Intra-disciplinary bridges for multi-dimensional patterns: Part II

Priya Subramanian

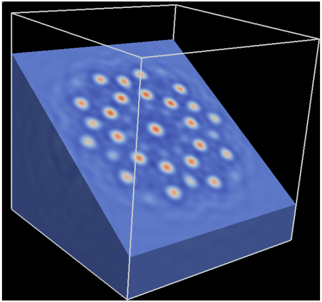
By Frits Ahlefeldt

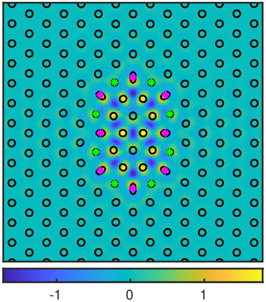
with many collaborators: AMR, AJA, EK, VR, CL, MC, etc.

University of Auckland
Waipapa Taumata Rau
New Zealand

A small recap...

- Pattern formation often requires techniques to simulate/analyse nonlinear PDEs
- Things we can do: numerical simulations (IVP), numerical continuation (root finding), weakly nonlinear analysis
- Things we can prove in 1D: Existence proofs for specific families of patterns, fronts and waves, spatially localisation of patterns and pinned defects





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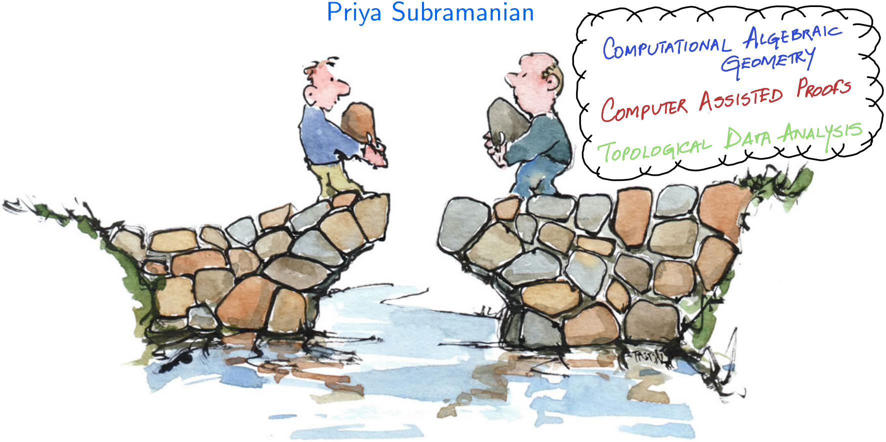

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UNIVERSITY OF AUCKLAND
Waipapa Taumata Rau
NEW ZEALAND

Computer assisted proofs (CAPs) in nonlinear analysis

We want to construct algorithms that provide an approximate solution to a problem together with precise and possibly efficient bounds within which a rigorous exact solution is guaranteed to exist.

This area uses ideas from

- scientific computing
- functional analysis
- approximation theory
- numerical analysis
- topological methods

We will use a contraction mapping argument on a Newton-like operator to identify closed balls in a Banach space with bounds on error and on uniqueness.

Based on slides from the SIAM Gene Golub Summer School 2025

Preliminaries 1: existence theorem

Let X, Y are Banach spaces together with a smooth $F : X \to Y$. We want solutions $x \in X$ such that

$$F(x) = 0$$

- Solutions can be an equilibrium, periodic solution, a bifurcating solution, a connecting orbit, etc.
- Often we have multiple efficient numerical methods to obtain a finite approximation of a solution as $\bar{x} \in X$ with $F(\bar{x}) \approx 0$
- *a-posteriori existence theorem*: We want to prove the existence of a unique true solution $x \in X$ 'near' a 'good' approximate solution $\bar{x} \in X$ that we already know

Preliminaries 2: Newton's method

- Let a scalar function $f(x)$ that is C^2 have a solution x^* such that $f(x^*) = 0$ and $f'(x^*) \neq 0$.
- Then there exists $\epsilon > 0$ such that for all $a \in (x^* - \epsilon, x^* + \epsilon)$, Newton iterations
$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)},$$
initialised at $x = a$ will converge to x^* with contraction property
$$|x_{n+1} - x^*| \leq \alpha |x_n - x^*|^2$$
- Every iterate gets closer to the true solution $\rightarrow$ contraction
- What if we do not know x^* and do not know about properties of f, but only have an approximate solution x_0 with a small $f(x_0)$?

