An introduction to computer-assisted proofs via a posteriori validation

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 - eigenvalues/eigenfunctions
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- Possible motivation: prove theorems that cannot be proven by "classical" pen-and-paper methods.
- Alternate viewpoint: these computer-assisted techniques can be seen as a way to guarantee/certify the output of some numerical simulations.



2 Validated integration of ODEs using Chebyshev series

3 Alternate strategy

1 A simple example

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Theorem [Sharkovsky '64, Li York '75]

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Theorem [Sharkovsky '64, Li York '75]

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► For a given value of µ, how can we prove the existence of a period 3 orbit, in order to apply the above theorem?

Maxime Breden

Computer-assisted proofs

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- ▶ To do so, we can consider the map $F : \mathbb{R}^3 \to \mathbb{R}^3$ defined by

$$F(x_0, x_1, x_2) = \begin{pmatrix} \mu x_0(1 - x_0) - x_1 \\ \mu x_1(1 - x_1) - x_2 \\ \mu x_2(1 - x_2) - x_0 \end{pmatrix}.$$

If we manage to find a zero of *F* (such that $x_0 \neq x_1 \neq x_2$), we then have a period 3 orbit.

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Numerically, it is easy to find an "approximate solution" $\bar{X} = (\bar{x}_0, \bar{x}_1, \bar{x}_2)$ such that $F(\bar{X}) \approx 0$.

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How to rigorously prove the existence of this zero of *F*?

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Theorem (à la Newton-Kantorovich) Let $\varepsilon, K, L > 0$ such that $\|F(\bar{X})\| < \varepsilon$ $\|DF(\bar{X})^{-1}\| < \kappa$ $\forall X \in \mathbb{R}^3$. $||DF(X) - DF(\bar{X})|| < L||X - \bar{X}||$ lf $\varepsilon < \frac{1}{2\kappa^2 I},$ then F has a unique zero X* satisfying $||X^* - \bar{X}|| \le r$, $r = \frac{1 - \sqrt{1 - 2\kappa^2 L \varepsilon}}{r}$

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Proof: $T : X \mapsto X - DF(\bar{X})^{-1}F(X)$ is a contraction on the closed ball of center \bar{X} and radius r.

A frightening example

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$$g(a,b) = 333.75b^6 + a^2(11a^2b^2 - b^6 - 121b^4 - 2) + 5.5b^8 + \frac{a}{2b},$$

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- ▶ We have to be wary of round-off errors, especially if we claim to have proven a theorem based on some numerical computations!
- ▶ In our "proof" of existence of a period 3 orbit, how can we be certain that the quantity ε that we numerically evaluated really bounds $||F(\bar{X})||$, or that $\varepsilon < \frac{1}{2\kappa^2 L}$?

▶ Let F bet a set of floating point numbers, corresponding to the (finite!) set of real numbers that the computer can represent with a given precision, and

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Example: consider x = 0.1. In base 2, x writes

 $x = (1.100110011001100...)_2 \times 2^{-4}.$

With 8 bits of precision (for the mantissa), we have

 $\nabla(x) = (1.1001100)_2 \times 2^{-4}$ and $\triangle(x) = (1.1001101)_2 \times 2^{-4}$.

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► On can then extend the elementary operations (+, -, ×, ÷) to intervals, in such a way that the result always contain the true value:

$$x + y \rightarrow [x] [+] [y],$$

where [+] is defined as follows

$$[x] [+] [y] := [\bigtriangledown (\bigtriangledown (x) + \bigtriangledown (y)) , \bigtriangleup (\bigtriangleup (x) + \bigtriangleup (y))].$$

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• We then have $\mathbf{x} + \mathbf{y} \in [\mathbf{x}] [+] [\mathbf{y}]$.
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- Reformulate the problem we are interested in (ODE, PDE, etc) in the form F(X) = 0.
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• The main difficulty lies in controlling $\|DF(\bar{X})^{-1}\|$.

A new validation criteria

Theorem à la Newton-Kantorovich bis

Let $\varepsilon, \kappa, L, \delta > 0$ such that

lf

 $\|F(\bar{X})\| \le \varepsilon, \quad \|A\| \le \kappa, \quad \|DF(X) - DF(\bar{X})\| \le L\|X - \bar{X}\|,$ $\|I - ADF(\bar{X})\| < \delta < 1.$ $\varepsilon < \frac{(1-\delta)^2}{2\kappa^2 I},$ then F has a unique zero X^{*} satisfying $||X^* - \bar{X}|| \le r$, $r = \frac{1 - \delta - \sqrt{(1 - \delta)^2 - 2\kappa^2 L}}{r}$.

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An equivalent way to interpret this strategy is to say that we replace the former fixed-point operator $T: x \mapsto x - DF(\bar{x})^{-1}F(x)$ by

$$\tilde{T}: x \mapsto x - AF(x).$$

$$\begin{cases} u'(t) = f(u(t)) & t \in [0, 2\tau] \\ u(0) = u^{in} \end{cases}$$

with $f : \mathbb{R}^d \to \mathbb{R}^d$ smooth and $\tau > 0$ fixed.

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▶ Goal: given an approximate solution $\bar{u} : [0, 2\tau] \to \mathbb{R}^d$, prove that the exact solution u satisfies $||u - \bar{u}|| \le r$ for some explicit r.

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- ▶ Main idea for the zero-finding problem:

$$F(u)(t) = u(t) - \left(u^{in} + \int_0^t f(u(s)) \mathrm{d}s\right).$$

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Key observation:

$$DF(\overline{u})(h)(t) = h(t) - \int_0^t Df(\overline{u}(s))h(s)\mathrm{d}s,$$

i.e., $DF(\bar{u})$ is a compact perturbation of the identity.

