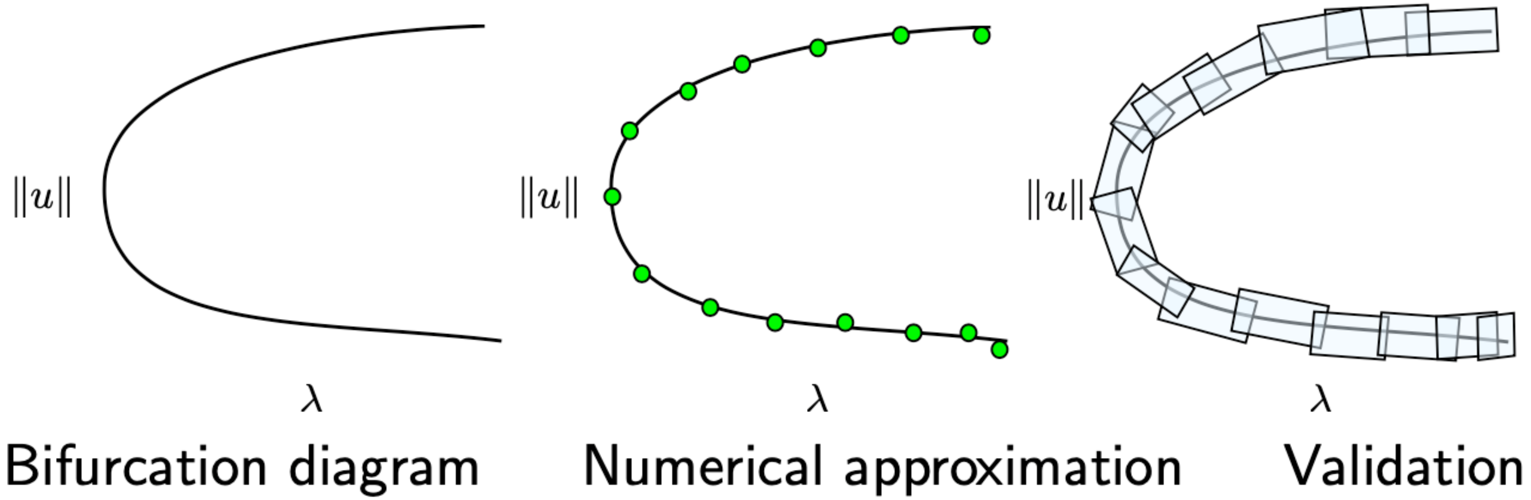
Computer-Assisted Proofs in Applied Mathematics



Organizers

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New Jersey Institute of Technology

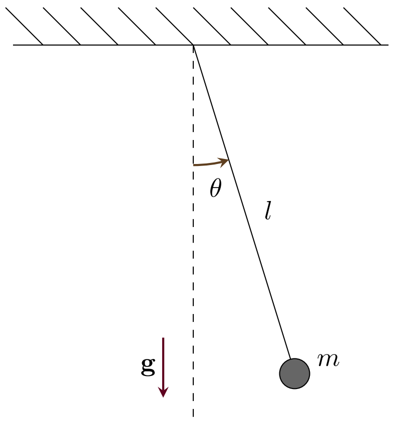


Image Credit: Wikipedia

$$\theta(t) = \theta_0 \cos\left(\sqrt{\frac{g}{\ell}}\, t\right)$$

Natural World

Pendulum	Weather

Scientific Model

$\frac{d^2}{dt^2}\theta + \frac{g}{\ell}\sin\theta = 0$	Navier-Stokes; Rayleigh-Bénard convection

Toy Model

$\frac{d^2}{dt^2}\theta + \frac{g}{\ell}\theta = 0$	Lorenz System (ODE)

?

?

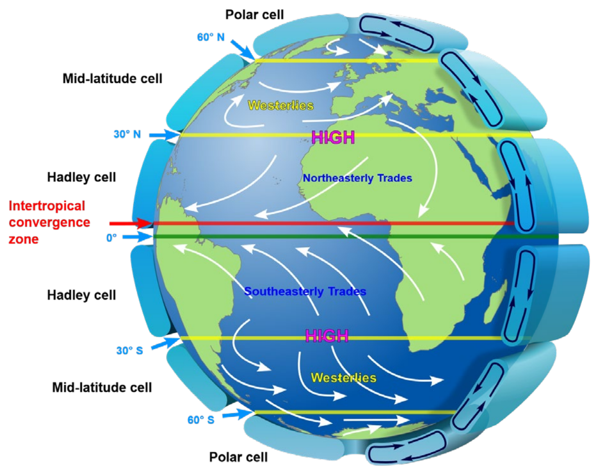
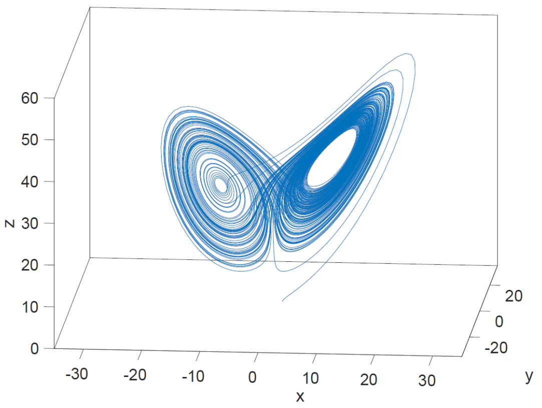
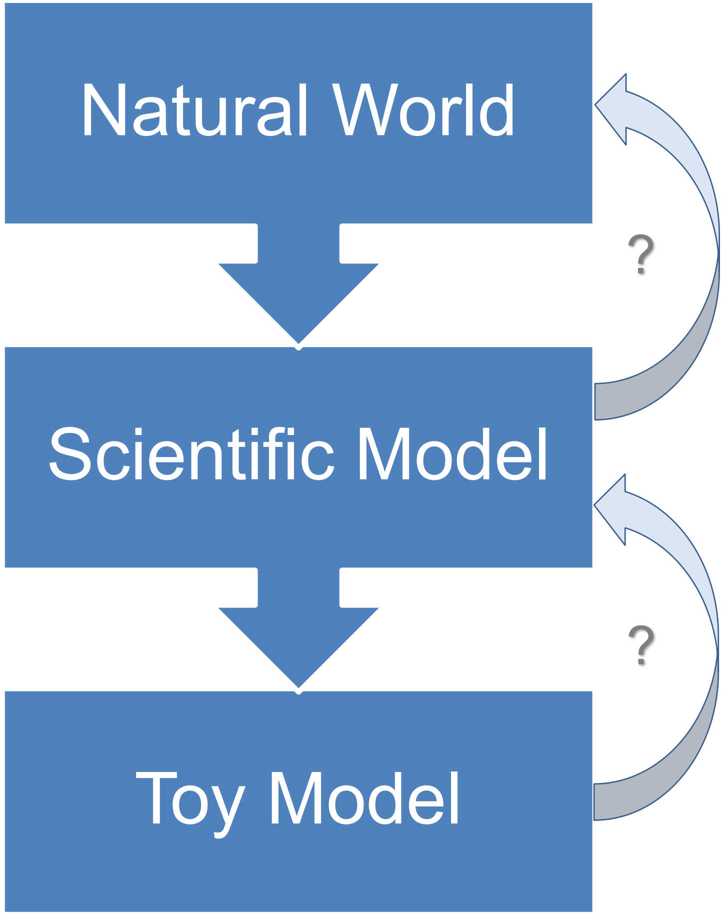


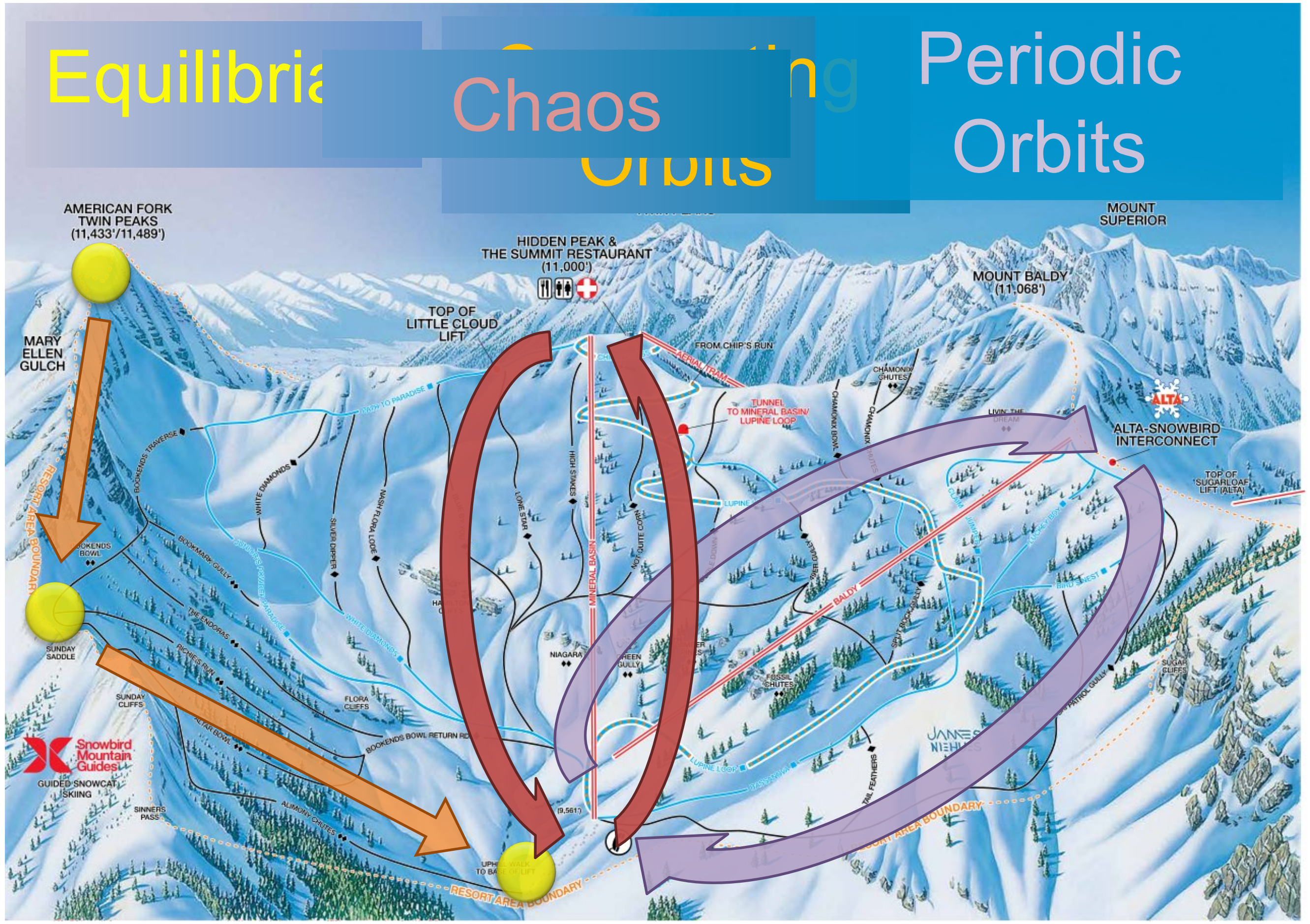
Image Credit: Wikipedia

Image Credit: Scientific Background on the Nobel Prize in Physics 2021; Weady et al. '18

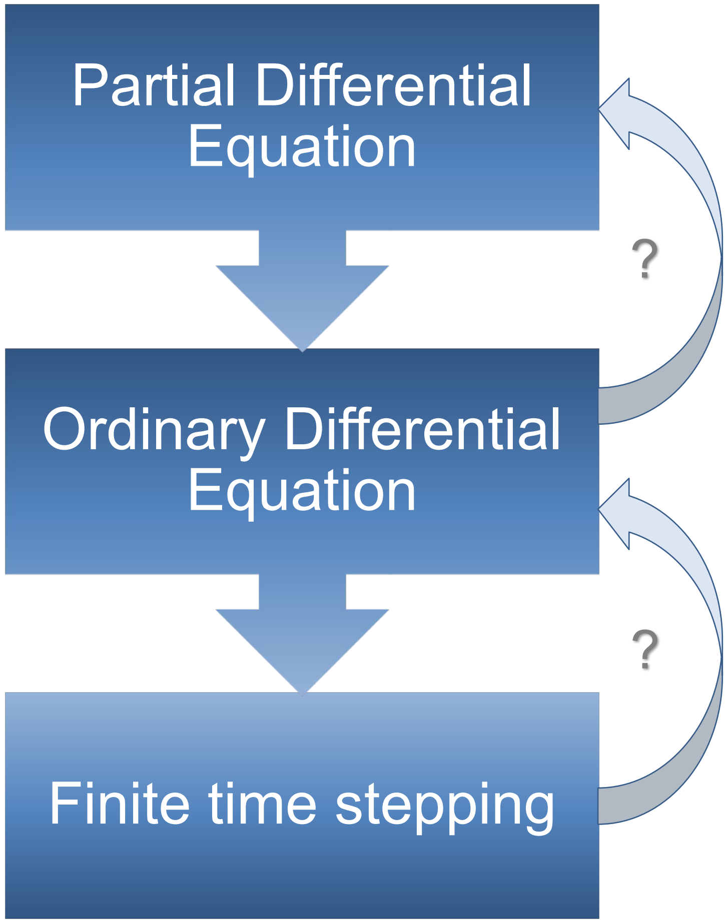


Which dynamical features are important?

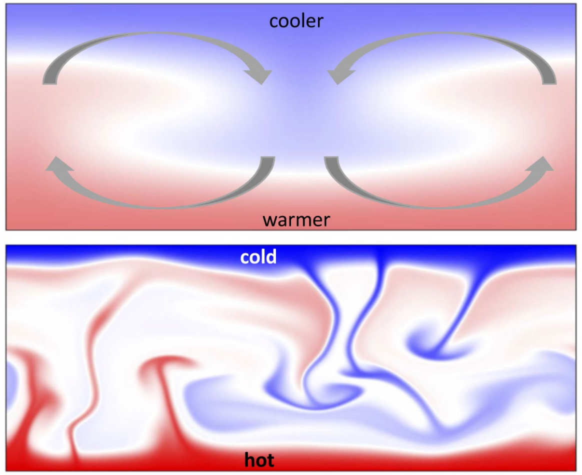




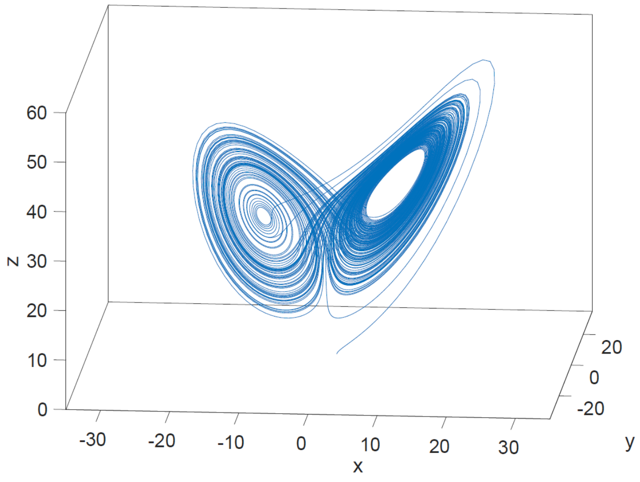
Which dynamical features persist?



- Numerical approximations converge in the limit
  - How accurate is a particular computation?



Temperature field in 2D Rayleigh-Bénard convection simulations. Image Credit: Doering 2020



The Lorenz attractor, a 3-mode approx. of Rayleigh-Bénard convection. Image Credit: Weady et al. ‘18

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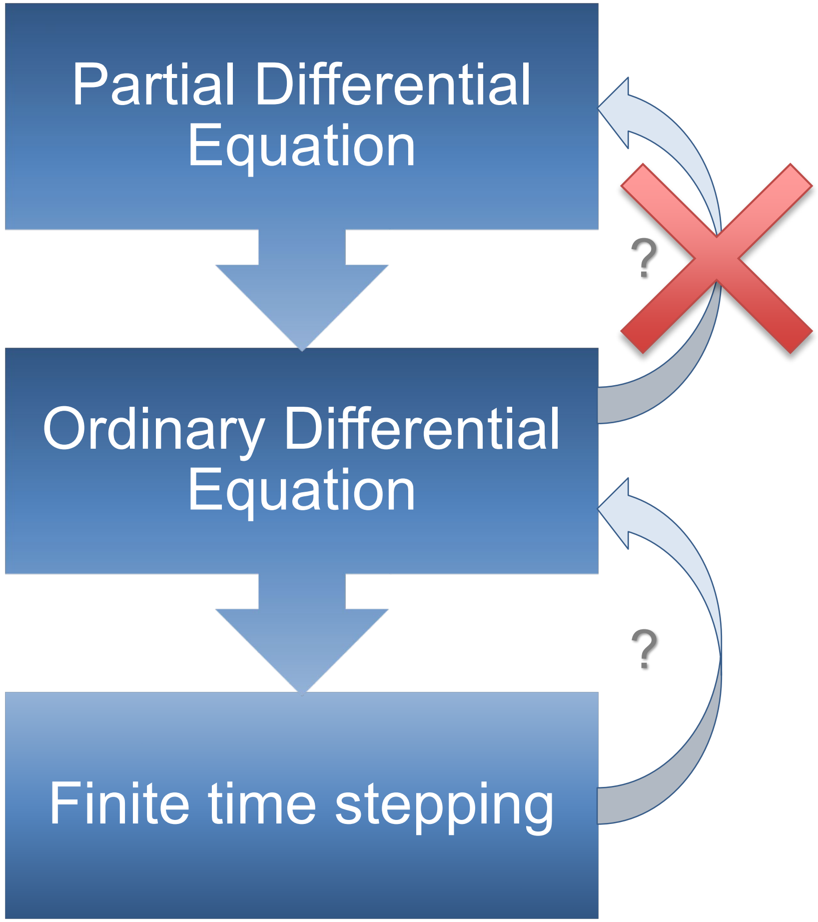

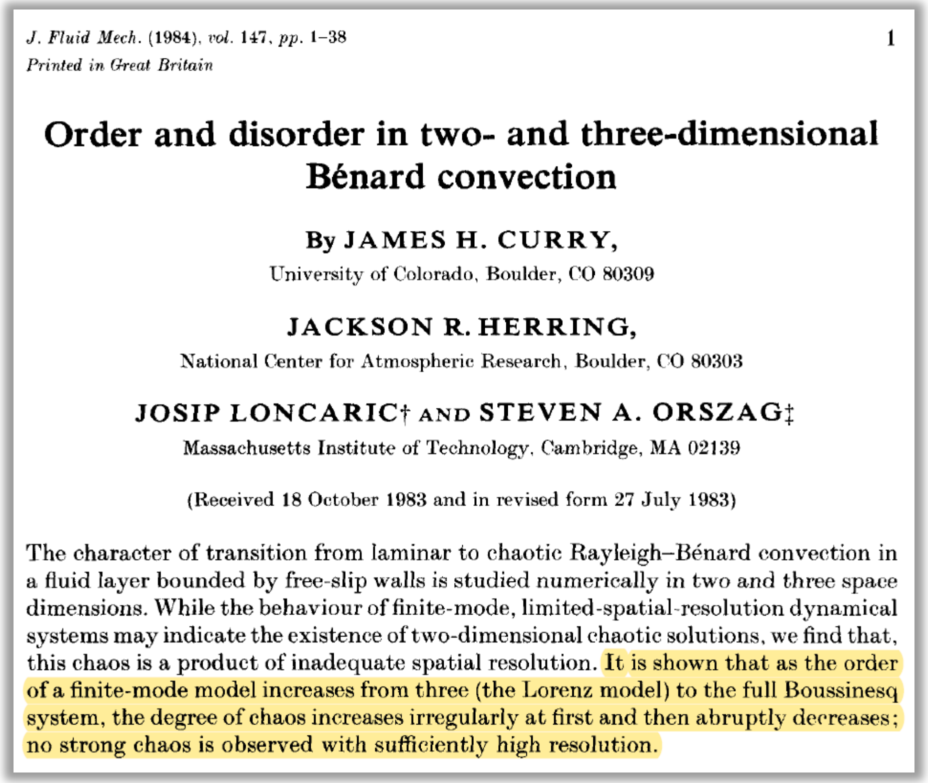

J. Fluid Mech. (1984), *vol.* 147, *pp.* 1–38 1
Printed in Great Britain

Order and disorder in two- and three-dimensional Bénard convection

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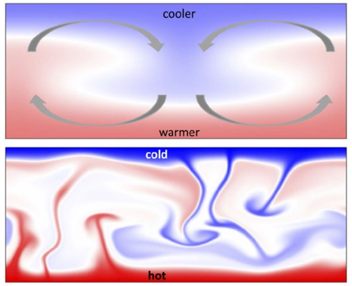
(Received 18 October 1983 and in revised form 27 July 1983)

The character of transition from laminar to chaotic Rayleigh–Bénard convection in a fluid layer bounded by free-slip walls is studied numerically in two and three space dimensions. While the behaviour of finite-mode, limited-spatial-resolution dynamical systems may indicate the existence of two-dimensional chaotic solutions, we find that, this chaos is a product of inadequate spatial resolution. It is shown that as the order of a finite-mode model increases from three (the Lorenz model) to the full Boussinesq system, the degree of chaos increases irregularly at first and then abruptly decreases; no strong chaos is observed with sufficiently high resolution.



