Taylor series revisited

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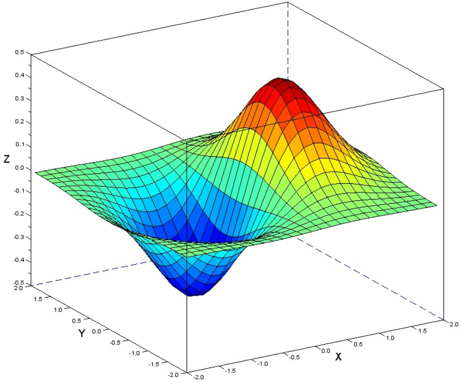
Industrial problematics



- Search of optimums
- Certified integration (ODE / PDE)
- Computation of invariants in dynamical systems

Motivations

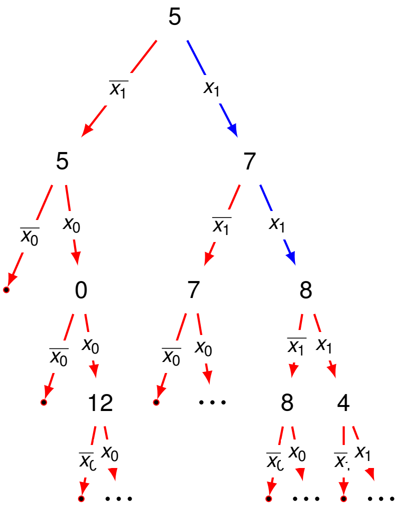
- Functions approximations (multivariate Taylor series)
- ODE/PDE solving (directly, no numerical scheme)

- Optimal in computation
- Type guarantees
- Certified errors
- On demand computations

Solution

- Functions approximations with Taylor series
- based on a previous work from X. Thirioux
- $f(x) = \sum_{|\alpha|<R} D_f^{(\alpha)}(0)\frac{x^\alpha}{\alpha!} + \sum_{|\alpha|=R} D_f^{(\alpha)}(\lambda * x)\frac{x^\alpha}{\alpha!}$
- Example : $sin(y + x^2) = 0 + 1.y + 1.x^2 - \frac{1}{6}.y^3 - \frac{1}{2}.x^2y^2 + \frac{1}{120}.y^5 - \frac{1}{2}.x^4y + ...$
- New notation : $f(X) = \sum_{n\in\mathbb{N}} T_n \odot X^n$

Solution : infinite trees



- $\sum_r T_r$ is a cotensor
- inspired from *Binary Decision Diagrams*
- and representing :

$$5 + 7.x_1 + 8.x_1^2 + 12.x_0^2 + 4.x_1^3 + \ldots$$

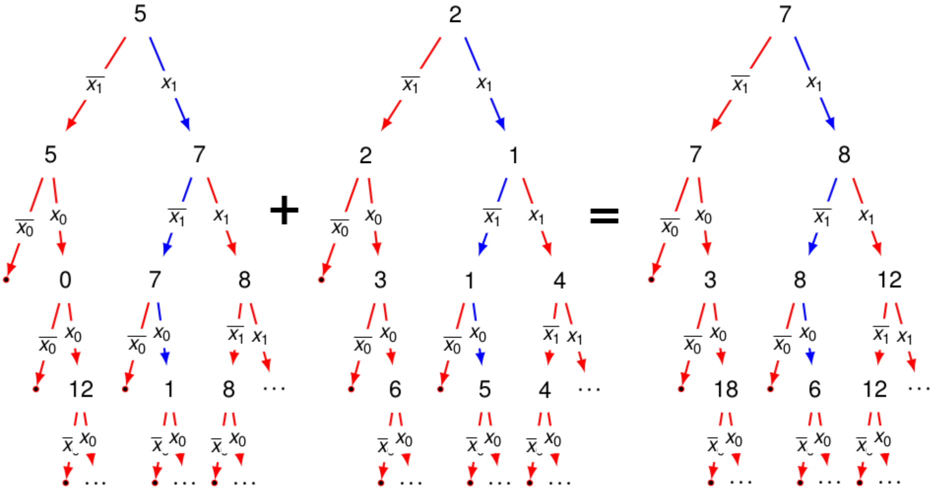
Taylor series approximations : related work

	COSY	Flowstar	Karczmarczuk	Pearlmutter	Proposal
	1997	2013	2000	2007	2019
On demand			x	x	x
Multivariate				x	x
Certified errors	x	x			x
Correction					x
Efficiency					x

Solution : infinite trees

- Linear operators
- Multiplication
- Composition
- Solving differential equations
- Experimentations

Linear operation : Sum



Multiplication

Définition

$$X = (x_0, ..., x_N)$$

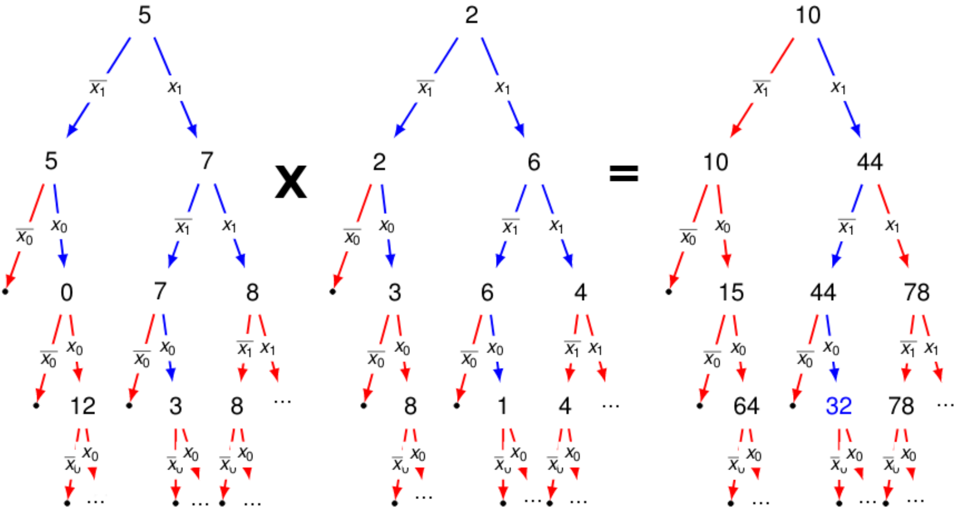
$$S(X) \times T(X) = (S_0 + ... + S_p X^p + ...) \times (T_0 + ... + T_q X^q + ...)$$
$$= R_0 + R_1 X + R_2 X^2 + ... + R_k X^k + ...$$

