Numerical Integration Methods Applied to Astrodynamics and Astronomy (IV)

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Validated computations

- Interval Arithmetics.
- Dependency problem and wrapping effect.
- Validated integration of ODE's.
  - Interval based methods.
  - Taylor based methods.
- Computer assisted proofs.

Why interval arithmetics?

Every time that a real number x is stored on a computer roundoff errors occur. This error is propagated in future computations.

Example. Consider the iteration

$$x_{k+1} = 4 * x_k * (1 - x_k),\ x_0 = 0.125 \text{ (logistic map).}$$

We have $x_{30} \in [0.27004609549825 81, 0.311312186930057 5]$ due to propagation of roundoff error.

Rounded Interval Arithmetic provides a tool to **bound the roundoff error in an automatic way**.

Real Interval Arithmetic

- The interval arithmetic is an extension of the real arithmetic.
- Real interval: $[a] = [a_l, a_u] = \{x \in \mathbb{R} \,|\, a_l \leq x \leq a_u\}$.
- Notation:

  $w([a]) = a_u - a_l$ is the *width* of the interval $[a]$.

  $m([a]) = (a_l + a_u)/2$ is the *mid point* of the interval $[a]$.

- Consider the set of real intervals:

  $$\mathbb{IR} = \{[a] = [a_l, a_u] \quad | \quad a_l, a_u \in \mathbb{R}, a_l < a_u\}.$$

Real Interval Operations

Given $[a], [b] \in \mathbb{IR}$, for any operation $\circ \in \{+, -, *, /\}$, we define

$$[a] \circ [b] = \{x \circ y \,|\, x \in [a], y \in [b]\}$$

Equivalently,

$$\begin{aligned}
[a] + [b] &= [a_l + b_l, a_u + b_u], \\
[a] - [b] &= [a_l - b_u, a_u - b_l], \\
[a] * [b] &= [\text{min}(a_l b_l, a_l b_u, a_u b_l, a_u b_u), \text{max}(a_l b_l, a_l b_u, a_u b_l, a_u b_u)], \\
[a]/[b] &= [a_l, a_u] * [1/b_u, 1/b_l], \text{ if } b_l > 0.
\end{aligned}$$

- The $+$ and $*$ inverses only exist for real numbers.
- $+$ and $*$ are both associative and commutative but...

  Sub-distributive law: $[a] * ([b] + [c]) \subseteq [a] * [b] + [a] * [c]$

Interval Arithmetic: drawbacks

- Interval arithmetic is usually affected by overestimation, mainly due to the **Dependency Problem** and the **Wrapping Effect**.

- Our validated methods have to deal with these problems in a suitable way to make rigorous computations with small overestimation.

Dependency problem

The Dependency Problem is due to the use of interval arithmetic in computations. The computation with interval arithmetic treats two different occurrences of the same variable as if they were different variables. In general, the order in which the operations are made also plays a role.

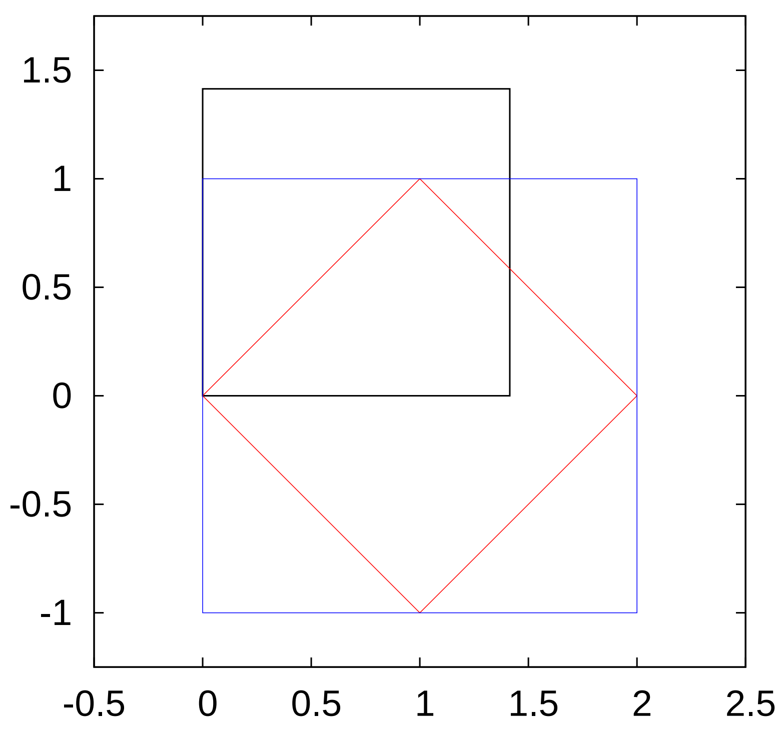
Examples:

