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Validated numerics

and the art of dividing by zero

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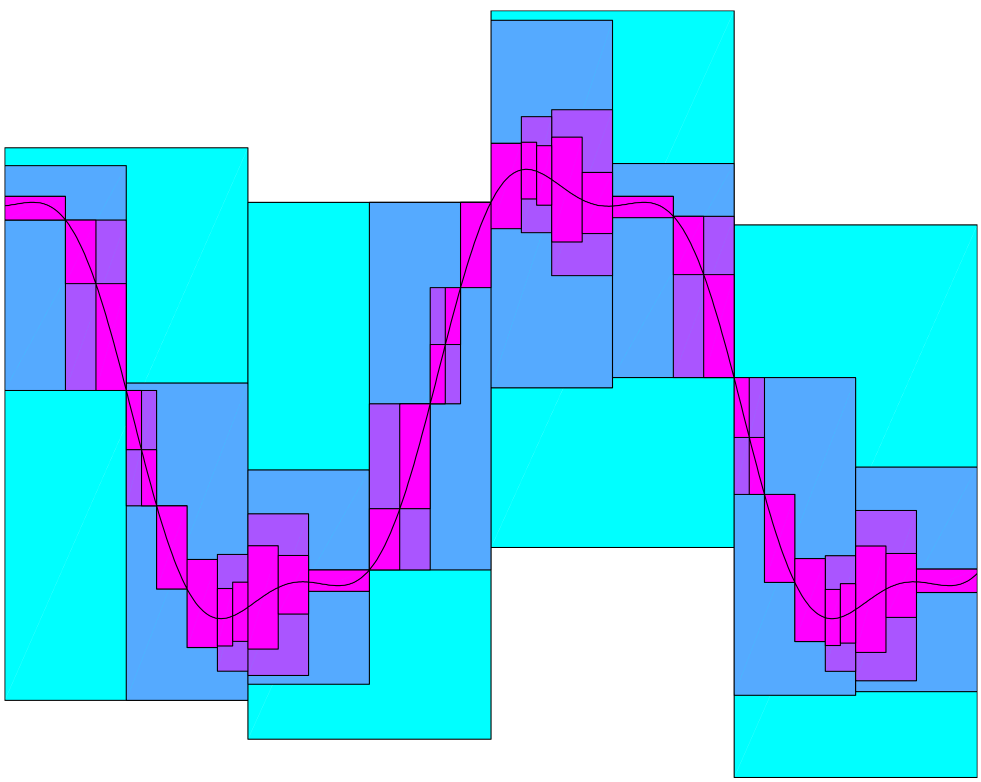


What is validated numerics?

- set-valued mathematics;
- intervals replace real numbers.

Why use validated numerics?

- provides rigorous error bounds;
- models uncertainty;
- may produce faster numerical methods.

Early work: R. C. Young (1931), M. Warmus (1956), T. Sunaga (1958), R. E. Moore (1959) *Interval Analysis* (1966).

Intervals

We will adopt the short-hand notation

$$[a] = [\underline{a}, \bar{a}] = \{x \in \mathbb{R} \colon \underline{a} \le x \le \bar{a}\},$$

and let $\mathbb{IR}$ denote the set of all compact intervals of the real line:

$$\mathbb{IR} = \{[a] \colon \underline{a}, \bar{a} \in \mathbb{R}; \underline{a} \le \bar{a}\}.$$

We allow for *thin* intervals with $\underline{a} = \bar{a}$.

Example: $[1, \pi] \in \mathbb{IR}$, but not $[2, 1]$ or $[1, \infty]$.

As sets, intervals inherit relations such as

$$= \qquad \subseteq \qquad \subset \qquad \neq \qquad \not\subset \ldots$$

Furthermore, we can define the operations

$$[a] \sqcup [b] = [\min\{\underline{a}, \underline{b}\}, \max\{\bar{a}, \bar{b}\}],$$

$$[a] \cap [b] = \begin{cases} \emptyset & : \text{if } \bar{a} < \underline{b} \text{ or } \bar{b} < \underline{a}, \\ [\max\{\underline{a}, \underline{b}\}, \min\{\bar{a}, \bar{b}\}] & : \text{otherwise.} \end{cases}$$

Useful functions

Functions from $\mathbb{IR}$ to $\mathbb{R}$:

$$\text{rad}([a]) = \tfrac{1}{2}(\bar{a} - \underline{a}); \qquad \text{mid}([a]) = \tfrac{1}{2}(\bar{a} + \underline{a}),$$

$$\text{mig}([a]) = \begin{cases} 0 & : \text{ if } 0 \in [a], \\ \min\{|\underline{a}|, |\bar{a}|\} & : \text{ otherwise;} \end{cases}$$

$$\text{mag}([a]) = \max\{|\underline{a}|, |\bar{a}|\}.$$

Functions from $\mathbb{IR}$ to $\mathbb{IR}$:

$$\text{abs}([a]) = \{|a| : a \in [a]\} = [\text{mig}([a]), \text{mag}([a])].$$

$\mathbb{IR}$ as a metric space:

We can turn $\mathbb{IR}$ into a metric space by equipping it with the Hausdorff distance:

$$d([a], [b]) = \max\{|\underline{a} - \underline{b}|, |\bar{a} - \bar{b}|\}.$$

Using the metric, we can define the notion of a convergent sequence of intervals:

$$\lim_{k \to \infty} [a_k] = [a] \quad \Leftrightarrow \quad \lim_{k \to \infty} d([a_k], [a]) = 0.$$

Arithmetic over $\mathbb{IR}$:

Definition: If $\star$ is one of the operators $+, -, \times, \div$, and if $[a], [b] \in \mathbb{IR}$, then

$$[a] \star [b] = \{a \star b \colon a \in [a], b \in [b]\},$$

except that $[a] \div [b]$ is undefined if $0 \in [b]$.

Uncountable many cases to consider!

Continuity, monotonicity, and compactness $\Rightarrow$

$$\begin{aligned}
[a] + [b] &= [\underline{a} + \underline{b}, \bar{a} + \bar{b}] \\
[a] - [b] &= [\underline{a} - \bar{b}, \bar{a} - \underline{b}] \\
[a] \times [b] &= [\min\{\underline{ab}, \underline{a}\bar{b}, \bar{a}\underline{b}, \bar{a}\bar{b}\}, \max\{\underline{ab}, \underline{a}\bar{b}, \bar{a}\underline{b}, \bar{a}\bar{b}\}] \\
[a] \div [b] &= [a] \times [1/\bar{b}, 1/\underline{b}], \quad \text{if } 0 \notin [b].
\end{aligned}$$

On a computer we use *directed rounding*:

$$[a] + [b] = [\bigtriangledown(\underline{a} \oplus \underline{b}), \triangle(\bar{a} \oplus \bar{b})].$$

We then have $[a] \star [b] \supseteq \{a \star b \colon a \in [a], b \in [b]\}$.

Properties of interval arithmetic

(1) IA is associative and commutative.