where

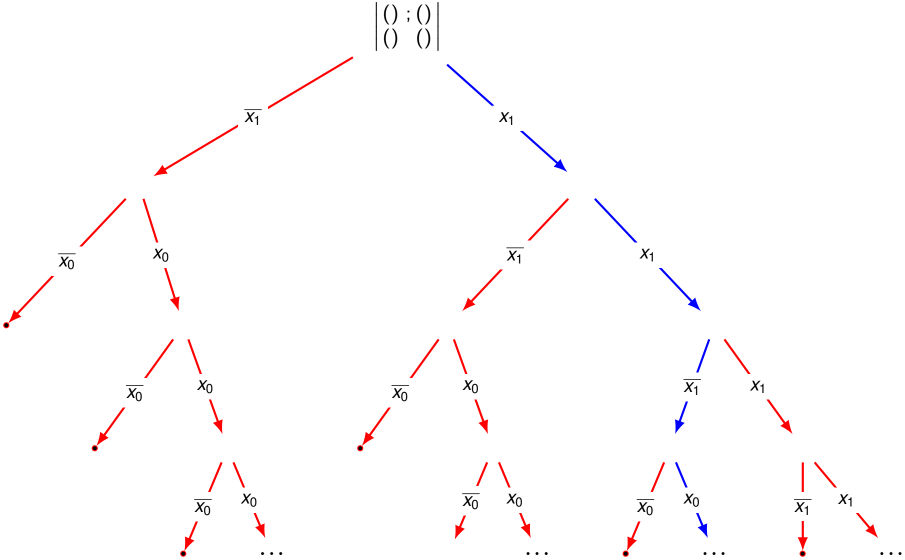
$$\forall k \in \mathbb{N}, R_k = \sum_{i=0}^{k} S_i T_{k-i}$$

- Multiplication is a performance bottleneck
- Efficient implementation through optimal convolution structure

