

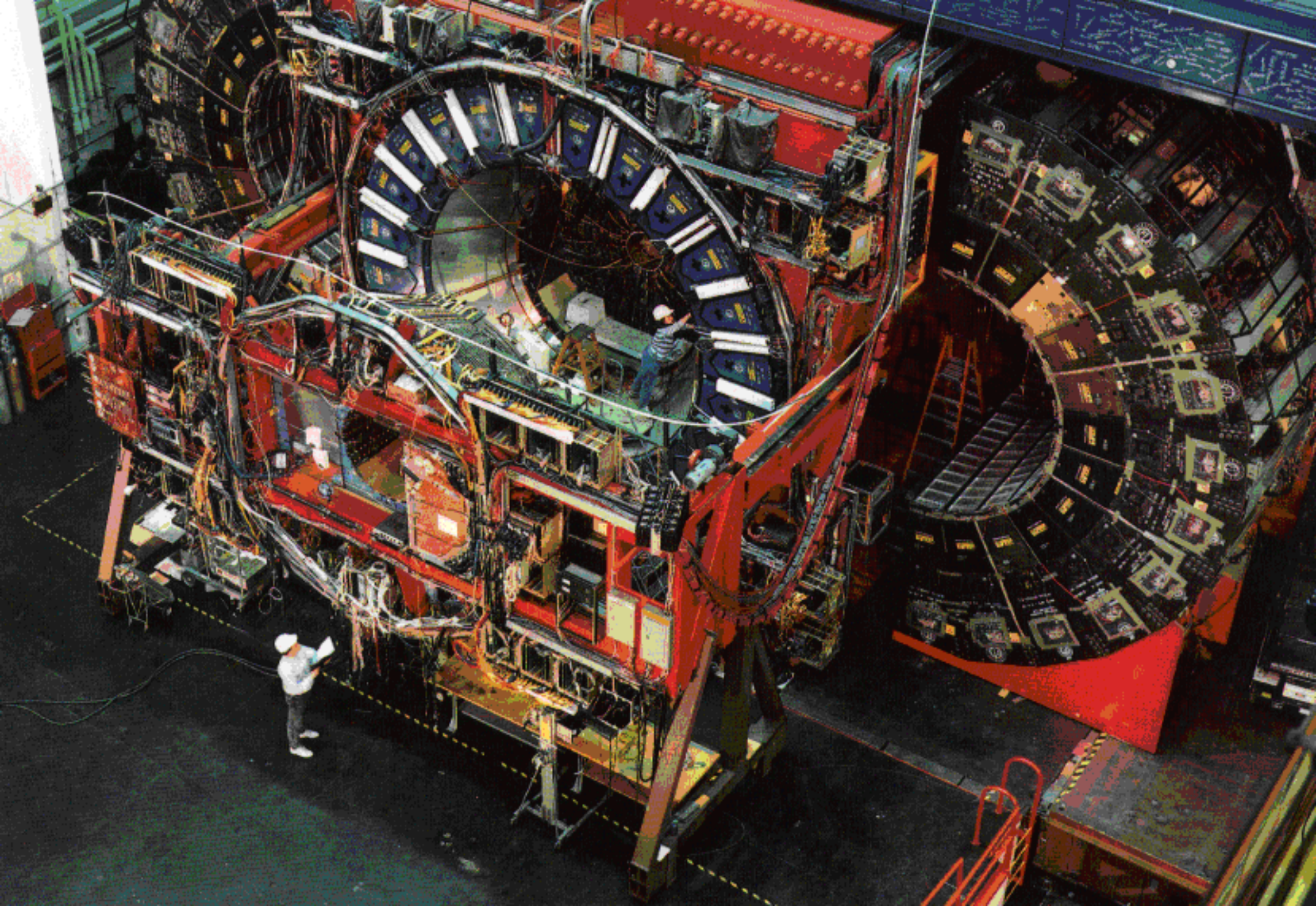
Verified Computations Using Taylor Models and Their Applications

Kyoko Makino and Martin Berz

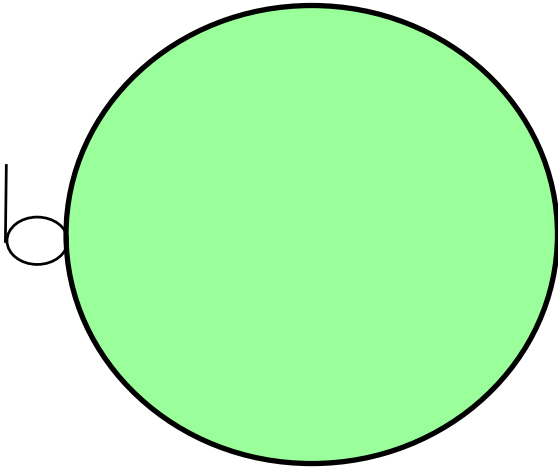
Department of Physics and Astronomy
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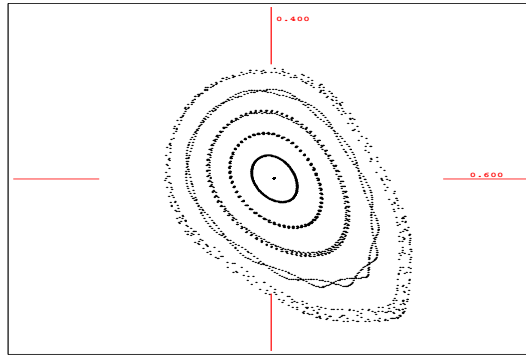
Motion in the Tevatron



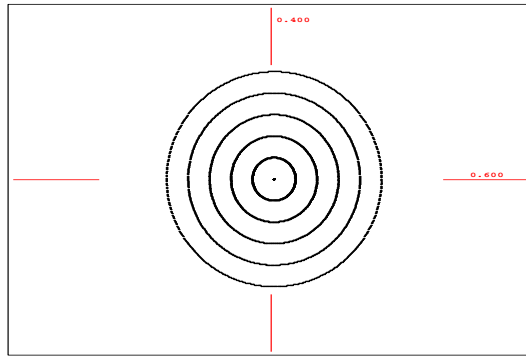
- Speed of Light: 3×10^8 m/sec
- Circumference: 6.28×10^3 m
➡ 4×10^4 revs/sec.
- Need to store about 10 hours, or 4×10^5 sec
➡ 2×10^{10} revolutions total.
- 10,000 magnets in ring
➡ 2×10^{14} contacts with fields!

- Extremely challenging computationally
- Need for several State-Of-The-Art Methods:
 - Phase Space Maps
 - Perturbation Theory
 - Lyapunov- and other Stability Theories
 - High-Performance Verified Methods