(2) IA is *not* distributive:

$$[-1,1]([-1,0]+[3,4]) = [-1,1][2,4] = [-4,4],$$

$$[-1,1][-1,0]+[-1,1][3,4] = [-1,1]+[-4,4] = [-5,5].$$

We do, however, always have

$$[a]([b]+[c]) \subseteq [a][b]+[a][c].$$

(3) IA has no multiplicative or additive inverse:

$$0 \in [a]-[a]; \qquad 1 \in [a]\div[a].$$

(4) IA is *inclusion monotonic*, i.e., if $[a] \subseteq [a']$, and $[b] \subseteq [b']$, then

$$[a] \star [b] \subseteq [a'] \star [b'],$$

where we demand that $0 \notin [b']$ for division.

Interval extensions

One of the the main goals is to enclose the *range* of a function f:

$$R(f;D) = \{f(x) \colon x \in D\}.$$

This is achieved by constructing an *interval extension* $F \colon \mathbb{IR} \to \mathbb{IR}$ of the real-valued function $f \colon \mathbb{R} \to \mathbb{R}$.

Monotone functions are easy!

$$\begin{array}{lcll} e^{[x]} & = & [e^{\underline{x}}, e^{\bar{x}}] & \\ \sqrt{[x]} & = & [\sqrt{\underline{x}}, \sqrt{\bar{x}}] & \text{if } 0 \le \underline{x} \\ \log\,[x] & = & [\log \underline{x}, \log \bar{x}] & \text{if } 0 < \underline{x} \\ \arctan\,[x] & = & [\arctan \underline{x}, \arctan \bar{x}]\,. & \end{array}$$

Piecewise monotone functions are also OK!

$$[x]^n = \begin{cases} [\underline{x}^n, \bar{x}^n] & : \text{ if } n \in \mathbb{Z}^+ \text{ is odd,} \\ [\mathrm{mig}([x])^n, \mathrm{mag}([x])^n] & : \text{ if } n \in \mathbb{Z}^+ \text{ is even,} \\ [1, 1] & : \text{ if } n = 0, \\ [1/\bar{x}, 1/\underline{x}]^{-n} & : \text{ if } n \in \mathbb{Z}^-;\ 0 \notin [x]. \end{cases}$$

Standard/elementary functions

We define the class of *standard* functions to be the set

$$\mathfrak{S} = \{e^x, \log x, x^a, \operatorname{abs} x, \sin x, \cos x, \tan x, \ldots$$
$$\ldots, \arccos x, \arctan x, \sinh x, \cosh x, \tanh x\}.$$

For any $f \in \mathfrak{S}$, we can construct a *sharp* interval extension F, i.e.,

$$f \in \mathfrak{S} \Rightarrow R(f; [x]) = F([x]).$$

Building new functions is easy...

We use finite combinations of constants, elements of $\mathfrak{S}$, $\{+, -, \times, \div\}$, and $\circ$ to build the *elementary* functions $\mathfrak{E}$. Interval versions of $\mathfrak{S}$ and $\{+, -, \times, \div\}$ provide the corresponding interval extensions.

... but we may now overestimate the range.

If $f(x) = \frac{x}{1+x^2}$, then $F([x]) = \frac{[x]}{1+[x]^2}$. For the interval $[x] = [1, 2]$, we have

$$R(f; [1,2]) = [\tfrac{2}{5}, \tfrac{1}{2}] \subseteq [\tfrac{1}{5}, 1] = F([1,2]).$$

Looks are important!

$$f_1(x) = 1 - x^2 = (1-x)(1+x) = f_2(x),$$

but

$$F_1([x]) = 1 - [x]^2 \neq (1 - [x])(1 + [x]) = F_2([x]),$$

since

$$\begin{aligned} F_1([-1,1]) &= 1 - [-1,1]^2 = [1,1] - [0,1] = [0,1], \\ F_2([-1,1]) &= (1 - [-1,1])(1 + [-1,1]) \\ &= [0,2] \times [0,2] = [0,4]. \end{aligned}$$

Different representations – different functions.

Interval enclosures

Theorem 1: If $f \in \mathfrak{E}$, and $F([x])$ is well-defined, then

$$R(f;[x]) \subseteq F([x]).$$

How tight is the enclosure?

Theorem 2: If $f \in \mathfrak{E}$, $[x] = [x_1] \cup \cdots \cup [x_k]$, and $F([x])$ is well-defined, then

$$R(f;[x]) \subseteq \bigcup_{i=1}^{k} F([x_i]) \subseteq F([x]).$$

If f is Lipschitz on $[x]$ there is a $K \geq 0$ s.t.

$$\mathrm{rad}\left(\bigcup_{i=1}^{k} F([x_i])\right) - \mathrm{rad}\Big(R(f;[x])\Big) \leq K \max_i \mathrm{rad}\left([x_i]\right).$$

I.A. (almost) gives us access to $R(f;[x])$.

Computer-aided proofs

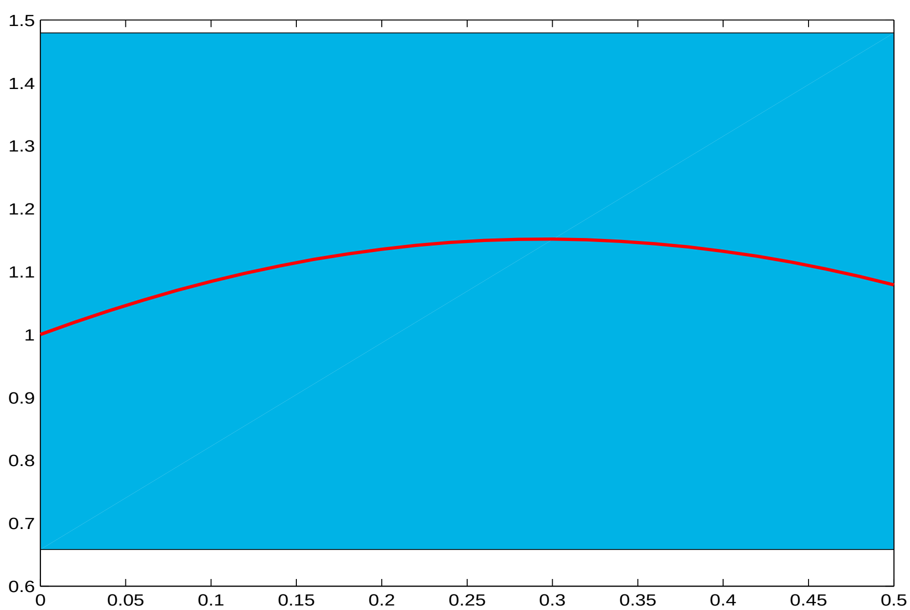
An important consequence of Theorem 1 is

$$y \notin F([x]) \Rightarrow y \notin R(f; [x]).$$

Exercise: Let $f(x) = (\sin x - x^2 + 1)\cos x$. Prove that $f(x) \neq 0$ for $x \in [0, \frac{1}{2}]$.