- Clearly $x - x = 0$ for all $x \in [1, 2]$.
  Using interval arithmetics we have $[1, 2] - [1, 2] = [-1, 1]$.
- It is $x^2 - x \in [-1/4, 0]$ for all $x \in [0, 1]$.
  Using interval arithmetics directly: $[0, 1] * [0, 1] - [0, 1] = [-1, 1]$.
  Using $x^2 - x = x(x - 1)$: $[0, 1] * ([0, 1] - 1) = [-1, 0]$.
  Dividing $[0, 1]$ in 10 equal parts: $[-0.35, 0.1]$ (quite poor estimation still).

The wrapping effect

The Wrapping Effect concerns with the problem of including rotated boxes in interval sets. Our validated computations have to confront it by adapting the coordinates to the geometry of the problem as much as possible.

Example (Moore):



Consider $f(x,y)=\frac{\sqrt{2}}{2}(x+y,y-x)$. The image of the square $[0,\sqrt{2}]\times[0,\sqrt{2}]$ is the rotated square of corners $(0,0),(-1,1),(2,0)$ and $(1,1)$. Interval arithmetics gives $[0,2]\times[-1,1]$, a square that doubles the size.

Rounded Interval Arithmetic

For validated computations roundoff errors on the operations must be considered. We can extend the real interval arithmetic by rounding positive at the right end and negative at the left end.

$$[a] + [b] = [(a_l + b_l)_\blacktriangledown, (a_u + b_u)_\blacktriangle]$$
$$[a] - [b] = [(a_l - b_u)_\blacktriangledown, (a_u - b_l)_\blacktriangle],$$
$$[a] * [b] = [\text{min}(a_l b_l, a_l b_u, a_u b_l, a_u b_u)_\blacktriangledown, \text{max}(a_l b_l, a_l b_u, a_u b_l, a_u b_u)_\blacktriangle],$$
$$[a]/[b] = [a_l, a_u] * [1/b_u, 1/b_l], \text{ if } b_l > 0.$$

A real number x is represented by an interval $[x] = [x_\blacktriangledown, x_\blacktriangle]$, where $x_\blacktriangledown$ is the negative rounding of x and $x_\blacktriangle$ is the positive rounding of x.

In this way, interval arithmetic provides a tool to bound roundoff errors in computations in an automatic way.

Bibliography & Libraries

R.E. Moore, *Interval Analysis*. Prentice-Hall, Englewood Cliffs, N.J., 1966.

N.S. Nedialkov, *Computing rigorous bounds on the solution of an initial value problem for ordinary differential equation*, PhD Thesis, University of Toronto, 1999.

N.S. Nedialkov and K.R. Jackson. A new perspective on the wrapping effect in interval methods for initial value problems for ordinary differential equations. In *Perspectives on enclousure methods (Karlsruhe, 2000)*, pages 219–264. Springer, Vienna, 2001.

Available interval arithmetics:

FILIB/FILIB++:

`http://www.math.uni-wuppertal.de/~xsc/software/filib.html`.

List of libraries of interval arithmetics:

`http://www.cs.utep.edu/interval-comp/intsoft.html`.

Validated Integration of ODE's

- Interval based methods.
  - Moore's direct algorithm.
  - Parallelepiped method.
  - QR-Lohner method.
- Taylor based methods.

Initial value problem (ISVP)

We consider the problem

$$\begin{cases} u' = f(u), \\ u(t_0) = u_0 \in \{u_0\}, \end{cases}$$

where $f : \mathbb{R}^m \longrightarrow \mathbb{R}^m$, $u_0 \in \mathbb{R}^m$ and $\{u_0\}$ is a set of $\mathbb{R}^m$.

Given $h > 0$ we look for a set $\{u_1\} \subset \mathbb{R}^m$ such that

$$u(t_0 + h; u_0) \in \{u_1\} \text{ for all } u_0 \in \{u_0\}.$$

Main goal: The validated integrator should provide $\{u_1\}$ as close as possible to the set

$$\{u(t_0 + h, u_0), u_0 \in \{u_0\}\}.$$

Different approaches

In the literature mainly two different approaches can be found:

- **Interval methods**: They represent the set $\{u_1\}$ using admissible sets which can be intervals, parallelepipeds, cuboids,...