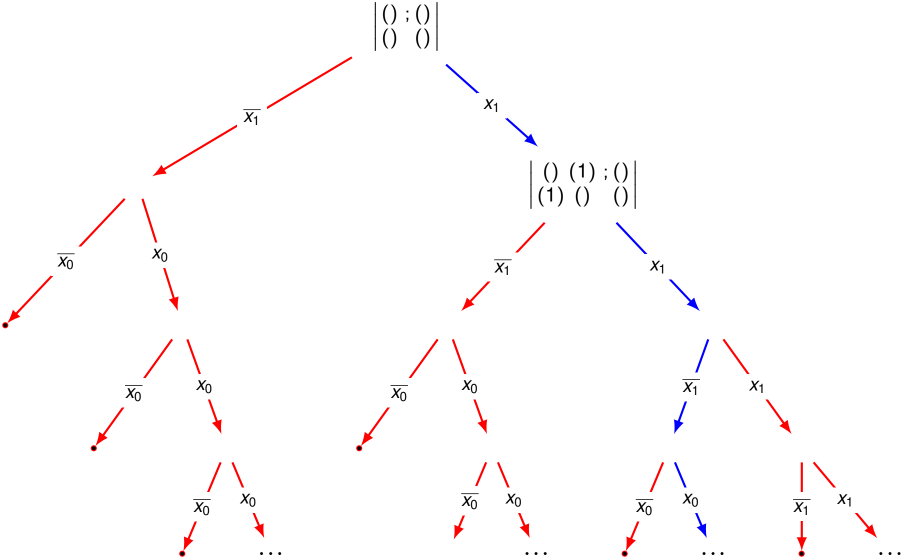
Multiplication



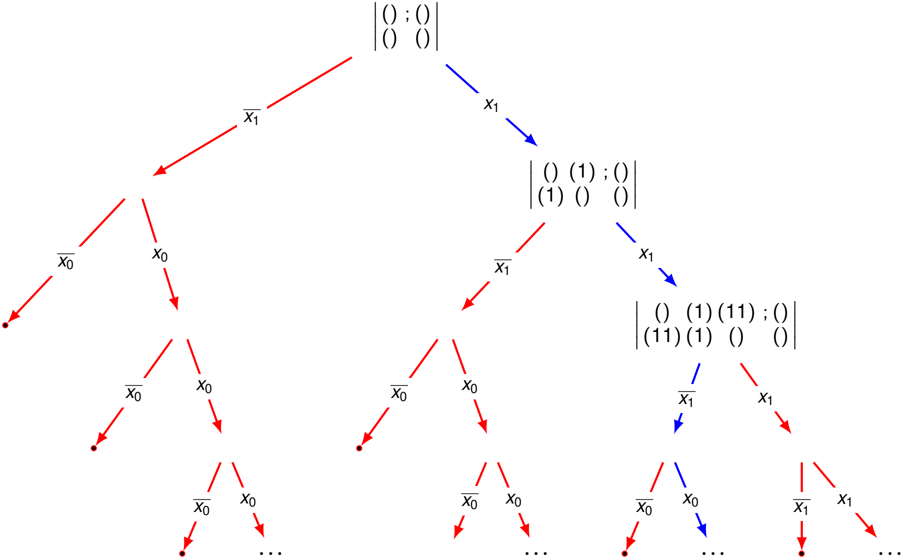
Multiplication



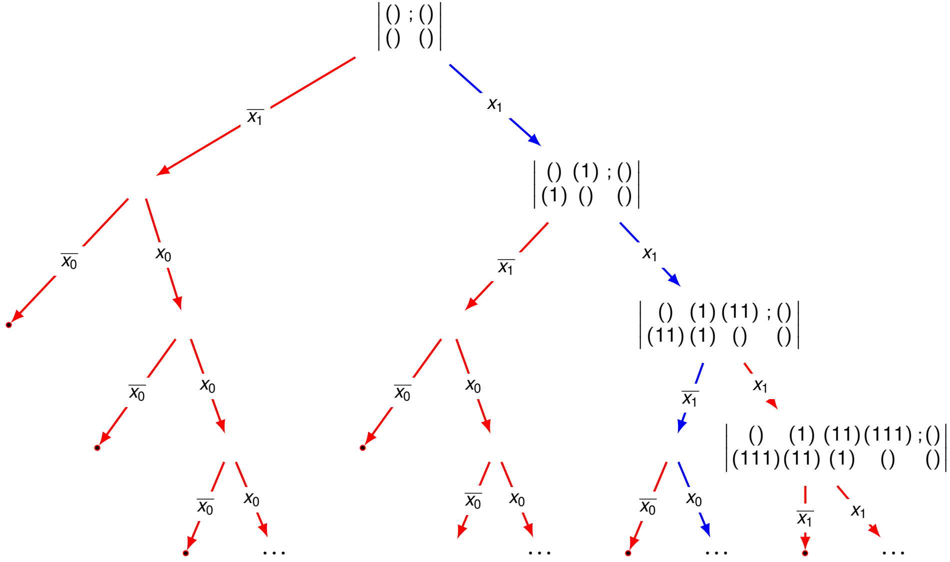
Multiplication



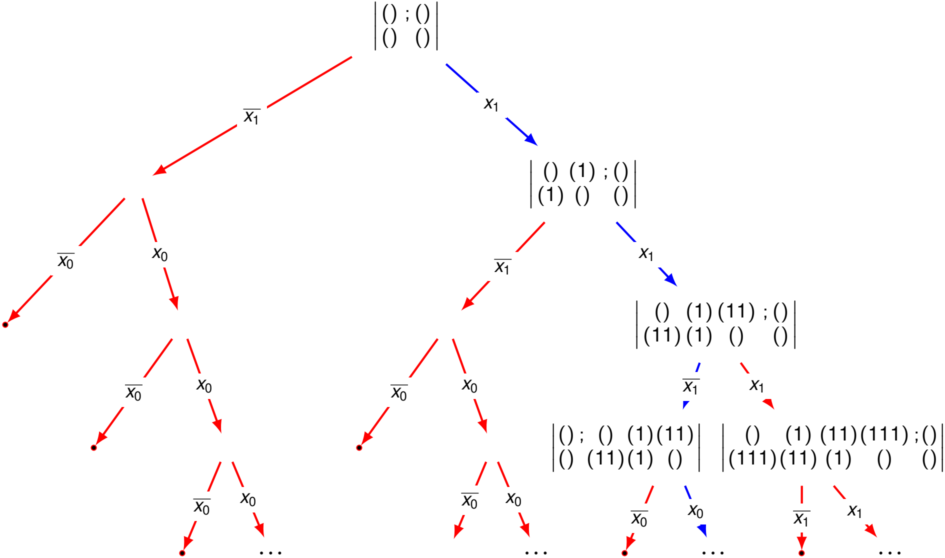
Multiplication



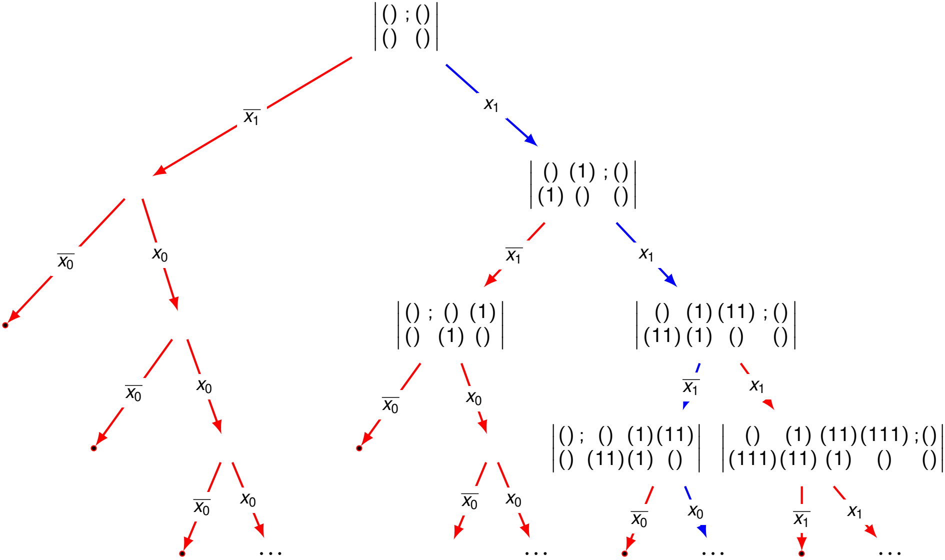
Multiplication



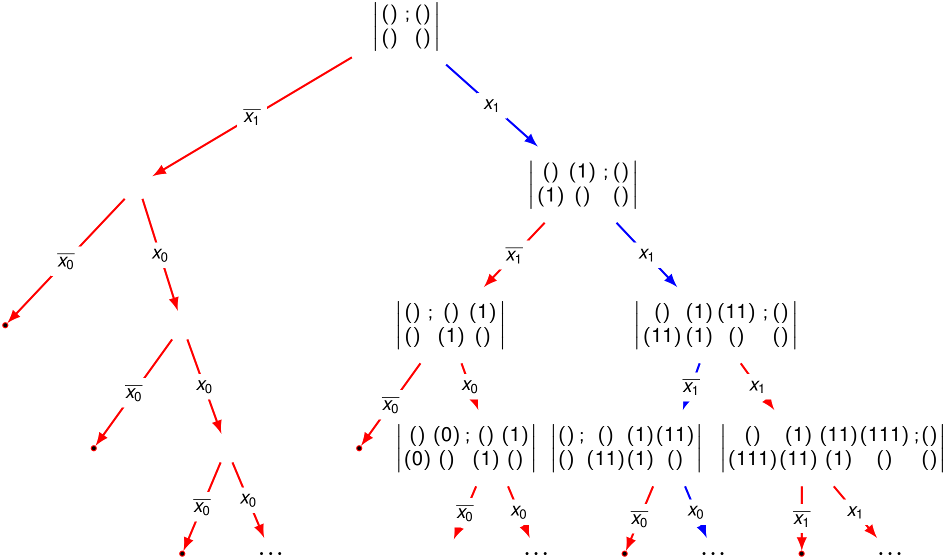
Multiplication



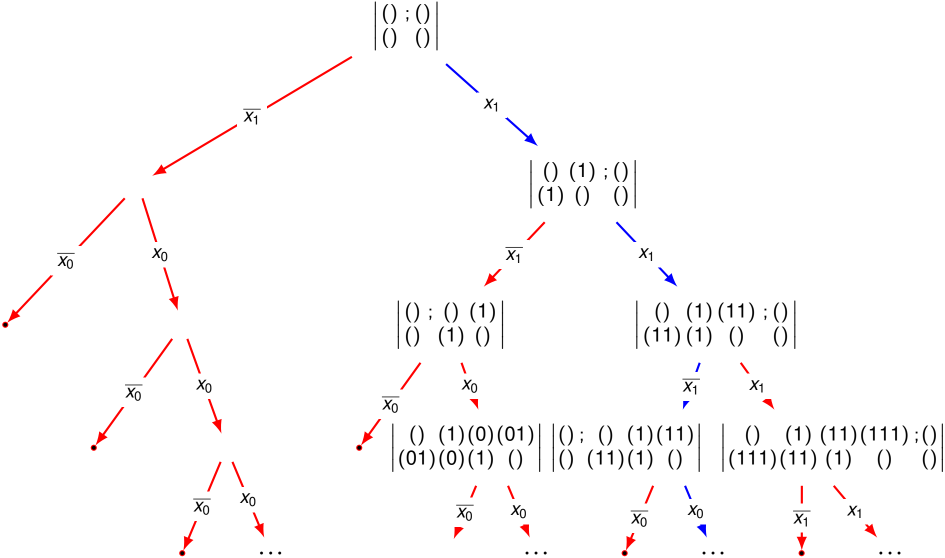
Multiplication



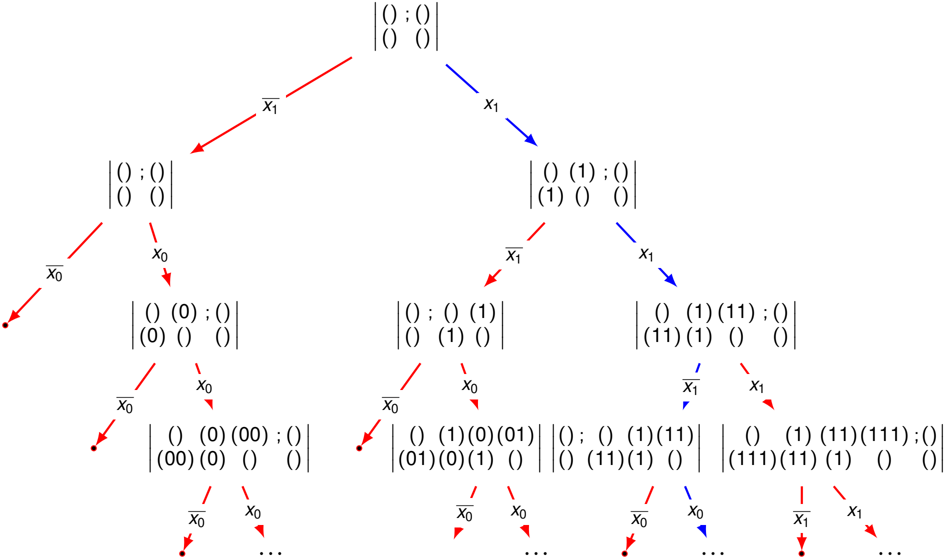
Multiplication



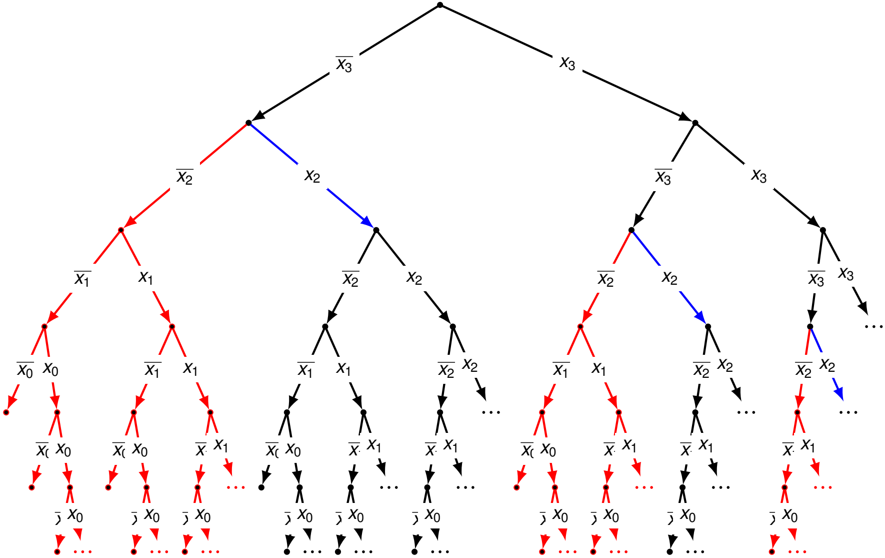
Multiplication



Multiplication



Integro-differential operators : `set` and `lift`



Integro-differential operators

- Polynomial expansion only (errors will be treated afterwards)
- With $(\Delta_k)_{(o_0,\ldots,o_{N-1})} \triangleq 1 + o_k,\;$ for $\sum_i o_i = R$

Differentiation

$$\frac{\partial f}{\partial X_k} \triangleq f[k] \odot \Delta_k = (\texttt{set}\ f\ k) \odot \Delta_k$$

Integration

$$\int_0^{X_k} f dx_k \triangleq (\mathbf{S} \odot \Delta_k^{-1})\!\uparrow\! k = (\texttt{lift}\ f\ k) \odot \Delta_k^{-1})$$

Composition

Motivations

- Apply univariate elementary functions to multivariate functions
- to create multivariate elementary functions
- Example : $$sin(y + x^2) = 0 + 1.y + 1.x^2 - \frac{1}{6}.y^3 - \frac{1}{2}.x^2y^2 + \frac{1}{120}.y^5 - \frac{1}{2}.x^4y + ...$$