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- Every iterate gets closer to the true solution $\rightarrow$ contraction
- What if we do not know x^* and do not know about properties of f, but only have an approximate solution x_0 with a small $f(x_0)$?
- Hand wave!

Preliminaries 3: extending to infinite dimensions

- Given X a Banach space, $F : X \to Y$ a smooth map and $B \subset X$ is closed
- B is a complete metric space - inherits norm from X
- $F : X \to Y$ is Fréchet differentiable at $x_0 \in X$, if there exists a bounded linear operator $A : X \to Y$ having

$$lim_{h \to 0} \frac{||F(x_0 + h) - F(x_0) - Ah||_Y}{||h||_X} = 0$$

- A if it exists, is unique
- Therefore we define,

$$DF(x_0) := A$$

  and call A the derivative of F at x_0

Preliminaries 4:

- Every point $x \in X$ has an associated $DF(x)$ in a Banach space $G(X, Y)$. If this correspondence is continuous, we say $F \in C^1(X, Y)$
- If $F \in C^1(X, Y)$, $M \geq 0$ and has

$$\sup_{w \in B} ||DF(w)||_{G(X,Y)} \leq M \qquad B \subset X\,, B \text{ is convex}$$

then for $x_1, x_2 \in B$,

$$||F(x_1) - F(x_2)||_Y \leq M||x_1 - x_2||_X$$

- Given $B \subset X$ and B is convex, if

$$\sup_{w \in B} ||DF(w)||_{G(X,Y)} < 1$$

then F is a contraction on the complete metric space B

- *Fixed point theorem*: If B is a complete metric space and F is a contraction mapping, then F has a unique fixed point within B

a-posteriori existence theorem setup

- Let X, Y be Banach spaces and $F = C^1(X, Y)$
- We have an approximate solution $\bar{x} \in X$ with $||F(\bar{x})||_X \ll 1$
- NOTE: there is no generic reason why F should be a contraction near $\bar{x}$
- For the Newton method in Banach space, $x_{n+1} = x_n + h_n$ where h_n is a solution to the linear equation

$$DF(x_n)h_n = -F(x_n)$$

- This suggests that we look for fixed points of near $\bar{x}$ for

$$T(x) = x - DF(x)^{-1}F(x) \qquad \text{(Newton operator)}$$

- T might be a contraction near $\bar{x}$!

a-posteriori existence theorem setup

- Problem 1: Computing $DF(x)^{-1}$ might be problematic
- Approximation 1: Replace inverse of derivative at x with a quantity independent of x, say the inverse of derivative at $\bar{x}$ to define

$$T(x) = x - DF(\bar{x})^{-1}F(x) \qquad \text{(Newton-like operator)}$$

- Problem 2: $DF(\bar{x})$ might still be hard to invert
- Approximation 2: Replace $DF(\bar{x})$ with any $A^{\dagger} \in G(X, Y)$ and $DF(\bar{x})^{-1}$ with $A \in G(Y, X)$
- This lets us define $T = x - AF(x)$ as the Newton-like operator
- If A is injective, then fixed points of T correspond to zeros of F
- Approximation 3: Actually we would like it better if $A^{\dagger} \approx DF(\bar{x})$ and if $A \approx inv(A^{\dagger})$

Newton-Kantorovich theorem

Suppose $F : X \to Y$ is continuously differentiable and $\bar{x} \in X$,
$A^\dagger \in G(X, Y)$ and $A \in G(Y, X)$ and A is one-to-one
We want scalar bounds for