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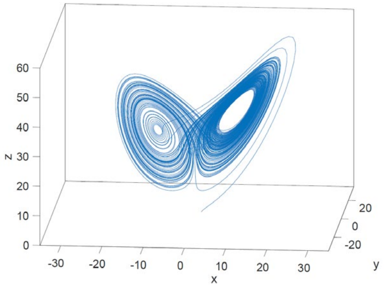

The Lorenz attractor, a 3-mode approx. of Rayleigh-Bénard convection. Image Credit: Weady et al. ‘18

What is a Computer Assisted Proof?

My Definition: *A proof involving computations.*

e.g. 109 is prime; $9 < \pi^2 < 10$

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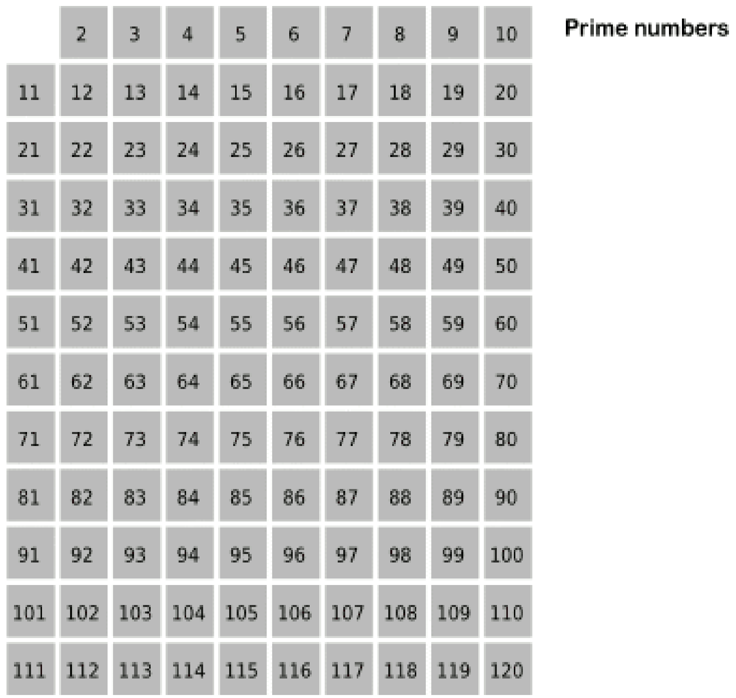
Sieve of Eratosthenes

`input`: integer n

`output`: primes between 2 & n

$S \coloneqq \{2,3,4 \ldots, n\}$
$p \coloneqq 2$
`while` $p \leq \sqrt{n}$
    remove $2p, 3p, 4p, \ldots$ from S
    $p \leftarrow$ smallest $x \in S, x > p$
`return` S



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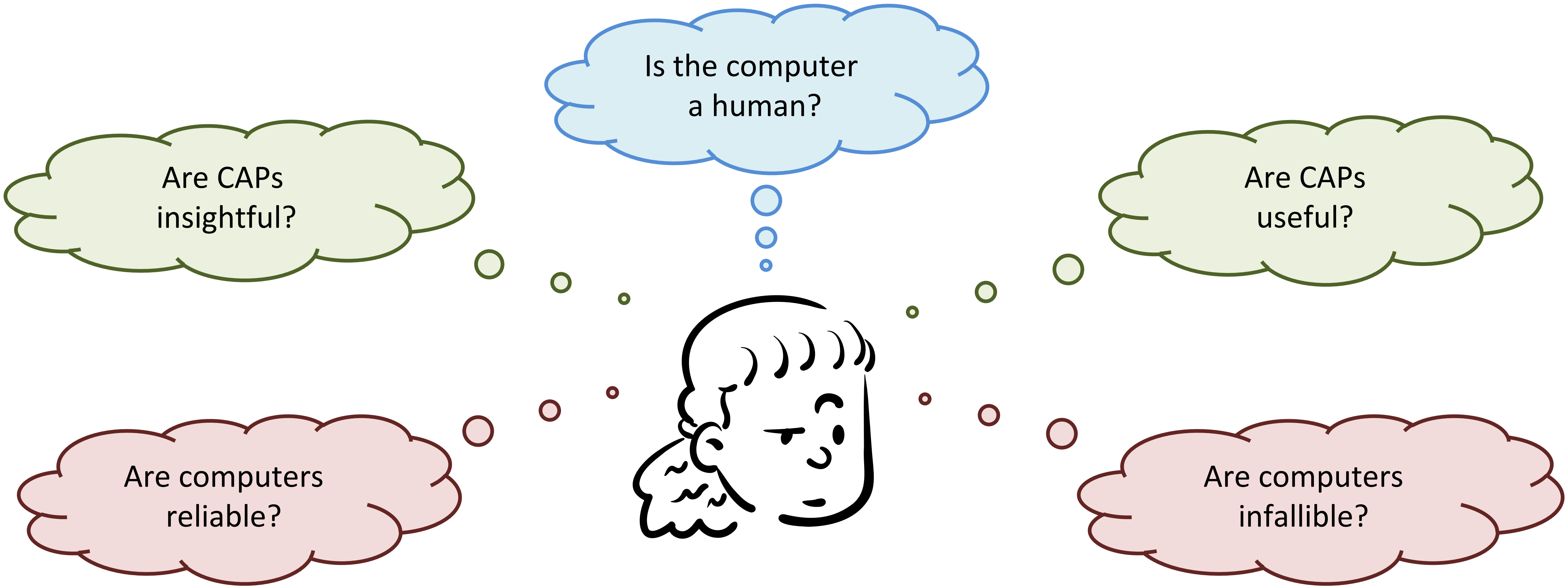


What is a Computer Assisted Proof?

Neumaier's Definition

Stage 1
- Qualitative understanding reduces the problem to a finite number of subproblems

Stage 2
- Reduce each subproblem to a finite number of equations and/or inequalities to be checked

Stage 3
- A specialized computational algorithm is executed

A.I. Is Coming for Mathematics, Too

For thousands of years, mathematicians have adapted to the latest advances in logic and reasoning. Are they ready for artificial intelligence?

By Siobhan Roberts July 2, 2023

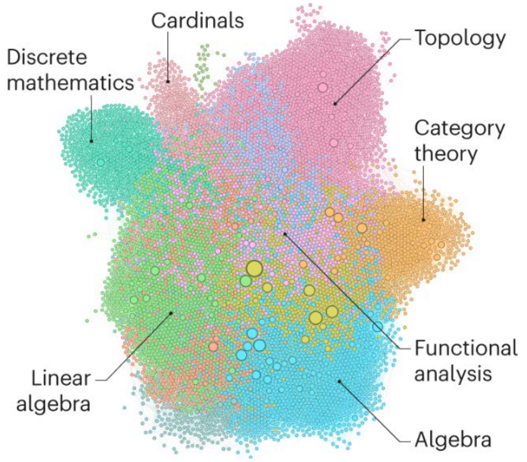
nature

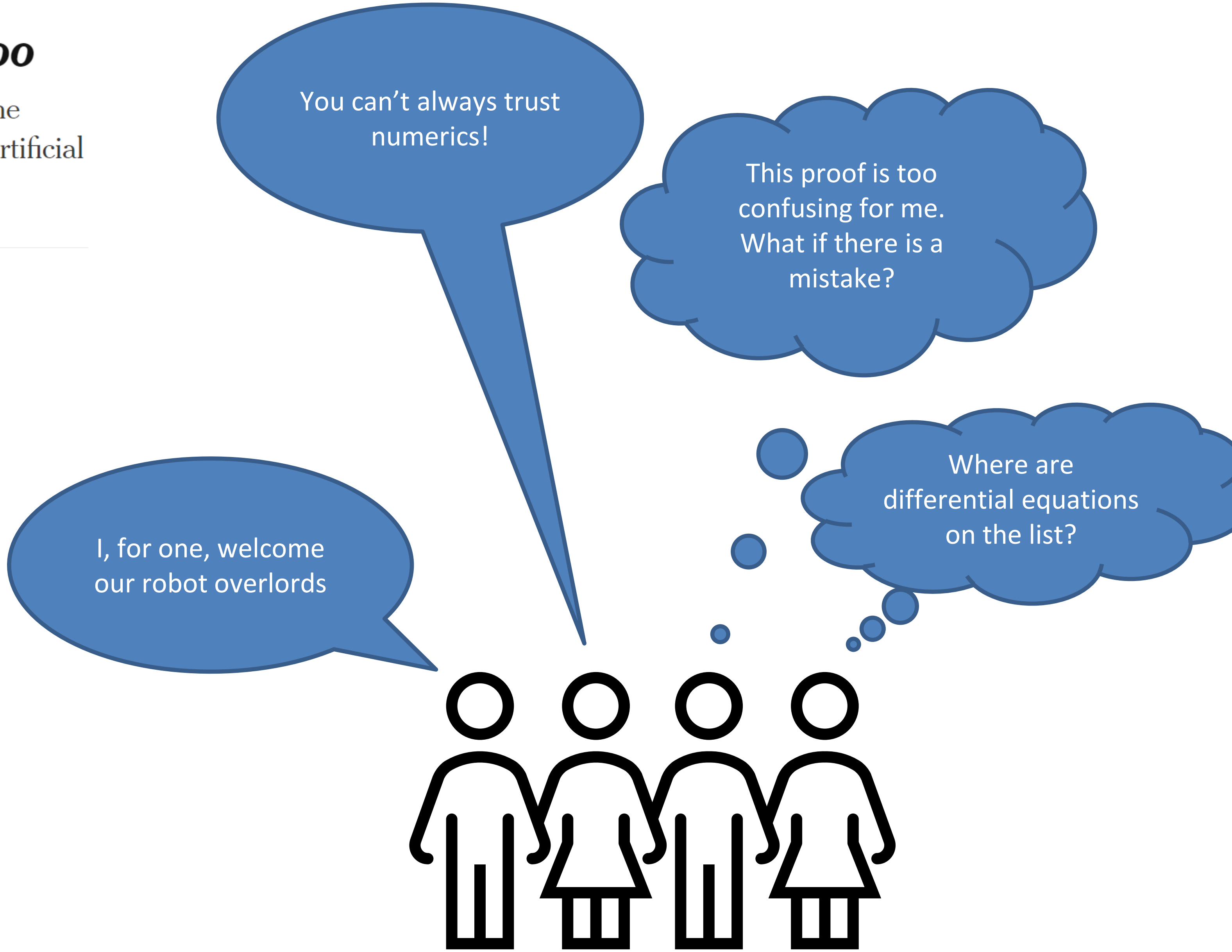
NEWS | 18 June 2021

Mathematicians welcome computer-assisted proof in 'grand unification' theory

Proof-assistant software handles an abstract concept at the cutting edge of research, revealing a bigger role for software in mathematics.

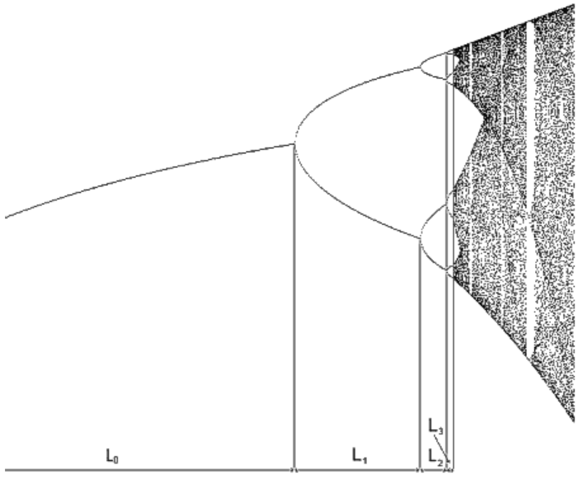
Davide Castelvecchi

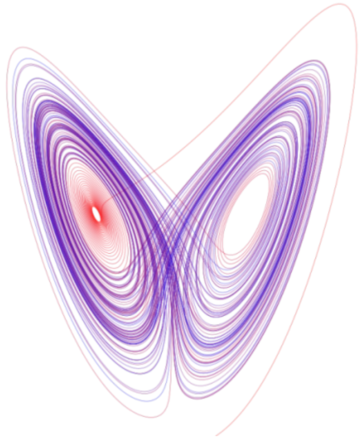


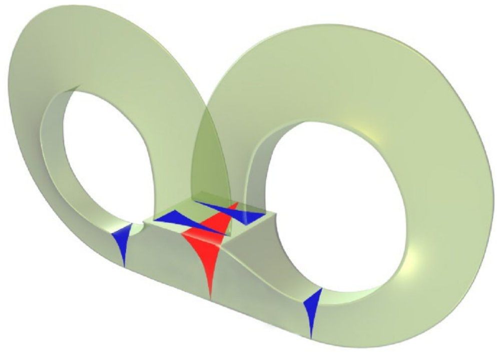


Computer Assisted Proofs in Dynamics

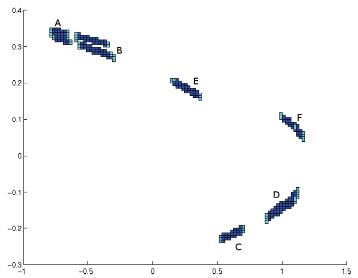
- Feigenbaum Conjectures
  - All unimodal maps undergo period doubling cascades at the same rate
    - *Lanford 1982*
- Early work in PDEs
  - Solving nonlinear BVPs with finite element method
    - *Nakao 1991; Plum 1992*
- Lorenz equation & Smale's 14th problem
  - The Lorenz eq. is chaotic and its attractor is strange
    - *Mischaikow & Mrozek 1998; Tucker 2002*
- Wright's conjecture (1955)
  - Characterizes the global attractor of Wright's delay differential equation
    - *v/d Berg & **JJ** 2018; **JJ** 2019*



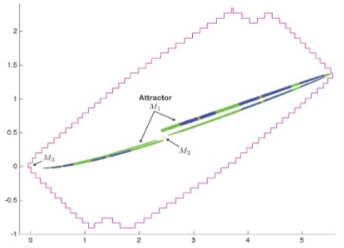




Global Dynamics

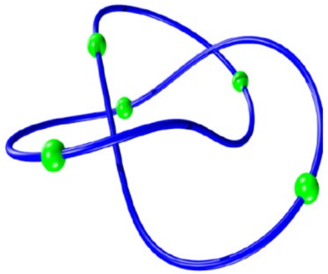


Henon Attractor, Bounds on Topological Entropy
Day, Frongillo, Treviño 2008

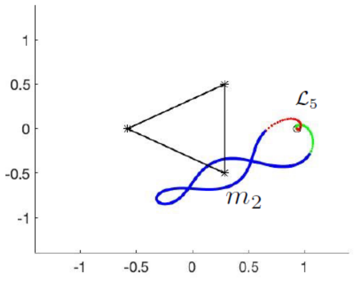


Kot-Schaffer attractor
Day, Kalies (2013)

Celestial Mechanics

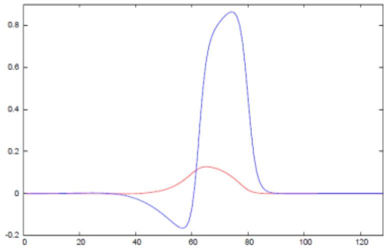


Choreography of n-bodies
Calleja et al. 2019

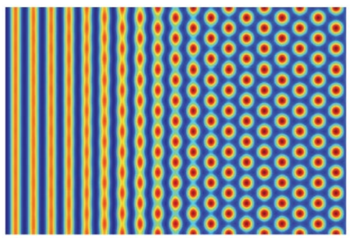


Homoclinic Tangles in CRFBP
Murray, Mireles-James 2020

Traveling Waves

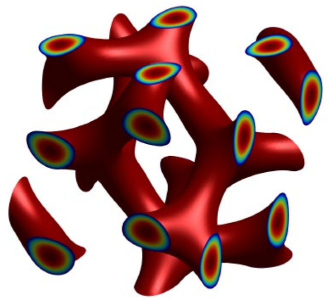


Existence & Stability of Pulses in FitzHugh-Nagumo PDE
Arioli, Koch 2015

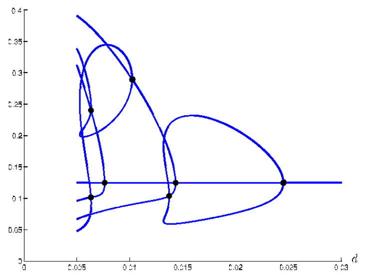


Coexistence of Hexagons & Rolls
v.d. Berg et al. 2015

Equilibria in PDE



Equilibria of 3D Ohta-Kawasaki
v.d. Berg, Williams 2019

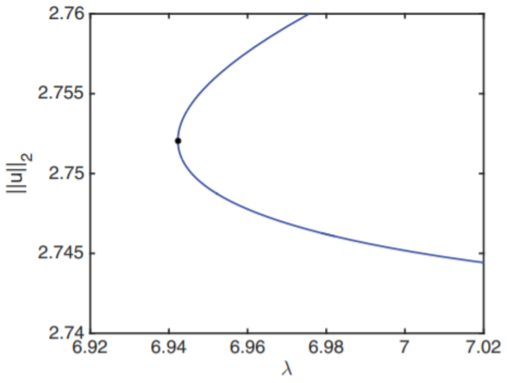


Validated Bifurcation Diagram
Breden, Lessard, Vanicat 2013

Why use *validated* numerics?