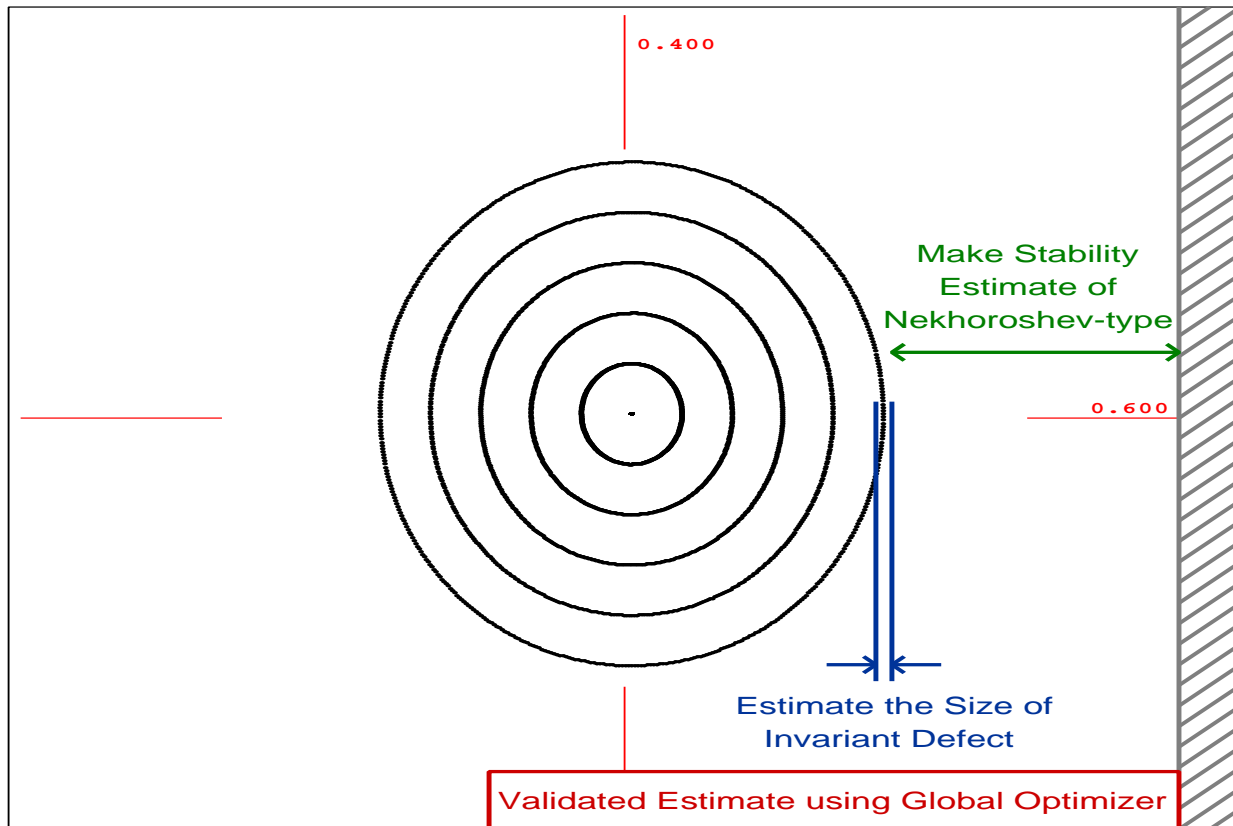
Example of Phase Space Motion



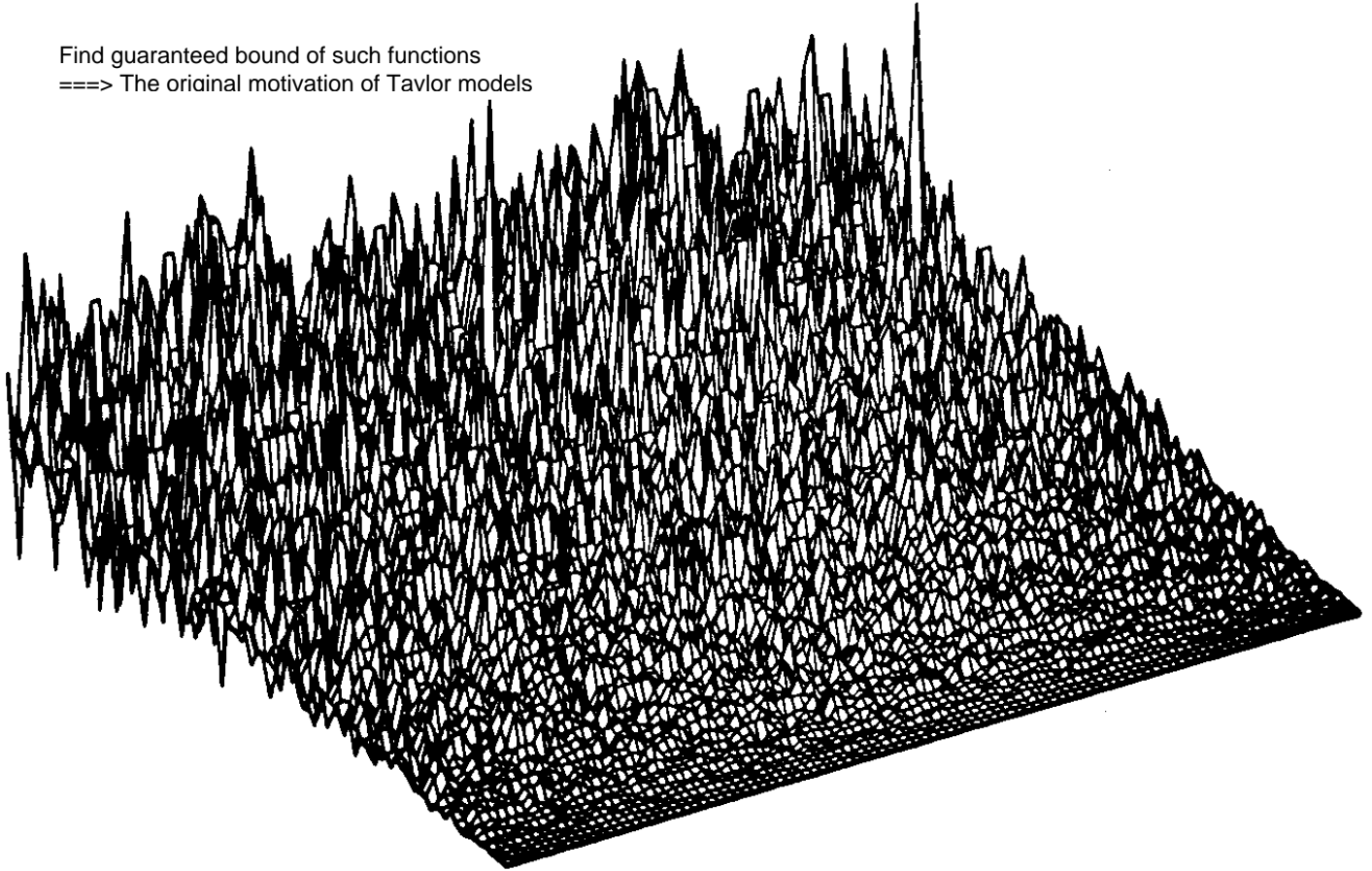
Tracking Phase Space Motion of 5 Particles in Regular Coordinates



Tracking Phase Space Motion of 5 Particles in Normal Form Coordinates



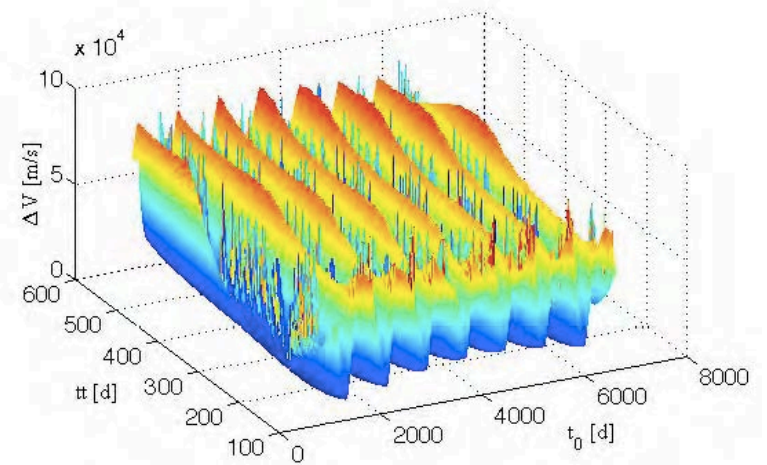
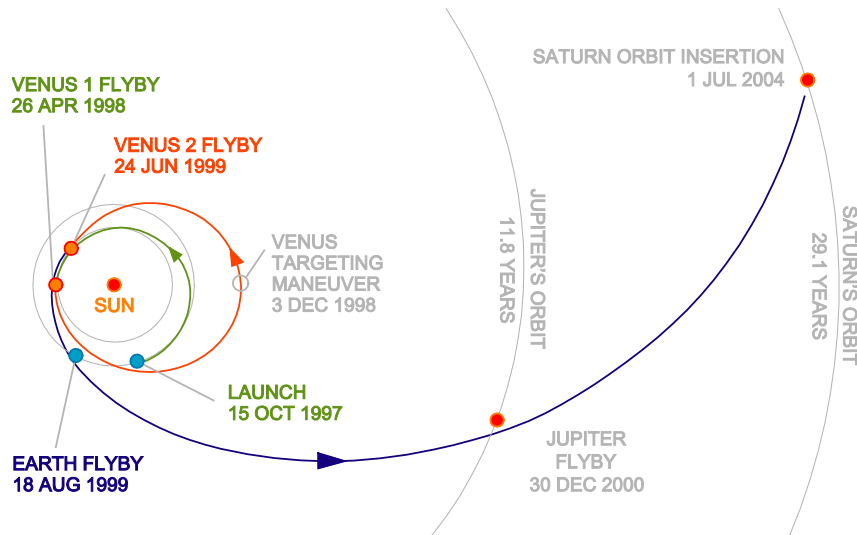
Find guaranteed bound of such functions
==> The original motivation of Taylor models



Impacts by Near Earth Asteroids



Astro-dynamical Transfer Problems



A Simple and Yet Challenging Example

Bound the function

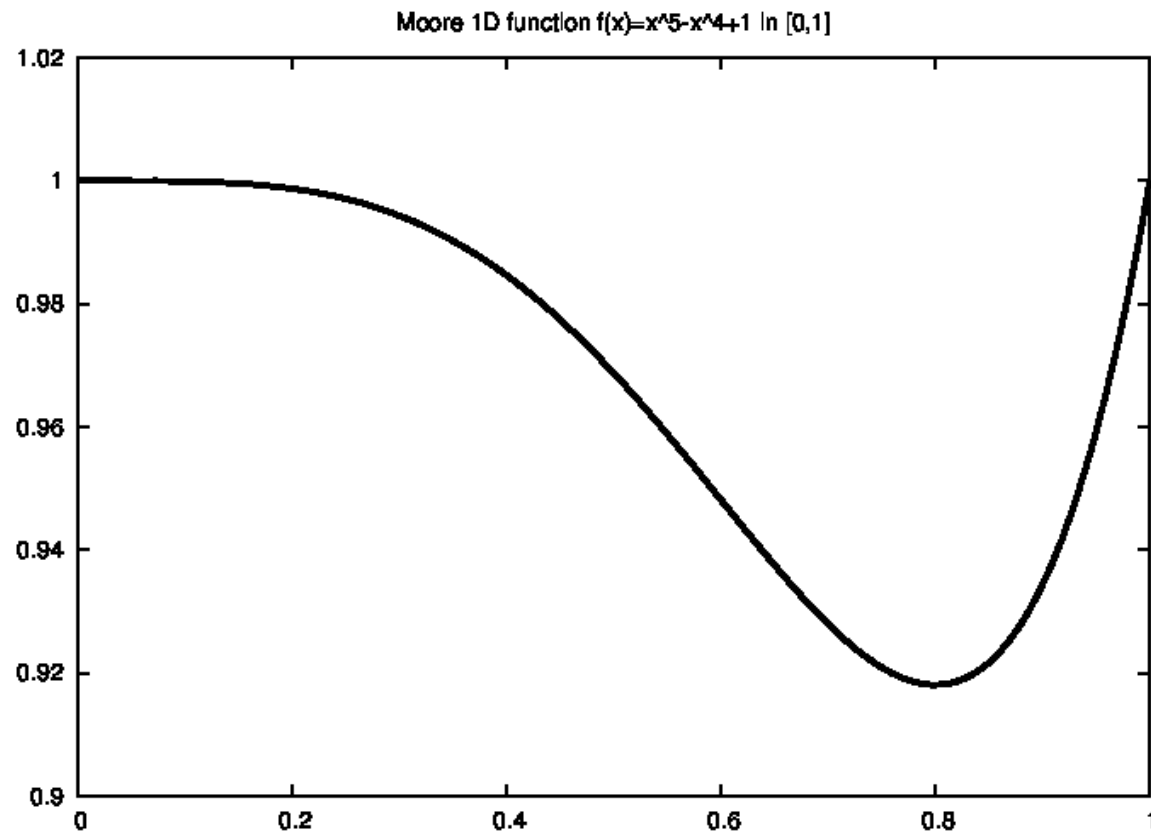
$$f(x) = 1 + x^5 - x^4 \quad \text{in } [0, 1].$$

– The problem was proposed by Ramon Moore.

A Simple and Yet Challenging Example

Bound the function

$$f(x) = 1 + x^5 - x^4 \quad \text{in } [0, 1].$$



A Simple and Yet Challenging Example – Exact Bound

Bound the function

$$f(x) = 1 + x^5 - x^4 \quad \text{in } [0, 1].$$

The derivative is

$$f'(x) = 5x^4 - 4x^3 = x^3(5x - 4),$$

so the extrema can happen at $x = 0$ and $x = 4/5 = 0.8$. In $[0, 1]$, the function takes the maxima at the end points $x = 0$ and $x = 1$, and the minimum at $x = 4/5$. Thus, the exact bound is

$$\begin{aligned} B_{\text{exact}} &= \left[f\left(\frac{4}{5}\right), f(0) = f(1) \right] = \left[1 + \left(\frac{4}{5}\right)^5 - \left(\frac{4}{5}\right)^4, 1 \right] \\ &= \left[1 - \frac{4^4}{5^5}, 1 \right] = [0.91808, 1], \\ w(B_{\text{exact}}) &= \frac{4^4}{5^5} = 0.08192. \end{aligned}$$

A Simple and Yet Challenging Example – Exact Bound

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But, normally one cannot evaluate exact bounds except for trivial problems.

Interval Arithmetic

Basic operations for intervals $I_1 = [L_1, U_1]$, $I_2 = [L_2, U_2]$.

$$I_1 + I_2 = [L_1 + L_2, U_1 + U_2],$$

$$I_1 - I_2 = [L_1 - U_2, U_1 - L_2],$$

$$I_1 \cdot I_2 = [\min\{L_1L_2, L_1U_2, U_1L_2, U_1U_2\}, \max\{L_1L_2, L_1U_2, U_1L_2, U_1U_2\}],$$

$$1/I_1 = [1/U_1, 1/L_1], \quad \text{if } 0 \notin I_1.$$

Rigorous range bounding by evaluating a function in interval arithmetic.

