithmetic.
- Taylor Models
  - An optimisation method computing with sets of functions of the form "polynomial + error interval"
- Formal
  - Both the optimisation algorithm (-Cal) and its correctness proof (Logi-) are Coq terms. To obtain a formal proof for a particular problem it suffices to execute the algorithm (proof by reflection).

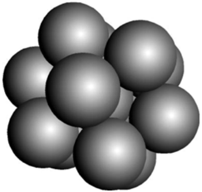
What Is Global Optimisation Good for?

- Engineering: aeronautics, robotics, ...
- Experimental physics: particle motion in accelerators
- Geometry: volumes of cells in space decomposition occuring in T. Hales' proof of the Kepler conjecture

$$x_1 \in [4; 2.168^2] \wedge x_2 \in [6.3001; 2.696^2] \wedge x_3 \in [4; 2.168^2] \wedge$$
$$x_4 \in [4; 6.3001] \wedge x_5 \in [4; 6.3001] \wedge x_6 \in [4; 6.3001] \rightarrow$$
$$\frac{\pi}{2} + \arctan\left(- \frac{-x_1^2 - (x_3 - x_5)(x_2 - x_6) + (x_1(x_2 + x_3 - 2x_4 + x_5 + x_6))}{\sqrt{\begin{array}{l} 4x_1(-x_1^2 * x_4 - x_2^2 * x_5 - (x_3 - x_4)(x_3 - x_5)x_6 - \\ \quad x_3 x_6^2 + x_2((x_3 - x_5)(x_5 - x_4) + (x_3 + x_5)x_6) + \\ \quad x_1((x_3 - x_4)(x_4 - x_5) + (x_3 + x_4)x_6 + x_2(x_4 + x_5 - x_6))) \end{array}}} \right) > 0.74$$

The Kepler Conjecture (1611)

- The maximal density of any sphere packing in 3-space is $\frac{\pi}{\sqrt{18}}$.



- In 1998 Thomas C. Hales has found a proof, which is large in every sense: article of 300 pages, 40.000 lines of code, several weeks of computation
- The "**Flyspeck**" project aims at formalising this proof, in order to eliminate any doubt about its correctness.

Interval Arithmetic

- The set of intervals: $\mathbb{I} = (\mathbb{R} \cup \{-\infty\}) \times (\mathbb{R} \cup \{\infty\})$
- Let $f : \mathbb{R}^n \to \mathbb{R}$. The function $\hat{f} : \mathbb{I}^n \to \mathbb{I}$ is called ...
  - an *extension* of f iff $\quad \forall X \in \mathbb{I}^n.\ \hat{f}(X) \supseteq \{f\ x \mid x \in X\}$
  - a *sharp extension* of f iff $\quad \forall X \in \mathbb{I}^n.\ \hat{f}(X) = \{f\ x \mid x \in X\}$
- Some sharp extensions:

$$
\begin{aligned}
[a;b] \mathbin{\hat{+}} [c;d] &:= (a+c, b+d) \\
[a;b] \mathbin{\hat{-}} [c;d] &:= (a-d, b-c) \\
[a;b] \mathbin{\hat{*}} [c;d] &:= (\min\{ac, ad, bc, bd\}, \max\{ac, ad, bc, bd\}) \\
1 \mathbin{\hat{/}} [a;b] &:= \begin{cases} (\frac{1}{b}, \frac{1}{a}) & \text{if } a \geq 0 \vee b \leq 0 \\ (-\infty, \infty) & \text{if } a \leq 0 \leq b \end{cases}
\end{aligned}
$$

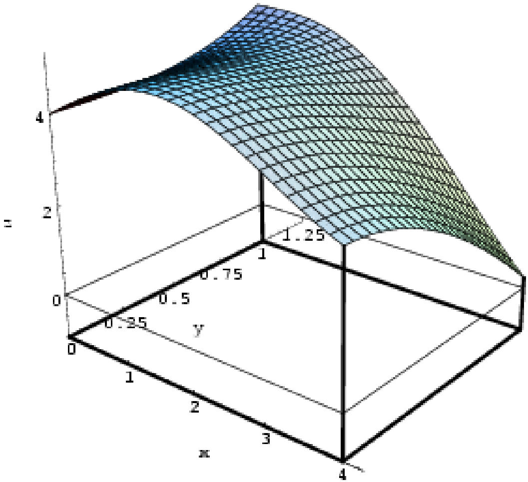
- Structural recursion with these extensions over a term yields its *natural extension*.

