Application: study of NLS on metric graphs

Introduction to computer-assisted proofs in nonlinear analysis Séminaire doctorant du LAMFA

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Joint work with Colette De Coster (CERAMATHS/DMATHS) and Christophe Troestler (UMONS)

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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

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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.

Floating-point computations

Interval arithmetic

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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

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

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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.

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Where are we now?

For us, an important question remains.

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

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

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

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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

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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

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

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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.

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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

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

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

$$\partial_t x_3 = -\beta x_3 + x_1 x_2$$

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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.

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What is a compact metric graph?

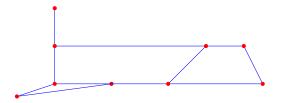
A compact metric graph is made of a finite number of vertices



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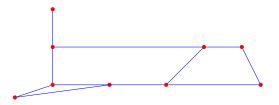
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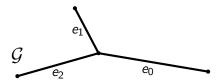
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Metric graphs: the lengths of edges are important.

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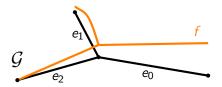
Functions defined on metric graphs



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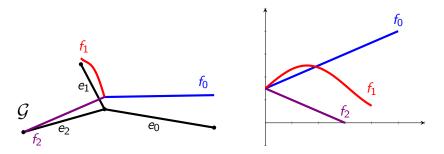
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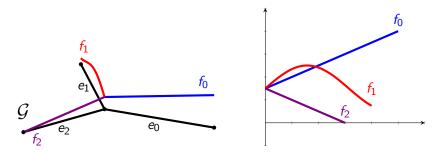
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A compact metric graph \mathcal{G} with three edges e_0 (length 5), e_1 (length 4) and e_2 (length 3), a function $f : \mathcal{G} \to \mathbb{R}$, and the three associated real functions.

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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 $f : \mathcal{G} \to \mathbb{R}$, and the three associated real functions.

$$\int_{\mathcal{G}} f \, \mathrm{d}x := \int_{0}^{5} f_{0}(x) \, \mathrm{d}x + \int_{0}^{4} f_{1}(x) \, \mathrm{d}x + \int_{0}^{3} f_{2}(x) \, \mathrm{d}x$$

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The spectral problem on metric graphs

$$\begin{cases} -u'' = \gamma u & \text{ on each edge } e \text{ of } \mathcal{G}, \end{cases}$$

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

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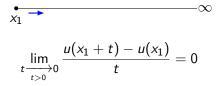
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Remark: we always have dim $E_1 = 1$ with $\gamma_1 = 0$, considering constant functions.

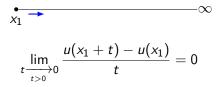
Application: study of NLS on metric graphs

Kirchoff's condition: degree one nodes



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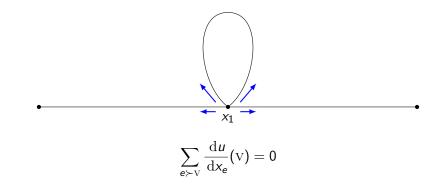
Kirchoff's condition: degree one nodes



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

Application: study of NLS on metric graphs

Kirchoff's condition in general: outgoing derivatives



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Question

What about p > 2?

Damien Galant

 (\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

Application: study of NLS on metric graphs

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Application: study of NLS on metric graphs

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Application: study of NLS on metric graphs

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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 $\mathcal{J}_*: \textit{E}_2 \rightarrow \mathbb{R}$

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

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

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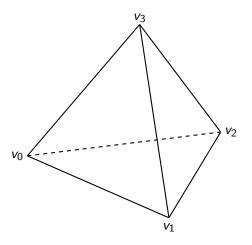
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Using a "Lyapunov-Schmidt" argument, we can show **existence and** uniqueness results around a nondegenerate critical point for (\mathcal{P}_p) , when $p \approx 2$.

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

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However, it cannot classify all critical points of J_* .

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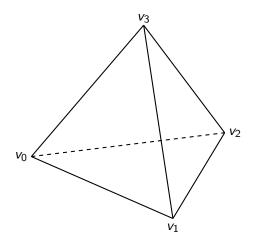
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After a careful implementation and some computing time... Things worked out!

Thanks for your attention!





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