Refer to the references in the proceedings paper.

Interval Arithmetic

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$$1/I_1 = [1/U_1, 1/L_1], \quad \text{if } 0 \notin I_1.$$

Rigorous range bounding by evaluating a function in interval arithmetic.

A trivial example of the blow-up phenomenon due to lack of the dependency information. Compute the subtraction from itself; $w(I) = U - L$.

$$\begin{aligned} I - I &= [L, U] - [L, U] = [L - U, U - L], \\ w(I - I) &= (U - L) - (L - U) = 2(U - L). \end{aligned}$$

$w(I - I) = 2 \cdot w(I)$, even though $x - x = 0$.

Interval Range Bounding of the Function $f(x) = 1 + x^5 - x^4$ in $[0, 1]$

Evaluate the function on the entire domain $[0, 1]$ via interval arithmetic:

$$\begin{aligned}f([0, 1]) &= 1 + [0, 1]^5 - [0, 1]^4 = 1 + [0, 1] - [0, 1] = [0, 2], \\w(f[0, 1]) &= 2.\end{aligned}$$

The interval range bound $f([0, 1]) = [0, 2]$ certainly encloses the exact bound $B_{\text{exact}} = [0.91808, 1]$, but it is uselessly overestimated.

Some issues in interval arithmetic:

Overestimation, the dependency problem, the dimensionality curse, etc.

$$I_1 - I_2 = [L_1 - U_2, U_1 - L_2],$$

$$I_1 \cdot I_2 = [\min\{L_1L_2, L_1U_2, U_1L_2, U_1U_2\}, \max\{L_1L_2, L_1U_2, U_1L_2, U_1U_2\}],$$

Taylor models

For $f : D \subset \mathbb{R}^v \rightarrow \mathbb{R}$ that is $(n + 1)$ times continuously partially differentiable,
 $P(x - x_0)$: the n -th order Taylor polynomial of f around $x_0 \in D$
 e : a small remainder bounding set of the deviation of P from f

$$f(x) - P(x - x_0) \in e, \quad \forall x \in D \text{ where } x_0 \in D.$$

We call the combination of P and e as a Taylor model.

$$T = (P, e) = P + e.$$

T depends on the order n , the domain D , and the expansion point x_0 .

Taylor Model Arithmetic

Define Taylor model addition, multiplication for $T_1 = (P_1, e_1)$, $T_2 = (P_2, e_2)$ with the same conditions $\{n, D, x_0\}$.

$$T_1 + T_2 = (P_1 + P_2, e_1 + e_2),$$

$$T_1 \cdot T_2 = (P_{1.2}, e_{1.2}).$$

$P_{1.2}$: the part of the polynomial $P_1 \cdot P_2$ up to the order n .

$$e_{1.2} = B(P_{>n}) + B(P_1) \cdot e_2 + B(P_2) \cdot e_1 + e_1 \cdot e_2.$$

$P_{>n}$: the higher order part from $(n + 1)$ to $2n$.

$B(P)$: an enclosure bound of P over D .

Operations on sets e_i follow set theoretical operations and outward rounding.

Taylor Model Arithmetic – and Intrinsic Functions

Define Taylor model addition, multiplication for $T_1 = (P_1, e_1)$, $T_2 = (P_2, e_2)$ with the same conditions $\{n, D, x_0\}$.

$$\begin{aligned}T_1 + T_2 &= (P_1 + P_2, e_1 + e_2), \\T_1 \cdot T_2 &= (P_{1.2}, e_{1.2}).\end{aligned}$$

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Operations on sets e_i follow set theoretical operations and outward rounding.

Intrinsic functions for Taylor models can be defined by performing various manipulations using these. The particularly nice is ∂_i^{-1} , antiderivation, being a Taylor model intrinsic function; because obtaining the integral with respect to variable x_i of P is straightforward, so is an integral of a Taylor model.

Refer to the references in the proceedings paper.

TM Range Bounding of the Function $f(x) = 1 + x^5 - x^4$ in $[0, 1]$

First, express the variable x on the entire domain $[0, 1]$ by a Taylor model as

$$x \in T_x = P_x + e_x \quad \text{with} \quad P_x = 0.5 + 0.5 \cdot x_0, \quad e_x = 0, \quad x_0 \in [-1, 1].$$

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A self-subtraction test: Subtract the Taylor model T_x from itself.

$$\begin{aligned} T_x - T_x &= (P_x - P_x, e_x - e_x) \\ &= ((0.5 + 0.5 \cdot x_0) - (0.5 + 0.5 \cdot x_0), 0 - 0) = (0, 0). \end{aligned}$$

Note that on computers, a tiny nonzero remainder error enclosure will result.

TM Range Bounding of the Function $f(x) = 1 + x^5 - x^4$ in $[0, 1]$

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$$x \in T_x = P_x + e_x \quad \text{with} \quad P_x = 0.5 + 0.5 \cdot x_0, \quad e_x = 0, \quad x_0 \in [-1, 1].$$

Next, evaluate f in Taylor model arithmetic. Try the fifth order.

$$\begin{aligned} T_{f,5} = f(T_x) &= 1 + (T_x)^5 - (T_x)^4 \\ &= 1 + (0.5 + 0.5 \cdot x_0 + 0)^5 - (0.5 + 0.5 \cdot x_0 + 0)^4 \\ &= 1 + 0.5^5 \cdot (1 + 5x_0 + 10x_0^2 + 10x_0^3 + 5x_0^4 + x_0^5 + 0) \\ &\quad - 0.5^4 \cdot (1 + 4x_0 + 6x_0^2 + 4x_0^3 + x_0^4 + 0) \\ &= 1 + 0.5^5 \cdot (-1 - 3x_0 - 2x_0^2 + 2x_0^3 + 3x_0^4 + x_0^5) + 0. \end{aligned}$$

On computers, a tiny nonzero remainder error enclosure will result.

In lower order Taylor model arithmetic,

the resulting P is truncated by the order,

the $P_{>n}$ contributions are lumped into the remainder error enclosure.

TM Range Bounding of the Function $f(x) = 1 + x^5 - x^4$ in $[0, 1]$

First, express the variable x on the entire domain $[0, 1]$ by a Taylor model as

$$x \in T_x = P_x + e_x \quad \text{with} \quad P_x = 0.5 + 0.5 \cdot x_0, \quad e_x = 0, \quad x_0 \in [-1, 1].$$

Next, evaluate f in Taylor model arithmetic. Try the fifth order.

$$\begin{aligned} T_{f,5} = f(T_x) &= 1 + (T_x)^5 - (T_x)^4 \\ &= 1 + 0.5^5 \cdot (-1 - 3x_0 - 2x_0^2 + 2x_0^3 + 3x_0^4 + x_0^5) + 0. \end{aligned}$$

The simplest range bounding (naive TM bounding):

Sum up the bound contributions from each monomial.

Utilize $x_0, x_0^3, x_0^5 \in [-1, 1]$, $x_0^2, x_0^4 \in [0, 1]$.

$$\begin{aligned} f_{TM_5} &\in 1 + 0.5^5 \cdot (-1 - 3 \cdot [-1, 1] - 2 \cdot [0, 1] + 2 \cdot [-1, 1] + 3 \cdot [0, 1] + [-1, 1]) \\ &\in 1 + 0.5^5 \cdot [-9, 8] = [0.71875, 1.25], \end{aligned}$$

$$w(f_{TM_5}) = 0.5^5 \cdot (8 + 9) = 0.53125.$$

Range Bounding of the Function $f(x) = 1 + x^5 - x^4$ in $[0, 1]$

Method	Division	Lower bound	Upper bound	Width
Exact	1	0.91808	1	0.08192
TM naive, 5th	1	0.71875	1.25	0.53125
Interval	1	0	2	2

Range Bounding of the Function $f(x) = 1 + x^5 - x^4$ in $[0, 1]$

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Exact	1	0.91808	1	0.08192
TM naive, 5th	1	0.71875	1.25	0.53125
Interval	1	0	2	2

As a common practice, **divide** the entire domain into smaller subdomains.

TM enhancements:

The Linear Dominated Bounder (LDB), the Fast Quadratic Bounder (QFB), utilizing the linear, and the quadratic part respectively.

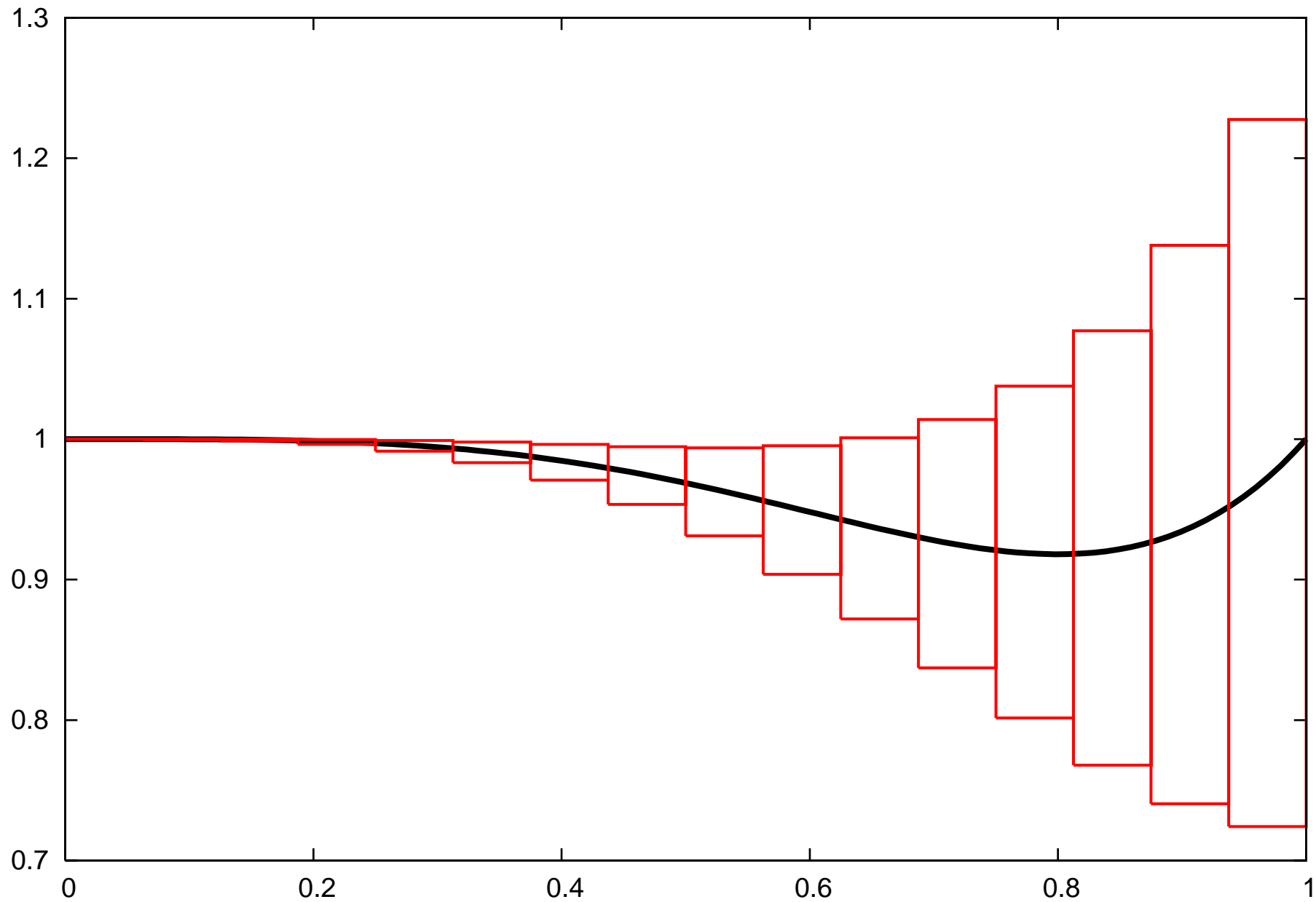
Applicable to multivariate cases. Economical, excellent range bounding.