- $||AF(\bar{x})||_X \leq Y_0$ — a-posteriori error
- $||I - AA^\dagger||_{G(X)} \leq Z_0$ — approximate inverse
- $||A(A^\dagger - DF(\bar{x})||_{G(X)} \leq Z_1$ — approximate derivative
- $\sup_{x \in B_r(\bar{x})} ||A(DF(\bar{x}) - DF(x))||_{G(X)} \leq Z_2(r)r$ — Lipschitz bound for first derivative
- We require $Y_0, Z_0, Z_1 > 0$ and $Z_2(r) : [0, \infty) \to [0, \infty)$ to define the function
$$p(r) = Z_2(r)r^2 - (1 - Z_0 - Z_1)r + Y_0$$
- Newton-Kantorovich theorem states that if there is an $r > 0$ such that $p(r) < 0$, then there exists a unique $x \in B_r(\bar{x})$ with $F(x) = 0$

Remarks

- In many applications, it can be arranged that $Z_2(r)$ and hence $p(r)$ are polynomial
- Therefore, this method is called the method of radii polynomials
- NOTE: This reduces infinite dimension zero finding problem to a one-dimensional zero finding problem
- We normally look for intervals $I = [r_-, r_+]$ such that any $r \in I$ implies $p(r) < 0$
- NOTE: Both limits of interval have to be finite ($p(r) \to \infty$ as $r \to \infty$) and non-zero ($p(0) = Y_0 > 0$)
- r_- gives the sharpest error bounds and r_+ gives the lower bound on isolation

Proof: Assume $r > 0$ has $p(r) < 0$

We can define operator $T: \overline{B_r(\bar{x})} \subset X \to X$ by

$$T(x) = x - AF(x), \quad x \in \overline{B_r(\bar{x})}$$

Step 1: Show T maps into $\overline{B_r(\bar{x})}$

Step 2: Show T is a contraction on $\overline{B_r(\bar{x})}$

Step 3: Use the Banach fixed point theorem to conclude T has a unique fixed point $x \in \overline{B_r(\bar{x})}$.

Step 4: Since A is one-to-one, zeros of T are zeros of F in $\overline{B_r(\bar{x})}$.

Step 1: T is continuously differentiable on $\overline{B_r(\bar{x})}$ as F is.

We want to bound the norm

$$\|DT(x)\|_{G(x)} = \|I - ADF(x)\|_{G(x)}$$

[Add & subtract $AA^{\dagger}$ and $ADF(\bar{x})$]

$$\Rightarrow \|DT(x)\|_{G(x)} = \|I - AA^{\dagger}\|_{G(x)} + \|A(A^{\dagger} - DF(\bar{x}))\|_{G(x)} + \|A(DF(\bar{x}) - DF(x))\|_{G(x)}$$

$$\leq Z_0 + Z_1 + Z_2(r)r$$

But $p(r) = Z_2(r)r^2 - (1 - Z_1 - Z_0)r + Y_0 < 0$

$$\Rightarrow Z_2(r)r^2 + (Z_1 + Z_0)r + Y_0 < r$$

or $Z_2(r)r + (Z_1 + Z_0) + \frac{Y_0}{r} < 1$

But $Y_0, r > 0$

$\Rightarrow \|DT(x)\|_{G(X)} \leq Z_2(r)r + Z_1 + Z_0 < 1, \; x \in \overline{B_r(\bar{x})}$

$\Rightarrow$ T maps into $\overline{B_r(\bar{x})}$. Step 1 proved.