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▶ Look for the solution as a Chebyshev series:

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 ▶ By plugging the Chebyshev series ansatz into

$$u(t)-\left(u^{in}+\tau\int_{-1}^{t}f(u(s))\mathrm{d}s\right)=0,$$

we obtain our $F(\mathbf{u}) = 0$ problem.

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The approximate solution *ū* is taken as a truncated Chebyshev series.
 We look for the exact solution in the space ℓ¹_ν := {*u*, ||*u*||_ν < ∞},

$$\|\boldsymbol{u}\|_{\nu} := |u_0| + 2\sum_{n=1}^{\infty} |u_n| \nu^n, \quad \nu \ge 1.$$

$$u(t) - \left(u^{in} + \tau \int_{-1}^{t} f(u(s)) \mathrm{d}s\right) = 0.$$

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Efficient computations of nonlinearities using the FFT.

- Computing $\|F(\bar{u})\|_{\nu}$ is rather straightforward.
- ▶ ℓ_{ν}^{1} is a Banach algebra: $\|\boldsymbol{u} \ast \boldsymbol{v}\|_{\nu} \leq \|\boldsymbol{u}\|_{\nu} \|\boldsymbol{v}\|_{\nu}$.
 - Simplifies the estimation of $||D^2F(u)||_{\nu}$ for u in a neighborhood of \bar{u} .







 $DF(\bar{u}) \approx$



A :=

Quality of this approximate inverse

▶ Using this constructing, when keeping the first *N* Chebyshev modes in the finite block, we get

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$$\|I - A DF(\bar{\boldsymbol{u}})\|_{\nu} \approx \frac{\tau \|f'(\bar{\boldsymbol{u}})\|_{\nu}}{N}.$$

▶ Up to taking *N* large enough, we can therefore get $||I - ADF(\bar{u})||_{\nu} < 1$, and hope to apply the entire *a posteriori validation* procedure.

▶ Using this constructing, when keeping the first *N* Chebyshev modes in the finite block, we get

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- ▶ Up to taking *N* large enough, we can therefore get $||I ADF(\bar{u})||_{\nu} < 1$, and hope to apply the entire *a posteriori validation* procedure.
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- [van den Berg Sheombarsing '21]

Some examples from [van den Berg Sheombarsing '21]



Integration time $\tau \approx 25$

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Integration time $\tau \approx 100$

Maxime Breden

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Integration time $\tau \approx 100$

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Computer-assisted proofs

Some related works

Chebyshev methods for linear ODEs, with special emphasis on studying and potentially reducing computational complexity [Benoit Joldes Mezzarobba '17; Brehard Brisebarre Joldes '18; Brehard '21].

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- Many other methods, some of which are more in the spirit of *traditional* numerical methods for ODEs. A particularly successful one is the CAPD::DynSys library [Kapela Mrozek Wilczak Zgliczynski '21].

A simple example

2 Validated integration of ODEs using Chebyshev series

3 Alternate strategy

$$\begin{cases} u'(t) = f(u(t)) & t \in [0, \tau] \\ u(0) = u^{in} \end{cases}$$

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• We started by converting the equation into an F(u) = 0 problem:

$$F(u)(t) = u(t) - \left(u^{in} + \int_0^t f(u(s)) \mathrm{d}s\right),$$

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$$\tilde{T}(u)(t) = u^{in} + \int_0^t f(u(s)) \mathrm{d}s.$$

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• $ilde{\mathcal{T}}$ has no reason to be contracting near $ar{u}$, except for au small.

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$$\widetilde{T}(u)(t) = e^{tL}u^{in} + \int_0^t e^{(t-s)L}\left(f(u(s)) - Lu(s)\right)\mathrm{d}s.$$

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$$\tilde{D}T(\bar{u})(h)(t) = \int_0^t e^{(t-s)L} \left(Df(\bar{u}(s)) - L \right) h(s) \mathrm{d}s,$$

we see that \tilde{T} should be contracting if $L \approx Df(\bar{u}(s))$.

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we see that \tilde{T} should be contracting if $L \approx Df(\bar{u}(s))$.

We again split the time interval 0 = τ₀ < τ₁ < ... < τ_M = τ, and take a different approximation on each smaller subinterval:

$$L^{(m)} \approx Df(\overline{u}^{(m)})(s), \qquad s \in [\tau_m, \tau_{m+1}].$$

Application to parabolic PDEs 1: Fisher-KPP

$$\begin{cases} \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u(1-u) \qquad (t,x) \in (0,4] \times \mathbb{T}_{4\pi}, \\ u(0,\cdot) = u^{in}. \end{cases}$$





$$N = 14$$
$$K = 2$$
$$M = 25$$

Application to parabolic PDEs 2: Swift-Hohenberg

$$\begin{cases} \frac{\partial u}{\partial t} = -\left(\frac{\partial^2}{\partial x^2} + 1\right)^2 u + 5u - u^3 \qquad (t, x) \in (0, 1.5] \times \mathbb{T}_{6\pi}, \\ u(0, \cdot) = u^{in}. \end{cases}$$



$$\frac{\|\bar{u} - u\| \le 4e^{-8}}{\|\bar{u} - u\| \le 4e^{-8}}$$

$$N = 30$$
$$K = 5$$
$$M = 100$$

MAX team seminar

Application to parabolic PDEs 2: Swift-Hohenberg

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THANK YOU FOR YOUR ATTENTION!