Great tools in verified global optimizations (GO) in the branch-and-bound approach, narrowing the search area by pruning and discarding subdomains.

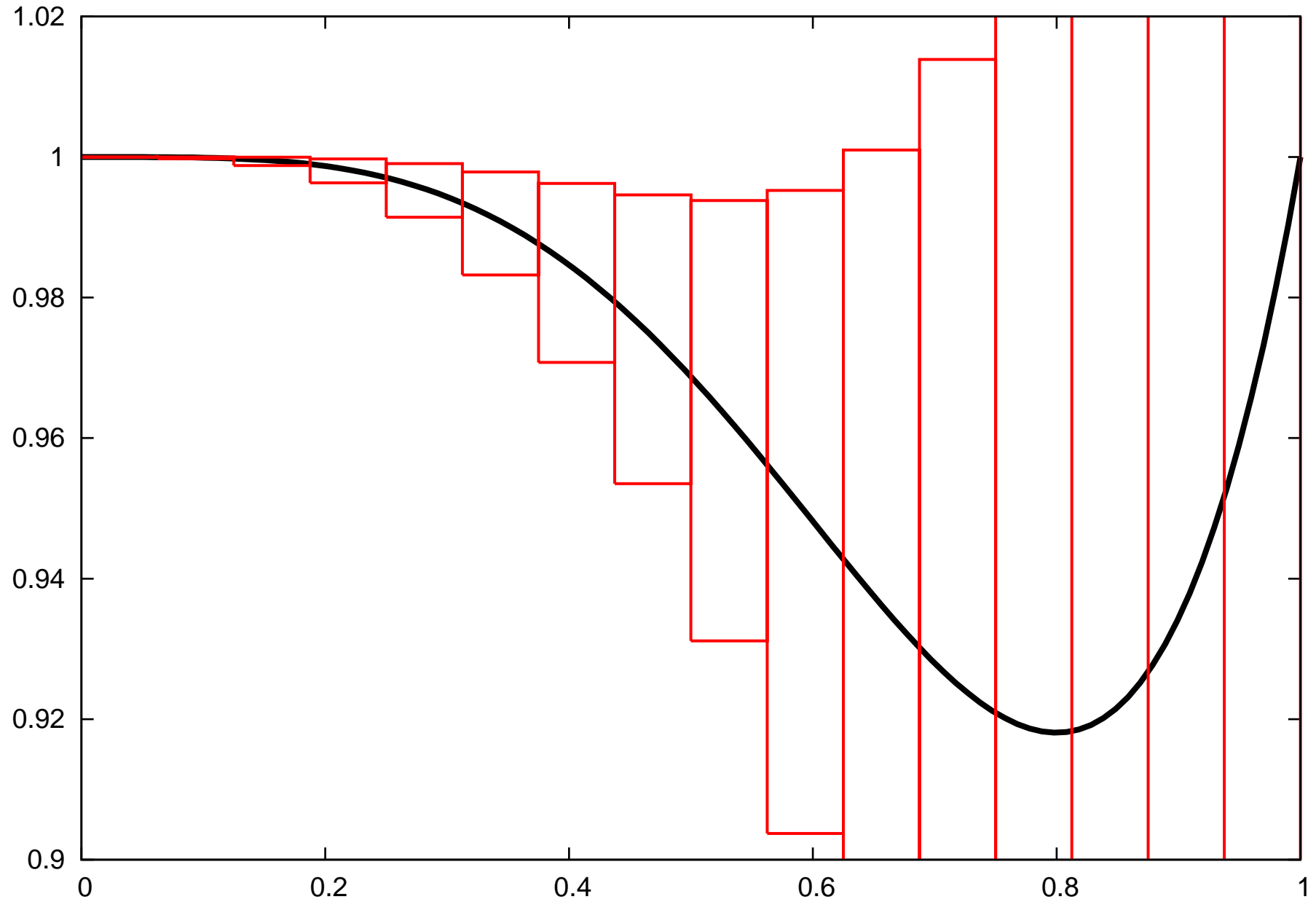
Range Bounding of the Function $f(x) = 1 + x^5 - x^4$ in $[0, 1]$

Method		Division	Lower bound	Upper bound	Width
Exact		1	0.91808	1	0.08192
TM	GO, 5th	3 (8 steps)*			
	LDB, 5th	16			
	naive, 5th	16			
	naive, 1st	16			
	naive, 5th	1	0.71875	1.25	0.53125
Interval		1024			
		128			
		16			
		1	0	2	2

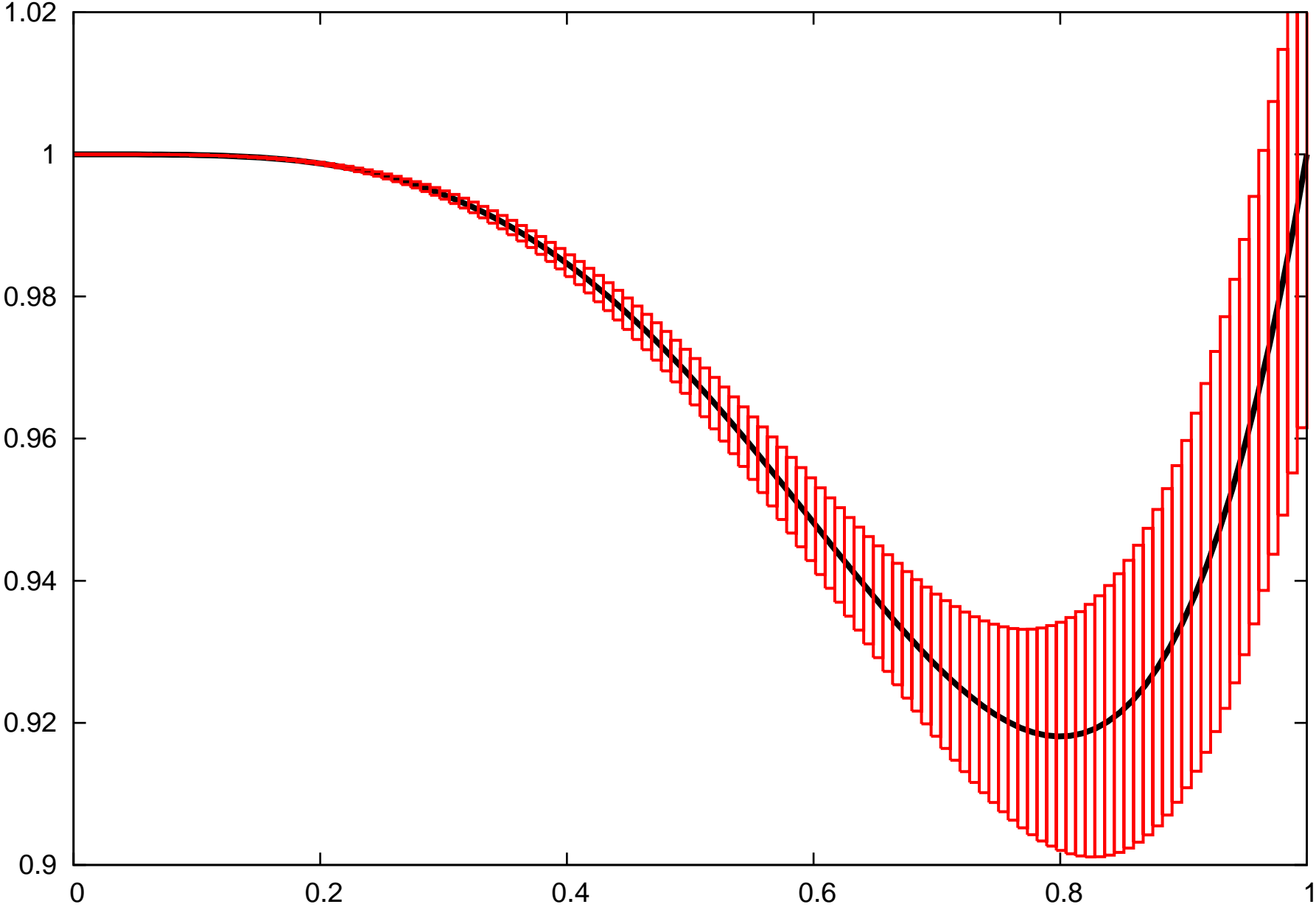
Moore 1D function $f(x)=x^5-x^4+1$ in $[0,1]$. Bounding by 16 intervals