The Dependence Problem

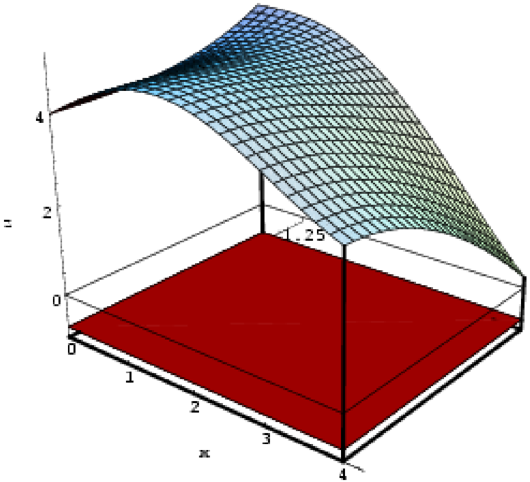
- Goal: $x \in [1;2] \wedge y, z \in [2;3] \rightarrow xy - z \geq -5$
  Proof: $[1;2] \mathbin{\hat{*}} [2;3] \mathbin{\hat{-}} [2;3] = [-1;3] \geq -5$
  structural induction; apply extension property. q.e.d.
- Goal: $x \in [3;5] \rightarrow x - x \geq -1$
  Proof: $[3;5] \mathbin{\hat{-}} [3;5] = [-2;2] \not\geq -1$
  :-(
- Why? For interval arithmetic the second goal looks like:
  $x, y \in [3;5] \rightarrow x - y \geq -1$

A Remedy: Branch & Bound

- If a simple evaluation of the natural extension fails, we split the domain X into X_1 and X_2. From the extension property follows: $x \in X_1 \vee x \in X_2 \to x \in \hat{f}(X_1) \cup \hat{f}(X_2)$
- Goal: $x \in [3;5] \to x - x \geq -1$
  Proof: $\left([3;4] \hat{-} [3;4]\right) \cup \left([4;5] \hat{-} [4;5]\right) = [-1,1]$
  ...structural induction; apply extension property. q.e.d.
- Algorithm for proving $x \in X \to f\ x \geq 0$:
  - $\hat{f}(X) \geq 0$: success
  - $\hat{f}(X) \not\geq 0$: split X into X_1 and X_2 and restart for each one



$$\sin x + y^2(y - x) + 4 > 0$$



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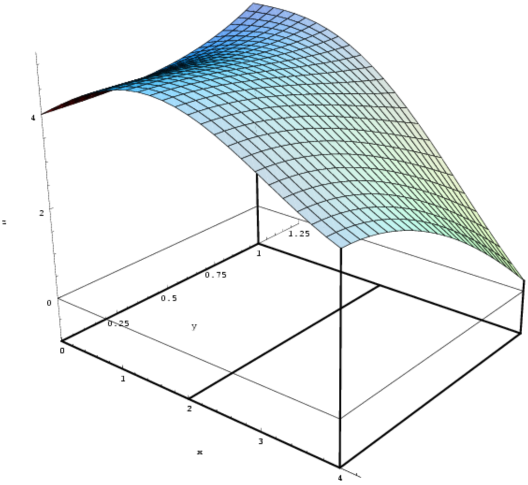