- Standard numerics don't come with error bounds
  - But they do converge "in the limit"
- Validated numerics & CAPs tell us when to turn off the computer

Continuation by *Auto*
(non-validated)

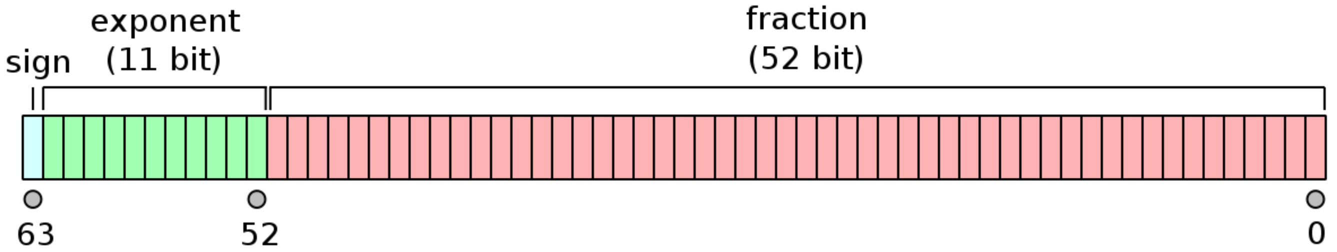


Sander & Wanner (2016)

How computers assist:

IEEE (double precision) floating point standard provides a useful model of a certain subset of $\mathbb{R}$.

64 bit representation



https://en.wikipedia.org/wiki/Double-precision_floating-point_format#:~:text=Double%2Dprecision%20floating%2Dpoint%20format%20(sometimes%20called%20FP64%20or,using%20a%20floating%20radix%20point.

In binary:

$\frac{1}{3} = 0.01010101\overline{10}$

$\frac{1}{10} = 0.0001100\overline{1100}$

Adding (subtracting/multiplying/dividing) two such numbers and forcing the result to have this form (typically) results in a rounding error.

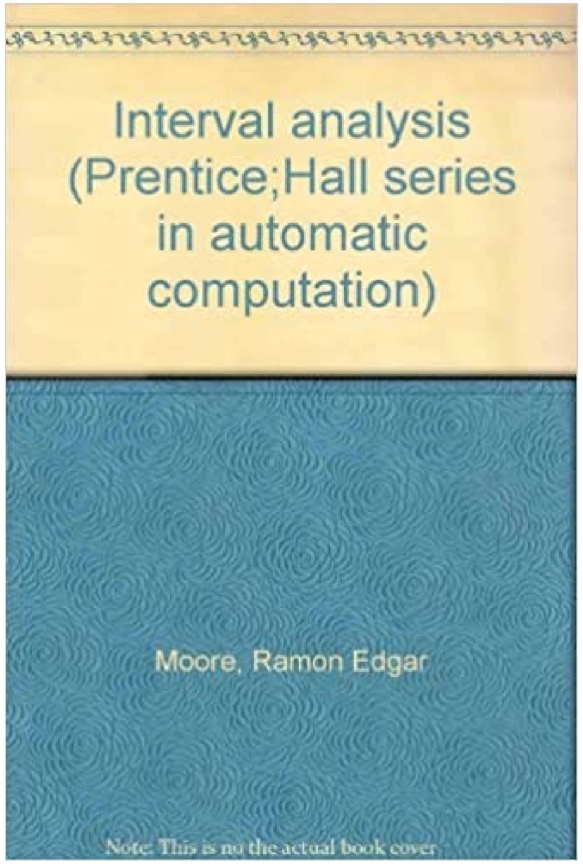
Our fancy computers are not even able to add!

But, IEEE standard requires that – if the numbers are in a certain range– then the result is wrong by at most one rounding operation.

That is, if you compute twice – once rounding up, and once rounding down – then you enclose the correct result.

This is the basis of interval arithmetic/interval analysis.

How computers assist:



- **ASIN : B0000CNI29**
- **Publisher :** Prentice Hall; First Edition (January 1, 1966)
- **Language : German**
- **Hardcover : 145 pages**
- **Item Weight : 2.14 pounds**

R. Moore - 1966

How computers assist:

Example: Consider the classical formula

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}$$

Using Rump's Intlab (using Matlab) we compute

$$1.643934566681450 \leq \sum_{n=1}^{1,000} \frac{1}{n^2} \leq 1.643934566681670 \quad (0.1\ sec)$$

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Bound the "tail" by comparing to an integral

$$\frac{1}{N+1} \leq \int_{N+1}^{\infty} \frac{1}{x^2}\,dx \leq \sum_{n=N+1}^{\infty} \frac{1}{n^2} \leq \int_{N}^{\infty} \frac{1}{x^2}\,dx \leq \frac{1}{N}$$

We then get bounds:

$$\frac{\pi^2}{6} \in [1.644933567680451, 1.644934566681670]$$

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Summary

- Computation time: $\approx 10^{-4} \times N\ sec$
- Error bound on the sum: $\approx 10^{-16} \times N$
- Error bound on the tail: $= \frac{1}{N} - \frac{1}{N+1} \approx \frac{1}{N^2}$

Improvements:

- Sum from smallest to largest!
- Use another formula, e.g.

$$\frac{1}{\pi} = \sum_{n=0}^{\infty}\binom{2n}{n}^3 \frac{42n+5}{2^{12n+4}}$$

Easy Part: living with rounding error

- **Interval arithmetic**
  - Define real intervals as
    $\mathbb{IR} = \{[a, b] \subseteq \mathbb{R} : a \leq b\}$
  - Define operations $\star \in \{+, -, \times, /\}$ as
    $A \star B = \{\alpha \star \beta : \alpha \in A, \beta \in B\}$
- It's not a bug, it's a feature!
  - Evaluates functions not just at points, but over sets!

Examples

$$[1,2] + [3,4] = [4,6]$$

$$[1,2] - [3,4] = [-3, -1]$$

$$[1]/[3] \in [\, 0.33, 0.34]$$

$$\pi \in [\, 3.1, 3.2]$$

$$\pi^2 \in [\, 9.61, 10.24]$$

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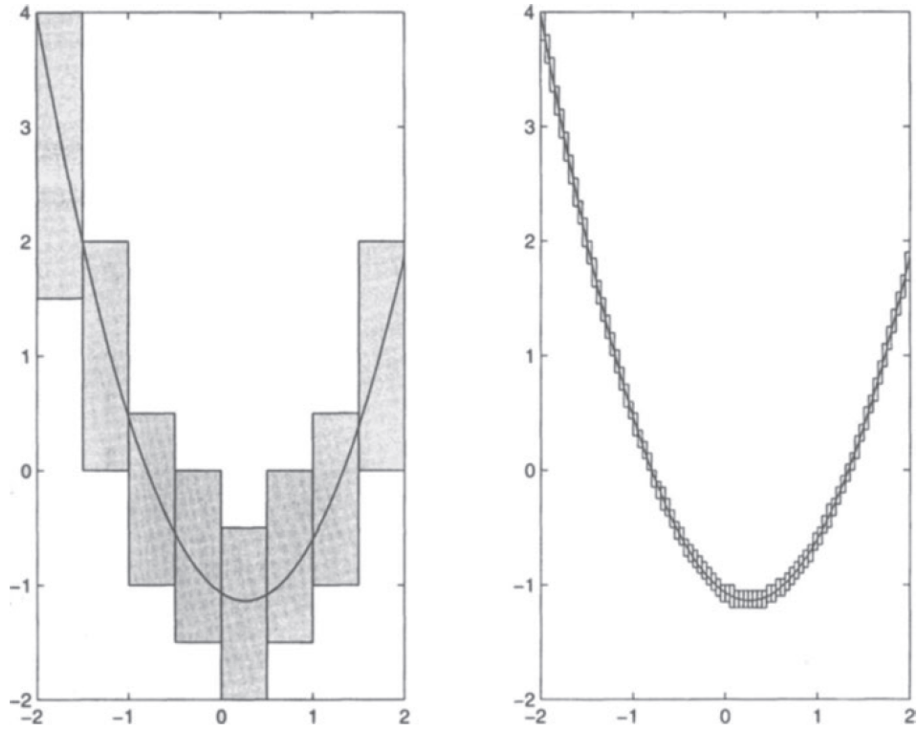


Fig. 5.3. Graphs of the multivalued approximation to $f(x) = (3x-4)(5x+4)/15$ obtained by means of interval arithmetic based on different basic lengths: 0.5 for the left graph and 0.05 for the right graph.

$f(x) = x^5 - x + 1$

- **Goal:** Solve $f(x) = 0$
- Consider interval $I = [-2, -1]$

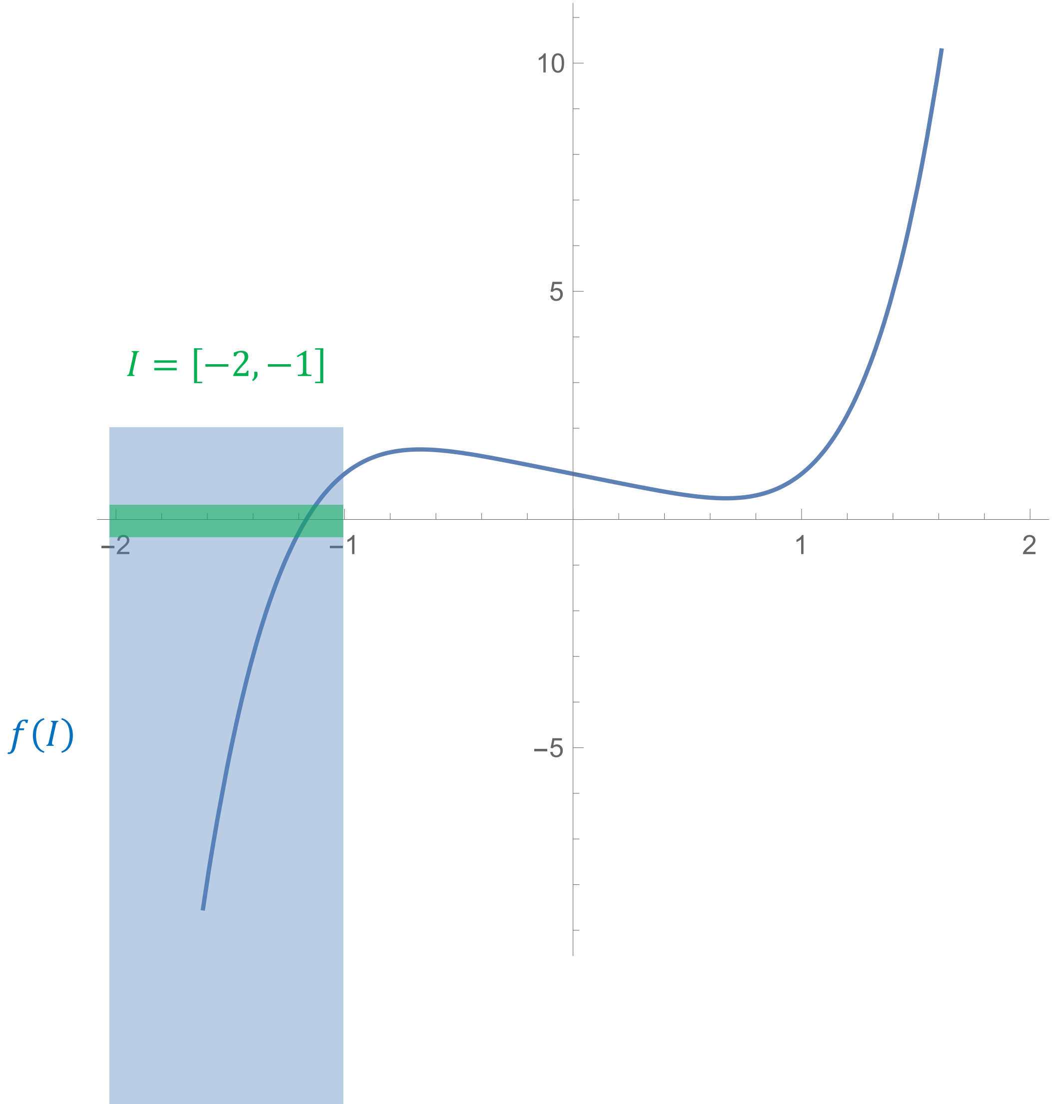
  $f(I) = [-2,-1]^5 - [-2,-1] + [1,1]$

  $= [-32,-1] + [2,3]$

  $= [-30, 2]$

Theorem (with computer assisted proof): There exists a unique $\tilde{x} \in [-2,-1]$ such that $f(\tilde{x}) = 0$.

- Use intermediate value theorem to show that a solution exists
  - $f(-2) = -29 < 0$
  - $f(-1) = +1 > 0$
- Uniqueness
  - $f'(I) = [\,4,\ 79\,] > 0$



Typical CAP of $f(x) = 0$

Approximate Solution

- Asymptotic expansion
- Standard numerics
- Machine learning

+

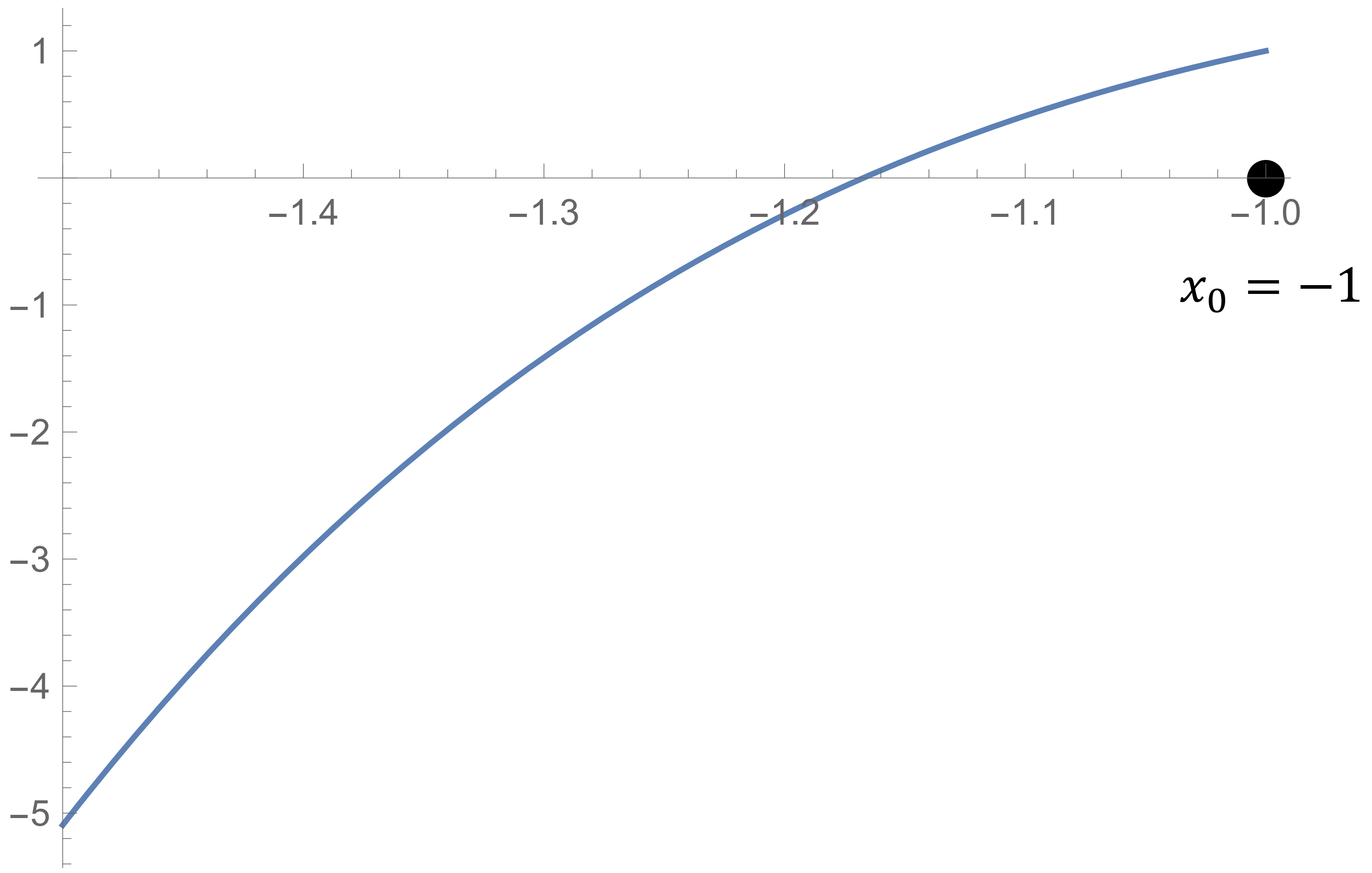
Explicit Theorem

- Proof checks a FINITE # of conditions / inequalities
- Not " … $\exists \epsilon > 0$ … "

→

Computer Assisted Proof

Newton's method: $x_{n+1} = x_n - f'(x_n)^{-1} f(x_n)$



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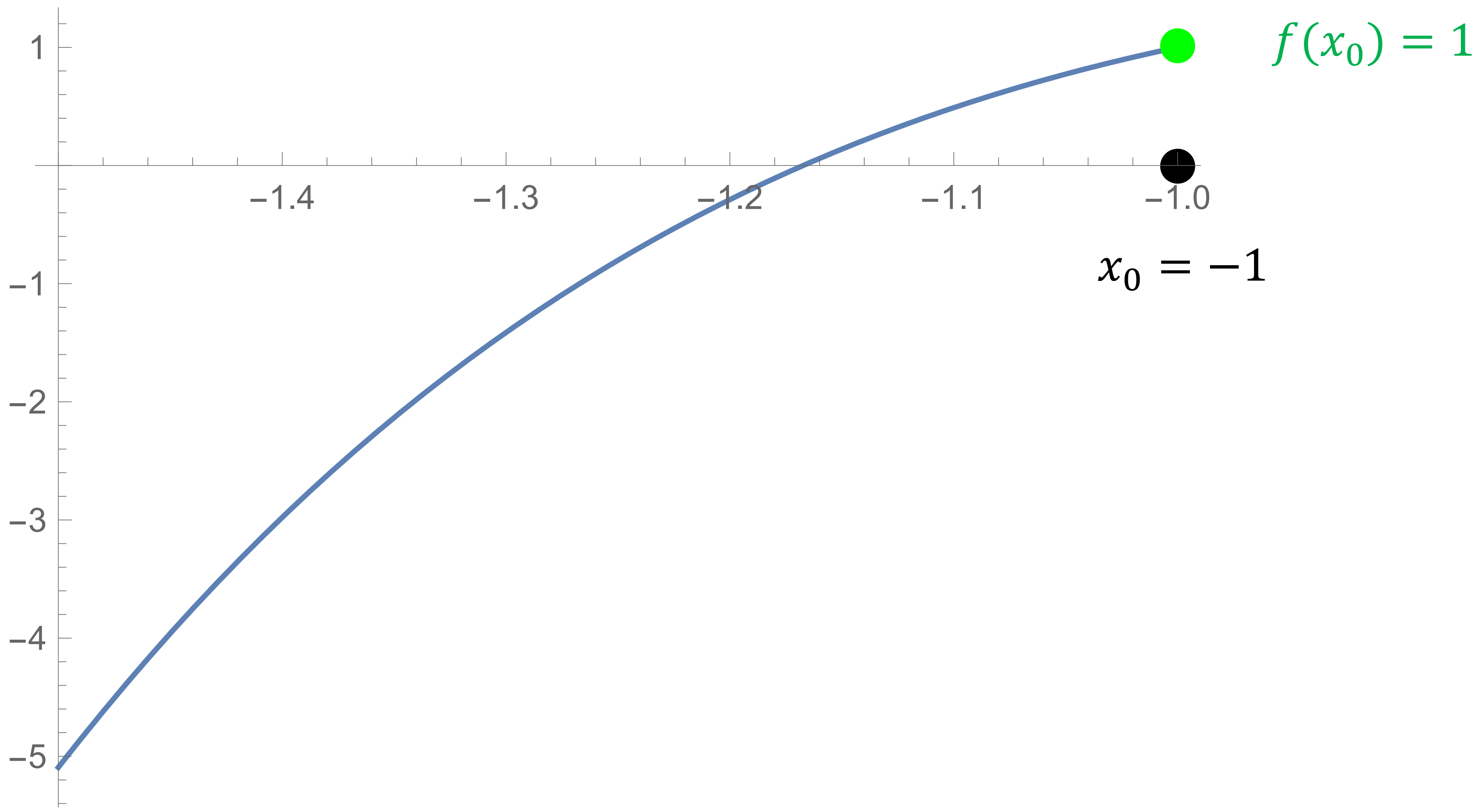