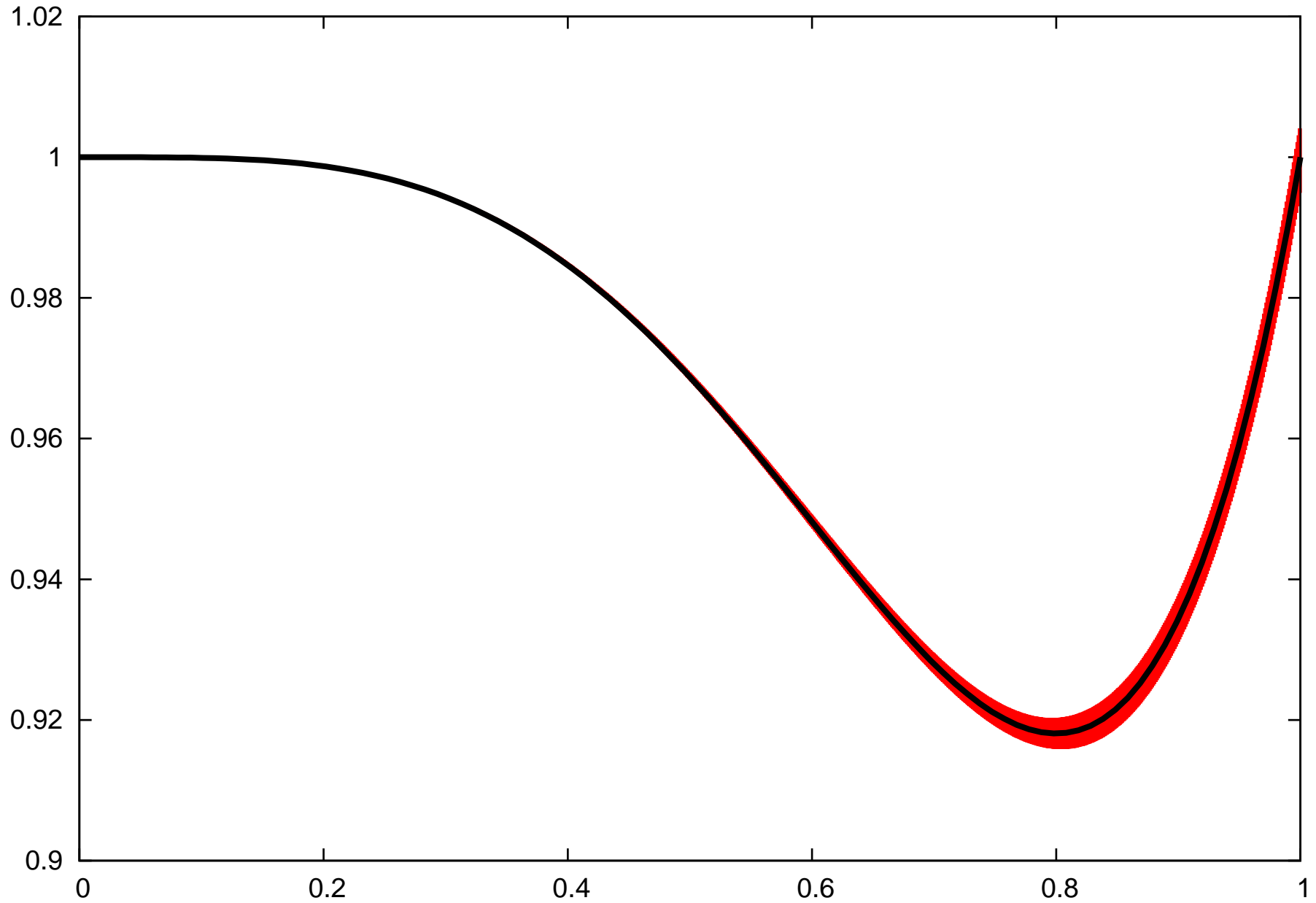
Moore 1D function $f(x)=x^5-x^4+1$ in $[0,1]$. Bounding by 16 intervals



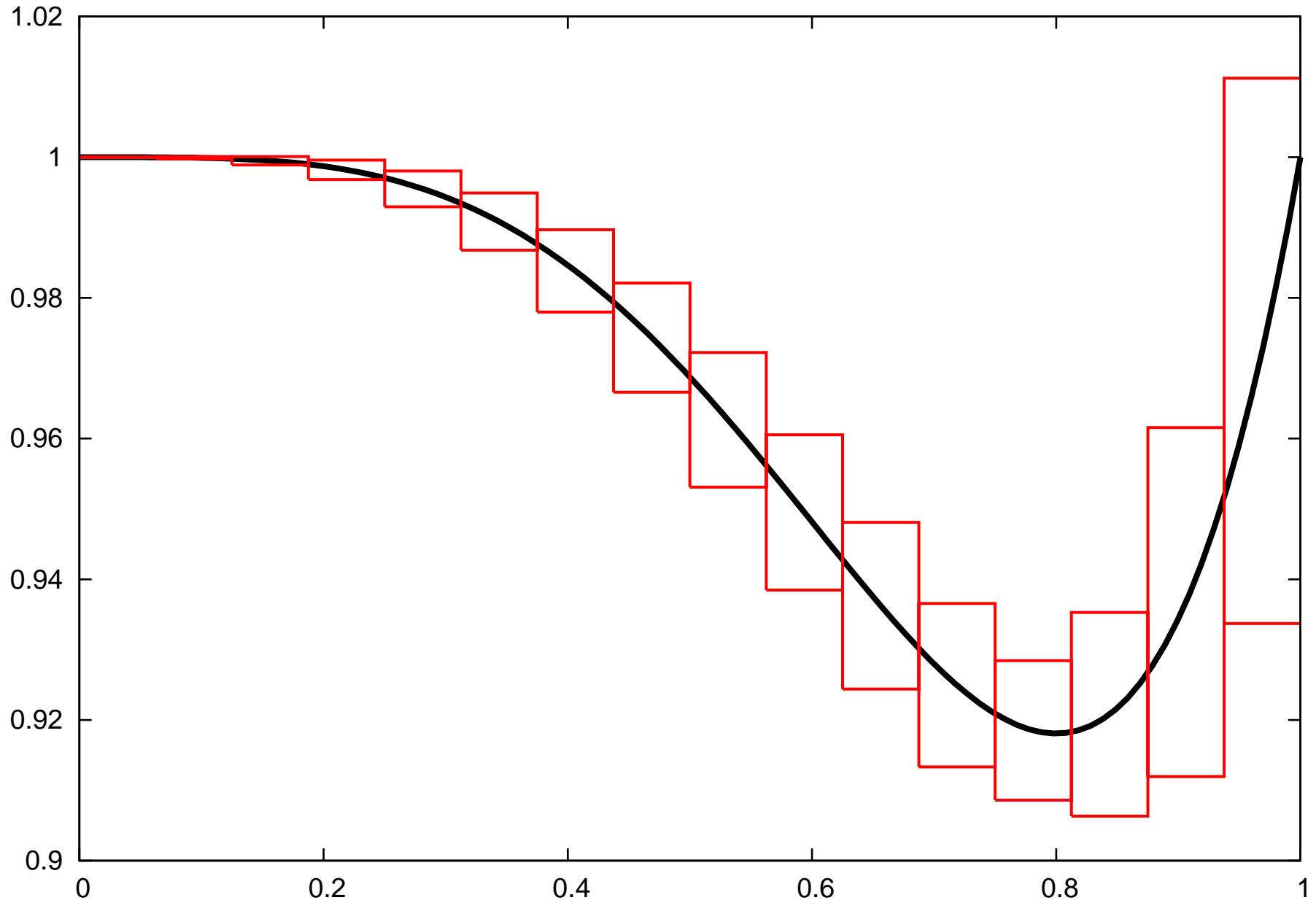
Moore 1D function $f(x)=x^5-x^4+1$ in $[0,1]$. Bounding by 128 intervals



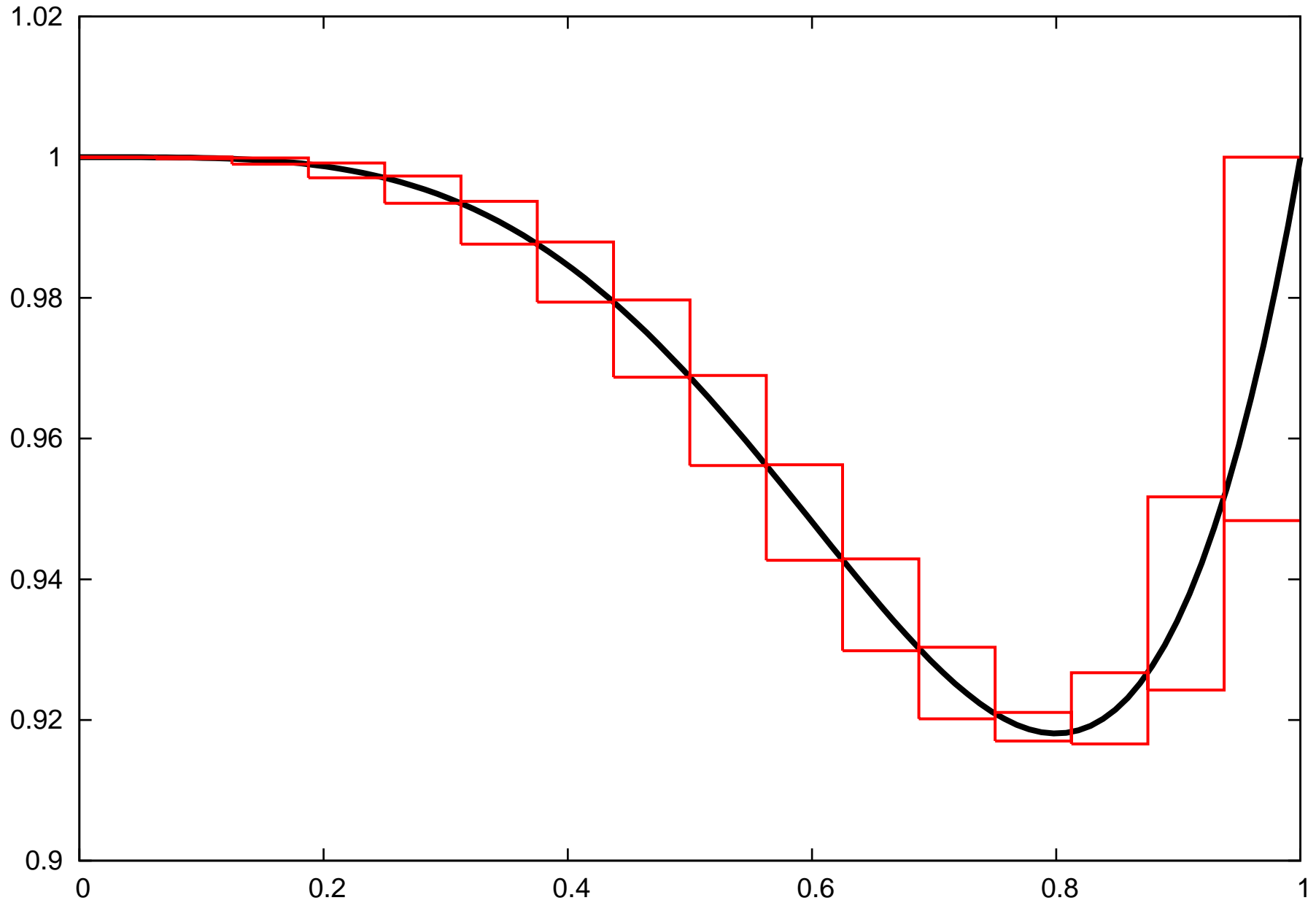
Moore 1D function $f(x)=x^5-x^4+1$ in $[0,1]$. Bounding by 1024 intervals