Solution: Define $F([x]) = (\sin [x] - [x]^2 + 1)\cos [x]$. Then, by Theorem 1, we have

$$R(f; [0, \tfrac{1}{2}]) \subseteq F([0, \tfrac{1}{2}]) = \dots$$
$$\dots = [\tfrac{3}{4}\cos\tfrac{1}{2}, 1 + \sin\tfrac{1}{2}] \subseteq [0.65818, 1.4795].$$



Graph enclosures

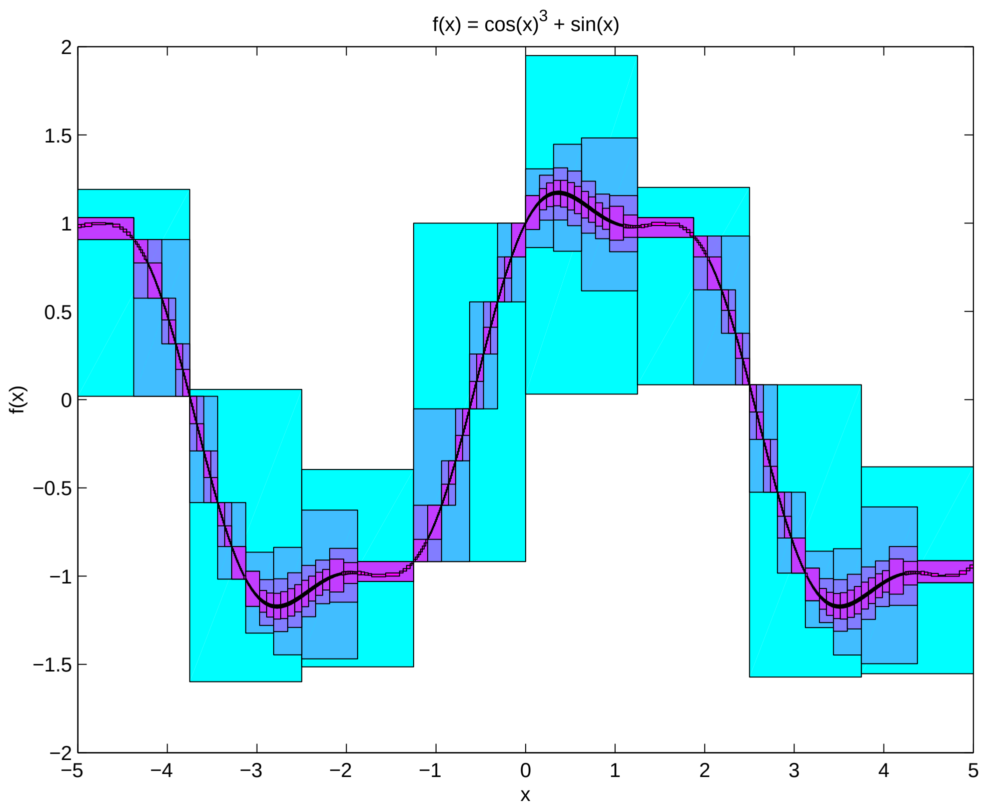
Exercise: Draw the graph of the function

$$f(x) = \cos^3 x + \sin x$$

over the interval $[-5, 5]$.

Solution: Define $F([x]) = \cos^3 [x] + \sin [x]$, and bisect the domain into smaller pieces until

$$\max_i \operatorname{rad}\Big(F([x_i])\Big) \leq \texttt{TOL}.$$

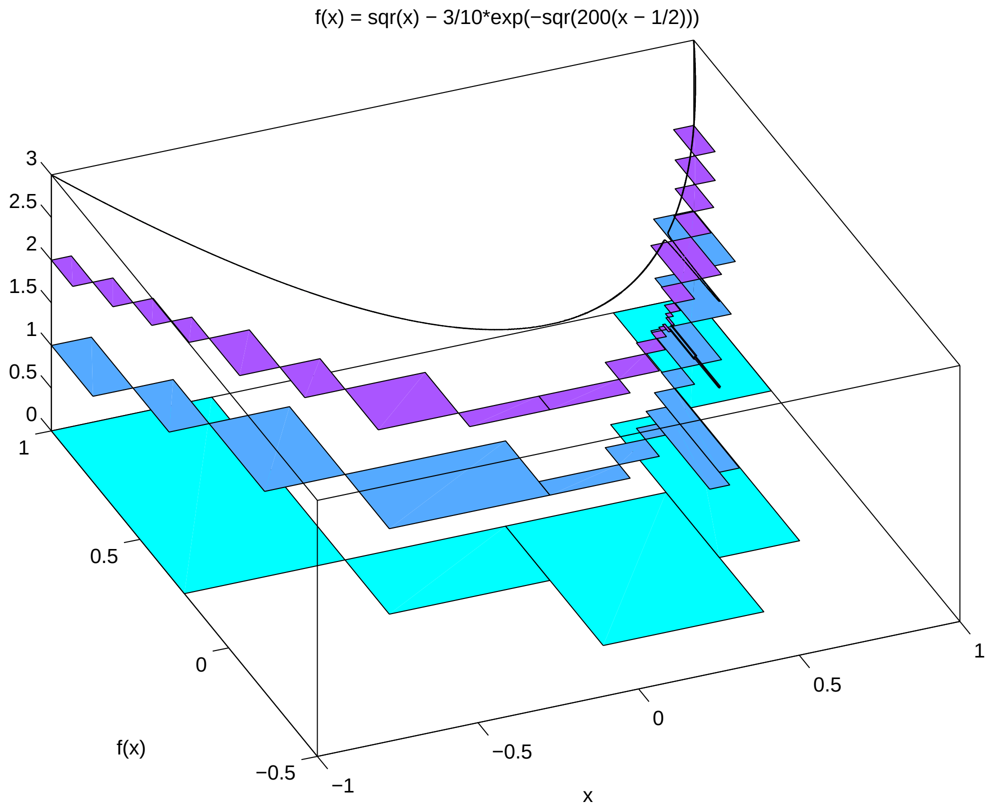


"Impossible" cases too

Exercise: Draw the graph of the function

$$f_a(x) = x^2 - \frac{3}{10} e^{-(a(x-\frac{1}{2}))^2}$$

for $a = 200$ over the interval $[-1, 1]$.



Even when a is huge, the I.A.-methods *cannot* miss the sharp bend! Conventional methods *must* miss it.

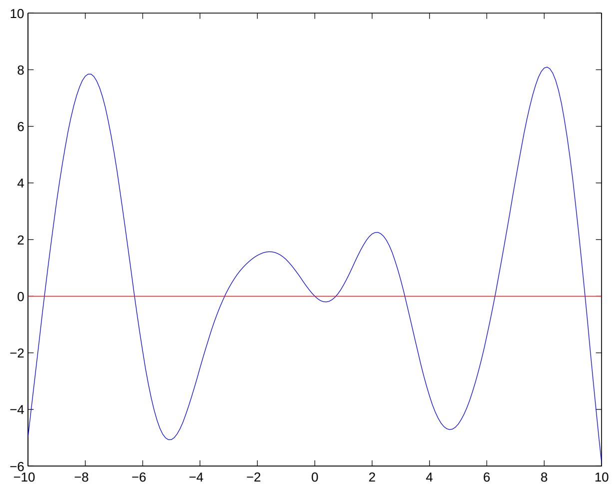
Root enclosures

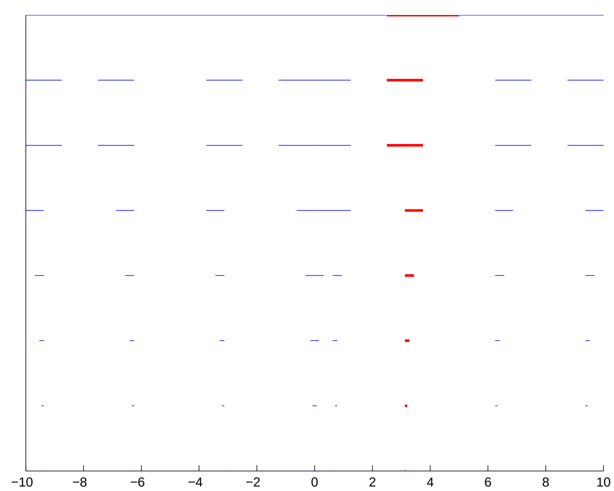
Exercise: Find all roots of the function

$$f(x) = \sin x(x - \cos x)$$

over the domain $[-10, 10]$.

