Qualitative properties of solutions of the nonlinear Schrödinger equation on metric graphs

Computer-assisted study of sign-changing solutions on the tetrahedron graph

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No Dirichlet vertices $\to \gamma_1 = 0$.

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When $p = 2$, the solutions of ($\mathcal{P}_p$) are the eigenfunctions in E_2.

Nodal action ground states

Among all solutions of $(\mathcal{P}_p)$ when $p > 2$, we are particularly interested in nodal action ground states, namely sign-changing solutions which minimize the action functional

$$\mathcal{J}_p(u) := \frac{1}{2}\|u'\|^2_{L^2(\mathcal{G})} + \frac{\lambda}{2}\|u\|^2_{L^2(\mathcal{G})} - \frac{\gamma_2}{p}\|u\|^p_{L^p(\mathcal{G})}$$

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Question

What is the behavior of nodal action ground states as $p \to 2$?

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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.

Variational formulation

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

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

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 $p \approx 2$. *But how to do goals 1 and 2?*

Geometry of $\mathcal{J}_*$

For any $\varphi \in E_2 \setminus \{0\}$, the map

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Its value can be computed explicitly and is given by

$$n_*(\varphi) = \exp\left(-\frac{\int_{\mathcal{G}} \varphi^2 \ln|\varphi| \,\mathrm{d}x}{\int_{\mathcal{G}} \varphi^2 \,\mathrm{d}x}\right).$$

The reduced Nehari manifold

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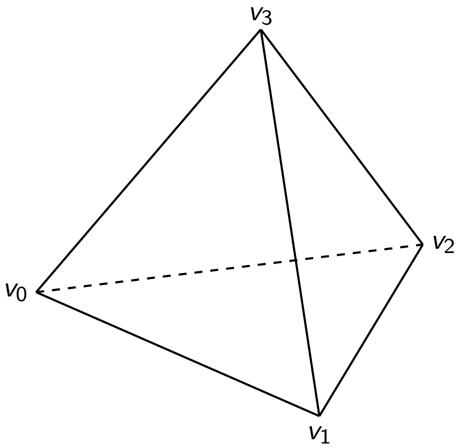
Theorem (Bonheure, Bouchez, Grumiau, Van Schaftingen (2008))

Weak limits of nodal action ground states minimize $\mathcal{J}_*$ over $\mathcal{N}_*$.

The tetrahedron

In the remainder of the talk, we will focus on the following graph $\mathcal{G}_{\mathrm{t}}$.



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where φ_a is such that

$$\varphi_a(x) = \frac{a_i \sin(\sqrt{\gamma_2}(1-x)) + a_j \sin(\sqrt{\gamma_2}x)}{\sin(\sqrt{\gamma_2})},$$

if x belongs to the edge $v_i v_j$.

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2. a encodes the values of φ_a at the vertices, in the sense that

$$\varphi_a(v_i) = a_i$$

   for all $i \in \{0, 1, 2, 3\}$.

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acts on E_2 due to the fact that "all vertices of the tetrahedron are the same" and that the functional $\mathcal{J}_*$ is even.

In this way, we obtain an *isometric group action*

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

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.

The families of critical points

Proposition

The following eigenfunctions are critical points of $\mathcal{J}_*$:

- $f_0 := \pi_{\mathcal{N}_*}\big(\varphi_{(1,-1,0,0)}\big)$;
- $f_1 := \pi_{\mathcal{N}_*}\big(\varphi_{(1,-1/3,-1/3,-1/3)}\big)$;
- $f_2 := \pi_{\mathcal{N}_*}\big(\varphi_{(1,1,-1,-1)}\big)$;
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Moreover, for every $g \in G_t$ *and every* $i \in \{0,1,2,3\}$, $g \cdot f_i$ *is a critical point of* $\mathcal{J}_*$.

For instance, f_1 is a critical point of $\mathcal{J}_*$ restricted to the one-dimensional subspace of E_2 taking equal values in v_1, v_2 and v_3.

A natural question

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Those are the only critical points as shown by a computer-assisted proof.

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

Floating-point numbers use the "scientific notation" on base 2, where both the significand and the exponent are written with a given number of bits (digits in base 2).

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

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- to analysts: this is a quantitative version of the ε's and the δ's;

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- to analysts: this is a quantitative version of the ε's and the δ's;
- to physicists: physical measurements are performed up to a finite precision anyway.

Interval arithmetic: a simple solution?

The main idea of *interval arithmetic* is very simple, yet powerful.