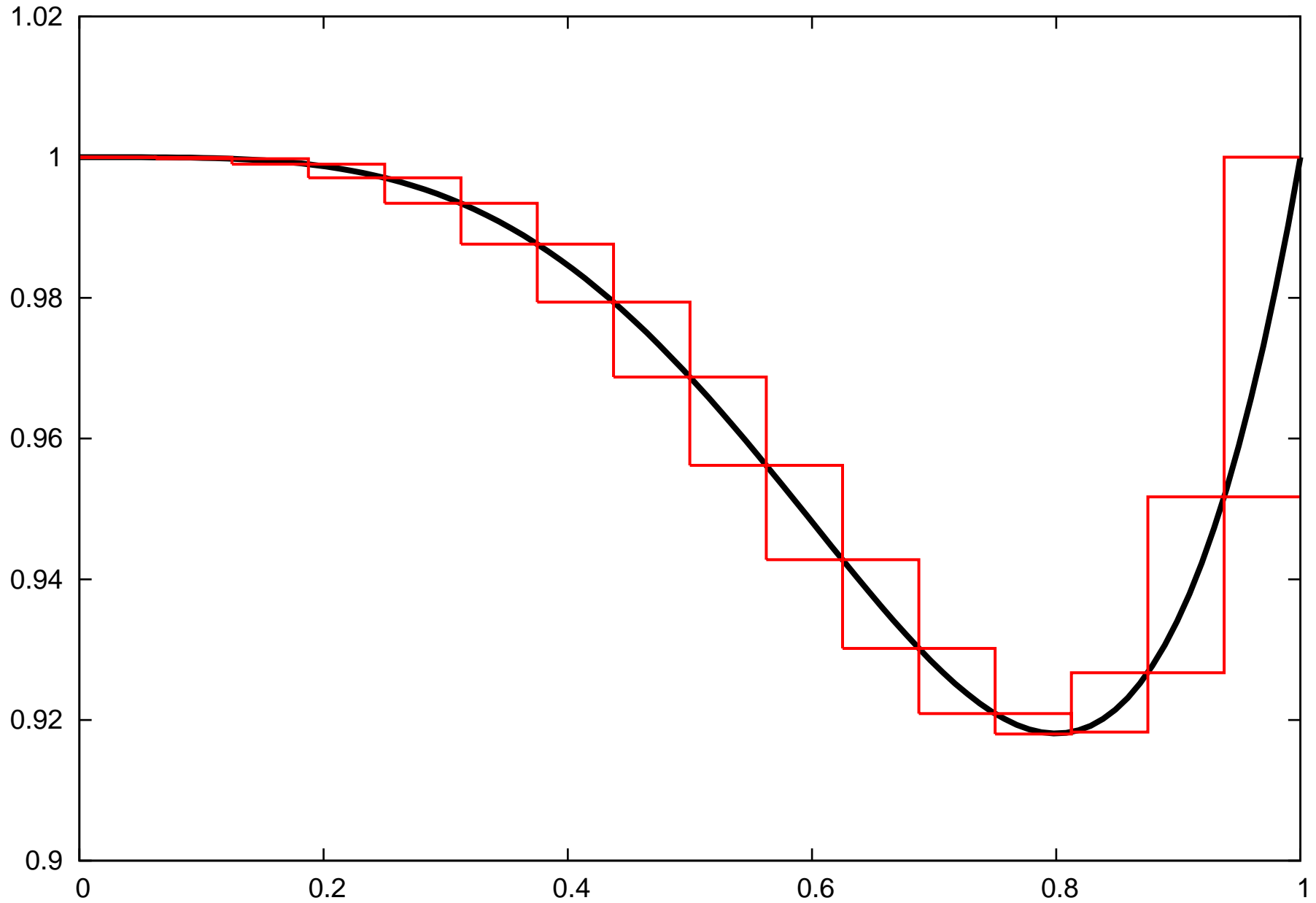
Moore 1D function $f(x)=x^5-x^4+1$ in $[0,1]$. Bounding by 16 naive linear TMs



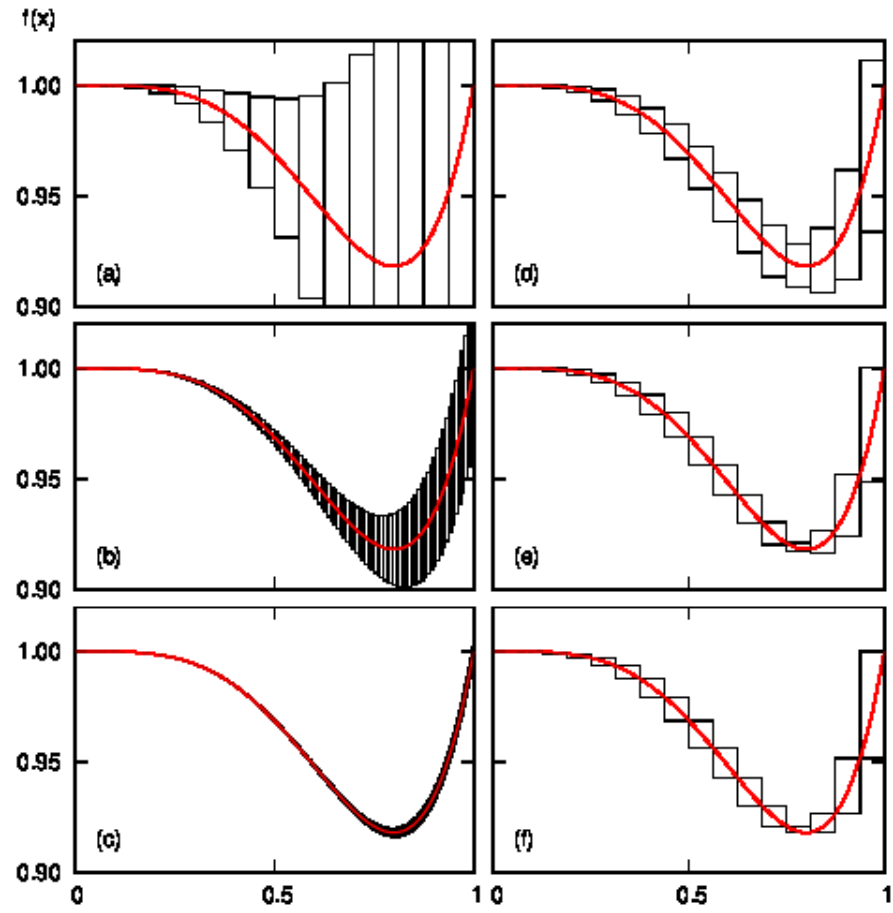
Moore 1D function $f(x)=x^5-x^4+1$ in $[0,1]$. Bounding by 16 naive 5th order TMs



Moore 1D function $f(x)=x^5-x^4+1$ in $[0,1]$. Bounding by 16 TM LDB



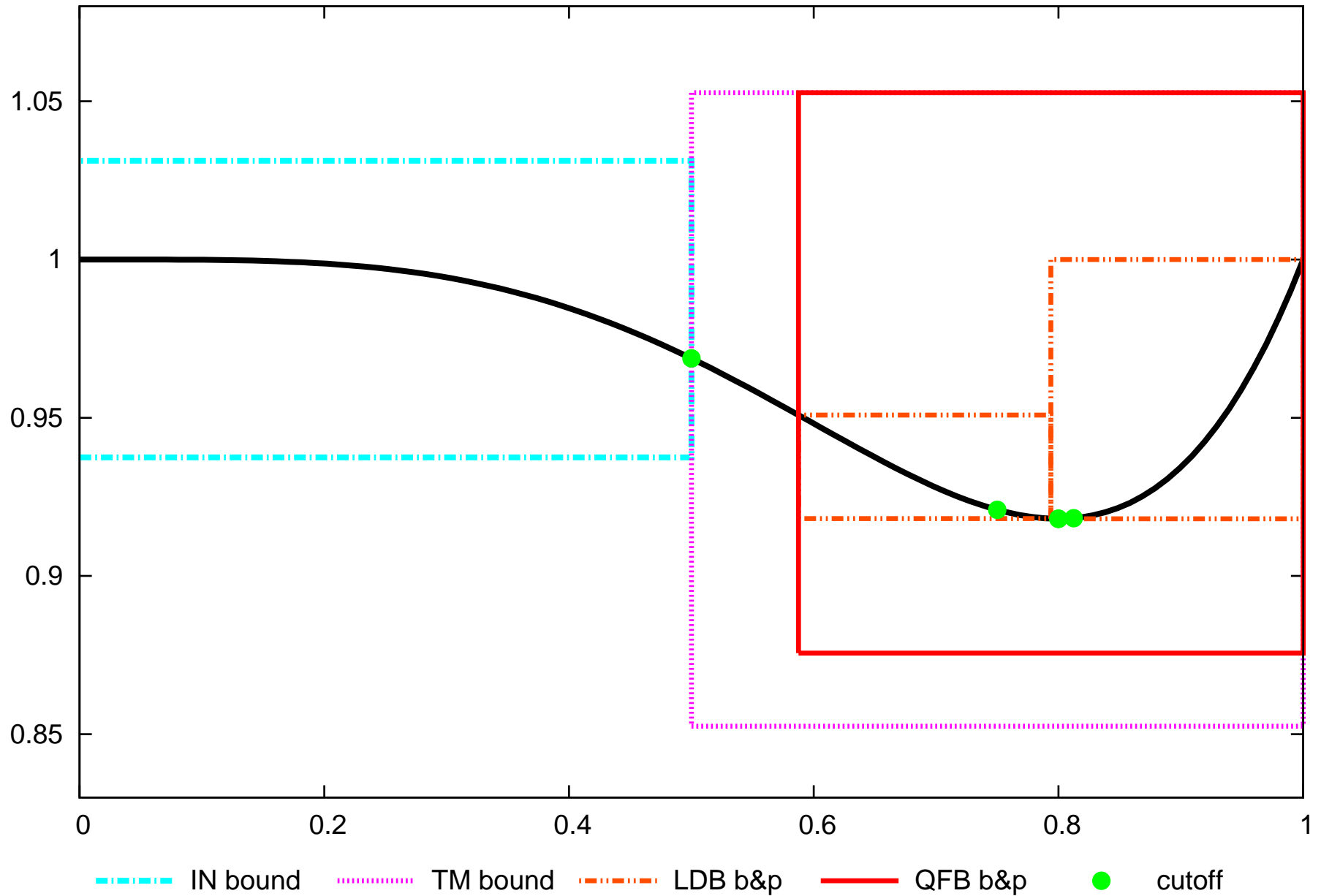
Range Bounding of the Function $f(x) = 1 + x^5 - x^4$ in $[0, 1]$



Intervals: (a) 16, (b) 128, (c) 1024 subdomains.

TMs: (d) 16 (1st, naive), (e) 16 (5th, naive), (f) 16 (5th, LDB).