Solution: Define $F([x]) = \sin [x]([x] - \cos [x])$, bisect the domain, and throw away all pieces that satisfy $0 \notin F([x_i])$.






```
#-------------------------------------------------------------#
Domain         : [-10,10]
Tolerance      : 0.001
Function calls: 227
Root list      :
 1: [-9.4251,-9.4244] 4: [-0.0007,+0.0000] 7: [+3.1414,+3.1421]
 2: [-6.2836,-6.2829] 5: [+0.0000,+0.0007] 8: [+6.2829,+6.2836]
 3: [-3.1421,-3.1414] 6: [+0.7385,+0.7392] 9: [+9.4244,+9.4251]
#-------------------------------------------------------------#
```

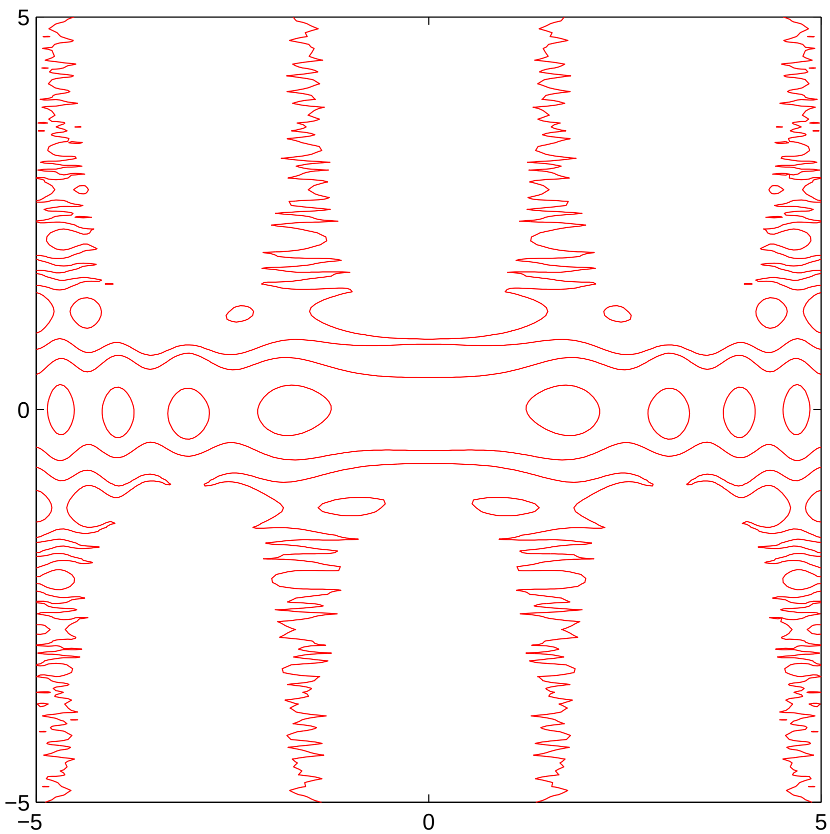
Implicit curves ($\mathbb{R}^2$)

Exercise: Draw the locus defined by

$$f(x,y) = \sin(\cos x^2 + 10 \sin y^2) - y \cos x = 0;$$

restricted to the domain $[-5,5] \times [-5,5]$.

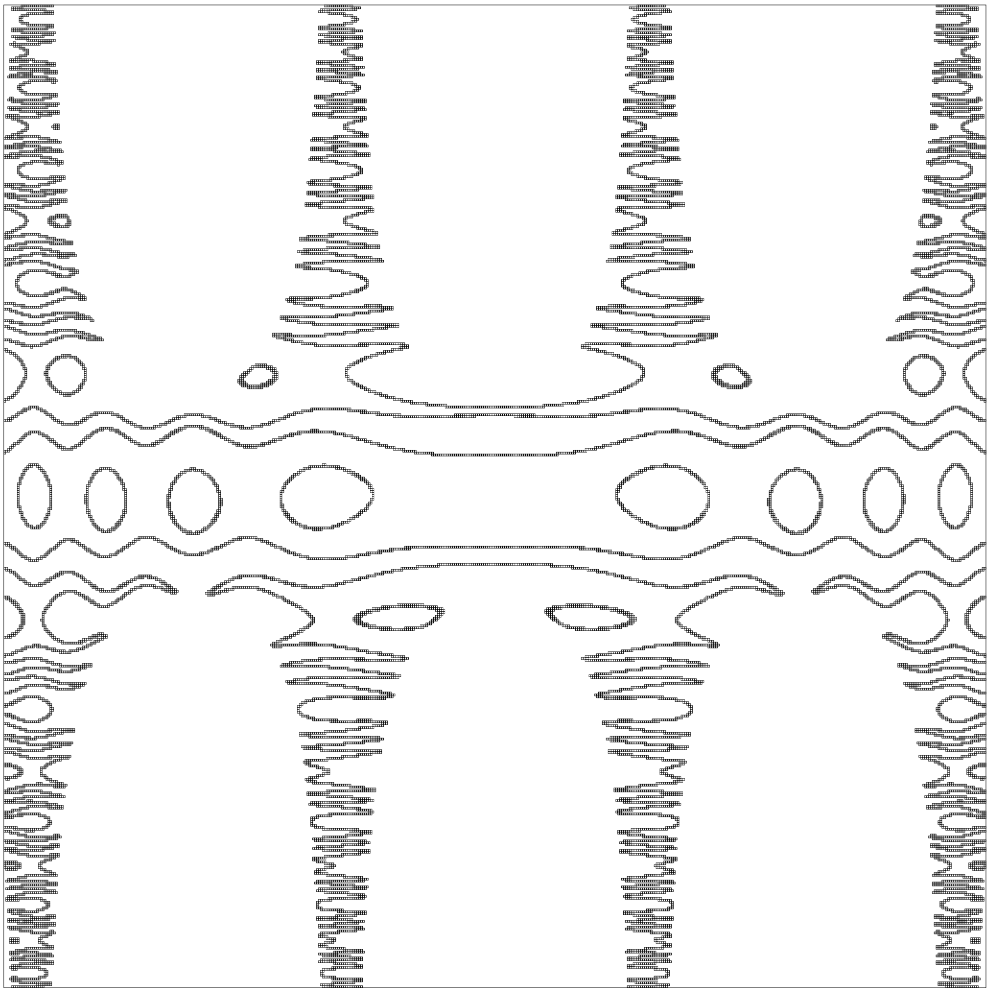
MATLAB produces the following picture:



The locus $|f(x,y)| = 0$, however, is empty!?!

Implicit curves...