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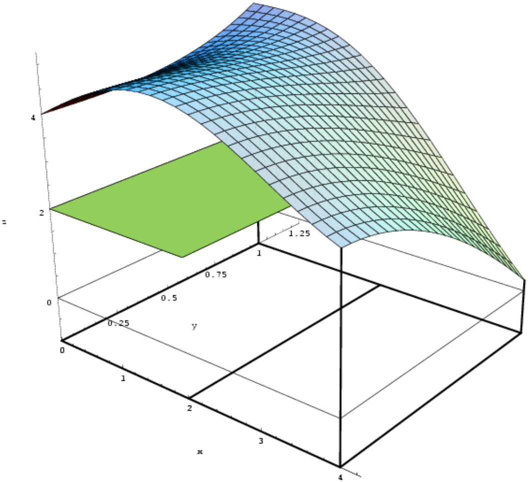

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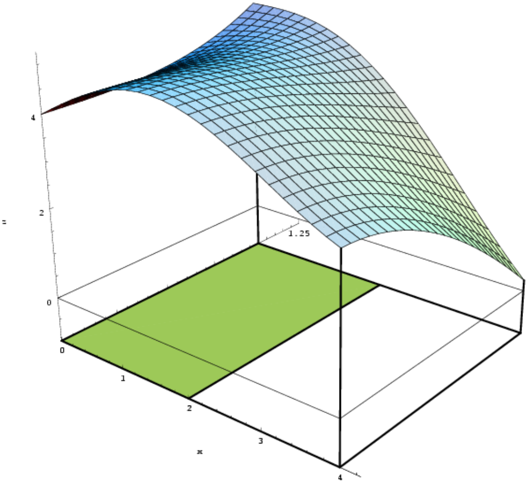

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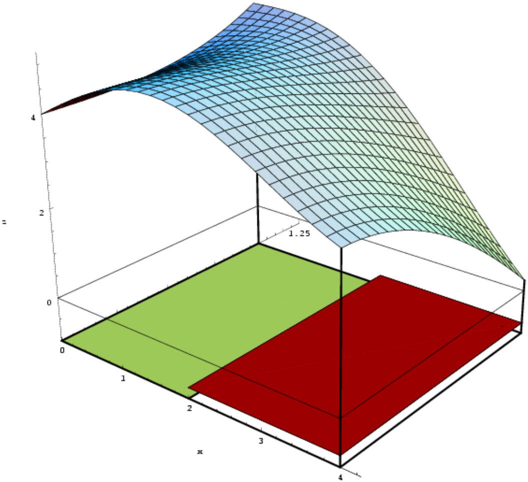

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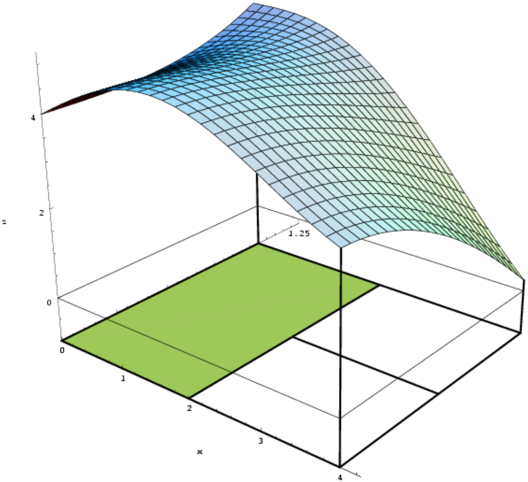

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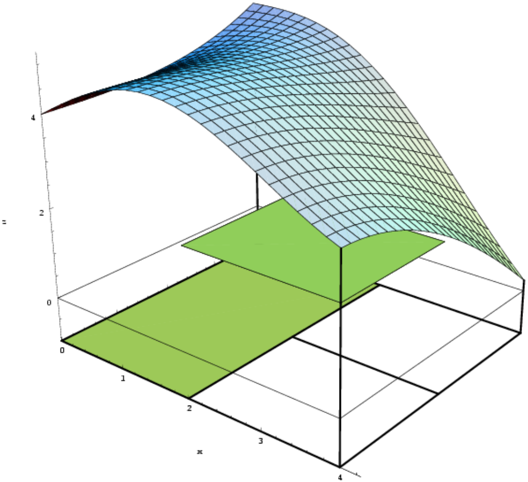