Composition

Principle

- Differential decomposition
- A function is the sum of the integrals of –almost– its derivatives :
- $$f : \mathbb{R}^N \to \mathbb{R}, \qquad f = f(0) + \sum_{i<N} \int^{X_i} \frac{\partial f}{\partial X_i}\Big|_{\substack{X_k=0 \\ k>i}} dX_i$$

Composition

Example

- $f : \mathbb{R}^3 \to \mathbb{R}, \qquad f(x,y,z) = x^3 + 2x^2y + xz + 5y^2 + 3yz^2$
- $$\begin{cases} \frac{\partial f}{\partial x} = 3x^2 + 4xy + z \\ \frac{\partial f}{\partial y} = 2x^2 + 10y + 3z^2 \\ \frac{\partial f}{\partial z} = x + 6yz \end{cases} \qquad \begin{array}{l} \int_0^x \frac{\partial f}{\partial x} dx = x^3 + 2x^2y + xz \\ \int_0^y \frac{\partial f}{\partial y} dy = 2x^2y + 5y^2 + 3yz^2 \\ \int_0^z \frac{\partial f}{\partial z} dz = xz + 3yz^2 \end{array}$$

Composition

Redundancies

- Eliminating redundant terms
- $$f(x,y,z) = f(0,0,0) + \int_0^x \frac{\partial f}{\partial x} dx + \int_0^y \frac{\partial f}{\partial y}\Big|_{x=0} dy + \int_0^z \frac{\partial f}{\partial z}\Big|_{\substack{x=0\\y=0}} dz$$

Composition

Chain rule

- $$\frac{\partial(f \circ g)}{\partial X_i}_{i<N} = (\frac{\partial g}{\partial X_i})_{i<N} \times (f' \circ g)$$

- Hence :

$$f \circ g = f \circ g(0) + \sum_{i<N} \int^{X_i} (\frac{\partial g}{\partial X_i} \times f' \circ g)\Big|_{\substack{X_k=0 \\ k>i}} dX_i$$

Applications : Differential equations

Airy equation

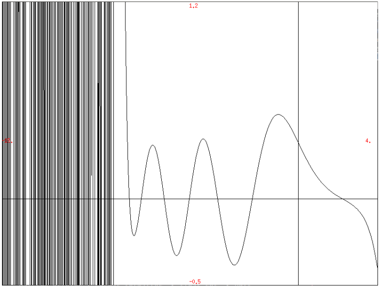
$$y'' - xy = 0$$

+ initial conditions

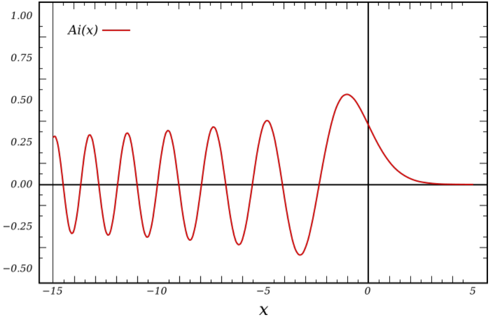
$$\equiv$$

$$\begin{cases} y\_dot = y\_dot_0 + \int^x xy \\ y = y_0 + \int^x y\_dot \end{cases}$$

Airy equation

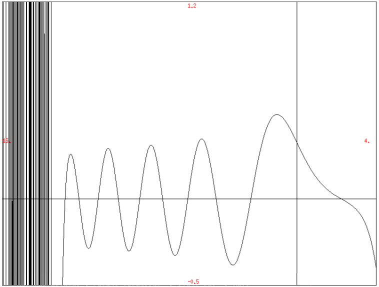


our result (at order 60)

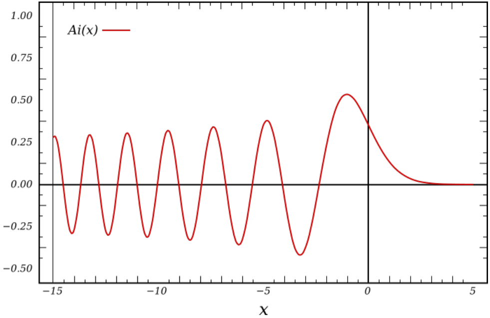


theorical result (wikipedia)

Airy equation

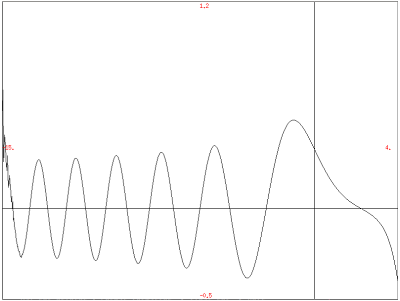


our result (at order 100)

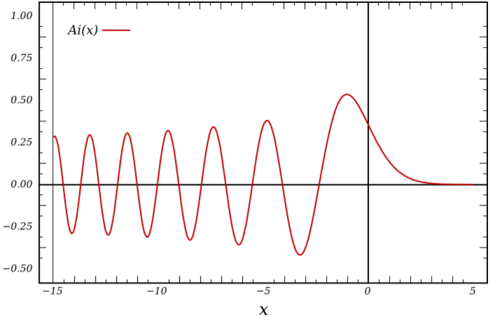


theorical result (wikipedia)

Airy equation



our result (at order 150)



theorical result (wikipedia)