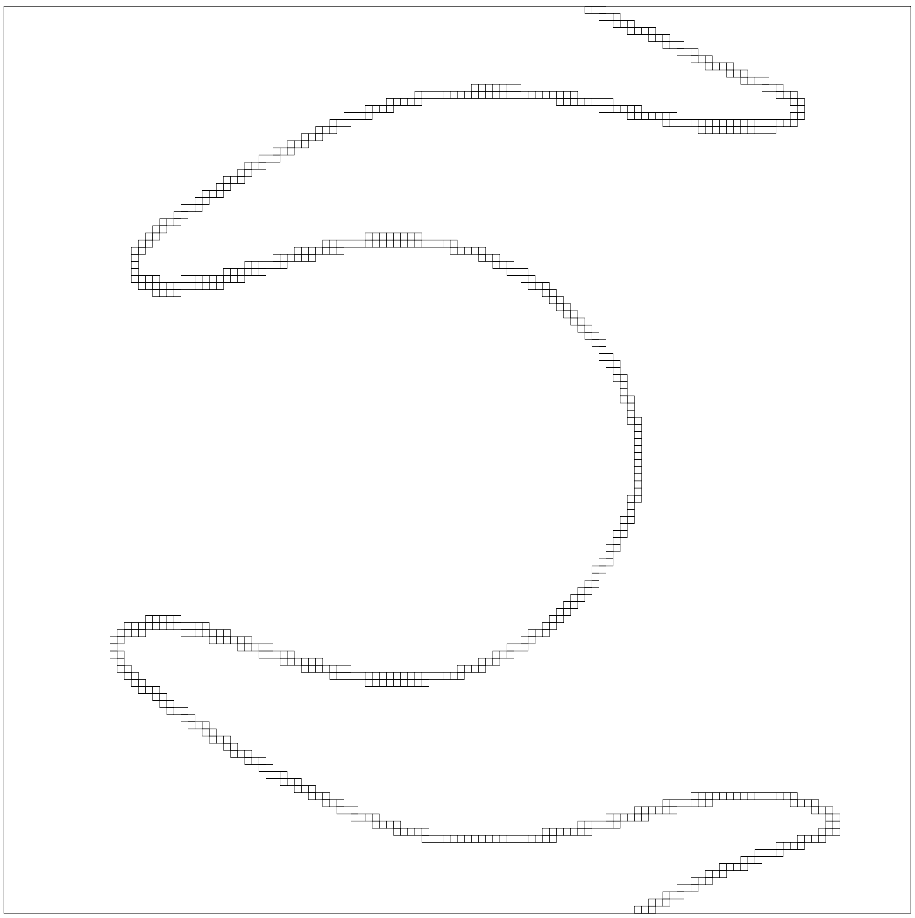
The validated enclosure in both cases is



```
#--------------------------------------------------------------#
Number of split calls    : 9
Number of function calls: 87550
Number of solution boxes: 19718
Maximal box diameter     : 0.0195312
#--------------------------------------------------------------#
```

Implicit curves...

A sharper look at the previous picture...



No zeroes can exist outside the boxes:

$$0 \notin F([x^{(i)}]) \Rightarrow 0 \notin R(f; [x^{(i)}]).$$

Optimization

Exercise: Find the minimum of the function

$$f_a(x) = x^2 - \tfrac{3}{10}e^{-(a(x-\frac{1}{2}))^2}$$

for $a = 10000$ over the interval $[-\frac{3}{2}, \frac{3}{2}]$.

Solution: Adaptive branch and bound.

```
#--------------------------------------------------------------#
Domain                 : [-1.5,1.5]
Tolerance              : 9.09495e-13 (2^-40)
Function calls         : 3810
Global minimizer       : [4.9999998318185e-01,4.9999998348404e-01]
Global minimum         : -5.000000833367428e-02 +- 3.412409245e-13
Non-rigorous estimate: 3.113063833543e-09
#--------------------------------------------------------------#
```

Prove that the minimum is negative:

```
#--------------------------------------------------------------#
Domain                 : [-1.5,1.5]
Tolerance              : 0.03125 (2^-5)
Function calls         : 67
Global minimizer       : [4.9996948242187e-01,5.0001525878907e-01]
Global minimum         : -4.914849425348847e-02 +- 8.820223934e-04
Non-rigorous estimate: 3.71e-04
#--------------------------------------------------------------#
```

Newton's method in $\mathbb{IR}$

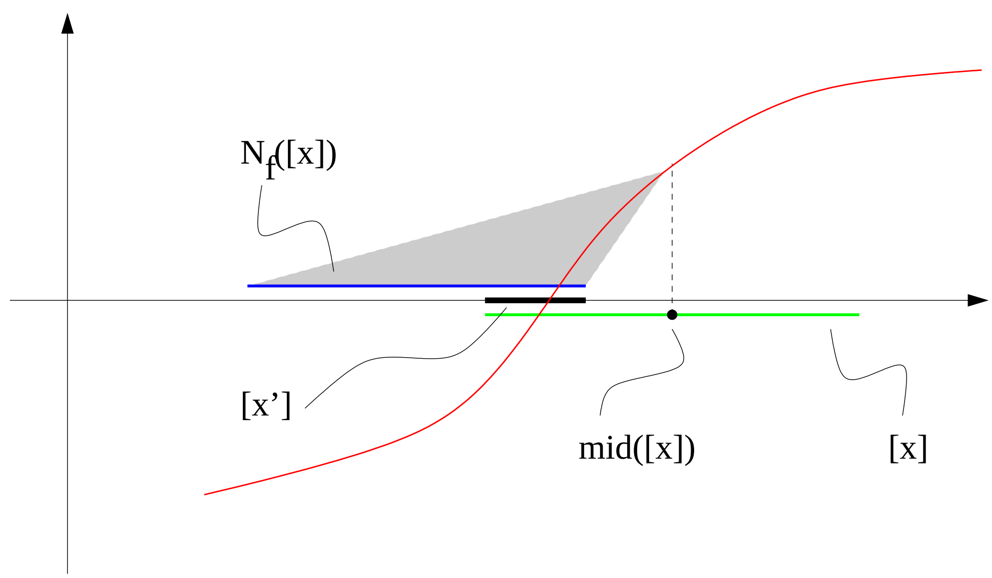
Assume that $f \in C^1([x], \mathbb{R})$, and that $x^* \in [x]$ is a root of f. Also assume that $0 \notin F'([x])$, and define

$$N_f([x]) = \text{mid}([x]) - \frac{f(\text{mid}([x]))}{F'([x])}.$$

Theorem 3: Assume that $N_f([x])$ exists. Then

$$N_f([x]) \cap [x] = \emptyset \Rightarrow f \text{ has no roots in } [x];$$

$$N_f([x]) \subseteq [x] \Rightarrow f \text{ has a unique root in } [x].$$



Newton's method in $\mathbb{IR}$

Set $[x^{(0)}] = [x]$, and consider the sequence

$$[x^{(k+1)}] = N_f([x^{(k)}]) \cap [x^{(k)}], \quad k \in \mathbb{N}.$$

Bonus: The iterates behave very regularly.

Theorem 4: If $N_f([x^{(0)}])$ exists, and $[x^{(0)}]$ contains a root x^* of f, then so do all $[x^{(k)}]$, $k \in \mathbb{N}$. Furthermore, the intervals $[x^{(k)}]$ form a nested sequence converging to x^*.

