Floating-point computations

Interval arithmetic

Application: study of NLS on metric graphs

Introduction to computer-assisted proofs in nonlinear analysis

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A first example

Let us compute sin(0) and $sin(\pi)$ using Python.



Image from https://fr.wikipedia.org/wiki/Fichier:Python-logo-notext.svg

Floating-point numbers in a nutshell

Rough idea

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 $\mathbb{F}:$ set of finite 64 bit (double precision) floating-point numbers.

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etc.

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How not to launch a rocket



Figure: An Ariane 5 launcher (click for the video)

Image from https://commons.wikimedia.org/wiki/File: Ariane_5_with_James_Webb_Space_Telescope_Prelaunch_(51773093465).jpg, video from https://www.youtube.com/watch?v=1qRUFg-Pte0

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To summarize:

A first (obvious) limitation of numerical computations

F is finite!

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Rounding modes

Since $\mathbb F$ is finite, not all real numbers may be represented by floating-point numbers.

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Rounding modes

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There are thus several *rounding modes*, depending on whether the result is to be rounded up, down, towards zero, etc.

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Accumulation of round-off errors

The Vancouver stock index



Figure: The BEL20 stock index

Image from https://commons.wikimedia.org/wiki/File:BEL_20.svg

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Accumulation of round-off errors The Vancouver stock index

Between 1982 and 1983, the Vancouver stock index dropped anomalously due to the accumulation of small round-off errors, due to the fact that quantities were always rounded *down* after each computation.



Figure: The BEL20 stock index

Image from https://commons.wikimedia.org/wiki/File:BEL_20.svg

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Accumulation of round-off errors Patriot missiles



Figure: A Patriot missile launch

Image from

https://upload.wikimedia.org/wikipedia/commons/f/f8/Patriot_missile_launch_b.jpg

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Accumulation of round-off errors Patriot missiles

In 1991, American Patriot missiles failed to intercept an incoming Scud missile, killing 28 soldiers and injuring 100 other people, due to a bad computation of internal time due to an accumulation of round-off errors.



Figure: A Patriot missile launch

Image from

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Approximation errors are typically studied by numerical analysts: rigorous error bounds, convergence results, etc.

As for round-off errors, in "practical applications" it is important to **be aware** of them and to **keep them small by design**. This typically involves a suitable **stability analysis** of the numerical methods. Floating-point computations

Interval arithmetic

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Where are we now?

For us, an important question remains.

How to obtain **mathematically rigorous** results based on numerical computations?

Floating-point computations

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How to obtain **mathematically rigorous** results based on numerical computations?

If only one could ignore round-off errors...

Interval arithmetic

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A simple solution?

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The idea of interval arithmetic

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- to physicists: physical measurements are performed up to a finite precision anyway.

Although this may seem a paradox, all exact science is dominated by the idea of approximation.

- Bertrand Russell, The Scientific Outlook

The class $\mathcal{I}_{\mathbb{R}}$ of intervals

The intervals we will consider are the topologically closed and connected subsets of \mathbb{R} (as specified in the standard IEEE-1788 devoted to interval arithmetic¹), i.e. they belong to the class $\mathcal{I}_{\mathbb{R}}$ of subsets of \mathbb{R} defined by

$$egin{aligned} \mathcal{I}_{\mathbb{R}} &:= \left\{ \emptyset
ight\} \cup \left\{ [a,b] \mid a,b \in \mathbb{R}, a \leq b
ight\} \ &\cup \left\{ [a,+\infty[\mid a \in \mathbb{R}
ight\} \ &\cup \left\{]{-\infty},b] \mid b \in \mathbb{R}
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¹See https://standards.ieee.org/ieee/1788/4431/.

Operations on intervals

Given two intervals \mathbf{x} and \mathbf{y} , their sum is given by

$$\mathbf{x} + \mathbf{y} := \Big\{ x + y \mid x \in \mathbf{x}, y \in \mathbf{y} \Big\},\$$

their *difference* by

$$\mathbf{x} - \mathbf{y} := \left\{ x - y \mid x \in \mathbf{x}, y \in \mathbf{y} \right\}$$

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Examples and surprises: on the blackboard!

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In general: interval extensions

Definition

Let $D \subseteq \mathbb{R}$ be a set and let $F : D \to \mathbb{R}$ be a map.

An *interval extension* of *F* is an application $\mathbf{F} : \mathcal{I}_{\mathbb{R}} \to \mathcal{I}_{\mathbb{R}}$ which satisfies the *containment property*, namely so that for all $\mathbf{x} \in \mathcal{I}_{\mathbb{R}}$, the set

$$F(\mathbf{x}) := \left\{ F(x) \mid x \in \mathbf{x} \cap D \right\}$$

is included in F(x).

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Examples on the blackboard! Compare extensions of $F : \mathbb{R} \to \mathbb{R} : x \mapsto x^2$ with the product operation.

Fundamental theorem of interval arithmetic

Theorem

If interval extensions of real functions f_1, \ldots, f_k are composed, the result is an interval extension of the composition $f_1 \circ \cdots \circ f_k$.

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Allows to obtain interval extensions of complicated functions by composing interval extensions of its subparts.

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In practice

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The set $\mathcal{I}_{\mathbb{R}}$ is a mathematical notion. In practice, the implementation will use intervals from the set

$$\mathcal{I}_{\mathbb{F}} := \Big\{ \mathbf{x} = [\underline{x}, \overline{x}] \mid \underline{x} \leq \overline{x} \text{ are two floating-point numbers} \Big\} \cup \Big\{ \emptyset \Big\}.$$

Interval arithmetic

Application: study of NLS on metric graphs

Back to the computation of $sin(\pi)$

Let us use the "mpmath" library² in Python3 and ask the value of

iv.pi

then

iv.sin(iv.pi).