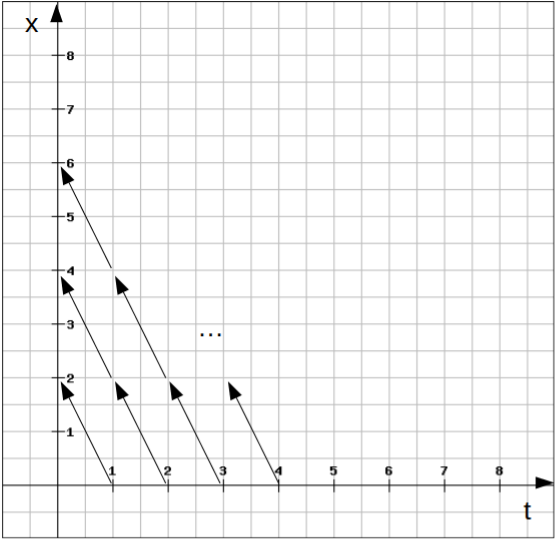
Applications : Differential equations

Heat equation

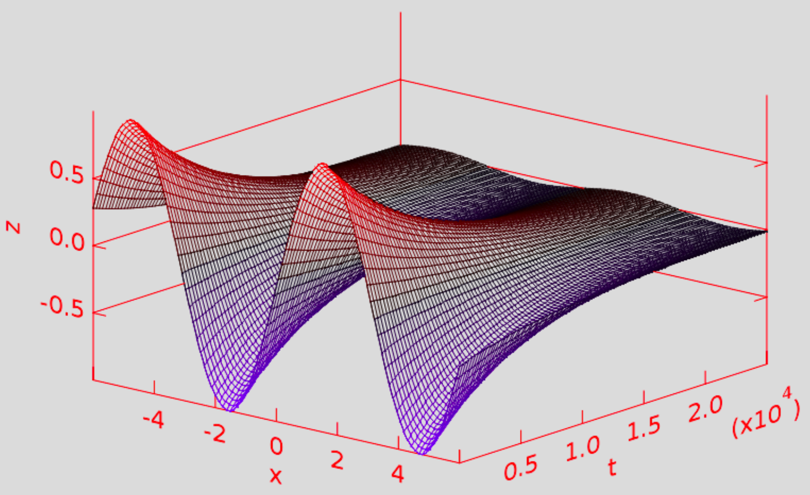
- $$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$
- $$u(x,t) = v(x) + \alpha \times \int^t \frac{\partial^2 u(x,t)}{\partial x^2}$$

Heat equation

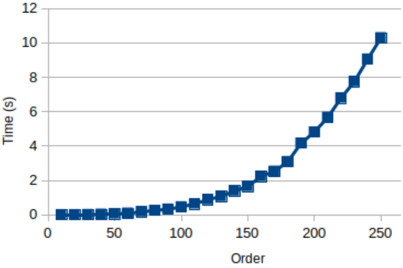
$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$$



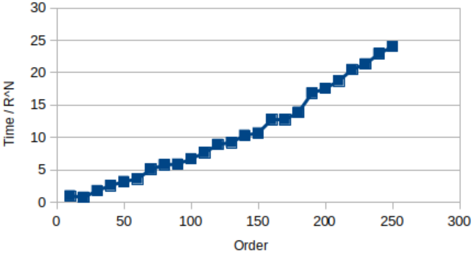
Heat equation



Some computation times

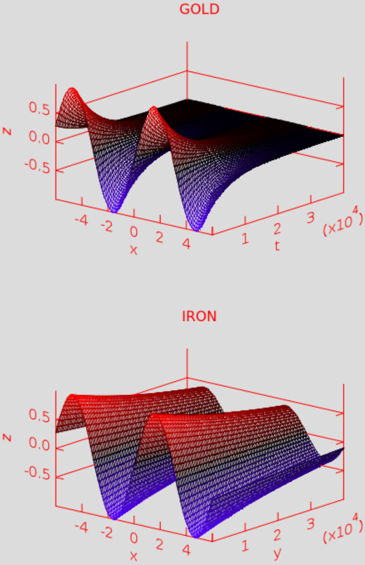


Computation time



Computation time / R^2

Heat equation



Errors

Définition

- $\mathbb{E} \triangleq \{f \in (\mathbb{K}^+)^N \to \mathbb{K}^+ \mid f(\mathbf{0}) = 0,\ f \text{ monotonic}\}$
- $[\![\langle v, \epsilon \rangle]\!] \triangleq \mathbf{X} \in (\mathbb{K}^+)^N \mapsto \{k \in \mathbb{K} \mid |k - v| \leq \epsilon(\mathbf{X})\}$
- $\langle v_1, \epsilon_1 \rangle + \langle v_2, \epsilon_2 \rangle \triangleq \langle v_1 + v_2, \epsilon_1 + \epsilon_2 \rangle$
- $\langle v_1, \epsilon_1 \rangle \times \langle v_2, \epsilon_2 \rangle \triangleq \langle v_1 \times v_2, |v_1| \times \epsilon_2 + |v_2| \times \epsilon_1 + \epsilon_1 \times \epsilon_2 \rangle$

- Other models of errors are also possible
- Works fine but for differential equations

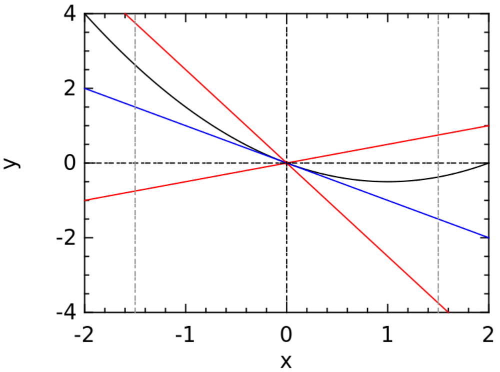
Taylor models

Taylor model predicate $\mathcal{TM}(f, R)$

at order R, in a neighbourhood of point **0** :

$$\mathcal{TM}(f, R) \triangleq \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^N . |\mathbf{x}| \leq \mathbf{y} \implies |f(\mathbf{x}) - \sum_{\alpha=0}^{|\alpha| \leq R} f_\alpha \mathbf{x}^\alpha| \leq \sum_{|\alpha|=R} \epsilon_\alpha(\mathbf{y}) |\mathbf{x}|^\alpha$$

Errors for polynomial forms



The **black** graph is the polynomial $P = \frac{1}{2}X^2 - X$.
The **blue** graph is the approximation of P at order 1.
The **red** graphs are the error bounds on interval $[-1.5, 1.5]$.