Major drawback: The Newton operator N_f is undefined when $0 \in F'([x])$.

Fix 1: Use bisection to single out subintervals $[\tilde{x}]$ on which $0 \notin F'([\tilde{x}])$. These are sent to the interval Newton method. Also keep all small $[\tilde{x}]$ with $0 \in F'([\tilde{x}])$ and $0 \in F([\tilde{x}])$.

Newton's method in $\mathbb{R}$

Example: Consider the function

$$f_a(x) = x^2 - \frac{3}{10}e^{-(a(x-\frac{1}{2}))^2}$$

with $a = 10000$ over the interval $[\frac{1}{4}, 1]$. Recall that this function has a *very* sharp bend.

```
#------------------------------------------------------------------#
Searching the domain [0.25,1] with TOL = 0.00390625 (2^-8).
After the adaptive bisection, we have:
  1 subdomain where f may have roots.

There may be roots within
  1: [0.496094,0.501953]
#------------------------------------------------------------------#
```

Decrease the tolerance...

```
#------------------------------------------------------------------#
Searching the domain [0.25,1] with TOL = 1.52588e-05 (2^-16).
After the adaptive bisection, we have:
  2 subdomains where f is strictly monotone.

Sending [0.500031,0.500122] to the Newton operator...
Finite convergence!
The unique root is within: +5.000426791339584e-01 +- 2.77556e-16

Sending [4.99939e-01,4.99985e-01] to the Newton operator...
Finite convergence!
The unique root is within: +4.999572808660400e-01 +- 1.38778e-16
#------------------------------------------------------------------#
```

Extended interval arithmetic

Fix 2: Extend the interval arithmetic to allow for division by zero.

Example: $[1,2] \div [-3,5] = ???$

$$\begin{aligned}[1,2] \div [-3,5] &= [1,2] \div ([-3,0] \cup [0,5]) \\ &= ([1,2] \div [-3,0]) \cup ([1,2] \div [0,5])\end{aligned}$$

Now we *define* the division as follows:

$$[1,2] \div [-3,0] \stackrel{\text{def}}{=} \lim_{\varepsilon \to 0^-} [1,2] \div [-3,\varepsilon] = [-\infty, -\tfrac{1}{3}]$$

and

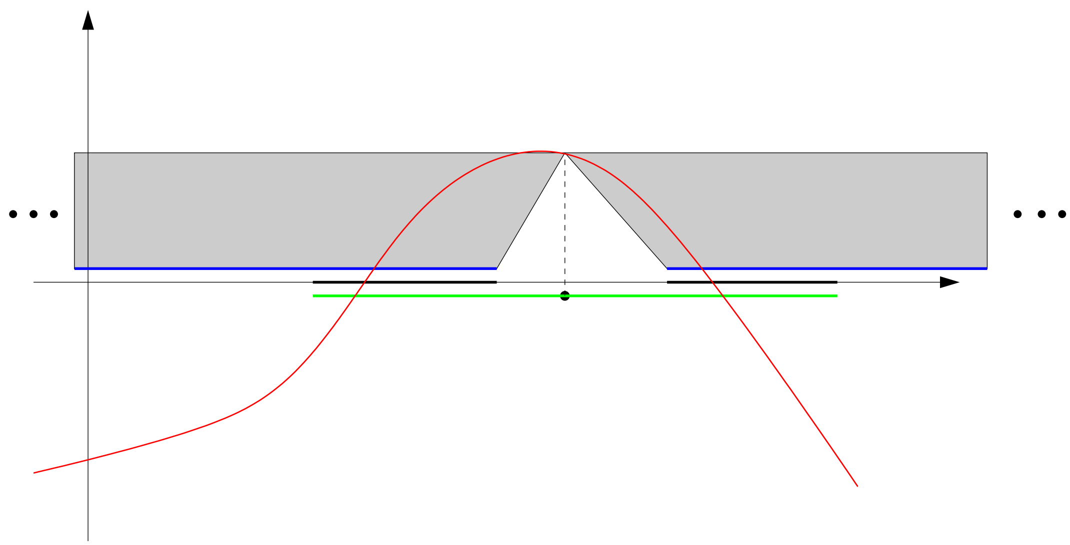
$$[1,2] \div [0,5] \stackrel{\text{def}}{=} \lim_{\varepsilon \to 0^+} [1,2] \div [\varepsilon,5] = [\tfrac{1}{5}, +\infty].$$

Answer: $[1,2] \div [-3,5] = [-\infty, -\frac{1}{3}] \cup [\frac{1}{5}, +\infty]$.

The extended interval Newton Method

When computing the Newton iterates, the unbounded intervals are intersected back to compact domains by the scheme

$$[x^{(k+1)}] = N_f([x^{(k)}]) \cap [x^{(k)}], \quad k \in \mathbb{N}.$$



Example: Again the function $f_{10000}(x)$.

```
#--------------------------------------------------------------#
Domain              : [2.500000e-01,1.000000e+00]
Tolerance           : 9.536743e-07 (2^-20)
Unique root within  : [+0.49995676466028721,+0.49995838064162701]
Unique root within  : [+0.50004262913481123,+0.50004274553256134]
Function calls      : 34
#--------------------------------------------------------------#
```

The Lorenz equations

Introduced in 1963 by Edward Lorenz.

$$\begin{aligned}\dot{x}_1 &= -\sigma x_1 + \sigma x_2\\ \dot{x}_2 &= \varrho x_1 - x_2 - x_1 x_3\\ \dot{x}_3 &= -\beta x_3 + x_1 x_2,\end{aligned}$$

Classical parameters: $\sigma = 10$, $\beta = 8/3$, $\varrho = 28$.

Symmetry: $S(x_1, x_2, x_3) = (-x_1, -x_2, x_3)$.

