Rigorous numerics and computer assisted proofs in dynamics of ODEs

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Plan of this talk

1. An incomplete list of computer assisted proofs in dynamics
2. What is a computer assisted proof.
3. Interval arithmetic
4. Dependency problem, wrapping effect
5. Lohner algorithm for rigorous integration of ODEs
6. Tools for fixed points, periodic orbits - interval Newton method, interval Krawczyk method
7. Rossler system - an example of chaotic dynamics

Some computer assisted proofs in dynamics

- Langford - 1982, the proof of Feigenbaum universality conjectures

- Eckmann, Koch, Wittwer - 1984, universality for area-preserving maps

- Grebogi, Hammel, Yorke 1987 - rigorous numerical shadowing of trajectories

- Neumaier, Rage, Schlier - 1994, - chaos in the molecular Thiele-Wilson model

- Mischaikow and Mrozek - chaos in Lorenz equations, 1995

- Palmer, Coomes, Kocak, Stoffer, Kichgraber - 1996-2003 - chaos via shadowing for Henon map, PCR3BP

- W. Tucker - 2001 - geometric model for Lorenz attractor

CAPD - Krakow/Rutgers group

- Mischaikow (Rutgers), Mrozek, Zgliczynski, Wilczak, Galias, Kapela, Pilarczyk

- proofs of chaos (semiconjugacy with Bernoulli shift) for Lorenz equations, Rössler equations, Hénon map, Chua circuit, PCR3BP

- homo- and heteroclinic orbits for PCR3BP, Hénon map, Michelson system

- Kuramoto-Sivashinsky PDE: existence of multiple steady states and its bifurcations, periodic orbits, heteroclinic connections between fixed points

- N-body problem: the existence of choreographies

- period doubling bifurcations for Rössler system

General scheme of CAP in dynamics

- a problem - $\mathcal{P}$, for example the question of existence of the horseshoe for Poincaré map for ODE

- abstract theorem, $\mathcal{T}$, implying a solution of problem $\mathcal{P}$, provided we can verify $\mathcal{Z}$ - the assumptions in $\mathcal{T}$

- the reduction $\mathcal{Z}$ to finite computations, $\mathcal{O}$

- finite rigorous computation of $\mathcal{O}$ checking $\mathcal{Z}$

- If $\mathcal{Z}$ is true, then theorem $\mathcal{T}$ gives positive answer to our problem $\mathcal{P}$

Some difficulties:

- computer is finite, the continuum can not be in rigorous way represented in computer (round-off errors)

- not every theorem can be verified in finite computations

- computer can be used to verification of theorems, whose assumptions can be reduced to a finite number of (strong) inequalities, which can be verified in finite computation

Interval arithmetics

Arithmetics on closed intervals. For example:

- $[1,3] \langle + \rangle [3,17] = [4,20]$
- $[-1,1] \langle \cdot \rangle [3,4] = [-4,4]$
- $1 \langle / \rangle 3 = [0.33333, 0.33334]$

Rigorous interval arithmetics can be realized on the computer i.e. for each arithmetic operator $\diamondsuit \in \{+, -, \cdot, /\}$ the following is true

$$[a_-, a^+] \diamondsuit [b_-, b_+] \subset [a_-, a^+] \langle \diamondsuit \rangle [b_-, b_+]$$

Interval arithmetics

Interval arithmetics does for us two things:

- takes care of round-off errors

- enables us to evaluate functions (maps) on sets (not just single points !!!)

Example: finding (proving) zero of an analytic function

$f(x) = \sum_{n=0}^{\infty} a_n x^n$

Problem: Prove that f has a zero in interval $(1, 2)$

Numerical simulation: Apparently $f(x)$ is increasing on $[1, 2]$ and $f(1) < 0$ i $f(2) > 0$. From the intermediate value thm. it follows that f has a zero in $(1, 2)$

Reduction to finite computation:

- $f_M(x) = \sum_{n=0}^{M} a_n x^n$ - a function computable in finite number of steps

- analytical estimate: $|f_M(x) - f(x)| < \epsilon$ dla $x \in [1, 2]$, this is done by a mathematician

- rigorous check on the computer that

$f_M(1) < -\epsilon$ i $f_M(2) > \epsilon$

Example: the existence of an attracting periodic orbit

$x' = f(x)$, $x \in \mathbb{R}^3$

Two-dimensional Poincaré map, P, on section Θ.

Numerical fact: Apparently, all orbits starting in some open set U converge to periodic orbit γ.

Brouwer Theorem: If D is homeomorphic with the closed ball, $D \subset \Theta$
and $P(D) \subset \text{int}D$ (interior of D), then there exists $x \in D$ such that $P(x) = x$.
In particular, the trajectory of x is periodic.