Errors for the integration operator

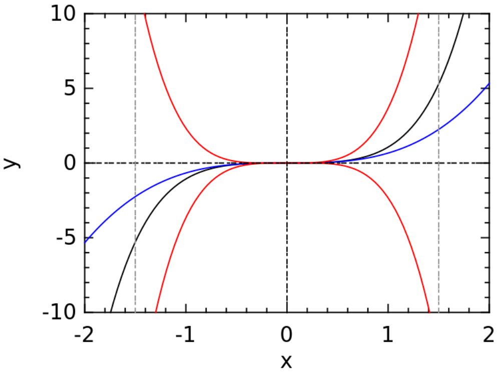
α-derivatives when $X_i \in \alpha$

$$\epsilon'_\alpha(X) = \epsilon'_{\alpha\setminus\{X_i\}}(X)$$

α-derivatives when $X_i \notin \alpha$

$$\begin{aligned} \epsilon'_\alpha(X) &= \frac{1}{\alpha!} \cdot \max_{\lambda\in[0,1]} \left| \frac{\partial^{|\alpha|}}{\partial X^\alpha}\Big(\int_0^{X_i} f\Big)(\lambda * X) - \frac{\partial^{|\alpha|}}{\partial X^\alpha}\Big(\int_0^{X_i} f\Big)(\mathbf{0}) \right| \\ &\leq (\mid v_\alpha^f \mid + \epsilon_\alpha^f(X)) * \mid X_i \mid \end{aligned}$$

Errors for the integration operator



The **black** graph is the integral of $2(X^4 + X^2)$, which is $\frac{2}{5}X^5 + \frac{2}{3}X^3$.
The **blue** graph is the approximation of this integral at order 4.
The **red** graphs are the error bounds on interval $[-1.5, 1.5]$.

Errors

Ordinary Differential Equations

- Assuming $f(X) \triangleq \langle f_0, \epsilon_0\rangle + X.\langle f_X, \epsilon_X\rangle + X^2.\langle f_{X^2}, \epsilon_{X^2}\rangle + \dots$
- Then $\int^X f = \langle 0, |X|.(|f_0| + \epsilon_0)\rangle + X.\langle f_0, \epsilon_0\rangle + \frac{X^2}{2}.\langle f_X, \epsilon_X\rangle + \dots$

- For a "causal" ODE, f depends on $\int^X f$
- That is : ϵ_0 depends on $|X|.(|f_0| + \epsilon_0)$, ϵ_{i+1} depend on ϵ_i

- Only an extra fixed-point computation for ϵ_0 is needed

Errors

Ordinary Differential Equations

- Assuming $f(X) \triangleq \langle f_0, \epsilon_0 \rangle + X.\langle f_X, \epsilon_X \rangle + X^2.\langle f_{X^2}, \epsilon_{X^2} \rangle + \dots$
- Then $\int^X f = \langle 0, |X|.(|f_0| + \epsilon_0) \rangle + X.\langle f_0, \epsilon_0 \rangle + \frac{X^2}{2}.\langle f_X, \epsilon_X \rangle + \dots$

- For a “causal” ODE, f depends on $\int^X f$
- That is : ϵ_0 depends on $|X|.(|f_0| + \epsilon_0)$, ϵ_{i+1} depend on ϵ_i

- Only an extra fixed-point computation for ϵ_0 is needed
- In the general case, only an extra fixed-point for a finite (and small) prefix of the ϵ_i sequence is needed

Errors

Partial Differential Equations

- The heat equation : $u(x,t) = v(x) + \alpha \times \int^t \frac{\partial^2 u(x,t)}{\partial x^2}$

- Assuming $u(x,t) = \langle u_0, \epsilon_0 \rangle + x.\langle u_x, \epsilon_x \rangle + t.\langle u_t, \epsilon_t \rangle + \dots$
- Then $\frac{\partial^2 u(x,t)}{\partial x^2} = 2.\langle u_{x^2}, \epsilon_{x^2} \rangle + 6x.\langle u_{x^3}, \epsilon_{x^3} \rangle + 2t.\langle u_{tx^2}, \epsilon_{tx^2} \rangle + \dots$
- And $\int^t \frac{\partial^2 u(x,t)}{\partial x^2} = 2t.\langle u_{x^2}, \epsilon_{x^2} \rangle + 6xt.\langle u_{x^3}, \epsilon_{x^3} \rangle + t^2.\langle u_{tx^2}, \epsilon_{tx^2} \rangle + \dots \quad + \langle 0, 2|t|.(|u_{x^2}| + \epsilon_{x^2}) \rangle + x.\langle 0, 6|tx|.(|u_{x^3}| + \epsilon_{x^3}) \rangle + \dots$

- In summary : ϵ_{x^i} depends on $\epsilon_{x^{i+2}}$ and $\epsilon_{t^{i+1}x^j}$ depends on $\epsilon_{t^i x^{2+j}}$
- Unsolvable without further assumptions

Errors and ODE

1. Fix `k`, the size of the finite prefix of error functions
2. Compute `let rec fix = lazy (Lazy.force (tie k (expr (untie k fix))))`

the `untie` function : extra fixed point through continuations

$$\texttt{untie}\ (k, \sum_{i \in \mathbb{N}} \langle v_i, \epsilon_i \rangle . X^i) = \sum_{i \in [0,k]} \langle v_i, \delta_i \rangle . X^i + \sum_{i > k} \langle v_i, \epsilon_i \rangle . X^i$$

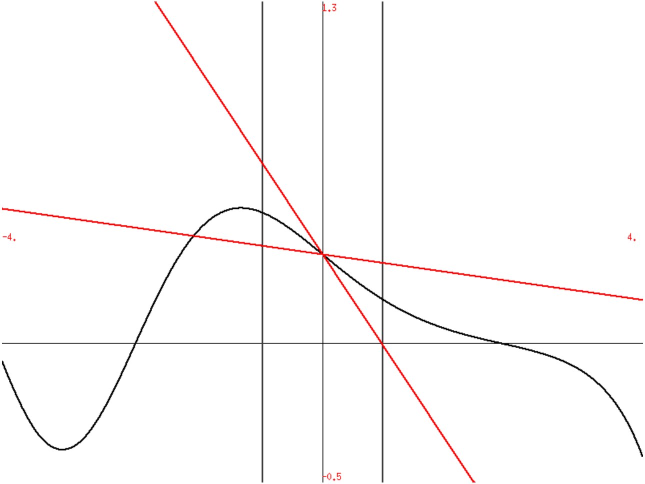
where $\delta_i(x) =$ `shift (fun k -> Request (i, k))`