Three fixed points: the origin 0 and

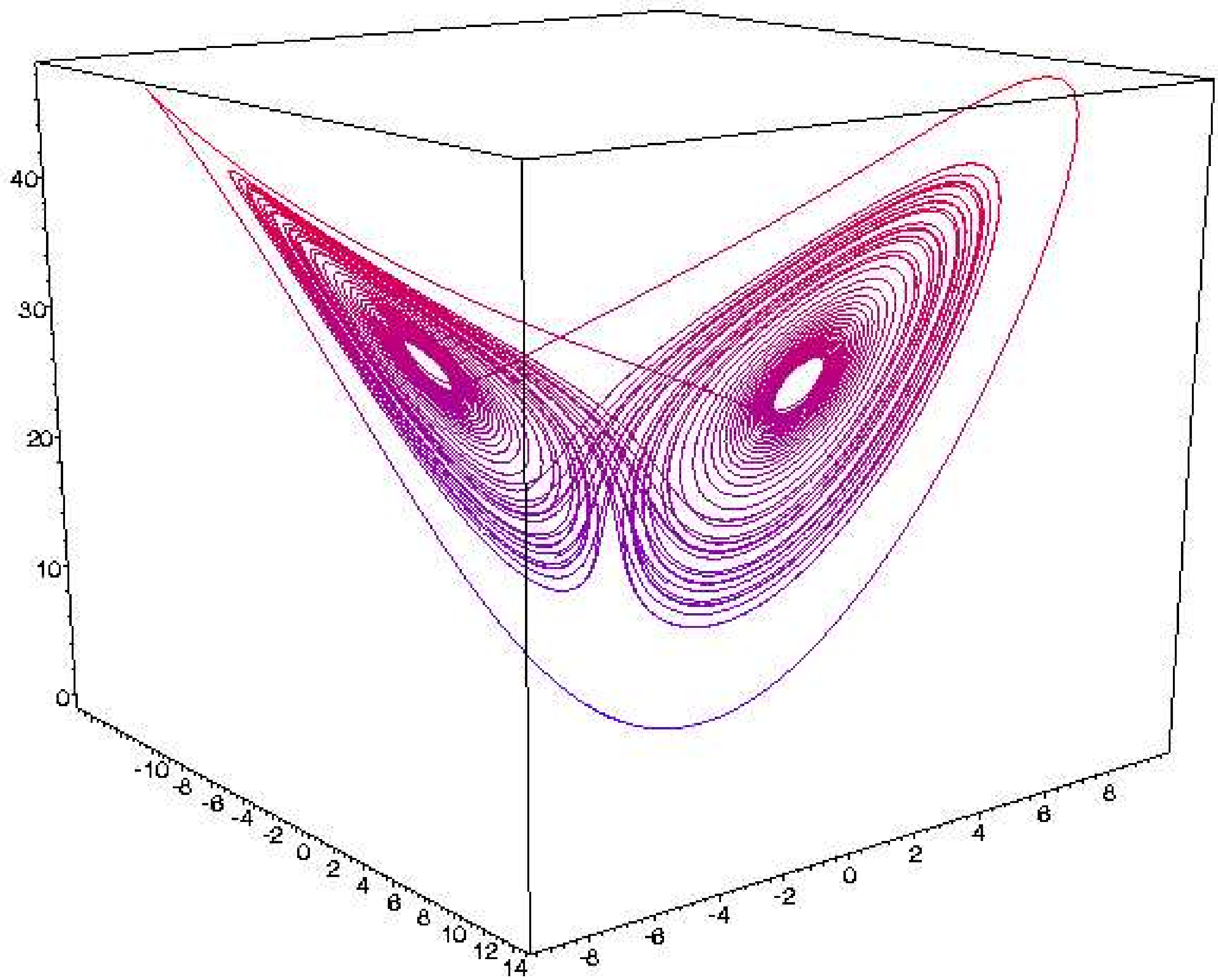
$$C^{\pm} = (\pm\sqrt{\beta(\varrho - 1)}, \pm\sqrt{\beta(\varrho - 1)}, \varrho - 1).$$

Stability: The origin is a saddle point with

$$0 < -\lambda_3 < \lambda_1 < -\lambda_2.$$

$C^{\pm}$ are unstable spirals.

Solutions of the Lorenz equations



The Lorenz equations...

Thus, the stable manifold of the origin $W^s(0)$ is two-dimensional, and the unstable manifold of the origin $W^u(0)$ is one-dimensional.

Constant divergence:

$$\frac{\partial \dot{x}_1}{\partial x_1} + \frac{\partial \dot{x}_2}{\partial x_2} + \frac{\partial \dot{x}_3}{\partial x_3} = -(\sigma + \beta + 1),$$

The volume of a solid at time t can be expressed as

$$V(t) = V(0)e^{-(\sigma+\beta+1)t} \approx V(0)e^{-13.7t},$$

for the classical parameter values.

Absorbing region: $\mathcal{U}$ containing the origin.

Maximal invariant set:

$$\mathcal{A} = \bigcap_{t \geq 0} \varphi(\mathcal{U}, t).$$

$\mathcal{A}$ must have zero volume, and $W^u(0) \subseteq \mathcal{A}$.

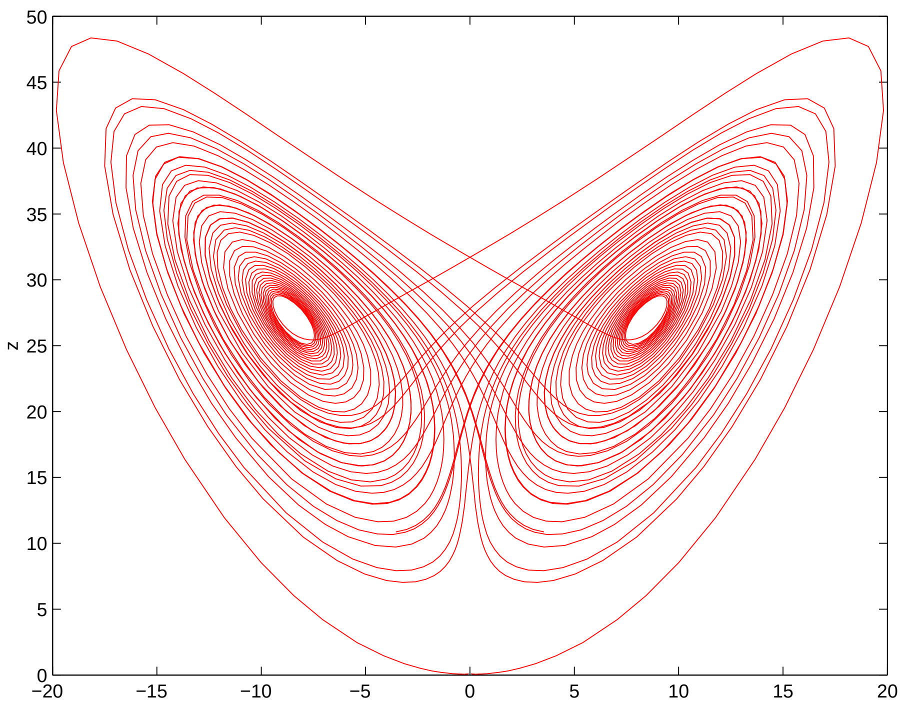
Lorenz observed:

[1] An attracting invariant set $\mathcal{A}$

[2] Sensitive dependence on i.c.

[3] Fractal structure of $\mathcal{A}$

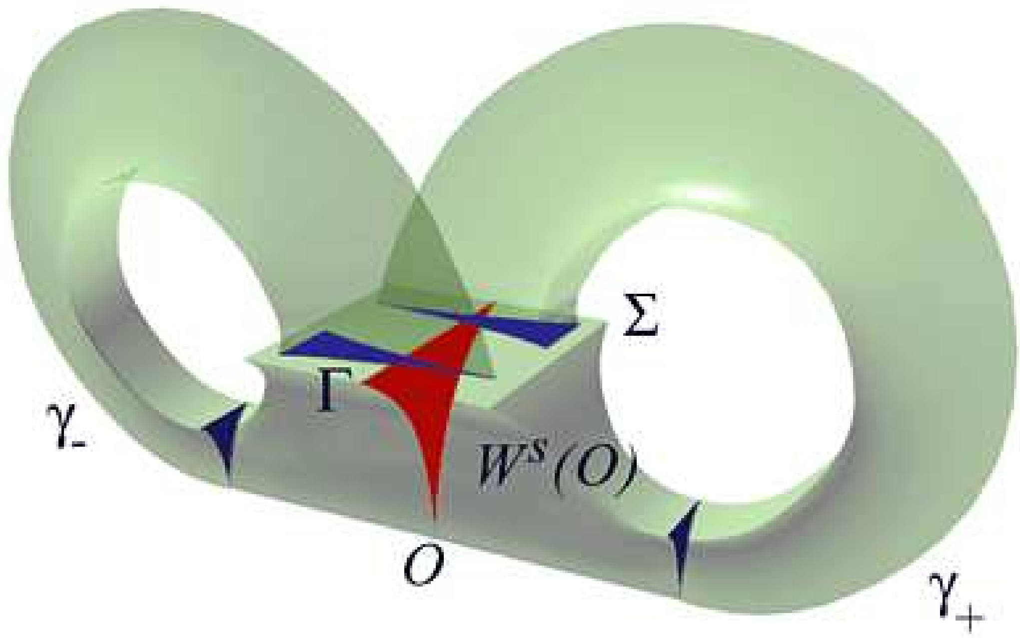
[4] Robustness of $\mathcal{A}$



He observed a strange attractor!