Moore 1D func. Process of COSY-GO - Step 2 through 8



Range Bounding of the Function $f(x) = 1 + x^5 - x^4$ in $[0, 1]$

Method		Division	Lower bound	Upper bound	Width
Exact		1	0.91808	1	0.08192
TM	GO, 5th	3 (8 steps)*	0.918079	1.000001	0.081922
	LDB, 5th	16	0.918015	1.000001	0.081986
	naive, 5th	16	0.916588	1.000030	0.083442
	naive, 1st	16	0.906340	1.011237	0.104897
	naive, 5th	1	0.71875	1.25	0.53125
Interval		1024	0.916065	1.003901	0.087836
		128	0.901137	1.030886	0.129749
		16	0.724196	1.227524	0.503328
		1	0	2	2

Unless exact, the bound values are rounded outward.

* No equi-sized subdomains – involving pruning and deleting of subdomains.

Important TM Algorithms

- **Range Bounding** (Evaluate f as TM, bound polynomial, add remainder bound. LDB, QFB etc.)
- **Global Optimization** (Use TM bounding schemes, obtain good cutoff values quickly by using non-verified schemes)
- **Quadrature** (Evaluate f as TM, integrate polynomial and remainder bound)
- **Implicit Equations** (Obtain TMs for implicit solutions of TM equations)
- **Superconvergent Interval Newton Method** (Application of Implicit Equations)
- **Implicit ODEs and DAEs**
- **Complex Arithmetic**
- **ODEs** (Obtain TMs describing dependence of final coordinates on initial coordinates)

The TM based Global Optimizer, COSY-GO

has utilized various algorithms based on Taylor models.

- LDB (Linear Dominated Bounding) bounding and domain reduction
- QFB (Quadratic Fast Bounding) bounding and domain reduction for positive definite cases (Quadratic pruning)
- Various cutoff value update schemes

And, we have

- Adjustment to parallel environments with low inter-processor communication rate
- Restart capability
- Continuation of computations while the underlying arithmetic fails

And, what we are doing further...

- High-order derivative based box rejection and the domain reduction
- Supporting high multiple precision computations for TMs

Applications

There are so many problems requiring optimizations.
Using COSY-GO, we have worked on

- Numerous challenging benchmark tests
- Design parameter optimizations
- Rump's Toeplitz problems
- Entropy estimates for chaotic dynamical systems
- Long-term stability estimates of the Tevatron
- Molecule packing problems
- Gravity assist interplanetary spacecraft trajectory designs

And more are, and will be, coming.

- Edge curvature design for FFAG magnets
- Complicated field computations for beam transfer maps
- ... Any problem you can imagine...

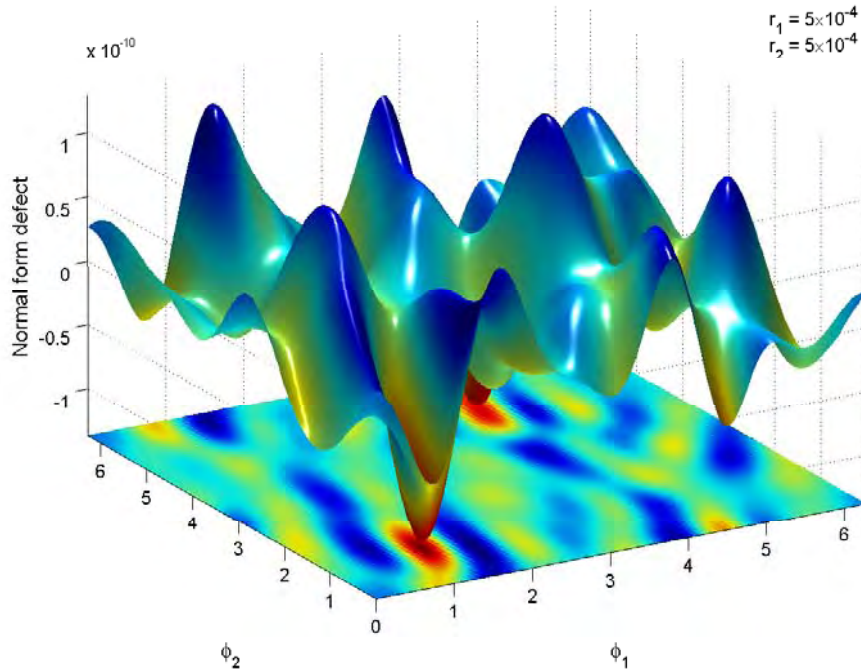


Fig. 9. Projection of the normal form defect function. Dependence on two angle variables for the fixed radii $r_1 = r_2 = 5 \cdot 10^{-4}$

Region	Boxes studied	CPU-time	Bound	Transversal Iterations
$[0.2, 0.4] \cdot 10^{-4}$	82, 930	30, 603 sec	$0.859 \cdot 10^{-13}$	$2.3283 \cdot 10^8$
$[0.4, 0.6] \cdot 10^{-4}$	82, 626	30, 603 sec	$0.587 \cdot 10^{-12}$	$3.4072 \cdot 10^7$
$[0.6, 0.9] \cdot 10^{-4}$	64, 131	14, 441 sec	$0.616 \cdot 10^{-11}$	$4.8701 \cdot 10^6$
$[0.9, 1.2] \cdot 10^{-4}$	73, 701	13, 501 sec	$0.372 \cdot 10^{-10}$	$8.0645 \cdot 10^5$
$[1.2, 1.5] \cdot 10^{-4}$	106, 929	24, 304 sec	$0.144 \cdot 10^{-9}$	$2.0833 \cdot 10^5$
$[1.5, 1.8] \cdot 10^{-4}$	111, 391	26, 103 sec	$0.314 \cdot 10^{-9}$	$0.95541 \cdot 10^5$

Table 8

Global bounds obtained for six radial regions in normal form space for the Tevatron. Also computed are the guaranteed minimum transversal iterations.

ODE Integration with Taylor Models

Idea: retain full **dependence on initial conditions** as Taylor model (Non-verified version: big breakthrough in particle optics and beam physics, 1984 - allows to calculate "aberrations" to any order, from earlier order three)

1. Different from other validated methods, the approach is **single step** - no need for a separate coarse enclosure and subsequent verification step
2. Error due to **time stepping** is $O(n_t + 1)$
3. Error due to **initial variables** is $O(n_v + 1)$, **not** $O(2)$ as in other methods
4. By choosing n_t and n_v appropriately, the error due to finite domain and time stepping can be made **arbitrarily small**.
5. Overall, **never** leave the TM representation until possibly the very end. Doing so may remove higher order dependence.

--> Talk by Martin Berz

Refer, also, to the references in the proceedings paper.

The Volterra Equation

Describe dynamics of two conflicting populations

$$\frac{dx_1}{dt} = 2x_1(1 - x_2), \quad \frac{dx_2}{dt} = -x_2(1 - x_1)$$

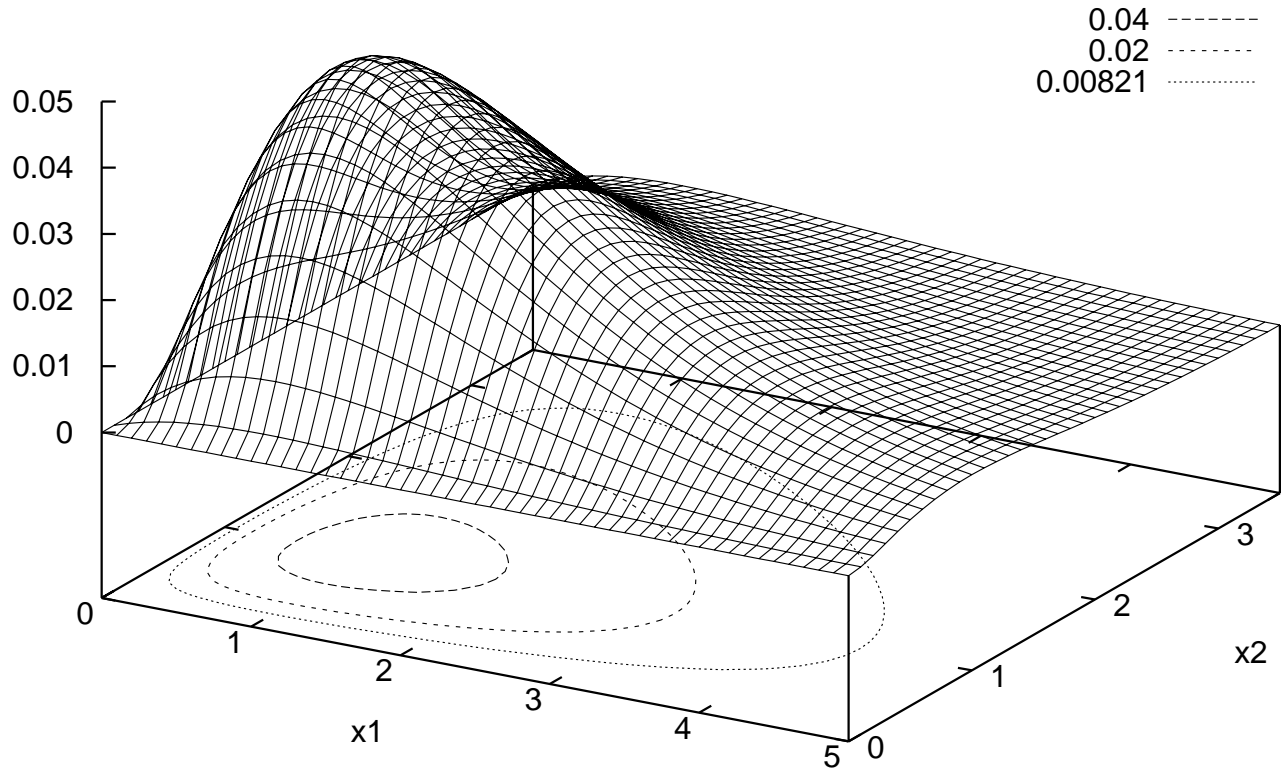
Interested in initial condition

$$x_{01} \in 1 + [-0.05, 0.05], \quad x_{02} \in 3 + [-0.05, 0.05] \quad \text{at } t = 0.$$