  Main Advantages:

  Fast,

  Easy to introduce uncertainties,

  More general: they can be applied to non-analytic cases.

- **Taylor-based methods**: They represent the set $\{u_1\}$ as a Taylor expansion with respect to the initial uncertainties in $\{u_0\}$.

  Main Advantage:

  Accurate.

Interval methods

Moore's direct algorithm (i)

In Moore's approach sets ($\{\ \}$) are represented by **intervals** ($[\ ]$).

Recall that:

For $u_0 \in \{u_0\}$, Taylor expansion of $u(t_0 + h; u_0)$ up to order n around $t = t_0$ gives

$$u(t_0 + h; u_0) = T(u_0) + R(\xi; u_0),$$

where

$$T(u_0) = u_0 + f(u_0)h + \cdots + \frac{d^{n-1}}{dt^{n-1}} f(u_0) \frac{h^n}{n!},$$

and

$$R(\xi; u_0) = \frac{d^n}{dt^n} f(u(\xi; u_0)) \frac{h^{n+1}}{(n+1)!},$$

with $\xi \in [t_0, t_0 + h]$.

Moore's direct algorithm (ii)

To make rigorous the evaluations:

If $\{u_0\} \subset [u_0]$, then

$$\boxed{T(\{u_0\}) \subset T([u_0])}$$

$$T(\{u_0\}) := \{T(u_0) | u_0 \in \{u_0\}\}$$

where

$$T([u_0]) = [u_0] + f([u_0])h + \cdots + \frac{d^{n-1}}{dt^{n-1}} f([u_0]) \frac{h^n}{n!}.$$

$$\boxed{R(\xi, u_0) \subset R([\hat{u}_0])}$$

where $[\hat{u}_0]$ is an interval box such that $u(t; u_0) \subset [\hat{u}_0]$ for all $t \in [t_0, t_0 + h]$ and for all $u_0 \in [u_0]$.

Moore's direct algorithm (iii)

Rough enclosure procedure:

To compute $[\hat{u}_0]$ the following iterative scheme was proposed by Moore

$$
\begin{aligned}
[\hat{u}_0^0] &= [u_0] + [\epsilon, \epsilon], \\
[\hat{u}_0^{k+1}] &= [u_0] + [0, h] f([\hat{u}_0^k]).
\end{aligned}
$$

Finally,

$$\boxed{[u_1] = T([u_0]) + R([\hat{u}_0]),}$$

gives a solution of the initial set value problem at time $t_0 + h$.

Moore's direct algorithm (iv)

Inconveniences:

- Small step size.

  The rough enclosure procedure requires Euler step-size.

- Dependency problem.

  $T([u_0])$ depends on the interval extension of f.

- Wrapping effect.

  The set $\{T(u_0), u_0 \in [u_0]\}$ is not an interval box and hence we need to include it in $T([u_0])$.

Show movie

First order interval methods

Note that

$$T(\{u_0\}) \subset T(m(u_0)) + \overbrace{DT([u_0])([r_0])}^{\text{"small" } wrapping},$$

where $m(u_0)$ denotes the center of the interval set and $[r_0] = [u_0] - m(u_0)$.

Moore's algorithm in centered form reads

$$[u_1] = T(m(u_0)) + DT([u_0])([r_0]) + [z_1], \qquad (1)$$

where $[z_1] = R([\hat{u}_0])$.

Idea: The first variational equation gives a linear change of coordinates that allows to represent the sets in a more accurate way than using interval representation.

Parallelepiped method

Sets are represented by parallelepipeds, that is, sets of the form

$$p + A[r],$$

where $p \in \mathbb{R}^n$ (point), $A \in \mathbb{R}^{n\times n}$ (matrix) and $[r] \subset \mathbb{R}^n$ (interval).
For $\{u_0\} = m(u_0) + A_0[\hat{r}_0]$, it should be

$$T(m(u_0)) + DT([u_0])A_0([\hat{r}_0]) + [z_1] \subset \{u_1\},$$

and if we require $\{u_1\} = m(u_1) + A_1[\hat{r}_1]$ it turns out that

$$\begin{aligned} m(u_1) &= T(m(u_0)) + m(z_1), \\ A_1 &= m(DT([u_0]A_0)), \\ [\hat{r}_1] &= [B_1][\hat{r}_0] + [A_1^{-1}]([z_1] - m(z_1)). \end{aligned}$$

($[B_1]$ is such that $DT([u_0])A_0 = A_1[B_1]$.)