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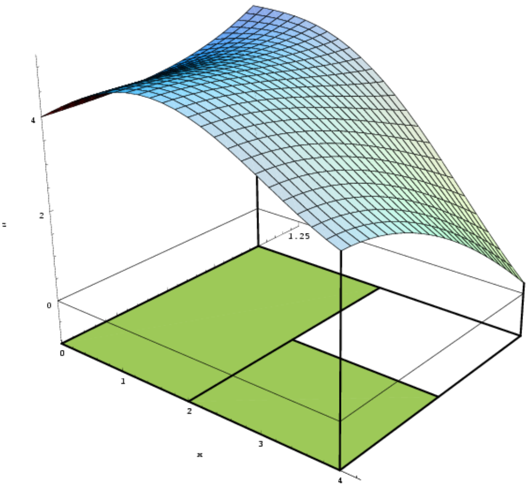

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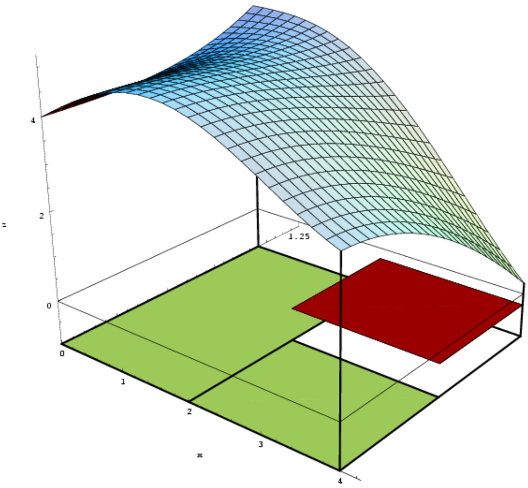

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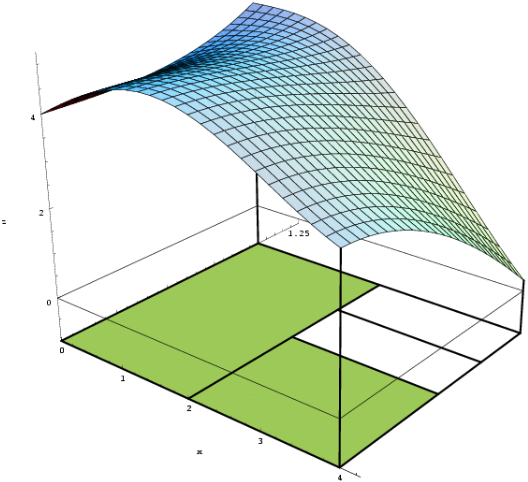

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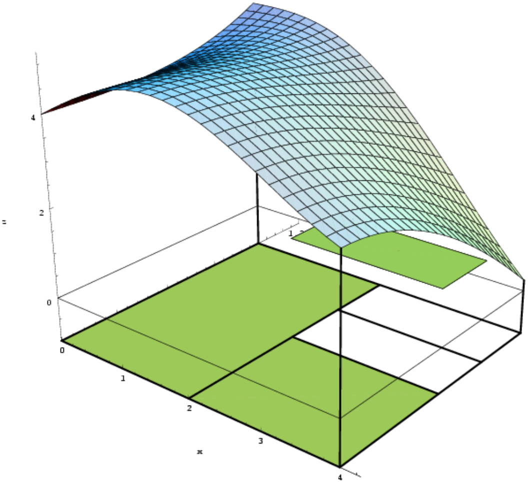

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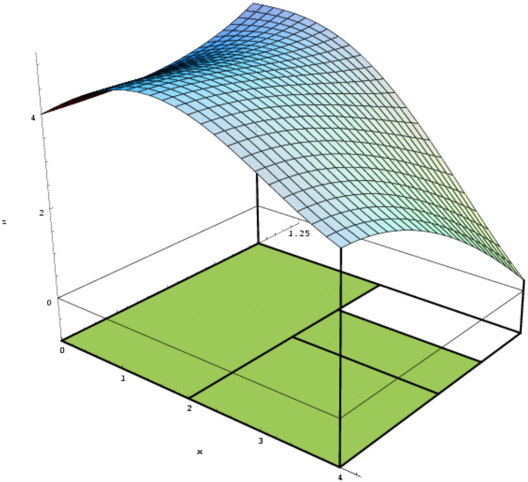