²See in particular the module iv, devoted to interval arithmetic at https://www.mpmath.org/doc/1.0.0/contexts.html.

Introduction to computer-assisted proofs in nonlinear analysis

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- If a returned interval is "too big", it is valid but useless.
 For instance, iv.sin(x) could return [-1, 1] regardless of the value of x, but this bound is useless.
- Nevertheless, it is in principle possible to show that given matrices are invertible, positive/negative definite... using interval arithmetic.

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We may thus divide [0, 1] into many "small" intervals and discard all those for which we are sure that F has no roots, this being determined by evaluating the interval extension **F**. We end up with (possibly many) small intervals such that all potential roots of F belong to one of those.

The system of ODEs

$$\partial_t x_1 = -\sigma x_1 + \sigma x_2$$

$$\partial_t x_2 = \rho x_1 - x_2 - x_1 x_3,$$

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This fact, though conjectured since the 1960s, was only proved by Warwick Tucker in 1999, using a computer-assisted proof using interval arithmetic.
Application: study of NLS on metric graphs

What is a compact metric graph?

A compact metric graph is made of a finite number of vertices



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Metric graphs: the lengths of edges are important.

Application: study of NLS on metric graphs

Functions defined on metric graphs



A compact metric graph G with three edges e_0 (length 5), e_1 (length 4) and e_2 (length 3)

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Functions defined on metric graphs



A compact metric graph \mathcal{G} with three edges e_0 (length 5), e_1 (length 4) and e_2 (length 3), a function $f : \mathcal{G} \to \mathbb{R}$

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$$\int_{\mathcal{G}} f \, \mathrm{d}x := \int_0^5 f_0(x) \, \mathrm{d}x + \int_0^4 f_1(x) \, \mathrm{d}x + \int_0^3 f_2(x) \, \mathrm{d}x$$

Application: study of NLS on metric graphs

The spectral problem on metric graphs

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We are interested in solutions (γ, u) , with $u \neq 0$, of the differential system

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Remark: we always have dim $E_1 = 1$ with $\gamma_1 = 0$, considering constant functions.

Application: study of NLS on metric graphs

Kirchoff's condition: degree one nodes



Application: study of NLS on metric graphs

Kirchoff's condition: degree one nodes



In other words, the derivative of u at x_1 vanishes: this is the usual Neumann condition.

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Kirchoff's condition in general: outgoing derivatives



We generalize the spectral problem by introducing a *nonlinear term* (which appears in models of optic fibers, Bose-Einstein condensates...).

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Question

What about p > 2?

 (\mathcal{P}_p)

Application: study of NLS on metric graphs

The quasilinear regime $p \approx 2 \ (p > 2)$

Proposition

Let $(p_n)_{n\geq 1} \subseteq]2, +\infty[$ be a sequence of exponents which converges to 2

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Application: study of NLS on metric graphs

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$$\int_{\mathcal{G}} u_* \ln |u_*| \varphi \, \mathrm{d} x = 0 \qquad \forall \varphi \in E_2.$$

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$$\int_{\mathcal{G}} u_* \ln |u_*| \varphi \, \mathrm{d} x = 0 \qquad \forall \varphi \in E_2.$$

We say that $u_* \in E_2$ is a solution of the reduced problem if the above condition holds.

The functional $\mathcal{J}_*: E_2 \to \mathbb{R}$

$$\mathcal{J}_*(\varphi) := rac{1}{4} \int_{\mathcal{G}} \varphi^2(x) (1 - 2 \ln |\varphi(x)|) \,\mathrm{d}x$$

is of class $\mathcal{C}^1,$ and the solutions of the reduced problem coincide with its critical points.

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Using a "Lyapunov-Schmidt" argument, we can show **existence and** uniqueness results around a nondegenerate critical point for (\mathcal{P}_p) , when $p \approx 2$.

Floating-point	computations

Application: study of NLS on metric graphs

The tetrahedron

In the remainder of the talk, we will only consider the following graph \mathcal{G}_t .


Second eigenspace and symmetries of \mathcal{G}_t

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In this way, we obtain an isometric group action

$$G_t \times E_2 \rightarrow E_2 : (g, \varphi) \mapsto g \cdot \varphi,$$

such that $J_*(g \cdot \varphi) = J_*(\varphi)$ for all $(g, \varphi) \in G_t \times E_2$.

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then u is a critical point of J.

Floating-point computations

Interval arithmetic

Application: study of NLS on metric graphs

A natural question

Critical point theory (using the principle of symmetric criticality, Morse theory, etc), will give relations on the number of critical points and the existence of some specific symmetric critical points.

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Question

Does \mathcal{J}_* possess critical points other than the ones of the four aforementioned families?

Theorem (De Coster, G., Troestler (2024))

All critical points of $\mathcal{J}_* : E_2 \to \mathbb{R}$ (for the tetrahedron graph) belong to one of the four families obtained thanks to the symmetries.

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1 locating small "boxes" containing all critical points of \mathcal{J}_* , by root finding methods.

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After a careful implementation and some computing time...

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After a careful implementation and some computing time... Things worked out!

Thanks for your attention!



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Soon: my PhD thesis (see in particular Chapter 5) and a corresponding paper related to the contents of the last section.