The idea of interval arithmetic

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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 arithmetic[1]), i.e. they belong to the class $\mathcal{I}_{\mathbb{R}}$ of subsets of $\mathbb{R}$ defined by

$$\begin{aligned}\mathcal{I}_{\mathbb{R}} := \Big\{\emptyset\Big\} &\cup \Big\{[a,b] \mid a,b \in \mathbb{R}, a \leq b\Big\} \\ &\cup \Big\{[a,+\infty) \mid a \in \mathbb{R}\Big\} \\ &\cup \Big\{(-\infty,b] \mid b \in \mathbb{R}\Big\} \\ &\cup \Big\{(-\infty,+\infty) := \mathbb{R}\Big\}.\end{aligned}$$

[1] See https://standards.ieee.org/ieee/1788/4431/.

Operations on intervals

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

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

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!

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

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

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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.

In practice

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In practice, the implementation will use intervals from the set

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

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

Let us use the "mpmath" library[2] in Python3 and ask the value of

```
iv.pi
```

then

```
iv.sin(iv.pi).
```

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

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- It may allow to prove that some values are nonzero, but it cannot prove that some values are equal to zero.

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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.

Locating roots of a function

Let $F : [0, 1] \to \mathbb{R}$. If $\mathbf{F}$ is an interval extension of F and if $\mathbf{x} \in \mathcal{I}_{\mathbb{R}}$ is included in $[0, 1]$, then

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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 $\mathbf{F}$. We end up with (possibly many) small intervals such that all potential roots of F belong to one of those.

What we use the computer for

The main thing we want to prove with the help of the computer is the following proposition.

Proposition

f_0, f_1, f_2 and f_3 are the only nonzero critical points of $\mathcal{J}_*$ up to symmetries, in the sense that

$$\forall \varphi \in E_2 \setminus \{0\}, \left[(\mathcal{J}_*'(\varphi) = 0) \implies (\exists i \in \{0,1,2,3\}, \exists g \in G_t, \varphi = g \cdot f_i) \right].$$

Moreover, f_1, f_2 and f_3 are nondegenerate.

Strategy of the proof

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At a high level, the strategy is rather "direct". It consists in the two following steps:

1. locating small "boxes" containing all critical points of $\mathcal{J}_*$, by root finding methods.
2. proving uniqueness of critical points inside each box using second order information.

Variational characterization of the critical points

Proposition

The action levels of the critical points we found are so that

$$\mathcal{J}_*(f_2) < \mathcal{J}_*(f_0) < \mathcal{J}_*(f_3) < \mathcal{J}_*(f_1).$$

Moreover,

- f_0 *is a* ***strict local minimum*** *of* $\mathcal{J}_*$ *on* $\mathcal{N}_*$*;*
- f_1 *is a strict* ***global maximum*** *of* $\mathcal{J}_*$ *on* $\mathcal{N}_*$*;*
- f_2 *is a strict* ***global minimum*** *of* $\mathcal{J}_*$ *on* $\mathcal{N}_*$*;*
- f_3 *is a* ***saddle point*** *of* $\mathcal{J}_*$ *on* $\mathcal{N}_*$*.*

Qualitative properties of nodal ground states as $p \to 2$

Theorem

There exists $\delta > 0$ such that, for every $p \in (2, 2+\delta]$, there exists $\tilde{u}_p$, a nodal action ground state of $(\mathcal{P}_p)$, such that

$$\tilde{u}_p(v_0) = \tilde{u}_p(v_1) = -\tilde{u}_p(v_2) = -\tilde{u}_p(v_3) > 0.$$

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Moreover, $\tilde{u}_p$ is unique up to symmetries, in the sense that

$$\forall u_p \in H^1(\mathcal{G}_\mathrm{t}), \Big[u_p \text{ is a nodal action ground state of } (\mathcal{P}_{p,2}) \implies (\exists g \in G_t, u_p = g \cdot \tilde{u}_p) \Big].$$

Take-home messages

Metric graphs allow to study interesting *one dimensional* problems and are much richer than the usual class of intervals of $\mathbb{R}$. In particular, one may study *highly symmetric examples*.

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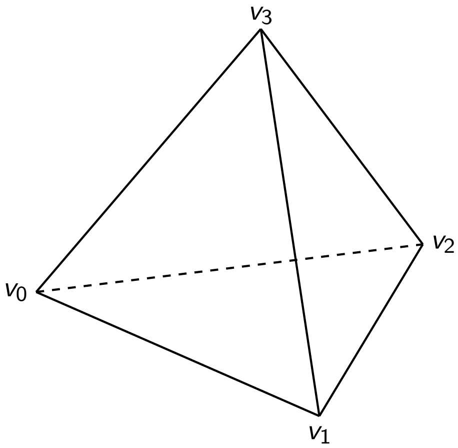
Computer-assisted methods may allow to prove difficult statements and can be very relevant to study in depth given examples.

Grazie mille!



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