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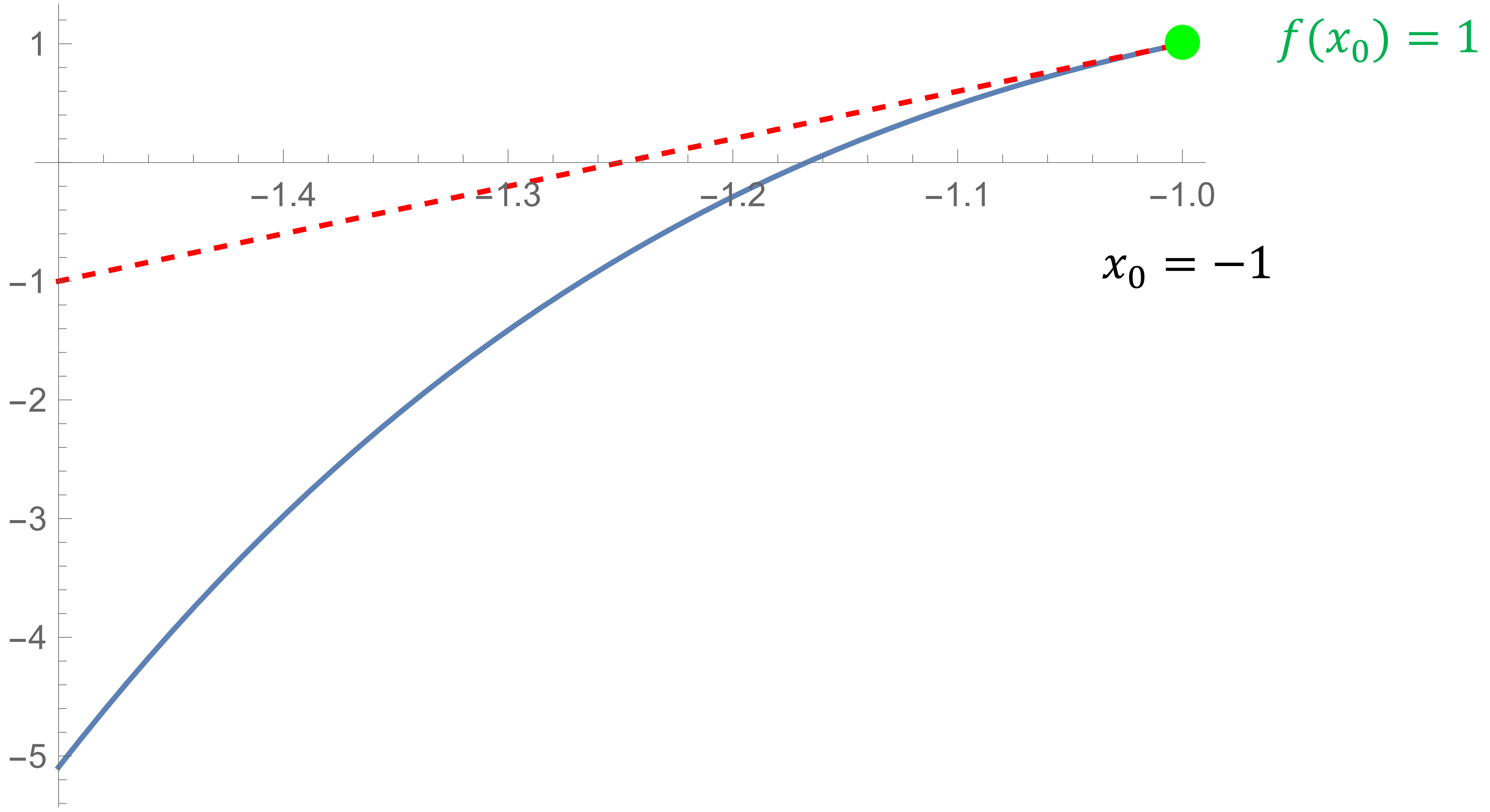

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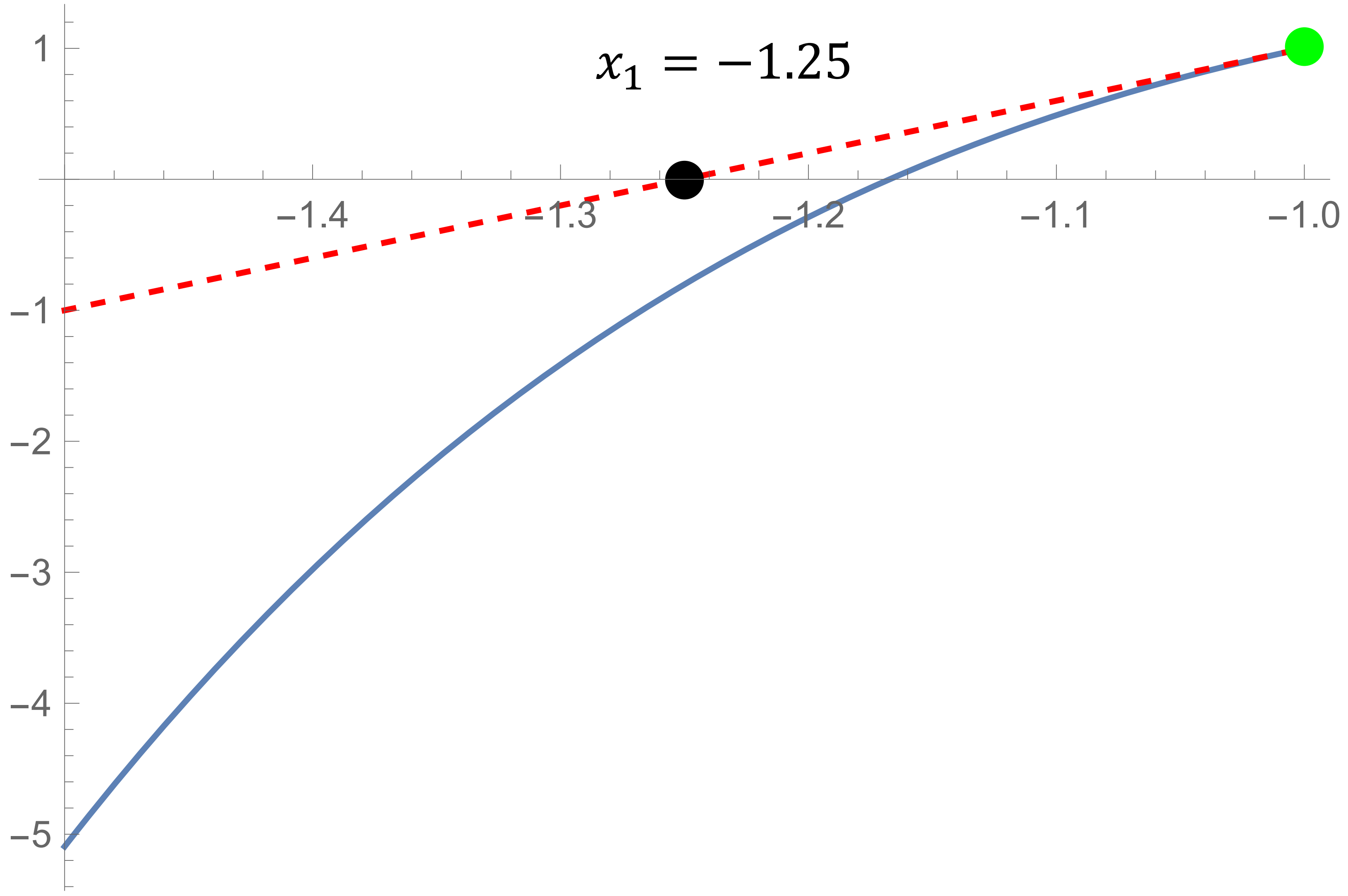

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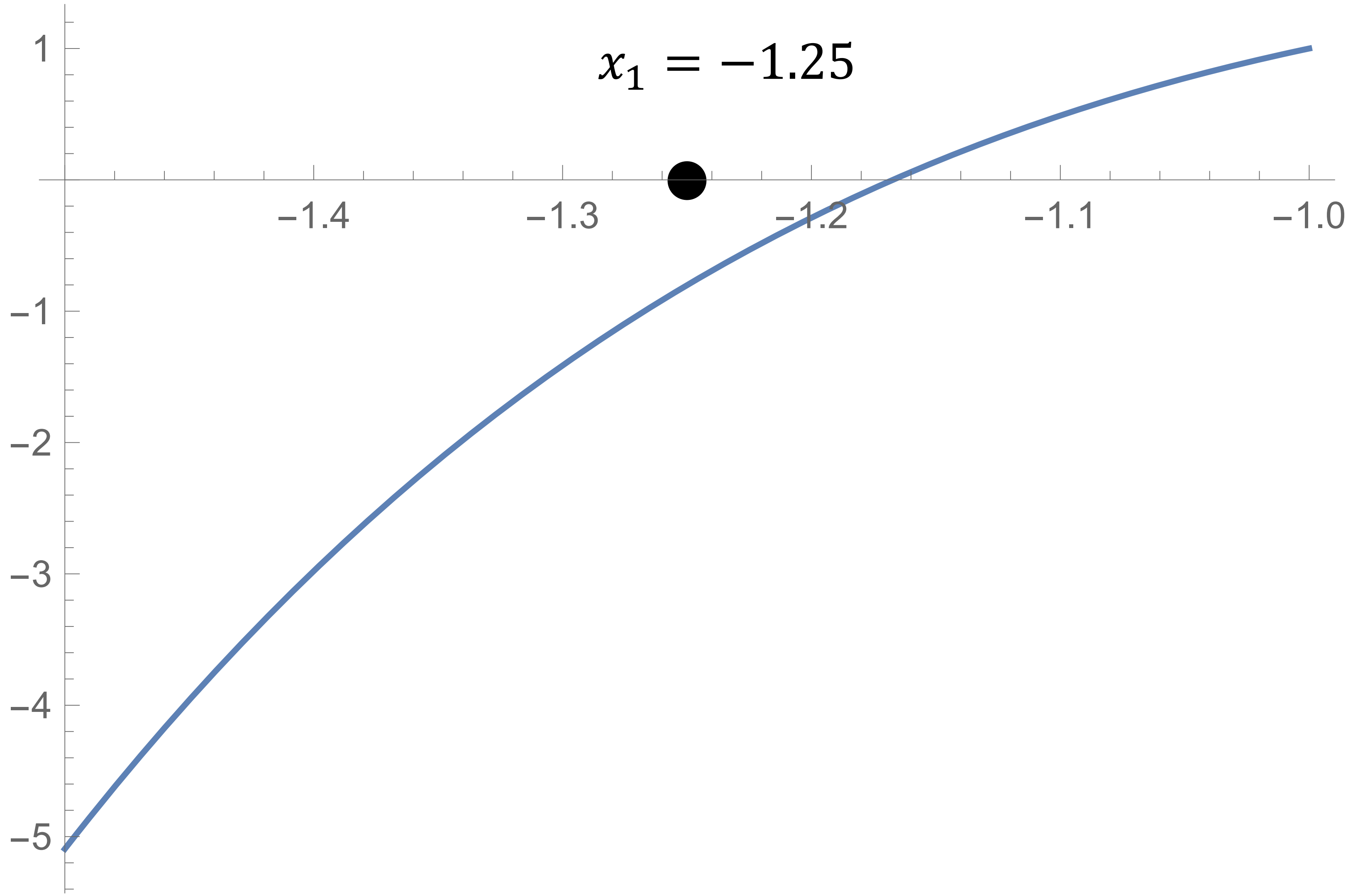

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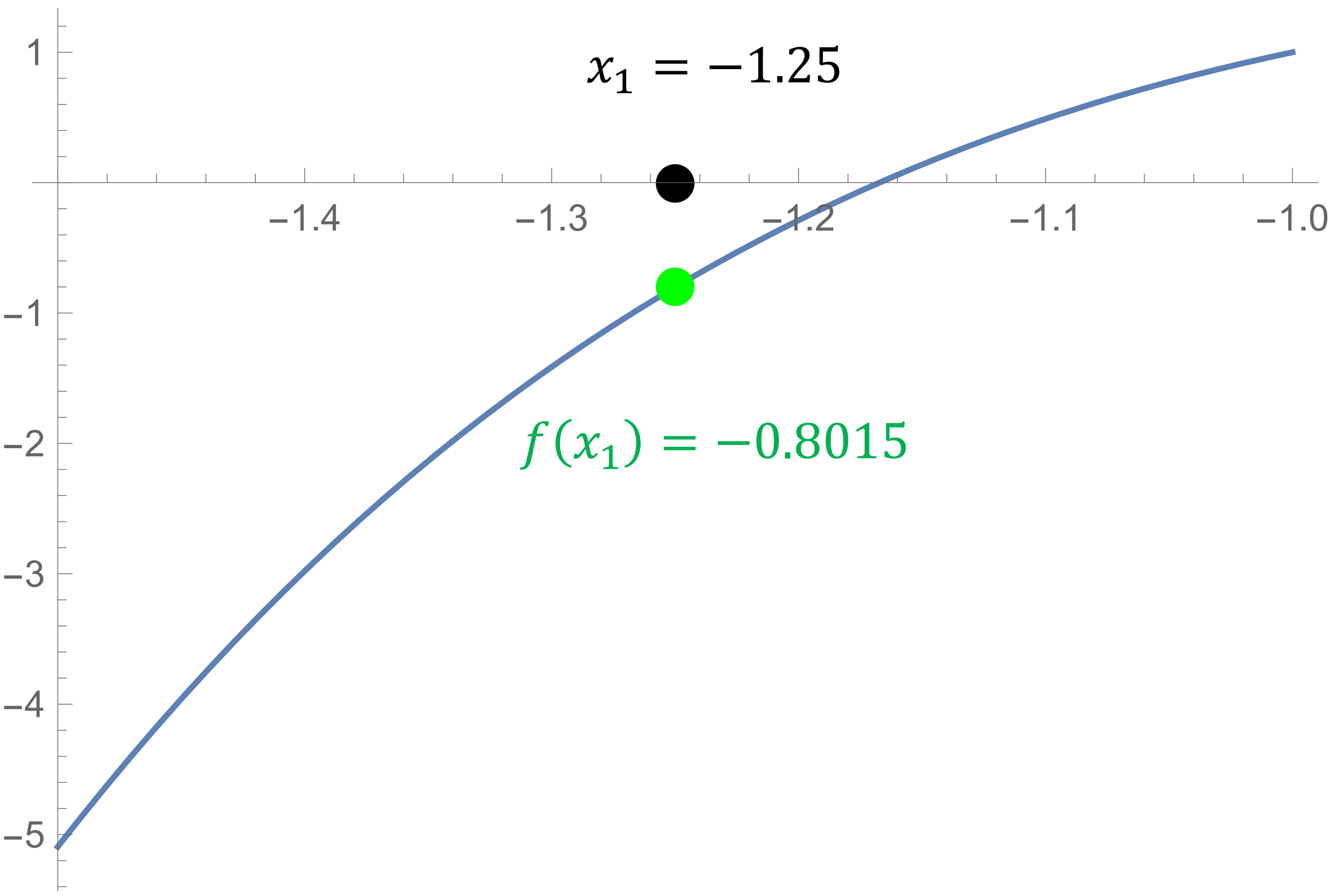
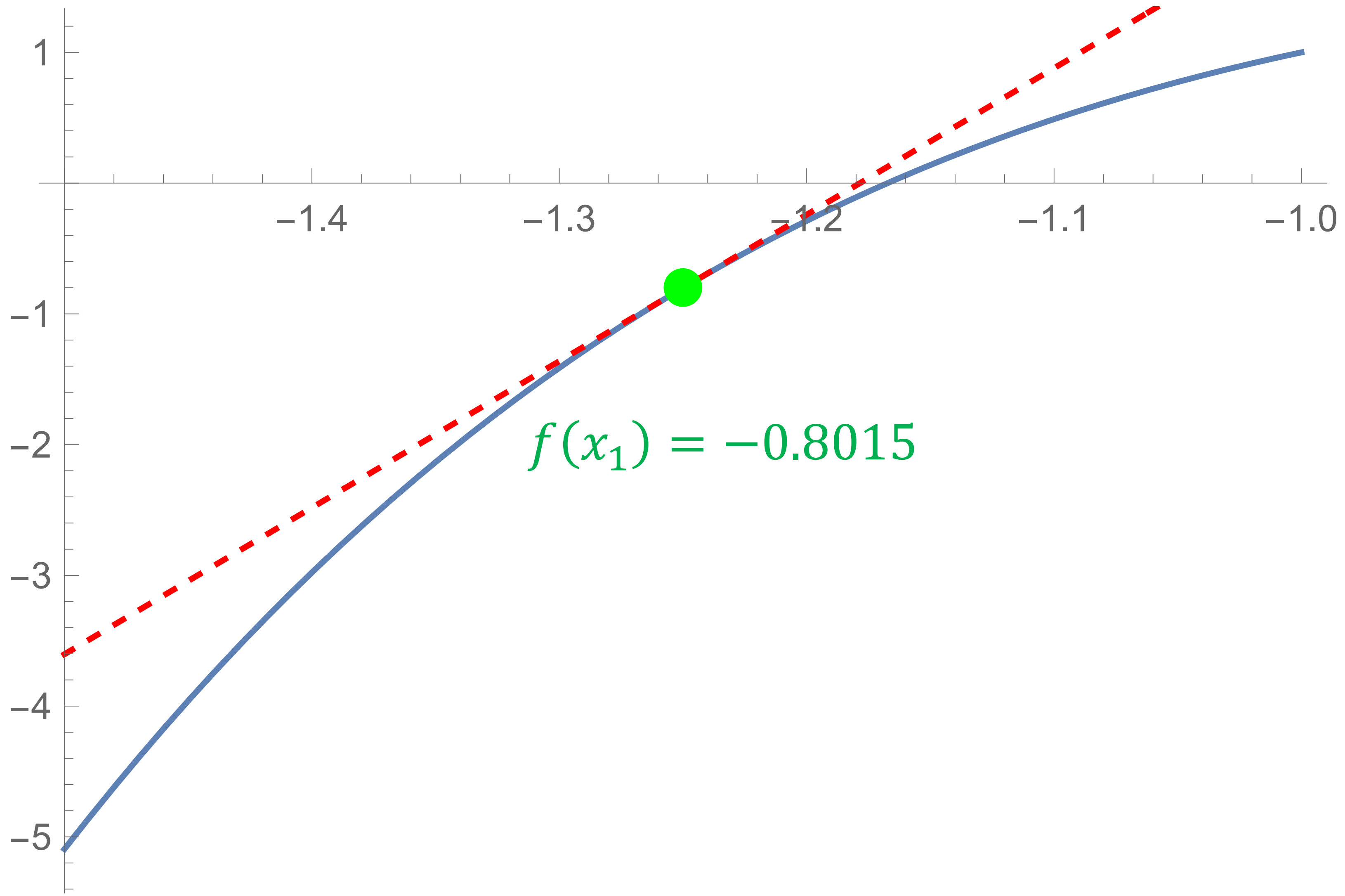