Show movie

QR-Lohner method

In general, the matrices A_1 of the parallelepiped method tend to be singular because of the errors. The inversion is, hence, a numerical problem.

To solve this inconvenience an alternative representation (cuboids) was proposed by Lohner. Instead of parallelepipeds $p + A[r]$ he proposed

$$p + Q[r],$$

with Q orthogonal matrix.

The adapted iteration reads (starting set $m(u_0) + Q_0[\hat{r}_0]$):

$$\begin{aligned} m(u_1) &= T(m(u_0)) + m(z_1), \\ Q_1 \text{ s.t. } Q_1 R_1 &= A_1 \quad = \quad m(DT([u_0]Q_0)), \\ [\hat{r}_1] &= R_1[B_1][\hat{r}_0] + [Q_1^{-1}]([z_1] - m(z_1)). \end{aligned}$$

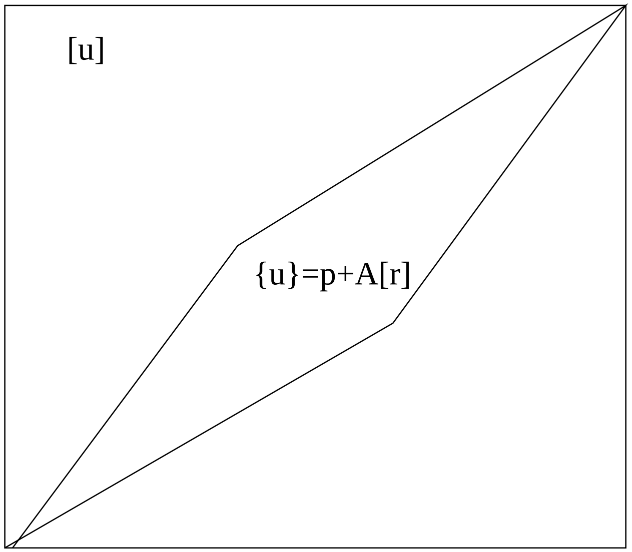
($[B_1]$ is such that $DT([u_0])Q_0 = A_1[B_1]$.)

Sum up: First order interval methods

- They are **fast** but produce **big overestimations**.
- They try to reduce overestimation by **adapting coordinates**.

In any case...

The methods described need DT to be evaluated in the **interval** set $[u_0] = m(u_0) + A_0[\hat{r}_0]$ which is not the set $\{u_0\}$ itself.



$\Rightarrow$ overestimation

2nd. order interval methods

Recall:

Direct method: $[u_1] = T([u_0]) + [z_1]$.

First order: $[u_1] = T(m(u_0)) + DT([u_0])A_0([\hat{r}_0]) + [z_1]$

We can compute the second order approximation (2nd order interval methods). In the parallelepiped case it reads,

$$
\begin{aligned}
[u_1] \quad = \quad & T(m(u_0)) + DT(m(u_0))A_0[\hat{r}_0] + \\
& \frac{1}{2}(A_0[\hat{r}_0])^t D^2 T([u_0])(A_0[\hat{r}_0]) + [z_1].
\end{aligned}
$$

This modification assures a good approximation of the dynamics in the interval set in a larger time interval.

Results: 1st order vs. 2nd. order

1st. order	268.75 days
2nd. order	893.75 days

Table 1: Maximum time of integration (in days) applying first and second order parallelepiped method to the Kepler's (Sun-Apophis) problem ($h = 0.625$ days). **Uncertainty** 10^{-6} **AU**.

1st. order	632.5 days
2nd. order	1529.375 days

Table 2: Maximum integration time obtained for Apophis in the $(N+1)$-JPL problem using first and second order parallelepiped validated methods. **Uncertainty** $\pm 5 \times 10^{-8}$ **AU**.

Bibliography on Interval methods

P. Zgliczynski. $\mathcal{C}^1$*-Lohner algorithm*. Foundations of Computational Mathematics, 2,429 – 465, 2002.

M. Mrozek and P. Zgliczynski. *Set arithmetic and the enclosing problem in dynamics*. Annales Pol. Math. 237–259. 2000.

AWA: Lohner.
http://www.math.uni-wuppertal.de/ xsc/xsc/pxsc_software.html#awa

CAPD'07: *Course given in Barcelona by P. Zgliczynski.*
http://www.imub.ub.es/cap07/slides.

E.M. Alessi, A. Farrés, A. Jorba, C. Simó, A. Vieiro. *Efficient Usage of Self-Validated Integrators for Space Applications.* ESA report, Ariadna ID: 07/5202.