Step 2:

Consider $\|\bar{x} - T(x)\|_X = \|\bar{x} - T(\bar{x})\|_X + \|T(\bar{x}) - T(x)\|_X$

$\leq \|AF(\bar{x})\|_X + \sup_{w \in B_r(\bar{x})} \|DT(w)\|_{G(X)} \|x - \bar{x}\|_X$

$\leq Y_0 + (Z_2(r)r + Z_1 + Z_0)\|x - \bar{x}\|_X$

$\leq Y_0 + (Z_2(r)r + Z_1 + Z_0) r$

$\leq Y_0 + Z_2 r^2 + (Z_1 + Z_0) r < r \; (p(r) < 0)$

Then $T(\overline{B_r(\bar{x})}) \subset B_r(\bar{x}) \subset \overline{B_r(\bar{x})}$

Since X is a Banach space, $\overline{B_r(\bar{x})}$ is a complete metric space.

Choose $x, y \in \overline{B_r(\bar{x})}$ and consider

$$\|T(y) - T(x)\|_X \leq \sup_{w \in \overline{B_r(\bar{x})}} \|DT(w)\|_{B(X)} \|x - y\|_X$$

$$\leq (Z_2(r) r + Z_1 + Z_0) \|x - y\|_X$$

with $Z_2(r) r + Z_1 + Z_0 < 1$

Then T is a strict contraction on the complete metric space $\overline{B_r(\bar{x})}$. Step 2 proved.

Given Step 1 & 2, we can use the fixed point theorem to conclude that T has a unique fixed point $x \in B_r(\bar{x})$, not on the boundary.

Again since A is one to one, $T(\bar{x}) = \bar{x}$ implies $F(\bar{x}) = 0$.

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In practice, we need...

- A numerical approximate solution $\bar{x} \in X$
- A numerical approximation $A^\dagger$ of $DF(\bar{x})$
- A numerical approximation A of $inv(A^\dagger)$
- Use some knowledge of the asymptotics of the derivative to define $A^\dagger$ and A
- An ability to check bounds – interval arithmetic

Swift-Hohenberg equation in 1D

$$\frac{\partial U}{\partial t} = \mu U - (1 + \partial_x^2)^2 U + \nu U^2 - U^3 \,.$$

Goal: Develop CAPS of existence of $2d$ spatially periodic even equilibrium solutions on the interval $\Omega_0 := (-d, d)$ for some $d > 0$

We want $F(U) = 0$ where $U : \Omega_0 \to \mathbb{R}$, U(x)=U(-x) and U is $2d$ periodic

So we can write

$$U(x) = \sum_{n \geq 0} \omega_n U_n \cos(2\pi(n/2d)x)$$

where $\omega_0 = 1$ and $\omega_n = 2$ for $n \geq 1$

Based on slides from the SIAM Gene Golub Summer School 2025

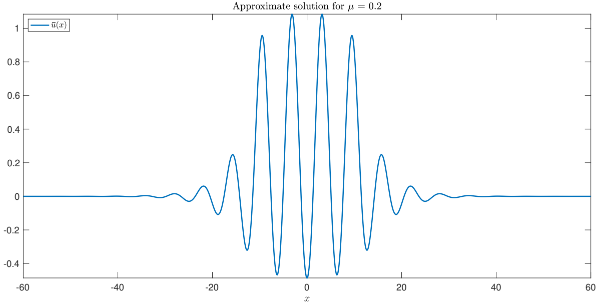
Numerical approximation

We fix $\mu \stackrel{\text{def}}{=} 0.2$, $\nu \stackrel{\text{def}}{=} 1.6$, $d = 60$ and $N = 300$.

The paper [Burke & Knobloch. Phys. Rev. E, 2006] provides the following ansatz u_{ini} to initialize Newton's method

$$u_{ini}(x) \stackrel{\text{def}}{=} 2\sqrt{\frac{2\mu}{\gamma}}\,\text{sech}\left(\frac{x\sqrt{\mu}}{2}\right)\cos(x), \quad \gamma \stackrel{\text{def}}{=} \frac{38\nu^2}{9} - 3$$

Applying the FFT to u_{ini} on $\Omega_0 = (-d, d)$ gave $U_{ini} \in \mathbb{R}^{N+1}$, which served as the initial guess for Newton's method on F^N, yielding the numerical approximation $\bar{U}$