Newton's method: $x_{n+1} = x_n - f'(x_n)^{-1} f(x_n)$



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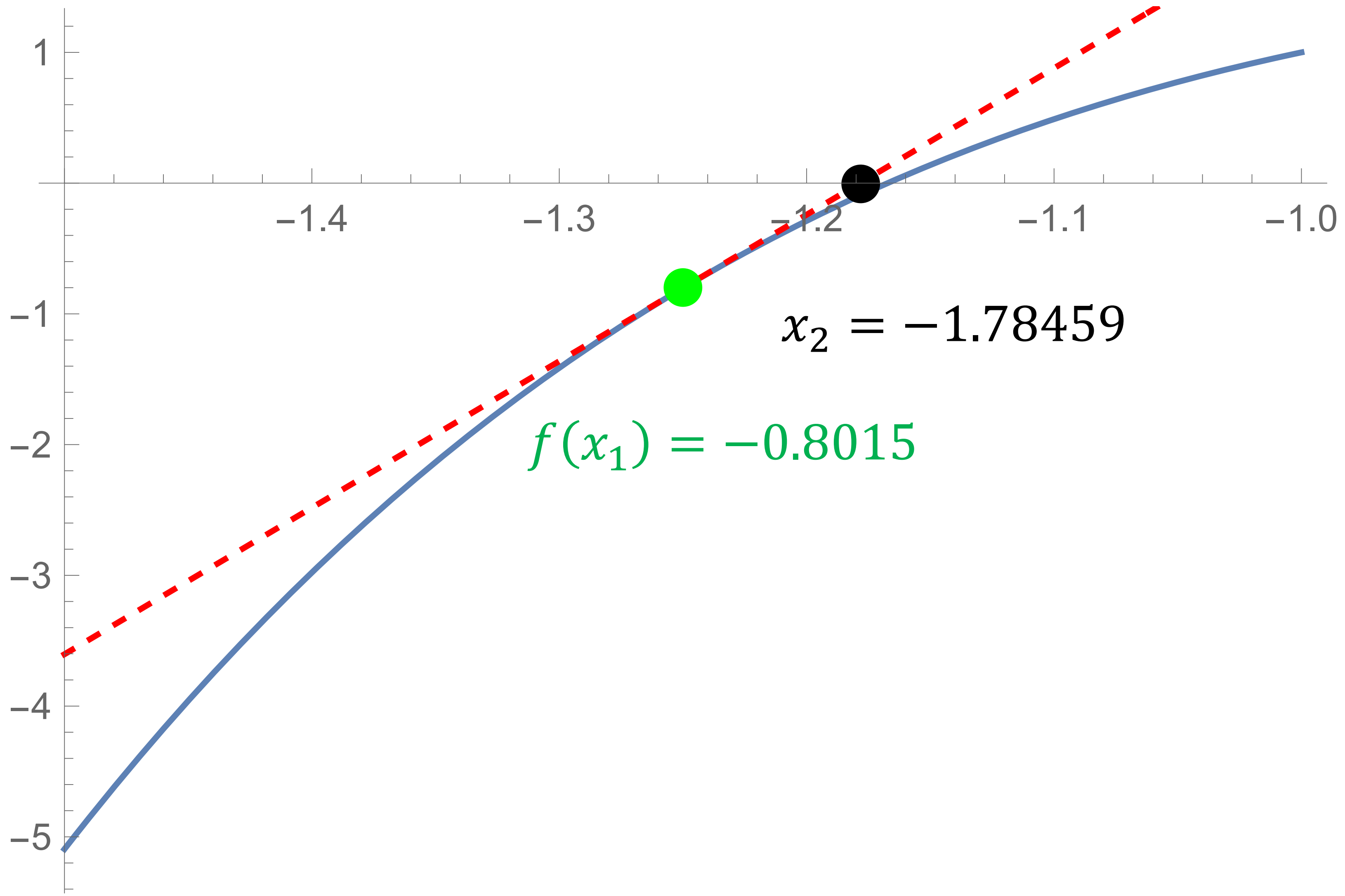

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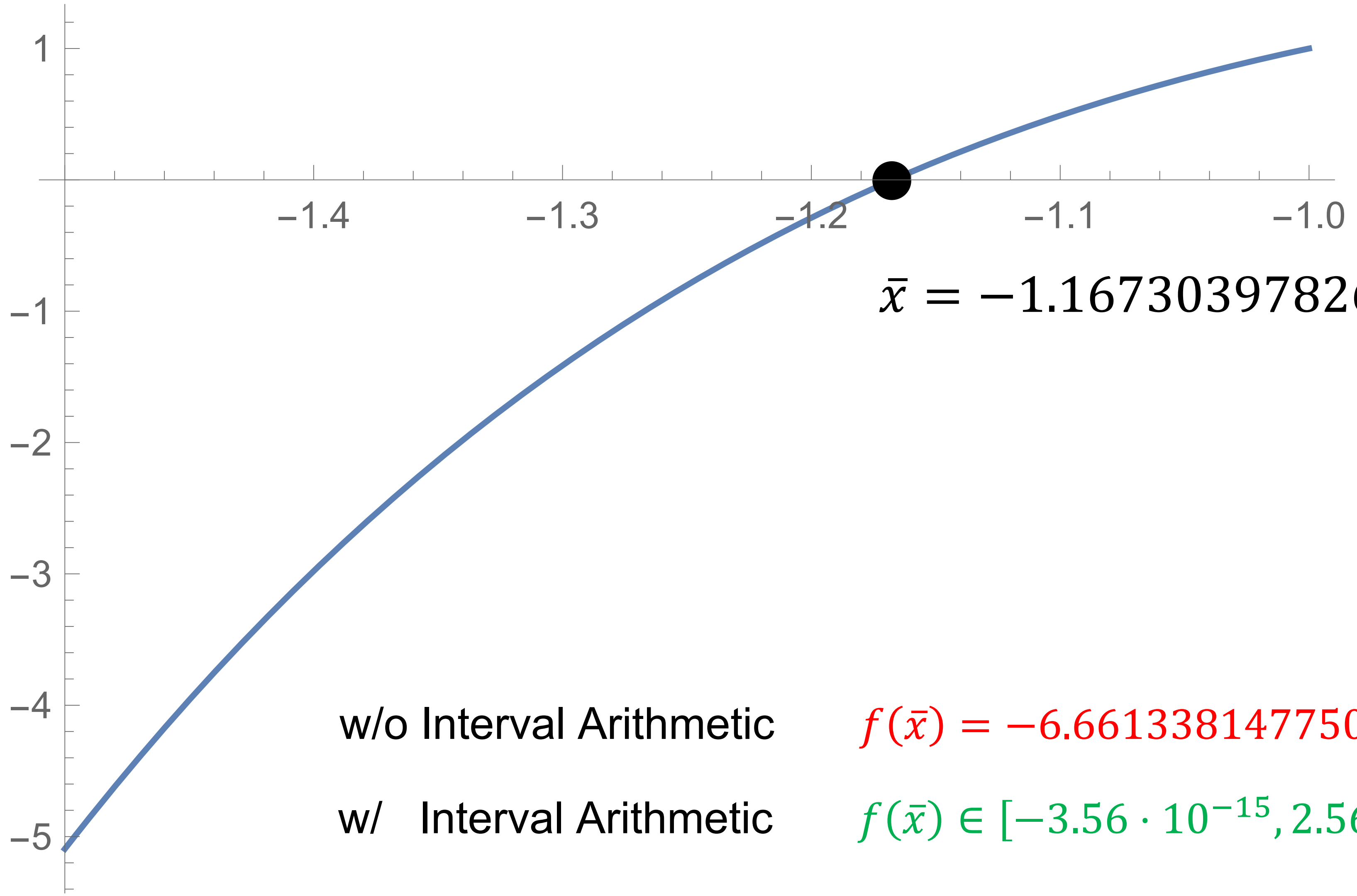


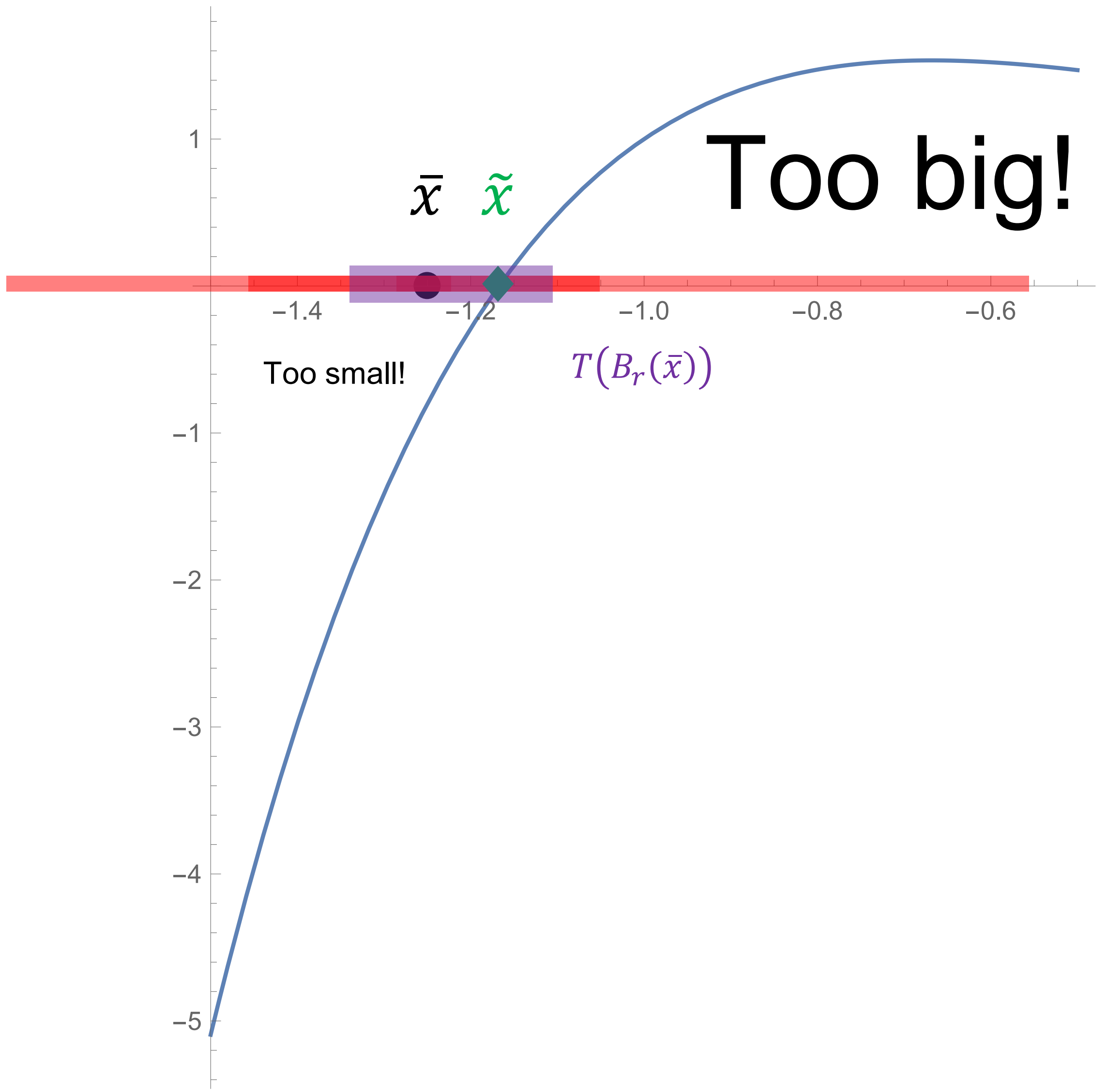
$\bar{x} = -1.1673039782614187$

w/o Interval Arithmetic $f(\bar{x}) = -6.661338147750939 \cdot 10^{-16}$

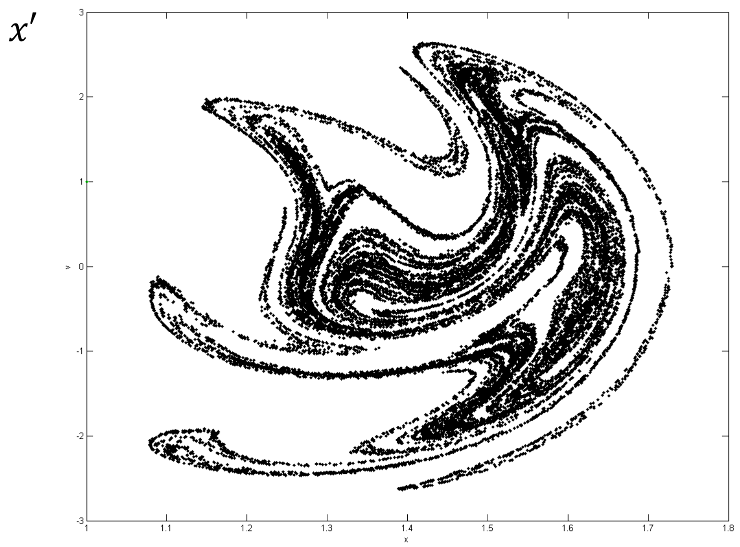
w/ Interval Arithmetic $f(\bar{x}) \in [-3.56 \cdot 10^{-15}, 2.56 \cdot 10^{-15}]$

How to prove $f(x) = 0$

- **Define:** Newton map
  $$T(x) = x - f'(x)^{-1} f(x)$$
- **Define:** $B_r(\bar{x})$, a closed ball about $\bar{x}$ of radius r
- **Goal:** Show that T is a **contraction mapping:**
  – T maps $B_r(\bar{x})$ into itself
  – points get closer together
- **Th'm:** If T is a contraction, then $B_r(\bar{x})$ contains a unique fixed point $\tilde{x}$
  $$T(\tilde{x}) = \tilde{x} \quad \Leftrightarrow \quad f(\tilde{x}) = 0$$
- How to choose the right value of $\boldsymbol{r}$?



Hard Part: ∞-dimensional problems



Poincare section of the Duffing equation with $\alpha = 1, \beta = 5, \epsilon = 0.02, \gamma = 8, \omega = 0.5.$
Image Credit: Wikipedia

Consider the Duffing equation for a **damped driven oscillator**

$$x'' + \epsilon\, x' + \alpha x + \beta x^3 = \gamma \cos \omega t$$

To look for 2π periodic solution ($\omega = 1$), expand $x(t)$ as a Fourier series

$$x(t) = \sum_{k \in \mathbb{Z}} a_k\, e^{ikt}$$

where $a_{-k} = (a_k)^*$. Inserting into the ODE, we obtain

$$\sum_{k\in\mathbb{Z}} (-k^2 + i\epsilon k + \alpha) a_k e^{ikt} + \beta \left(\sum_{k\in\mathbb{Z}} a_k e^{ikt} \right)^3 = \gamma\, (e^{it} + e^{-it})/2$$

Matching the e^{ikt} terms, we obtain equations $\forall k \in \mathbb{Z}$

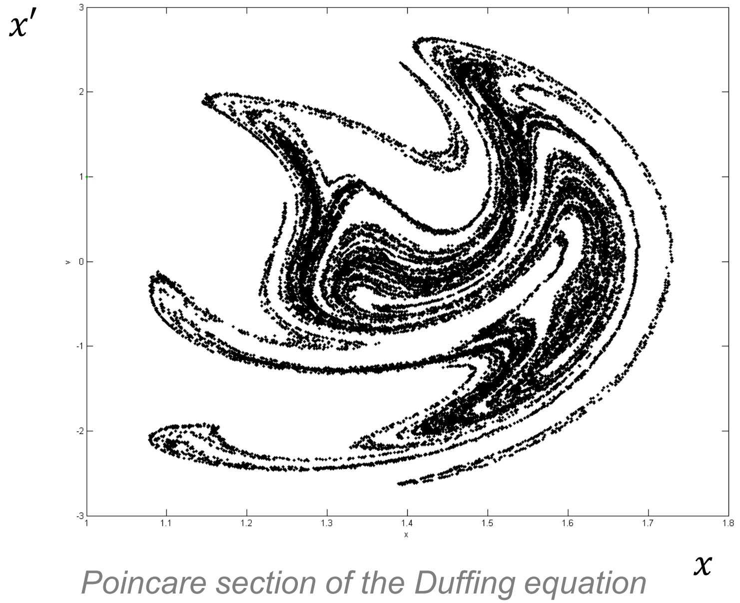
$$0 = (-k^2 + i\epsilon k + \alpha) a_k + \beta \sum_{\substack{k_1+k_2+k_3=k;\\ k_1,k_2,k_3\in\mathbb{Z}}} a_{k_1} a_{k_2} a_{k_3} - \gamma \delta_{1,k}/2$$

$$\stackrel{\text{def}}{=} f_k(a)$$

$$f_k(a) \approx (-k^2 + i\epsilon k) a_k + \mathcal{O}\left(\|a\|_{\ell^1}^3\right)$$

$$a_k = \mathcal{O}\left(\frac{1}{k^2}\right)$$

Hard Part: ∞-dimensional problems



Poincare section of the Duffing equation with $\alpha = 1, \beta = 5, \epsilon = 0.02, \gamma = 8, \omega = 0.5$.
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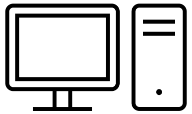
- **Theorem:** A periodic orbit $x(t)$ is equivalent to a solution $f(a) = 0$
- **Define:** Galerkin truncation $f^N: \mathbb{R}^{2N+1} \to \mathbb{R}^{2N+1}$
  - Find approximate solution $\hat{a} \in \mathbb{R}^{2N+1}$ such that $f^N(\hat{a}) \approx 0$
- **Define:** Quasi-Newton map on the whole ∞-dimensional space
  $$T(a) = a - Af(a),$$
  $$A \approx Df(\hat{a})^{-1}$$
- **Goal:** Show that T is a **contraction mapping**

Hard Part: ∞-dimensional problems

$$A^N = Df^N(\hat{a})^{-1} \in GL_{2N+1}(\mathbb{R})$$



$$A = \begin{pmatrix} A^N & 0 & 0 \\ 0 & (-k^2 + i\epsilon k)^{-1} & 0 \\ 0 & 0 & \ddots \end{pmatrix}$$

$$f_k(a) \approx (-k^2 + i\epsilon k)a_k + \mathcal{O}\left(\|a\|_{\ell^1}^3\right)$$

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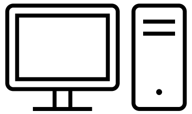


$$A = \begin{pmatrix} A^N & 0 & 0 \\ 0 & (-k^2 + i\epsilon k)^{-1} & 0 \\ 0 & 0 & \ddots \end{pmatrix}$$

$$f_k(a) \approx (-k^2 + i\epsilon k)a_k + \mathcal{O}\left(\|a\|_{\ell^1}^3\right)$$

$$a_k = \mathcal{O}\left(\frac{1}{k^2}\right)$$

Newton-Kantorovich Theorem:

Fix Banach spaces X & Y and $f: X \to Y$ Frechet differentiable, $A: Y \to X$ injective. Fix approx. solution $\hat{a} \in X$ and define

$$T(a) = a - Af(a)$$

with bounds

$$\|T(\hat{a}) - \hat{a}\|_X \leq \epsilon$$
$$\|DT(\hat{a})\|_{B(X)} \leq \delta$$
$$\|DT(c) - DT(\hat{a})\|_{B(X)} \leq \gamma(r)r$$

for all $c \in B_r(\hat{a})$ and $r > 0$.