Reduction to finite computations:

Condition: $P(D) \subset \text{int}D$ - represents a finite number of inequalities, if D - a parallepiped or ball

Phase space discretization: $D \subset \sum_{i=1}^{M} D_i$, D_i small enough, to compute $P(D_i)$ with a reasonable overestimation

$M \approx \frac{L^2 \cdot \text{Area}(D)}{4\epsilon^2}$, where
ϵ - an error margin
L - a Lipschitz constant (rigorous) for P

$|P(x) - P(y)| < L|x - y|$

L obtained in interval computations is usually much larger than L seen in nonrigorous simulations (the wrapping effect)

Total computation time: $= M \cdot$ computation time of $P(D_i)$

The sources of errors (overestimations) in rigorous computations of ODEs:

- round-off errors - *interval arithmetics*

- the numerical method error (the time discretization error) - *explicit formulas for error terms*

- the space discretizaton error and the propagation error (- *SERIOUS PROBLEM*)

- the errors connected to the intersection with the section in the computation of Poincaré map

Interval arithmetics - problems

• dependency:
for $x = [-1, 1]$ holds

$$x \langle - \rangle x = [-2, 2]$$

Another example:

$$e^{-x} = \sum_{n=0}^{\infty} \frac{(-1)^n x^n}{n!}$$

$$[1 - \sinh(t), \cosh(t)] \subset \langle e^{-[0,t]} \rangle$$

$$\mathrm{diam}(\langle e^{-[0,t]} \rangle) \geq e^t - 1, \quad \mathrm{diam}(e^{-[0,t]}) = 1 - e^{-t}$$

• wrapping
the result of evaluation of multidimensional map is product of intervals, disastrous results when considering f^n for n-large, ODEs

Wrapping effect

Harmonic oscillator

$$x' = -y, \qquad y' = x$$

Time shift by h, φ_h , rotation by h - ISOMETRY.

In the ideal (round-off error free) interval arithmetics we obtain

$$\lim_{n->\infty} \langle \varphi_{\frac{2\pi}{n}} \rangle ([-\delta,\delta]^2) = e^{2\pi}[-\delta,\delta]^2$$

($e^{2\pi} \approx 536$) while we would expect that

$$\lim_{n->\infty} \langle \varphi_{\frac{2\pi}{n}} \rangle = \varphi_{2\pi} = \text{identyczność}$$

DISASTER - SERIOUS OVERFLOW SOON

REASON:

- after each step the result is the following form $I_1 \times I_2$, where I_1, I_2 are intervals

These are not the reasons

- round-off errors

- the numerical method error

Hence increasing of the precision of the computations and improvement of numerical method via taking higher order and/or smaller time step does not guarantee any improvement.

Conclusion: Naive application of interval arithmetics to the integration of ODEs if very ineffective.

Propagation of errors according to the typical numerical analysis textbook:

$$x' = f(x) \tag{1}$$

$|f(x) - f(y)| \leq L|x - y|$.

Let $\varphi(t, x_0)$ be a solution of (1) with an initial condition $x(0) = x_0$. Then

$$|\varphi(t, x) - \varphi(t, y)| \leq e^{Lt}|x - y|, \qquad t \geq 0$$

This is very bad estimate

Could be considerably improved (but still not enough) by using logaritmic norms.

Examples:

• $x' = -10x$, predicts error-growth: e^{10t}

• for the Lorenz attractor (from the proof by Galias and P. Z.), gives an estimate for Lipschitz constant for the Poincare map $L > 10^9$, while from simulations it is clear that $L \approx 5 - 6$

• in the proof for Rössler system (P.Z.), gives an estimate for the Lipschitz constant of Poincare map $L > 5 \cdot 10^{41}$, while from simulations $L \approx 2 - 3$ **cosmic computation time**

Some methods for the reduction of the exponential error growth

• *set division*: Let $S_t = \varphi(t, S)$. When S_t becomes too large, one should divide it into smaller pieces and compute further the evolution of each piece separately

• *Lohner algorithm:* in order to avoid wrapping effect one should choose good coordinate frame in each step. *This is what we are using most of the time. Package CAPD*

• *Taylor models:* COSY - Berz, Makino. Propagate Taylor series of high order by ODE. Slow, but quite robust.

One step of the Lohner algorithm

$x' = f(x)$ induces $\varphi(t, x_0)$ - t-time, x_0 - initial condition,

$\Phi(h, x)$ - numerical method, Taylor method of order p

Input:

- t_k - time, h_k - time step
- $[x_k] \subset \mathbb{R}^n$, such that $\varphi(t_k, [x_0]) \subset [x_k]$

Output:

- $t_{k+1} = t_k + h_k$
- $[x_{k+1}] \subset \mathbb{R}^n$, such that $\varphi(t_{k+1}, [x_0]) \subset [x_{k+1}]$