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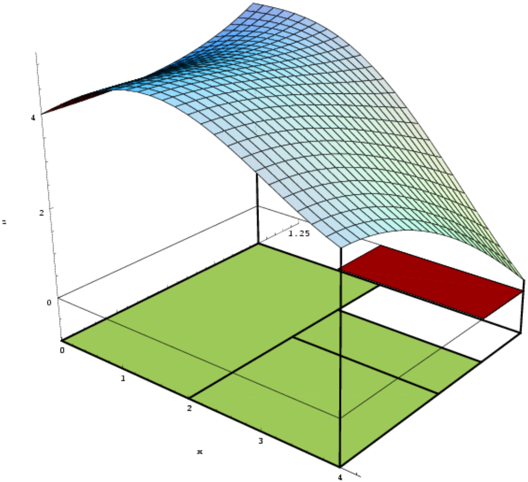

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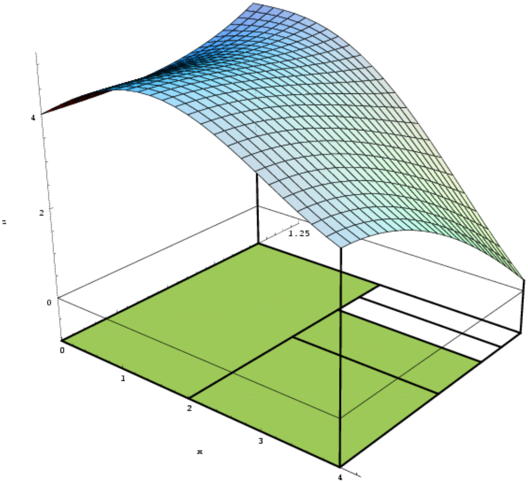

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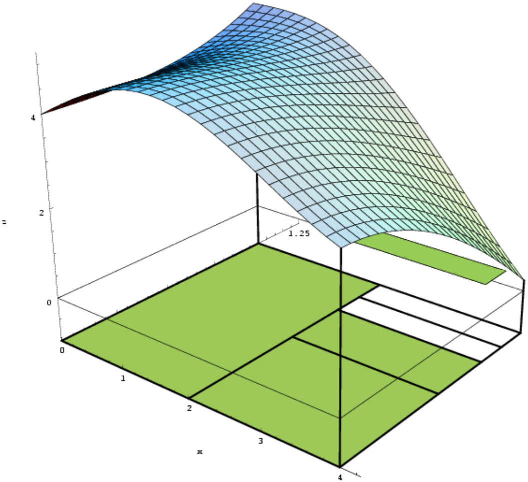

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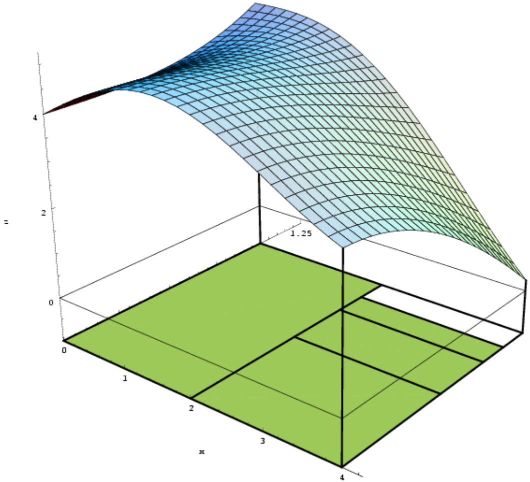