$f(\hat{a}) \approx 0$

$A \approx Df(\hat{a})^{-1}$

$\gamma \approx \|D^2 f\|$

If $\exists\, r_* > 0$ s.t.

$$\epsilon + \delta r_* + \gamma(r_*)r_*^2 < r_*$$

Then

- The map T is a contraction on $B_{r_*}(\hat{a})$
- There exists a unique $\tilde{a} \in B_{r_*}(\hat{a})$ s.t. $f(\tilde{a}) = 0$

Stages of the CAP

Neumaier's definition:

Stage 1
- Qualitative understanding reduces the problem to a finite number of subproblems

Stage 2
- Reduce each subproblem to a finite number of equations and/or inequalities to be checked

Stage 3
- A specialized computational algorithm is executed

Periodic orbits in Duffing oscillator

Stage 1
- Use Fourier analysis to convert the problem to a $F(x) = 0$

Stage 2
- Derive formulas for ϵ, δ, γ bounds so that a solution exists if $\exists\, r_* > 0$ s.t.

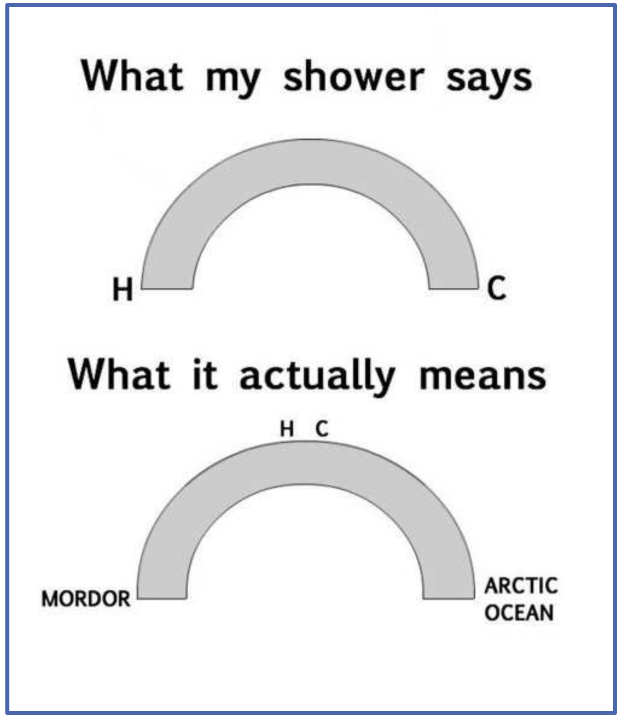
$$\epsilon + \delta r_* + \gamma(r_*) r_*^2 < r_*$$

Stage 3
- Compute everything with interval arithmetic

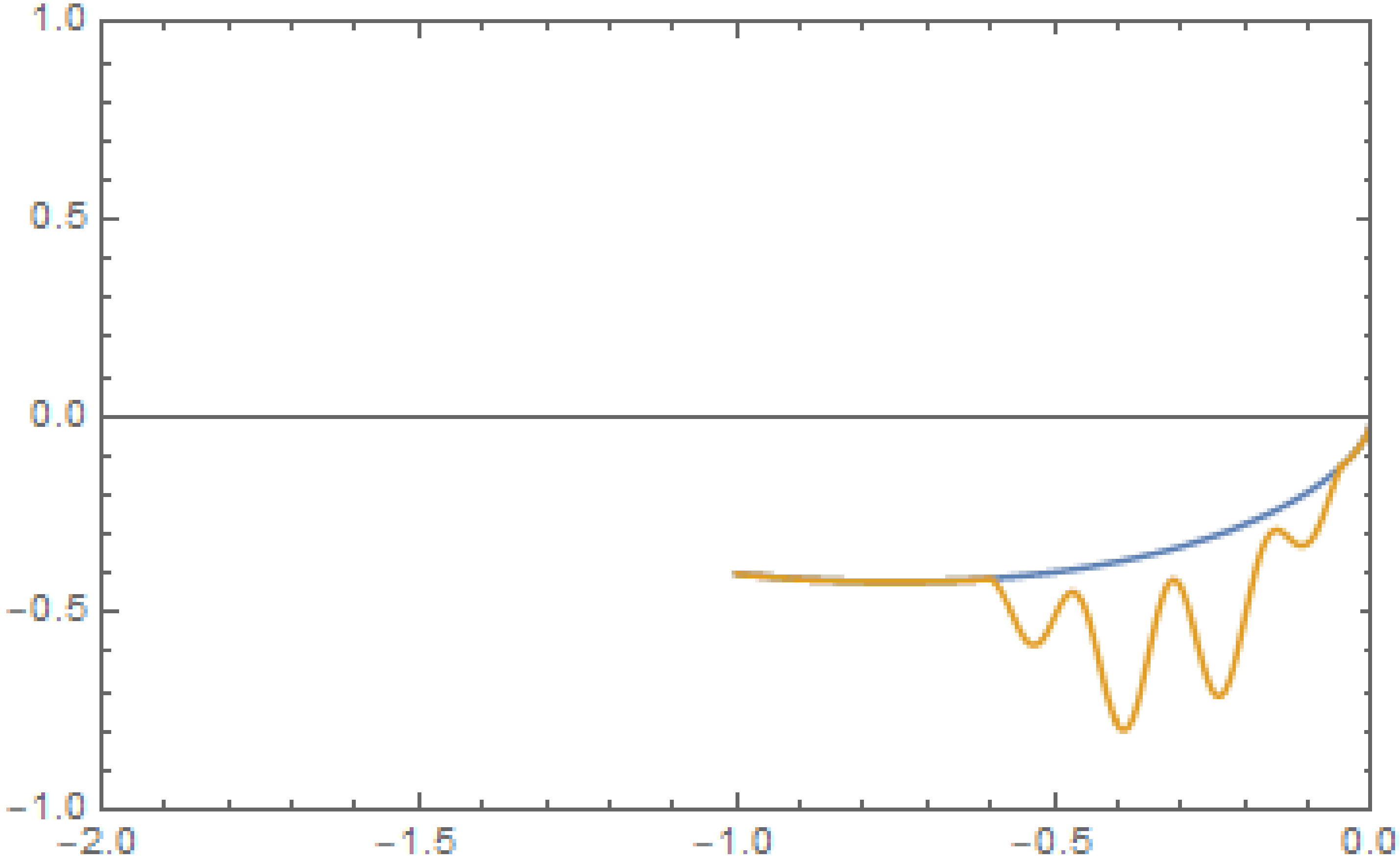
Computer-Assisted Proof of Wright's Conjecture

$$y'(t) = -\alpha\, y(t-1)[1 + y(t)]$$

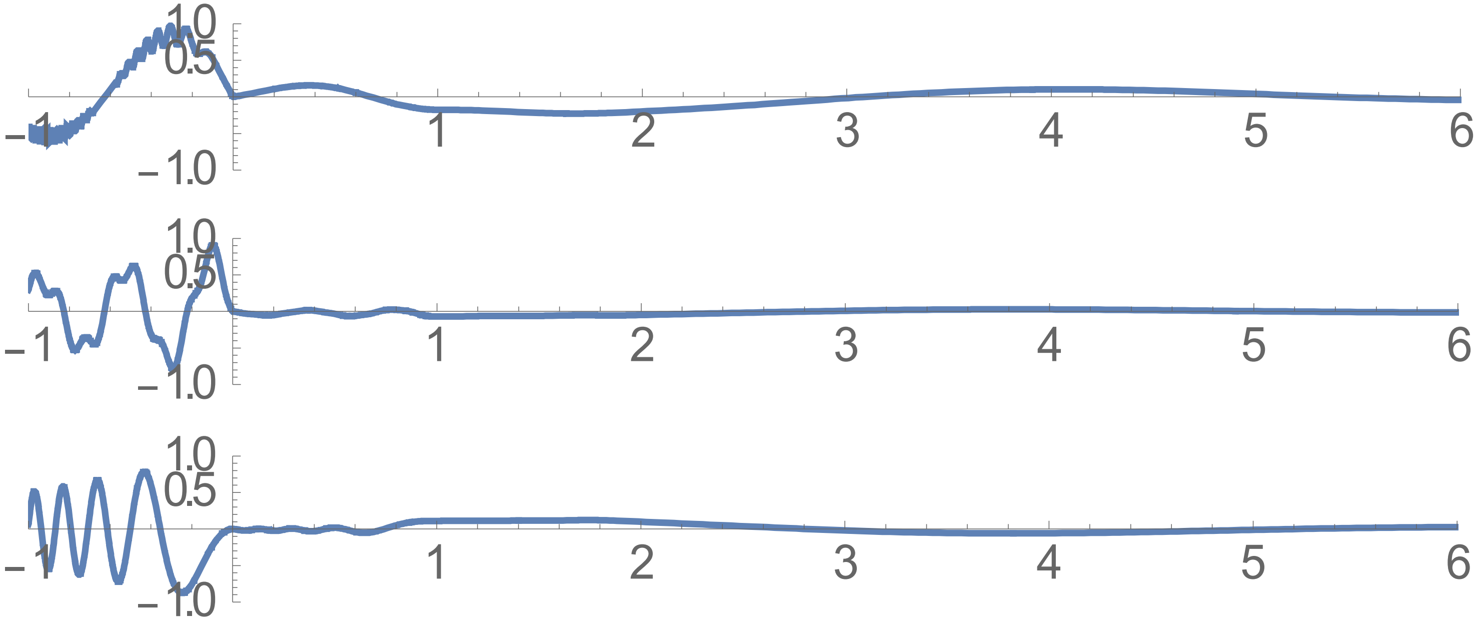
- Wright's equation is used to model
  - Delayed negative feedback
  - Distribution of prime numbers
- It is a Delay Differential Equation (DDE)
  - The derivative $y'(t)$ depends on $y(t)$ and $y(t-1)$
  - Describes the evolution of functions $y: [-1,0] \to \mathbb{R}$



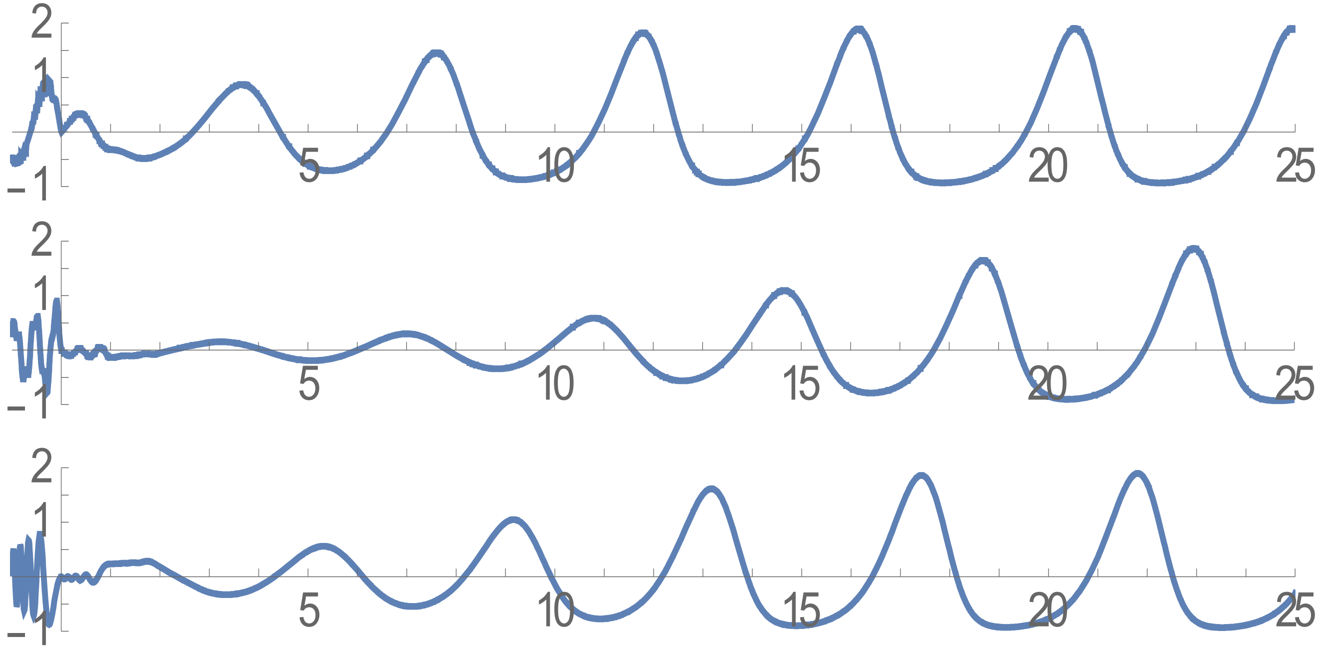
Wright’s Equation



$$y'(t) = -\alpha\, y(t-1)[1 + y(t)]; \qquad \alpha = 1$$



$\alpha = 1$



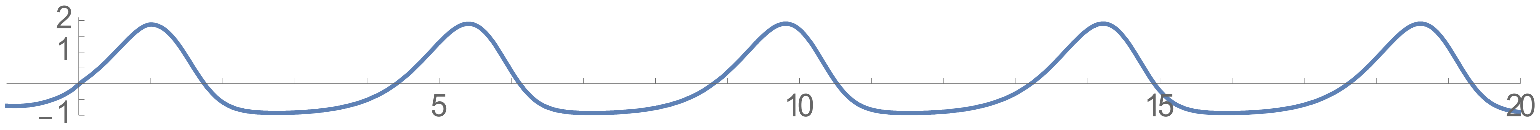
$\alpha = 2$

Wright's Equation

$$y'(t) = -\alpha\, y(t-1)[1 + y(t)]$$

A function is a Slowly Oscillating Periodic Solution (SOPS) if

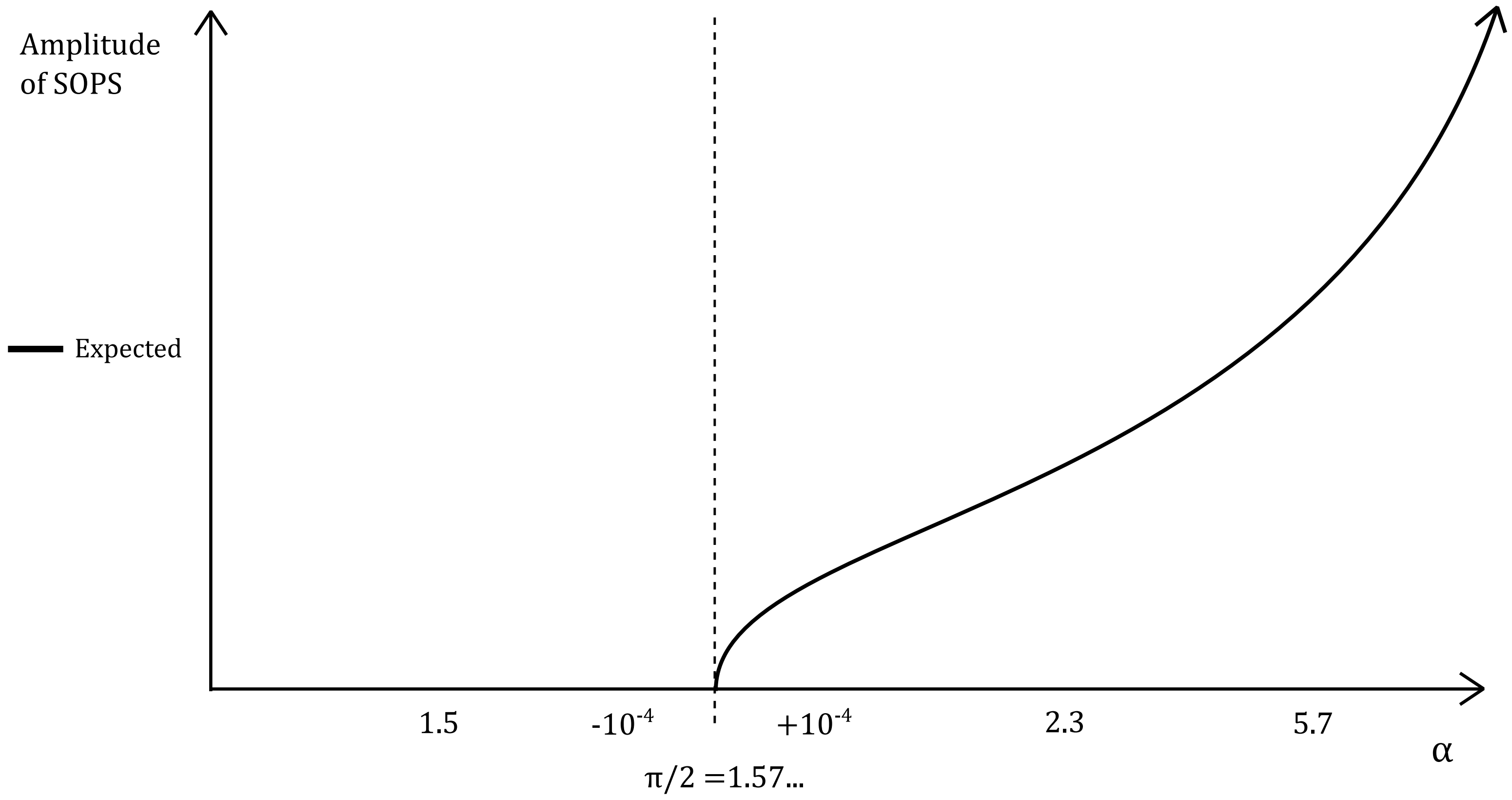
- It is a periodic solution to Wright's equation
- It is **positive** for at least one time unit
- It is **negative** for at least one time unit