Fourier series representation

Define $\ell : \mathbb{R} \to \mathbb{R}$, the Fourier transform of the differential operator as

$$\ell(\xi) := ((2\pi\xi)^2 - 1)^2 + \mu$$

for all $\xi \in \mathbb{R}$

Plugging in the Fourier series expansion in SH equation, we get

$$F(U) =:= \mathcal{L}U + U * U * U - \nu U * U = 0$$

with $\mathcal{L}U = ((\mathcal{L}U)_n)_{n\geq 0}$, $U * U = ((U * U)_n)_{n\geq 0}$ given component-wise by

$$(\mathcal{L}U)_n := \ell(\tilde{n})U_n \qquad \text{and} \qquad (U * U)_n := \sum_{k\in\mathbb{Z}} U_{|k|}U_{|n-k|}$$

We define a bounded linear map

$$F : X \to \ell^2, \quad \text{where} \quad ||U||_X = ||LU||_2$$

Finite numerical representation of a solution

- Numerical methods allow us to recover a finite number of Fourier coefficients of $\bar{U}$, in the vicinity of F close to a true zero $U \in X$
- We use projection operators to represent the finite dimensional objects

$$(\Pi^{\leq N} U)_n = \begin{cases} U_n, & |n| \leq N \\ 0, & |n| \leq N \end{cases}$$

and

$$(\Pi^{\geq N} U)_n = \begin{cases} 0, & |n| \leq N \\ U_n, & |n| \leq N \end{cases}$$

- We can identify elements in $\Pi^{\leq N}$ with vectors in $\mathbb{R}^{N+1}$
- The approximate solution $\bar{U}$ we assume $\bar{U} = \Pi^{\leq N} \bar{U}$ such that $\bar{U}$ has at most $N+1$ non-zero Fourier coefficients

Constructing an approximate inverse

We define M_U such that

$$M_U : X \to \ell^2 : V \to M_U W := U * W$$

it is the linear discrete convolution multiplication operator associated to U.

Given $\mathcal{N}(U) = U^3 - \nu U^2$, so

$$DF(\bar{U}) = \mathcal{L} + D\mathcal{N}[\bar{U}] = \mathcal{L} + 3M_{\bar{U}^2} - 2\nu M_{\bar{U}} = L + M_{\bar{V}}$$

$M_{\bar{V}}\mathcal{L}^{-1} : \ell^2 \to \ell^2$ is compact

This means that given a N big enough, we have

$$M_{\bar{V}}\mathcal{L}^{-1} \approx \Pi^{\leq N} M_{\bar{V}}\mathcal{L}^{-1}\Pi^{\leq N}$$

as a matrix

Computation of bounds - not shown here

In practice, we need...

- A numerical approximate solution $\bar{x} \in X$
- A numerical approximation $A^\dagger$ of $DF(\bar{x})$
- A numerical approximation A of $inv(A^\dagger)$
- Use some knowledge of the asymptotics of the derivative to define $A^\dagger$ and A
- An ability to check bounds – interval arithmetic

Introduction to interval arithmetic & rounding

- It is a technique designed to rigorously account for rounding errors by representing numbers as intervals rather than points
- The endpoints of the intervals are chosen so that they can be stored exactly on the computer
- Arithmetic operations on intervals produce new intervals that rigorously enclose all outcomes of the corresponding real-number operations, including propagation of numerical error
- If $\mathbb{F}$ is the set of representable real numbers that the computer can represent with a given precision, then $\triangle$ and $\bigtriangledown$ are functions $\mathbb{R} \rightarrow \mathbb{F}$, the corresponding round-up and round-down operators
- For every $x \in \mathbb{R}$,

$$\triangle = min\{y \in \mathbb{F}, y \leq x\}$$

$$\bigtriangledown = max\{y \in \mathbb{F}, y \geq x\}$$

- NOTE: The equality $\triangle(x) \geq x \geq \bigtriangledown(x)$ iff $x \in \mathbb{F}$