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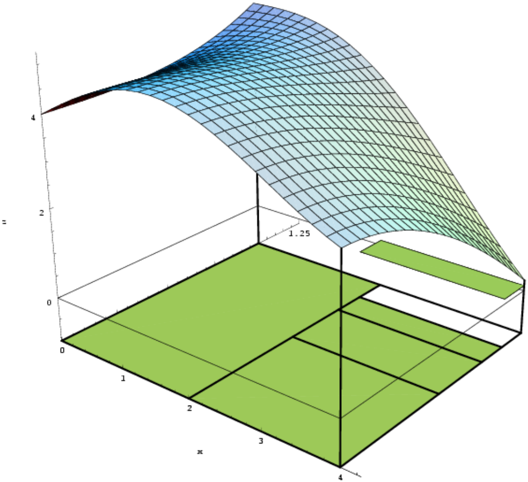

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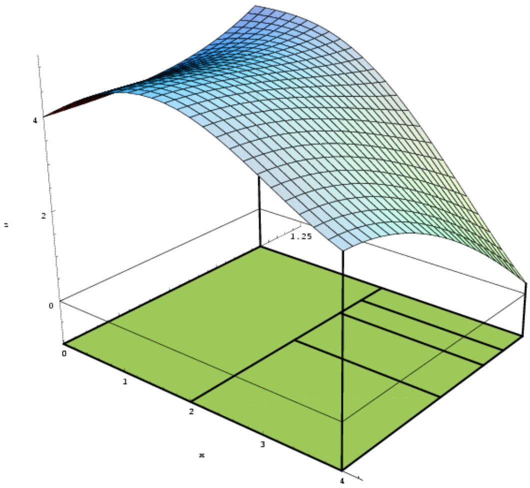

$$\sin x + y^2(y - x) + 4 > 0$$

Another Remedy: Use of The Gradient

- Fermat/Euler: x is a local extremum $\rightarrow \nabla f(x) = 0$
- $\widehat{\nabla f}(X) \not\ni 0 \rightarrow X$ does not contain a local extremum
- A *global* extremum is either a local one, or it lies on the border of the domain.
- If (after several splits) a sub-domain X does not touch the original domain's borders and $\widehat{\nabla f}(X) \not\ni 0$, then it can be safely forgotten.
- If $\widehat{\nabla f}(X) \not\ni 0$ and it still touches some borders, then there is some i with $\widehat{\partial_i f}(X) > 0$.
  So $x \in X \rightarrow x \in \hat{f}(X[i := \underline{X_i}]) \cup \hat{f}(X[i := \overline{X_i}])$

The Choice of Interval Bounds

- Most implementations use floating-point numbers as interval bounds.
- Therefore irrational functions have to be approximated with a *pre-defined* precision.
- For example with $\sqrt{(0,2)} = (\lfloor\sqrt{0}\rfloor, \lceil\sqrt{2}\rceil) = (0, 1.42)$ the inequality $x \in (0,2) \to \sqrt{x} \leq 1.416$ can't be proved.
- This is the floating-point numbers' fault!

Use of Constructive Real Numbers

- From Russell's talk: $\mathbb{R} \subset \mathbb{Q} \to \mathbb{Q}$
- With $\mathbb{I} = (\mathbb{R} \cup \{-\infty\}) \times (\mathbb{R} \cup \{\infty\})$ the united extension

$$\hat{f}_n\,[a;b] := \bigcup_{i=1}^{n} \hat{f}\,\left[a + (i-1)\frac{b-a}{n}; a + i\frac{b-a}{n}\right]$$

converges towards f's actual bounds, i.e.

$$X \mapsto \lim_{n\to\infty} \hat{f}_n\,X$$

is sharp.

- Constructive reals can be faster than rationals with fixed-precision operations (precisely when the precision actually necessary is less). But they can also be slower ...

Solving the Dependence Problem: Taylor Models

- For interval arithmetic $x - x$ on X looks like $x - y$ with $X := Y$
- A Taylor model represents a set of functions:

$$\mathbb{T} \ni (X, P, \Delta) \cong \{f : X \to \mathbb{R} \mid \forall x \in X.\, f\,x - P\,x \in \Delta\}$$

  - *domain* $X : \mathbb{I}^k$
  - *polynomial* $P : \mathbb{R}[k]$
  - *error bound* $\Delta : \mathbb{I}$
- Assuming we have some polynomial bounder B available, we can bound all functions in a Taylor model by $B\,X\,P + \Delta$
- How to obtain Taylor Models?
  - by Taylor's theorem with Lagrange remainder
  - by composition ...