The `tie` function : application of Schauder's fixed point theorem

$$\texttt{tie}\ (k, \sum_{i \in \mathbb{N}} \langle v_i, \epsilon_i \rangle . X^i) = \sum_{i \in [0,k]} \langle v_i, \delta_i \rangle . X^i + \sum_{i > k} \langle v_i, \epsilon_i \rangle . X^i$$

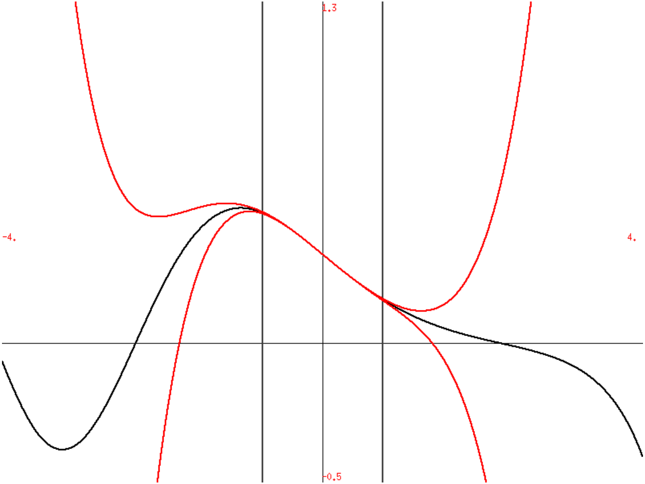
where $\delta_i(x) \geq$ `match reset` $\epsilon_i(x)$ `with Done r -> r | Request (j, k) -> k` $\delta_j(x)$

Certified ODE solving



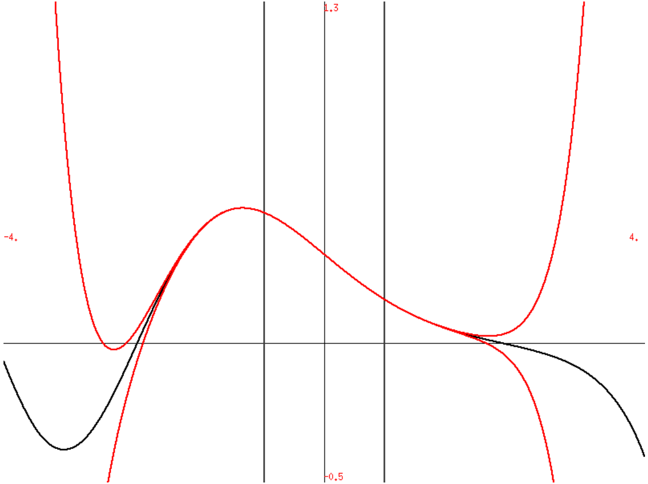
The **black** graph is the solution of Airy ODE.
The **red** graphs are the error bounds on interval $[-0.75, 0.75]$ (**grey** vertical bars) at order 1 (86.6% maximum relative error).

Certified ODE solving



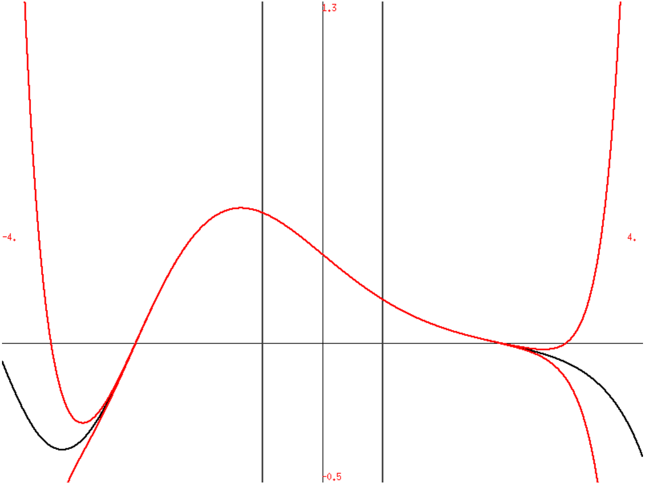
The **black** graph is the solution of Airy ODE.
The **red** graphs are the error bounds on interval $[-0.75, 0.75]$ (**grey** vertical bars) at order 5 (41.3% maximum relative error).

Certified ODE solving



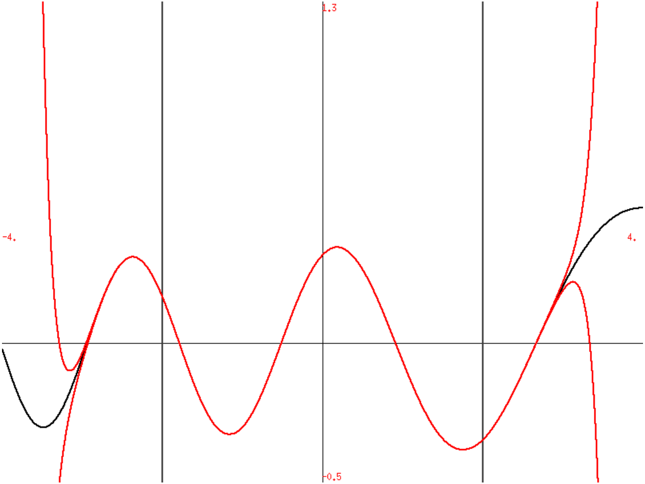
The **black** graph is the solution of Airy ODE.
The **red** graphs are the error bounds on interval $[-0.75, 0.75]$ (**grey** vertical bars) at order 10 (24.6% maximum relative error).

Certified ODE solving



The **black** graph is the solution of Airy ODE.
The **red** graphs are the error bounds on interval $[-0.75, 0.75]$ (**grey** vertical bars) at order 15 (1.1% maximum relative error).

Certified ODE solving



The **black** graph is the solution of Airy ODE, shifted at point -5.
The **red** graphs are the error bounds on interval $[-2.0, 2.0]$ (**grey** vertical bars) at order 15 (5×10^{-7} maximum relative error).

Conclusion

- Efforts towards efficiency
- “Solved” differential equations
- On-demand : refine sol. until precision and/or time limit
- Error bounds for PDE ?
- Optimal composition to define ?
- Poisson basis ?
- Formal verification ?