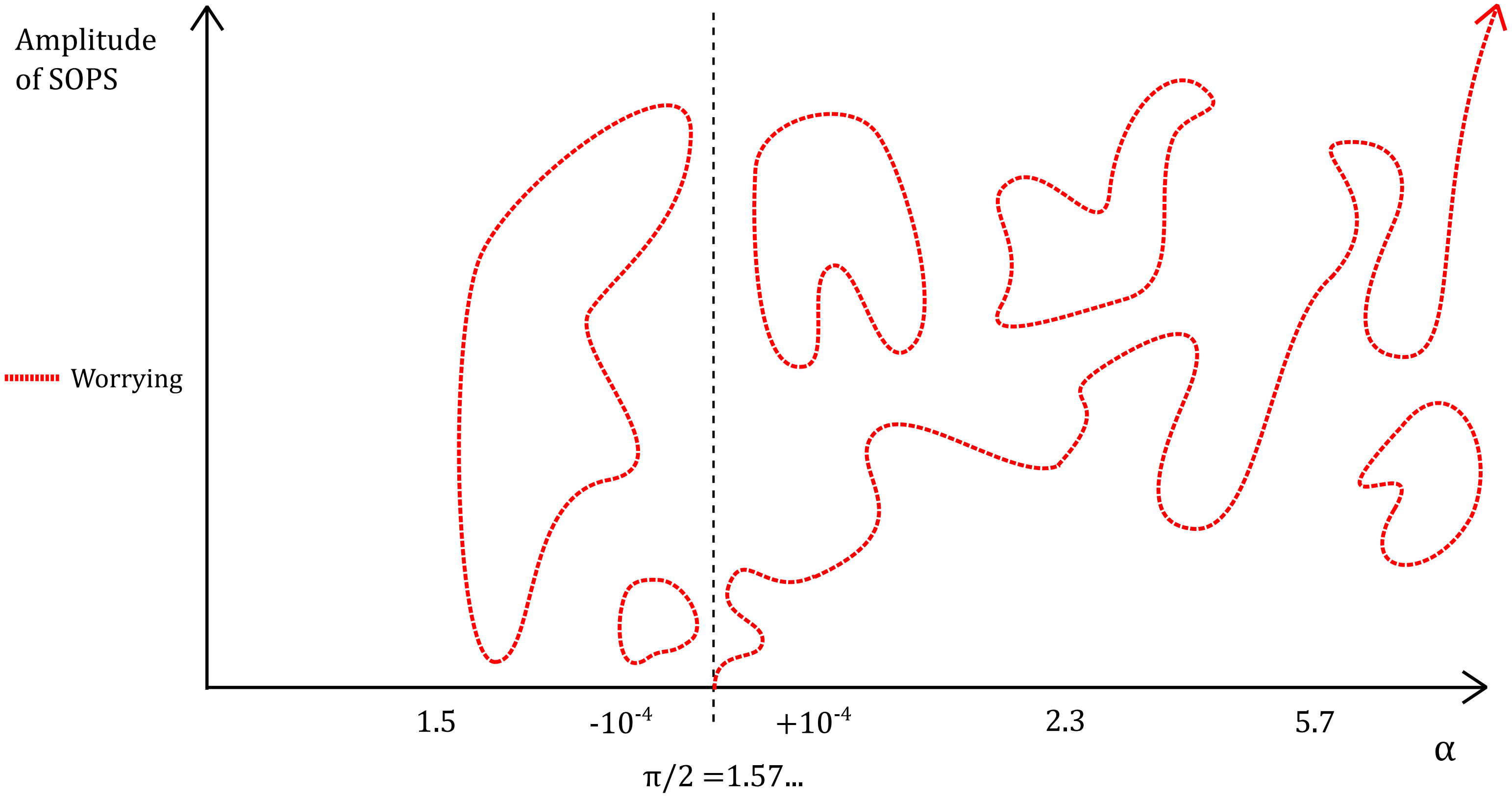
Old Conjectures

- **(1955) Wright's Conjecture:**
  For $\alpha < \pi/2$ zero is the global attractor
- **(1962) Jones' Conjecture:**
  For $\alpha > \pi/2$ there is a unique slowly oscillating periodic solution (SOPS)

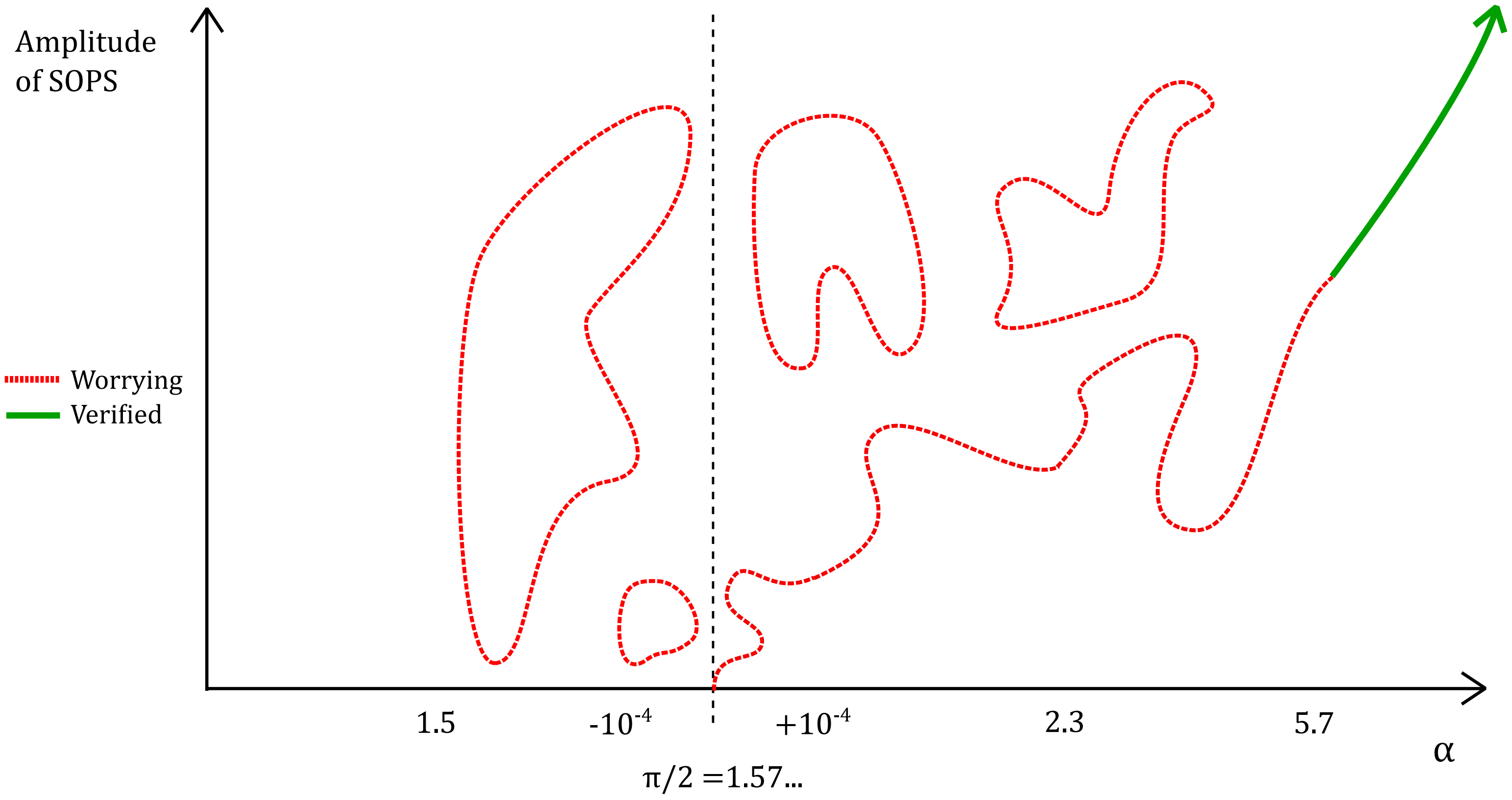
The conjectured bifurcation diagram for Wright's equation