A geometric model:

Introduced by Guckenheimer and Williams (1979)

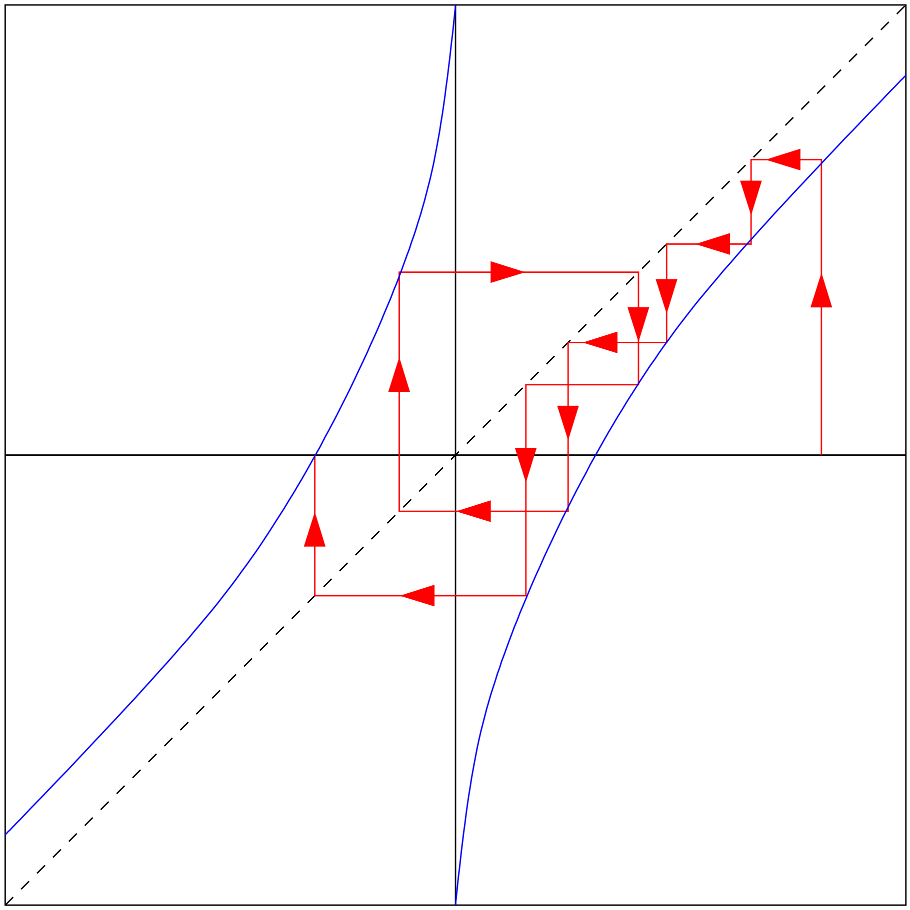


Return map: $R\colon \Sigma \setminus \Gamma \to \Sigma$.

The return plane Σ is foliated by stable leaves.

Projecting along these stable leaves induces a 1-d singular function:

$$f\colon [-1,1] \to [-1,1]$$



The function $f\colon [-1,1] \to [-1,1]$ satisfies:

[1] $f(-x) = -f(x)$;
[2] $\lim_{x\to 0} f'(x) = +\infty$;
[3] $f''(x) < 0$ on $(0,1]$;
[4] $f'(x) > \sqrt{2}$;

[1] - [4] $\Rightarrow$ f is topologically transitive on $[-1,1]$.

What is a strange attractor?

We need to prove:

(1) There exists a compact $N \subset \Sigma$, such that

$$R(N \setminus \Gamma) \subset N.$$

(2) On N, there exists a cone field $\mathfrak{C}$ such that for all $x \in N$,

$$DR(x) \cdot \mathfrak{C}(x) \subset \mathfrak{C}(R(x)).$$

(3) There exists $C > 0$ and $\lambda > 1$ such that for all $v \in \mathfrak{C}(x)$, $x \in N$, we have

$$|DR^n(x)v| \geq C\lambda^n |v|, \qquad n \geq 0.$$

Open conditions - Perfect for I.A.!

Computing R and DR requires solving interval-valued differential equations. This is still an open field of research.

How do we use these results?

(1) proves the existence of an attracting set. This *could* be a single periodic orbit.

(2)+(3) rule out the possibility of just observing a stable periodic orbit.

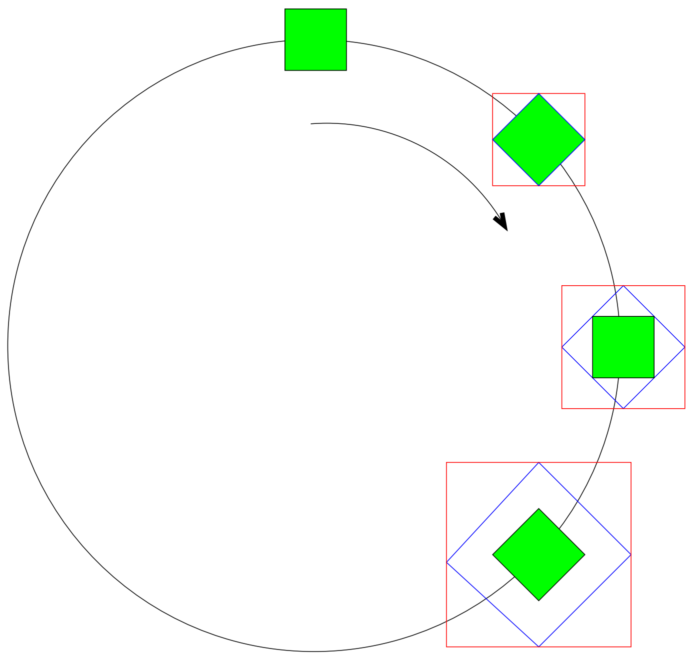
Strong enough expansion $\Rightarrow$ topological transitivity.

R area contracting + expansion in $\mathfrak{C}(x) \Rightarrow$ stable foliation.

Theorem: For the classical parameter values, the Lorenz equations support a robust strange attractor $\mathcal{A}$ – the Lorenz attractor!

The wrapping effect

Example: Solve the ODE $(\dot{x}_1, \dot{x}_2) = (x_2, -x_1)$.



Exponential growth of the solution set!

Fix: The Lorenz equations are strongly volume contracting. An adaptive bisection scheme dampens the overestimation of R and DR.

Analytic (non-numerical) techniques are needed near the fixed point of the flow.

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