Rigorous enclosures and elementary operations

- Standing-point arithmetic replaces a number x by the closest floating point approximation, i.e., either $\triangle(x)$ or $\triangledown(x)$
- Interval arithmetic replaces a real number x by the interval

$$[x] := [\triangledown(x), \triangle(x)]$$

- This interval contains the real number x even if it is not representable at the current precision
- We can extend basic operations to intervals by combining their definitions with suitable rounding to ensure that the outcome always encloses the value
- If $I = [a, b]$ and $J = [c, d]$ with $a, b, c, d \in \mathbb{F}$, then

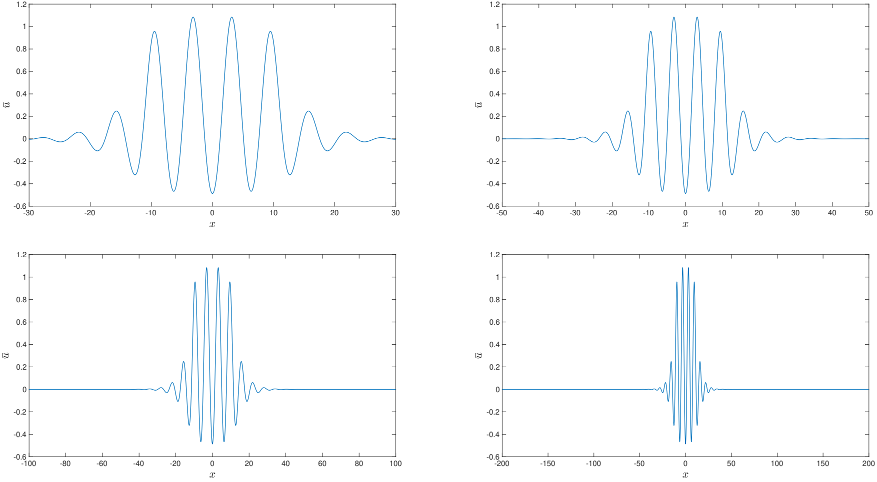
$$I + J = [\triangledown(a + c), \triangle(b + d)]$$

  and contains by construction $\{x + y, x \in I, y \in J\}$
- Many implementations exist: Intlab in Matlab, IntervalArithmetic.jl, etc.

d	N	Y	Z_1	$Z_2(r)$	r
30	200	3.52×10^{-11}	7.84×10^{-6}	249	3.56×10^{-11}
60	300	1.89×10^{-11}	2.42×10^{-5}	250	1.99×10^{-11}
100	500	3.24×10^{-11}	2.43×10^{-5}	251	3.34×10^{-11}
200	800	6.50×10^{-11}	5.91×10^{-5}	252	6.74×10^{-11}

Table 2.1: Computer-assisted proofs of periodic solutions for different half periods d.

Results for the Swift-Hohenberg Equation



In summary, CAP allows us to reduce an infinite dimensional zero finding problem to a one dimensional root finding problem

The way to do this involved proving contraction of a Newton-like operator and use the Banach fixed point theorem

- Let $\bar{x}$ be a numerical approximation to $\mathcal{F}(x) = 0$ using a finite dimensional reduction
- Construct a linear operator $\mathcal{A}$ that is the approximate inverse of $\mathcal{DF}(x)$
- Verify that $\mathcal{A}$ is an injective linear operator
- Define a Newton-like operator $T(x) = x - \mathcal{AF}(x)$ about the numerical approximation $\bar{x}$
- Consider $\mathcal{B}_{\bar{x}}(r) \in X$, the closed ball of radius r centered at $\bar{x}$
- Find a radius $r > 0$ such that the operator T is a contraction mapping

How can we extend a similar method to analyse spatial localisation in 2D/3D? Or to more complicated PDEs?

By Frits Ahlefeldt

CAP is agnostic to dimensions and might be a viable bridge to answer this question