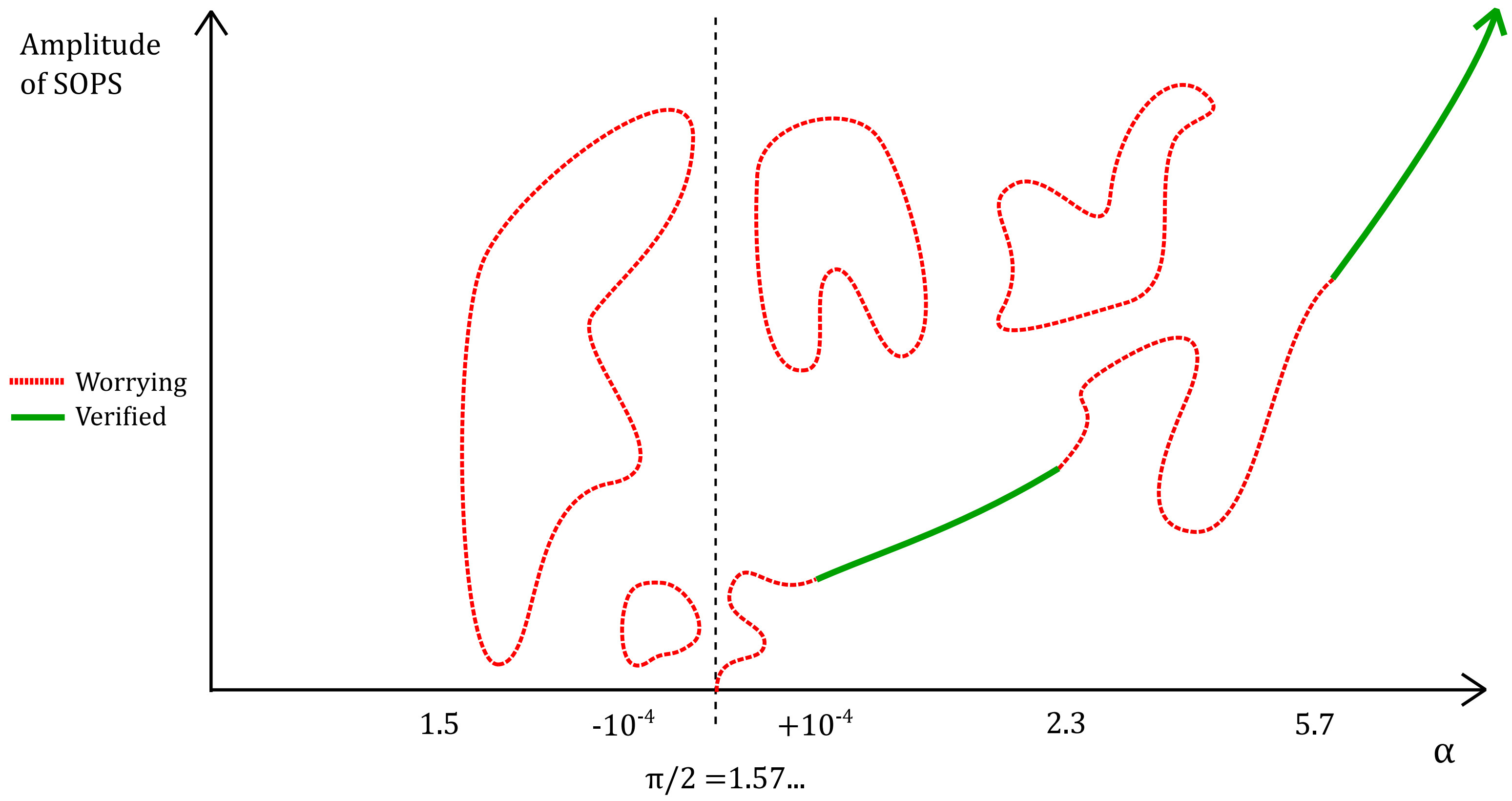
Things to worry about



(1991) Xie

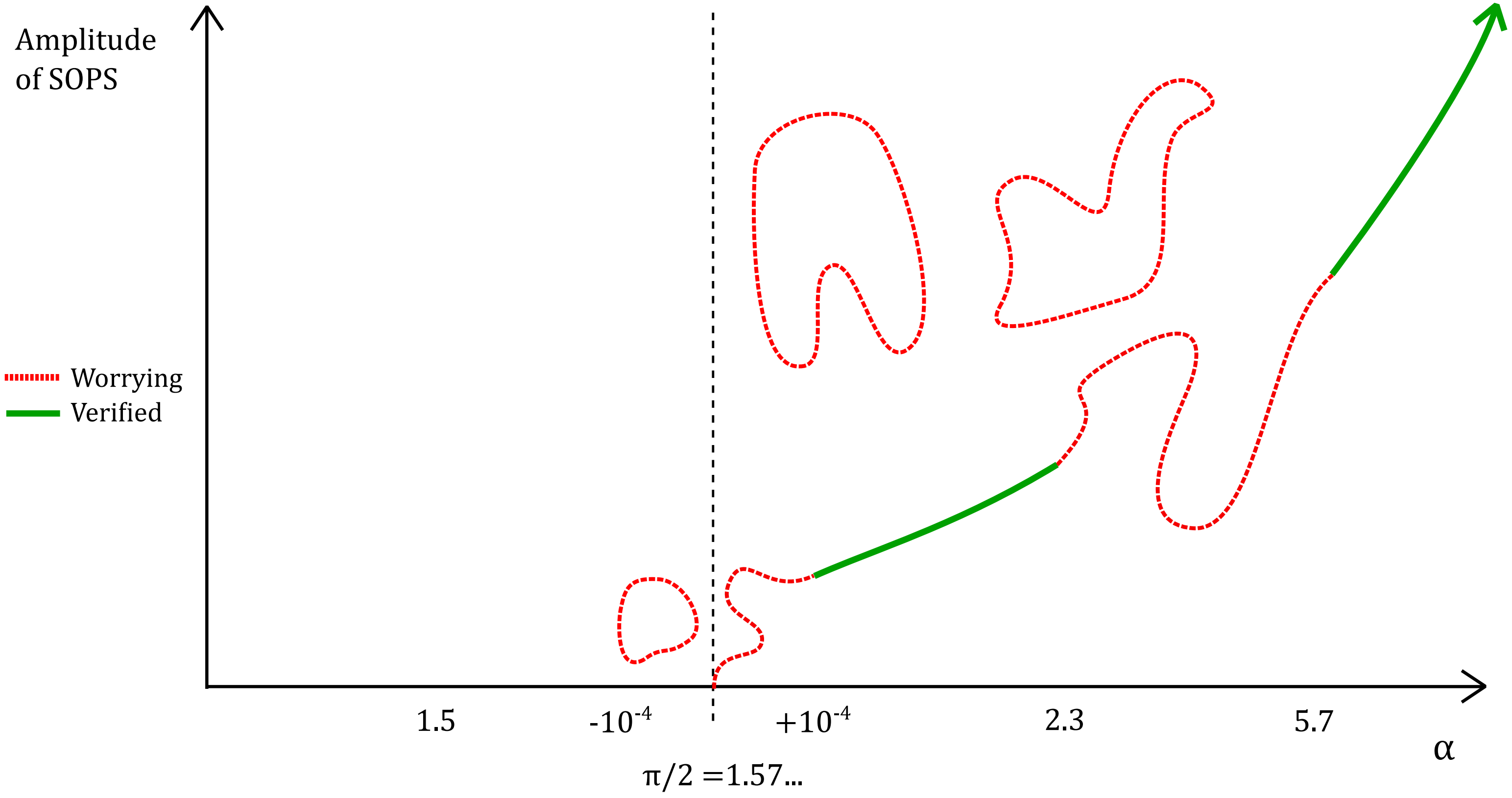


(2010)* Lessard



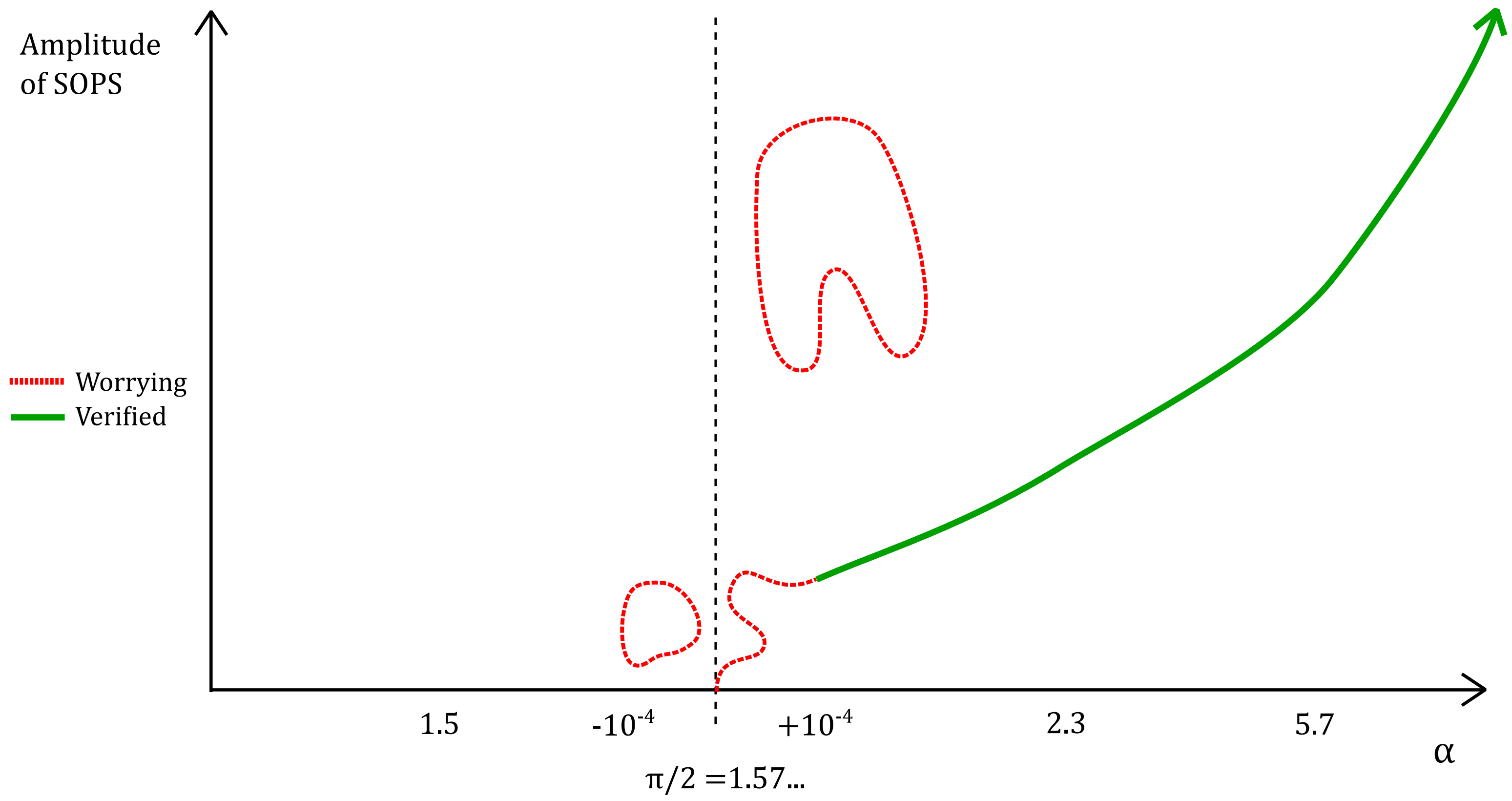
* Computer Assisted Proof

(2014)* Banhelyi, Csendes, Krisztin, Neumaier



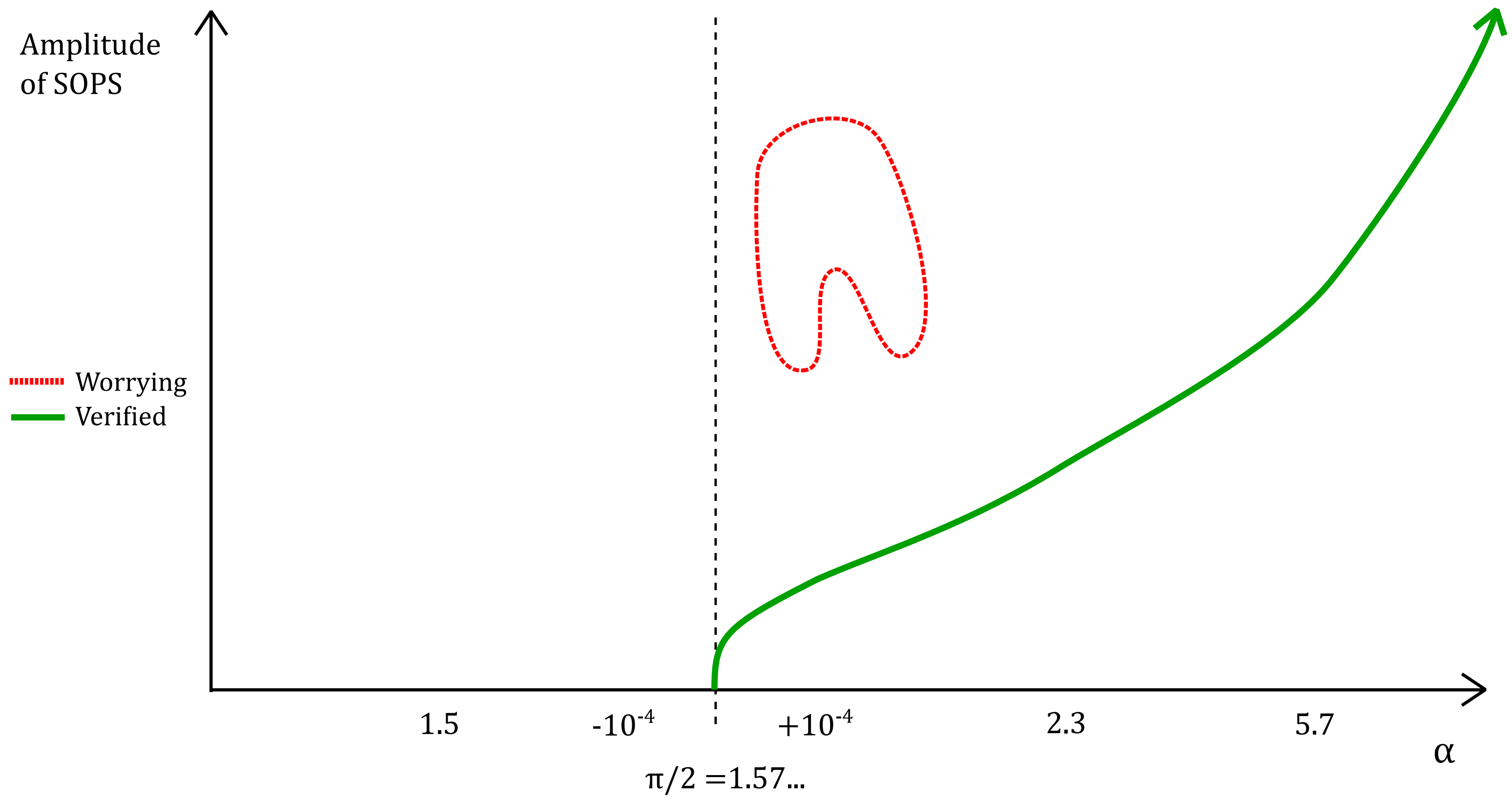
* Computer Assisted Proof

(2017)* **JJ**, Lessard, Mischaikow



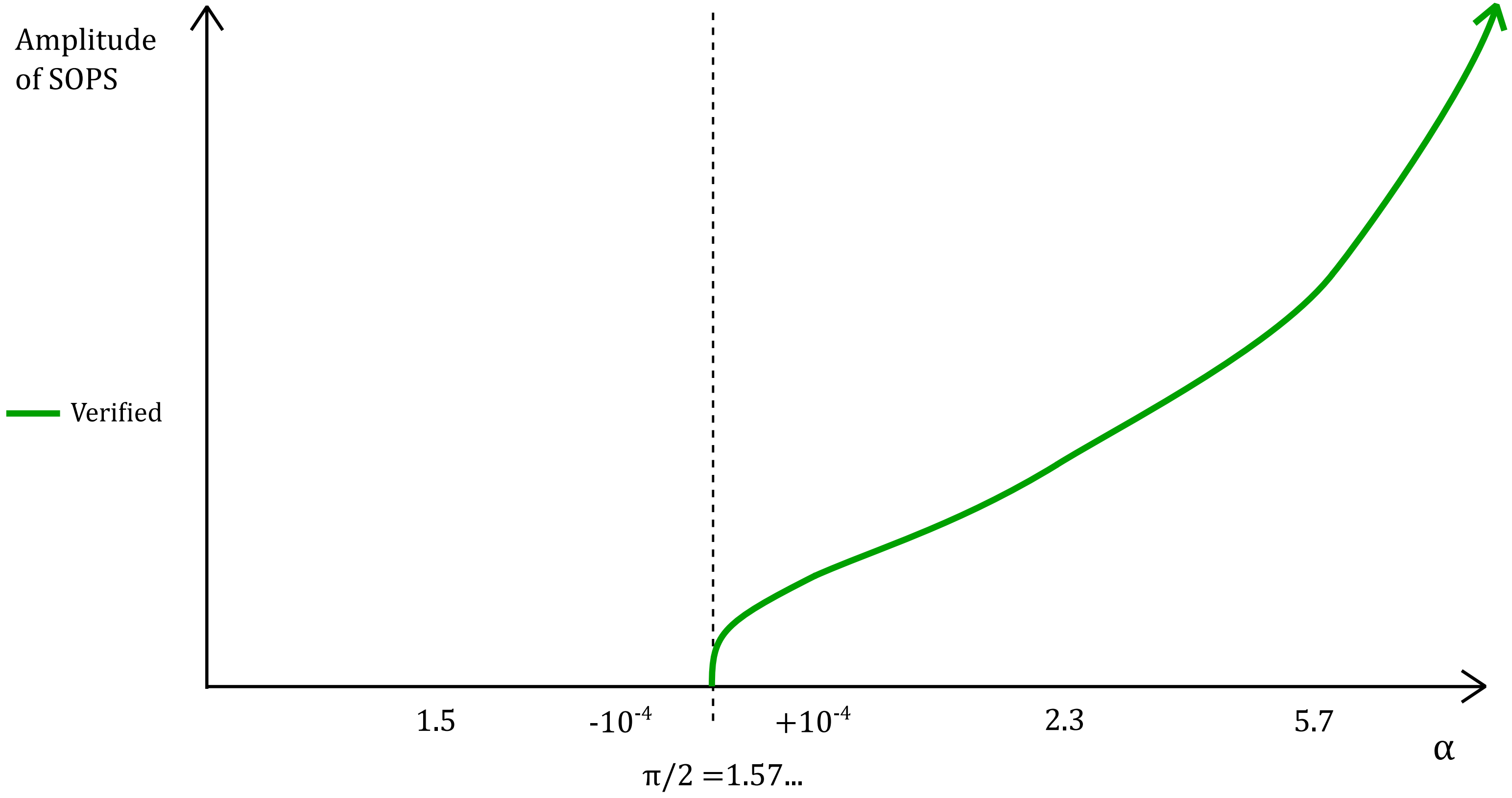
* Computer Assisted Proof

(2018)* van den Berg, **JJ**



* Computer Assisted Proof

(2019)* **JJ**



* Computer Assisted Proof

Conjectures

✓**(1955) Wright's Conjecture:**
For $\alpha \leq \pi/2$ zero is the global attractor

✓**(1962) Jones' Conjecture:**
For $\alpha > \pi/2$ there is a unique
slowly oscillating periodic orbit (SOPS)

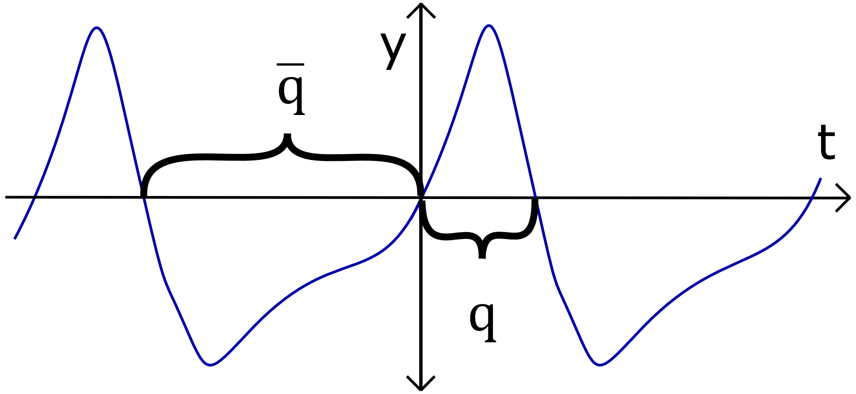
How to characterize all the SOPS?

- If $y(t)$ is a SOPS to Wright's equation at parameter $\alpha \geq \pi/2$, then*

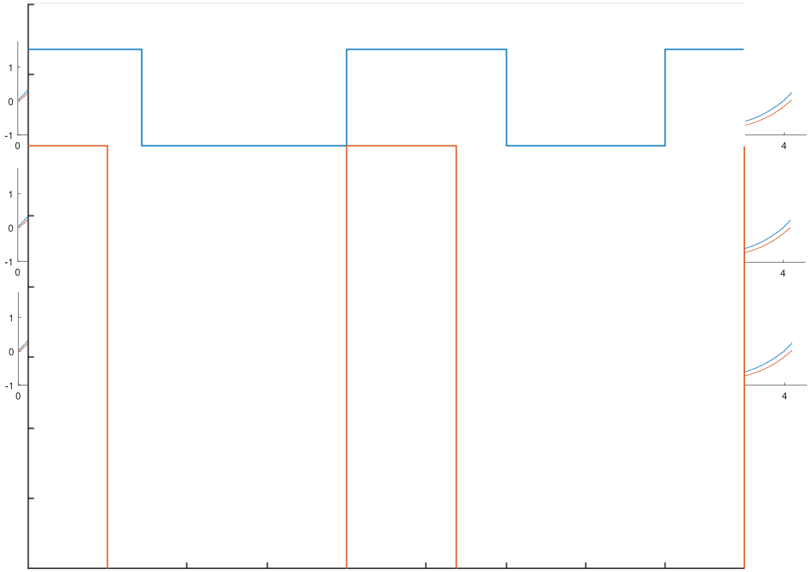
$$-1 \leq \boldsymbol{y(t)} \leq e^{\alpha} - 1$$

$$1 + \frac{1}{\alpha}\left(\frac{\alpha + e^{-\alpha} - 1}{\exp\{\alpha + e^{-\alpha} - 1\}}\right) < \boldsymbol{q} < 2 + \frac{1}{\alpha}$$

$$1 + \frac{1}{\alpha} < \boldsymbol{\bar{q}} < \max\left\{3, 2 + \frac{e^{\alpha} - 1}{1 - e^{-(\alpha - 1)}}\right\}$$



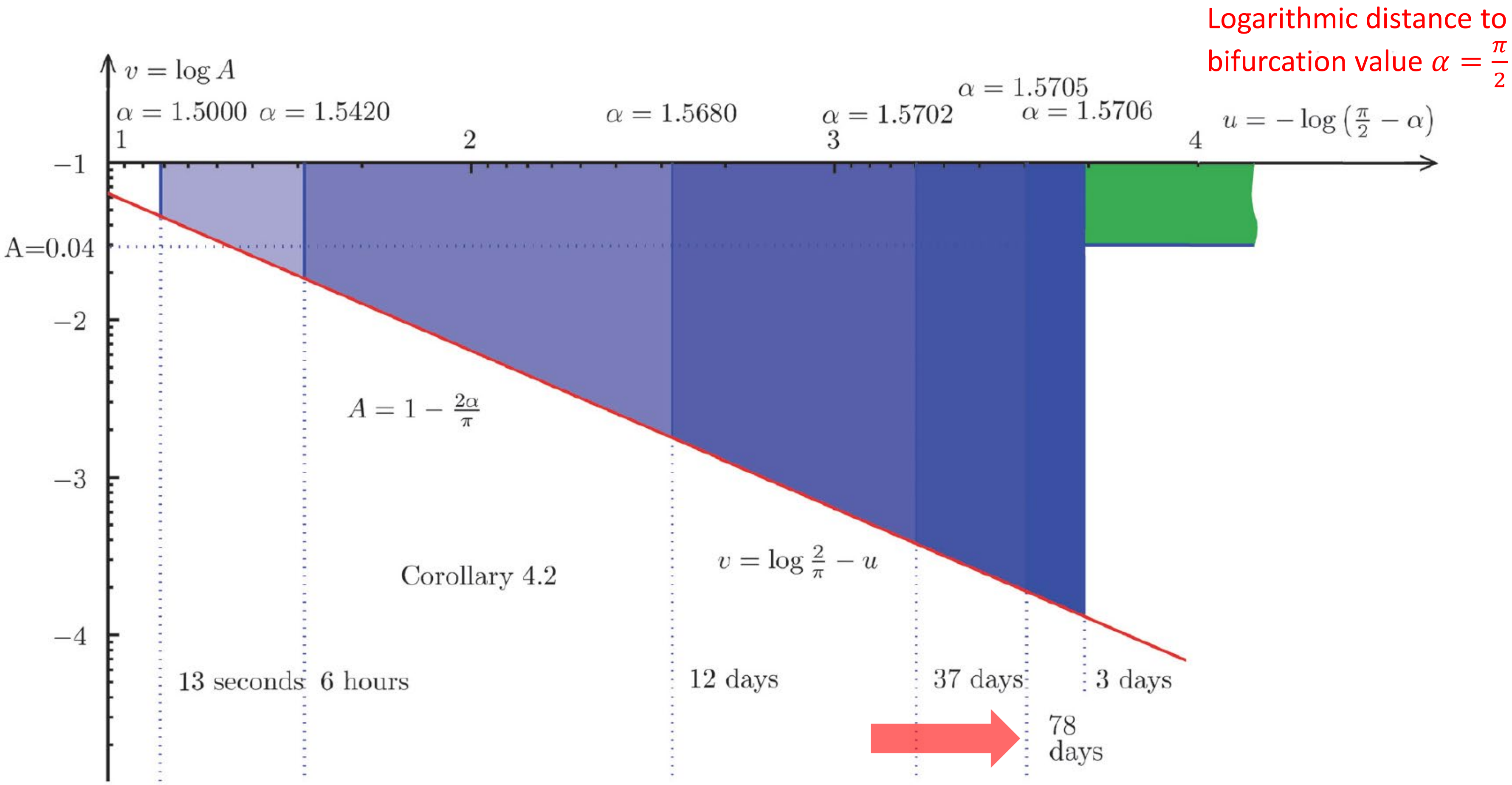
- Fix an interval α, and intervals $q, \bar{q}$ which could contain a SOPS**
  - Refine upper/lower bounds on the potential SOPS
    $$\ell_i(t) \leq y(t) \leq u_i(t)$$
  - Subdivide $q, \bar{q}$; discard contradictory cases
- Results in a collection of bounding functions
  - Contains any/all SOPS to Wright's equation
  - Prove uniqueness through stability argument



*Jones (1962)

****J.**, Lessard, Mischaikow (2017)

- Computation time in (BCKN 2014)
  - Moore Prize for Interval Arithmetic (Computer Assisted Proof)
  - Could not get all the way to the bifurcation value
    - Needs specialized analysis (v/d Berg, **JJ** 2018)



Week 1

- Essential Methods
  - Interval arithmetic, definite integrals, matrix algorithms
- Types of problems we'll solve
  - $\min_{x \in X} f(x)$
  - $f(x) = 0$
- Applications:
  - Trefethen's 100 digit challenge
  - Nonlinear ODEs
- Representing functions
  - Taylor series, Fourier series

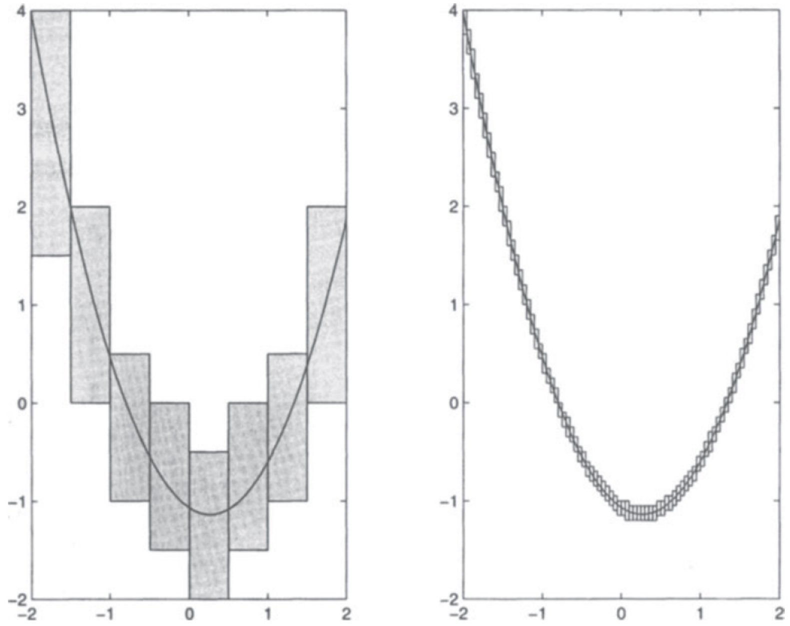


Fig. 5.3. Graphs of the multivalued approximation to $f(x) = (3x - 4)(5x + 4)/15$ obtained by means of interval arithmetic based on different basic lengths: 0.5 for the left graph and 0.05 for the right graph.

Week 2

- Additional Topics:
  - Infinite dimensional CAPs
  - Continuation, Bifurcation, PDEs
- Group Projects
  - Water waves, pattern formation, stability, bifurcations, blowup, chaos