Taylor Based methods

Taylor-based methods (I)

- When computing the set $\{u_1\}$ at time $t = t_0 + h$ of the ISVP with initial condition $\{u_0\}$ the interval computations give rise to wrapping and dependency phenomena.
- We have seen that the **dependency on initial conditions** up to first and second (or higher order) helps in reducing wrapping effect.

Idea: **Taylor-based methods**

Represent the set $\{u_1\}$ as a Taylor series with respect to the initial conditions.

Taylor-based methods (II)

- A set $\{u_1\}$ is included in a Taylor model

$$(p, I)$$

where p is a Taylor polynomial of order n with respect the initial condition and I is an interval bounding the errors of the approximation given by p.

- A step of integration:

$$(p_0, I_0) \longrightarrow (p_1, I_1).$$

- It requires operations on polynomials and bound the error.

Comments on Taylor-based methods

- Ability to deal with **non-convex sets**: it is not necessary to embed the approximated solution in an interval set at each step.
- The **wrapping effect** still plays a role in the interval part. We should use the same methods as for interval methods: parallelepiped representation, QR representation,... for the remainder interval part.
- They are **more accurate** but **more expensive**.

Bibliography on Taylor-based methods

K. Makino. *Rigorous analysis of nonlinear motion in particle accelerators* . PhD thesis. 1998.

M. Berz and K. Makino and J. Hoefkens. *Verified integration of dynamics in the solar system*. Nonlinear Analysis, 47, 179 – 190. 2001.

K. Makino and M. Berz *Suppression of the wrapping effect by Taylor model-based integrators: long-term stabilization by preconditioning*. International Journal of Differential Equations and Applications, 0, 1 – 36. 2006

M. Neher and R. Jackson and N.S. Nedialkov. *On Taylor model based integration of odes*. SIAM Journal, 45, 1, 236 – 262. 2007.

CAP08. *Course given in Barcelona by M. Berz and K. Makino.* http://www.imub.ub.es/cap08/ (slides not available but homepages links).

Computer Assisted Proofs

- What can be proved using interval arithmetics?
- Examples:
  - Fixed points / Periodic orbits.
  - List of some available proofs related with dynamical systems.

A Computer Assisted Proof

We need:

- A theoretical (mathematical) result which should be **computationally verifiable**, that is, the hypothesis reduce to check a **finite number of inequalities**.
- A **non-validated high accuracy computation** verifying what we want to prove.

Using interval arithmetics we...

- ... **check the hypothesis** of the theorem. If they hold then the theorem is proved.

Anything that fits within this general framework can be proved using interval arithmetics.

An example

Consider the Hénon map: $H_\alpha : \begin{pmatrix} x \\ y \end{pmatrix} \longrightarrow R_{2\pi\alpha} \begin{pmatrix} x \\ y - x^2 \end{pmatrix}$

(R_β rotation of angle β).