1. Rough estimate of $\varphi([0, h_k], [x_k])$

$[W_1] \subset \mathbb{R}^n$ compact and convex

$$\varphi([0, h_k], [x_k]) \subset [W_1]$$

2. $[A_k] = \frac{\partial \Phi}{\partial x}([x_k])$

3. $[x_{k+1}]$ ($m([x_k])$ - mid-point of $[x_k]$)

$$\begin{aligned}[x_{k+1}] &= \Phi(h_{k+1}, m([x_k])) + \\ &\quad [A_k]([x_k] - m([x_k])) + \text{Rem}([W_1])\end{aligned}$$

Reduction of the wrapping effect

$$[x_k] = x_k + [r_k], \qquad x_k = m([x_k]), [r_k] = [x_k] - x_k$$

The equation to evaluate:

$$[r_{k+1}] = [A_k][r_k] + [z_{k+1}]$$

We choose different coordinate frame: $[r_k] = B_k[\widehat{r}_k]$,

$$[r_{k+1}] = [A_k][r_k] + [z_{k+1}] =$$
$$B_{k+1}\left(B_{k+1}^{-1}[A_k]B_k[\widehat{r}_k] + B_{k+1}^{-1}[z_{k+1}]\right)$$

$$[r_0] = [B_0][\widehat{r}_0], \quad [B_0] = \{Id\}$$
$$[\widehat{r}_{k+1}] = \left([B_{k+1}^{-1}][A_k][B_k]\right)[\widehat{r}_k] + [B_{k+1}^{-1}][z_{k+1}]$$
$$[r_{k+1}] = [B_{k+1}][\widehat{r}_{k+1}]$$

Usually B_{k+1} is a Q-factor from QR decomposition of $U \in [A_k][B_k]$,

Even better:

$$[r_{k+1}] = C_{k+1}[r_0] + [\tilde{r}_{k+1}]$$
$$[\tilde{r}_{k+1}] = [A_k][\tilde{r}_k] + [z_{k+1}] + ([A_k]C_k - C_{k+1})[r_0],$$
$$[\tilde{r}_0] = 0$$
$$\text{and } C_0 = Id, \quad C_{k+1} \in [A_k]C_k$$

$[\tilde{r}_k]$ is evaluated using previous method

Interval tools for fixed points (periodic orbits):

Periodic orbit for ODE = fixed point (or periodic point) for Poincare map P

Topological methods: Brouwer Theorem, Miranda Theorem, covering relations - existence only, no uniqueness information

$C^1 - tools$: interval Krawczyk method, interval Newton method.

1. Find, $\bar{x}$, an approximate fixed point (periodic point) for P

2. define $F(x) = x - P(x)$ and use the interval Krawczyk (or Newton) method to equation $F(x) = 0$ in the neighborhood of $\bar{x}$.

Interval tools for fixed points: Interval Krawczyk Method

- $F : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is a C^1 function,
- $X \subset \mathbb{R}^n$ is an interval set, $\bar{x} \in X$
- $C \in \mathbb{R}^{n \times n}$ is a linear isomorphism.

Let

$K(\bar{x}, X, F) := \bar{x} - CF(\bar{x}) + (Id - C[DF(X)])(X - \bar{x})$

Thm *If $K(\bar{x}, X, F) \subset intX$, then there exists a unique $x^* \in X$ such that $F(x^*) = 0$.*

"Proof:" existence only. Let $N(x) = x - CF(x)$. Obviously $N(x) = x$ iff $F(x) = 0$. For any $x \in X$ holds

$$N(x) \approx \bar{x} - CF(\bar{x}) + (Id - CDF(\Theta))(x - \bar{x}) \subset$$

$$K(\bar{x}, X, F) \subset X$$

The existence now follows from Brouwer Theorem.

Interval Newton Method

- $F : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is a C^1 function,

- $X \subset \mathbb{R}^n$ is an interval set, $\bar{x} \in X$

Let

$$N(\bar{x}, X, F) := \bar{x} - [DF(X)]^{-1} F(\bar{x})$$

Thm *Assume* $[DF(X)]^{-1}$ *exists.*
If $N(\bar{x}, X, F) \subset X$*, then there exists a unique* $x^* \in X$ *such that* $F(x^*) = 0$*.*

It is even better, both the Krawczyk and Newton method can be used to rule out the existence of zeros and to find all zeros (if they are isolated) in a given region.

Interval Newton Method - cont.

$$N(\bar{x}, X, F) := \bar{x} - [DF(X)]^{-1} F(\bar{x})$$

Thm *Assume* $[DF(X)]^{-1}$ *exists.*

- *If* $N(\bar{x}, X, F) \subset X$, *then there exists a unique* $x^* \in X$ *such that* $F(x^*) = 0$.

- *if* $x^* \in X$ *and* $F(x^*) = 0$, *then* $x^* \in X \cap N(\bar{x}, X, F)$,

- *if* $X \cap N(\bar{x}, X, F) = \emptyset$, *then* $F(x) \neq 0$ *for all* $x \in X$

Analogous theorem is valid for the Krawczyk operator.