Arithmetic on Taylor Models

- Constants, variables: trivial ($\Delta := [0;0]$)
- Addition and multiplication:

$$
\begin{aligned}
(X, P_1, \Delta_1) \tilde{+} (X, P_2, \Delta_2) &= (X, P_1 +_{\mathbb{R}[k]} P_2, \Delta_1 \hat{+} \Delta_2) \\
(X, P_1, \Delta_1) \tilde{\cdot} (X, P_2, \Delta_2) &= (X, (P_1 \cdot_{\mathbb{R}[k]} P_2)_{\leq n}, B\, X\, (P_1 \cdot_{\mathbb{R}[k]} P_2)_{>n} \hat{+} \\
&\qquad B\, P_1\, X \hat{\cdot} \Delta_2 \hat{+} \Delta_1 \hat{\cdot} B\, P_2\, X \hat{+} \Delta_1 \hat{\cdot} \Delta_2)
\end{aligned}
$$

- $\tilde{f} : \mathbb{T}^m \to \mathbb{T}$ is a Taylor-extension of $f : \mathbb{R}^m \to \mathbb{R}$ iff:

$$\forall T.\ [|\tilde{f}\ T_1 \ldots T_m|] \supseteq \{x \mapsto f\ (t_1\, x) \ldots (t_2\, x) \mid \forall i \leq m.\ t_i \in [|T_i|]\}$$

Combining Smooth Functions with Taylor Models

Makino/Berz: First apply an addition theorem, depending on the function under consideration. Then apply Taylor's theorem with Lagrange's remainder.

$$
\begin{aligned}
\log \circ F &= \log \circ (c + \bar{F}) \stackrel{\textit{Heureka!}}{=} \log c + \log \circ \left(1 + \frac{\bar{F}}{c}\right) \\
&\in \log c + \sum_{k=1}^{n} \frac{(-1)^{k-1}}{k} \left(\frac{\bar{F}}{c}\right)^k + \frac{(-1)^n \left(\frac{B\,\bar{F}\,X}{c}\right)^{n+1}}{(n+1)\left(1 + \left[0, \frac{B\,\bar{F}\,X}{c}\right]\right)^{n+1}}
\end{aligned}
$$

where X the domain under consideration.
In [Makino/Berz] this procedure is applied to exp, log, inv, sqrt, sin, cos, sinh, cosh, arcsin, arccos, arctan.

Combining Smooth Functions with Taylor Models without Heureka

$$\log \circ F \subseteq \log y_0 + \sum_{k=1}^{n} \frac{(-1)^{k-1}}{k y_0^k} (F - y_0)^k + \frac{(-1)^n (B\,F\,X - y_0)^{n+1}}{(n+1)[y_0, B\,F\,X]^{n+1}}$$

- for $y_0 = c$ this is equivalent to Makino/Berz's version
- Advantages:
  - Implementation and proofs can be factorised.
  - Better choices for y_0 are possible.

Computational Proof by Reflection

- This approach has been successfully applied to the four colour theorem [Gonthier/Werner] and to Pocklington certificates for prime numbers [Grégoire/Thery/Werner]
- The tactic is a program written in Coq's term language:
  `test : list intvl -> term -> nat -> bool`
- ```
  test_correct :
    forall (X : list intvl) (t : term) (n : nat),
    test X t n = true ->
    forall x:R, contains x X ->
      interpR x t >= 0
  ```
- The trace does not need to be stored:
  ```
  test_correct X t n (refl_equal true) :
    forall x:R, contains x X -> interpR x t >= 0
  ```
  ```

Future Work

- Better polynomial bounding algorithms: vast choice
- `let x = pi^2 in x + x` performs two approximations of `pi^2`
- Provide a user-friendly Coq tactic.