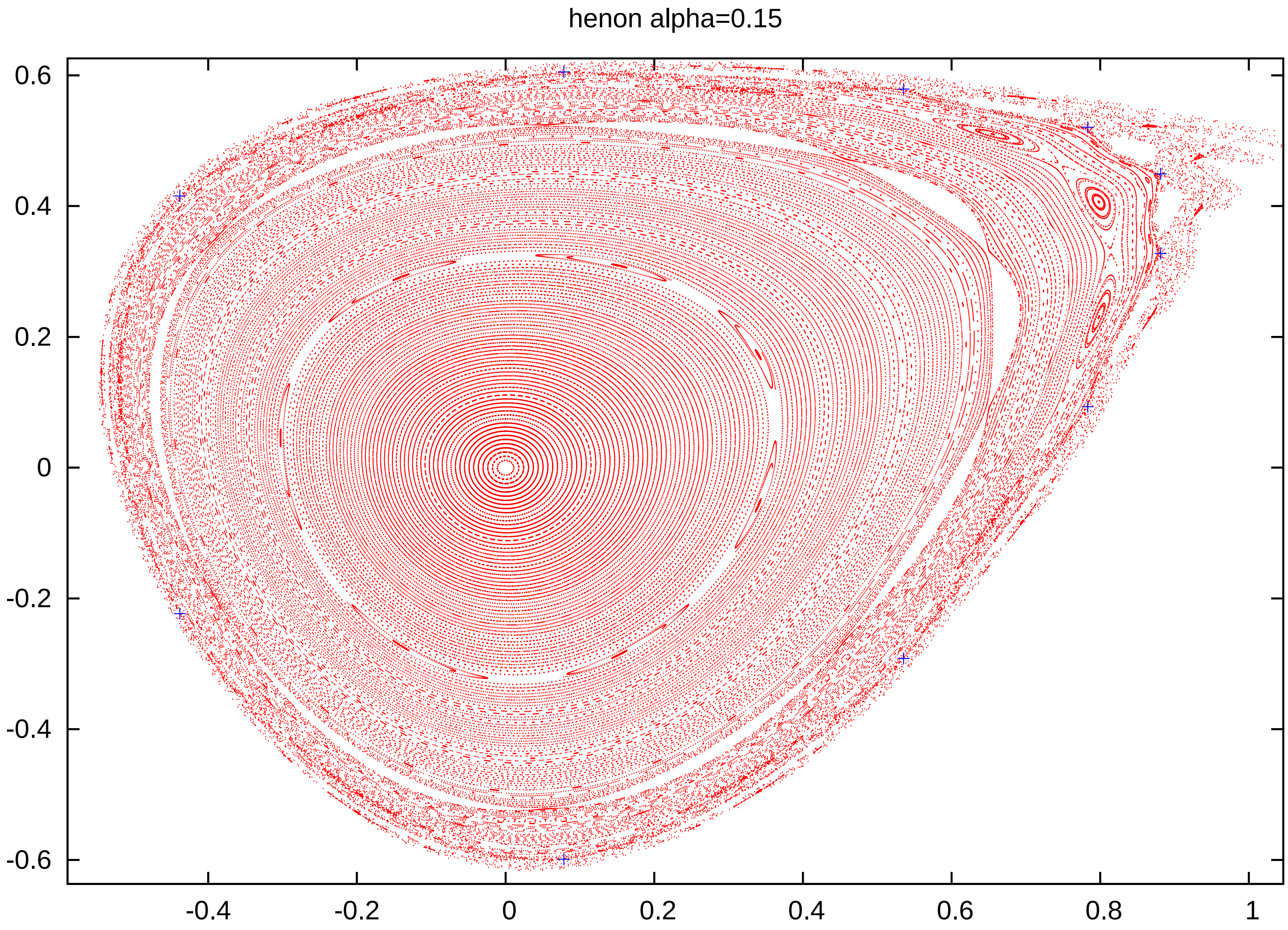
For $\alpha = 0.15$ computations gives an evidence that there is a periodic orbit of period 10.

Non-validated Newton method (error 10^{-12}) shows that it is located on the symmetry axis $y = \tan(\pi\alpha)x$ at the point

$$(0.8813697816675 2866, 0.4490803341749 5569)$$

$\longrightarrow$ **We want to prove it.**

Hénon map



The theoretical result

Theorem (Newton-Kantorovich).

Let $x_0 \in \mathbb{R}^n$ and $f : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ a function of class $\mathcal{C}^2$ such that $Df(x_0)$ is regular. Let a, b and c constants such that

1. $\|Df(x_0)^{-1}\| \leq a$,
2. $\|Df(x_0)^{-1}f(x_0)\| \leq b$, and
3. for all x verifying $\|x - x_0\| \leq 2b$ it is $\|D^2f(x)\| \leq c$.

Then, **if** $abc < 1/2$

there exists a unique zero in $B_{2b}(x_0)$**.**

The proof

1. We consider H_α^n, $n = 10$, and look for a fixed point.
2. We apply non-rigorous Newton method to get a good approximation.
3. Then we we apply interval arithmetics to find constants a, b and c of the theorem (we compute the 1st and 2nd differentials of the map, the inverse, and all the computations using interval arithmetics).

Conclusion: $a < 2.137772$, $b < 2.01205 \times 10^{-12}$ and $c < 31.0425$. Then $abc < 1.335232 \times 10^{-10}$ and there exist a unique 10-periodic point located inside the ball $B_r(x_0)$ of center

$$x0 = (0.8813697816675286\hat{6}, 0.4490803341749556\hat{9})$$

and radius

$$r = 4.024098e - 12.$$

List of examples of CAP available

Many different topics related with dynamical systems:

Langford - 1982, the proof of Feigenbaum universality conjectures

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

Mischaikow and Mrozek - chaos in Lorenz equations, 1995

Kapela and Simó, "Computer assisted proofs for nonsymmetric planar choreographies and for stability of the Eight" . Nonlinearity, 2007.

For a list of examples see:

http://www.imub.ub.es/cap07/slides/lect1.pdf