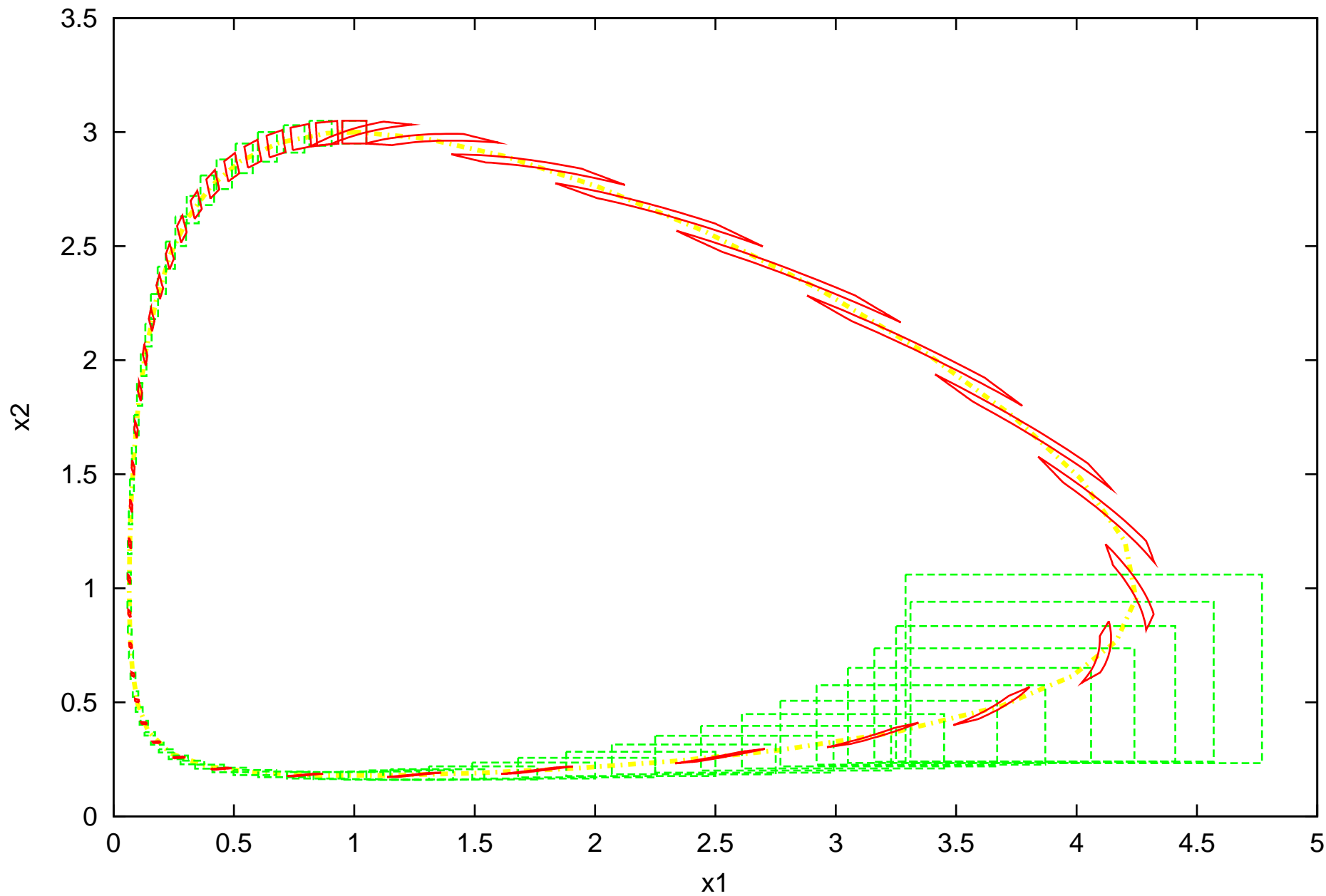
Satisfies constraint condition

$$C(x_1, x_2) = x_1 x_2^2 e^{-x_1 - 2x_2} = \text{Constant}$$

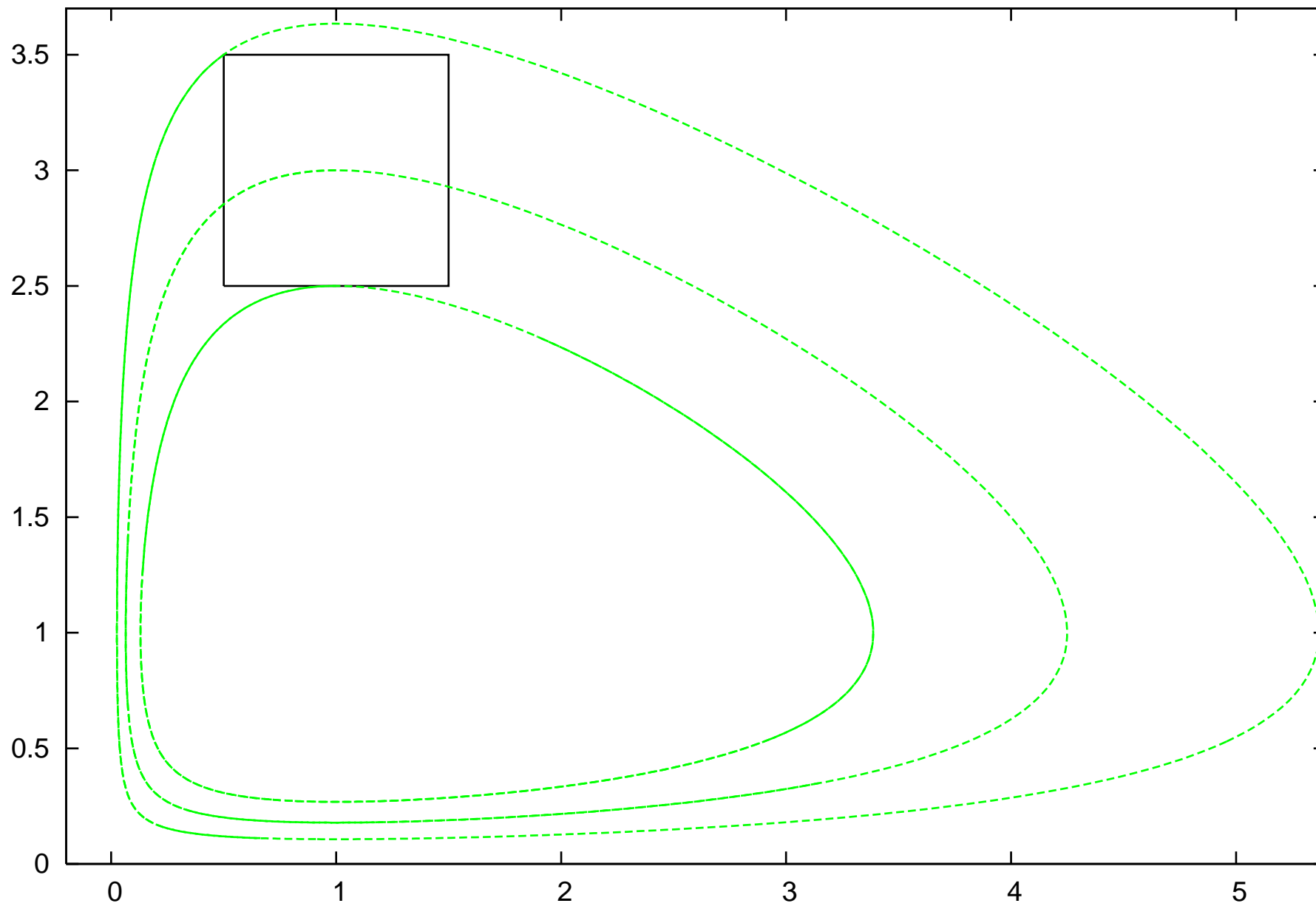
$f(x_1, x_2)$



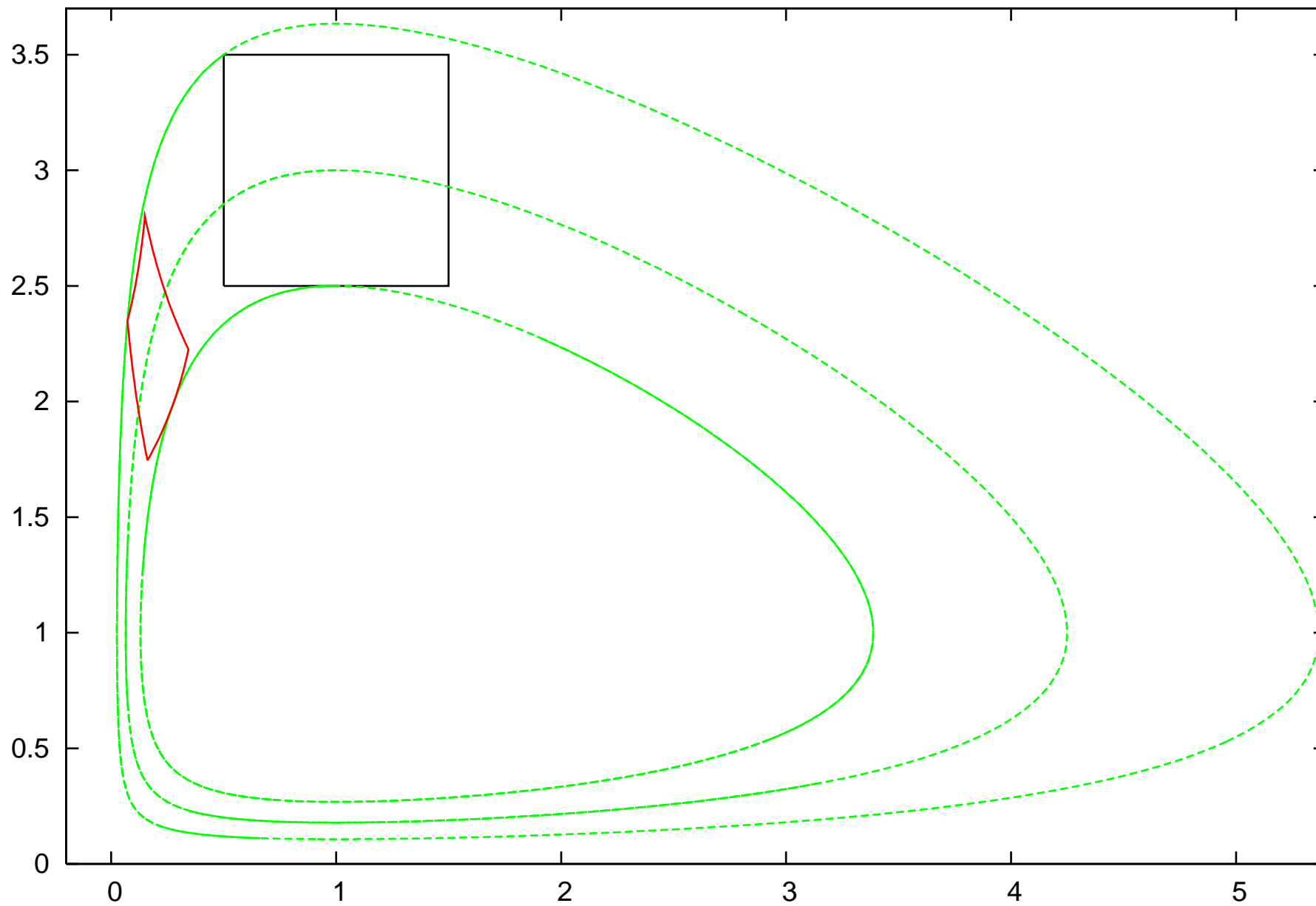
Integration of the Volterra eqs. COSY-VI and AWA



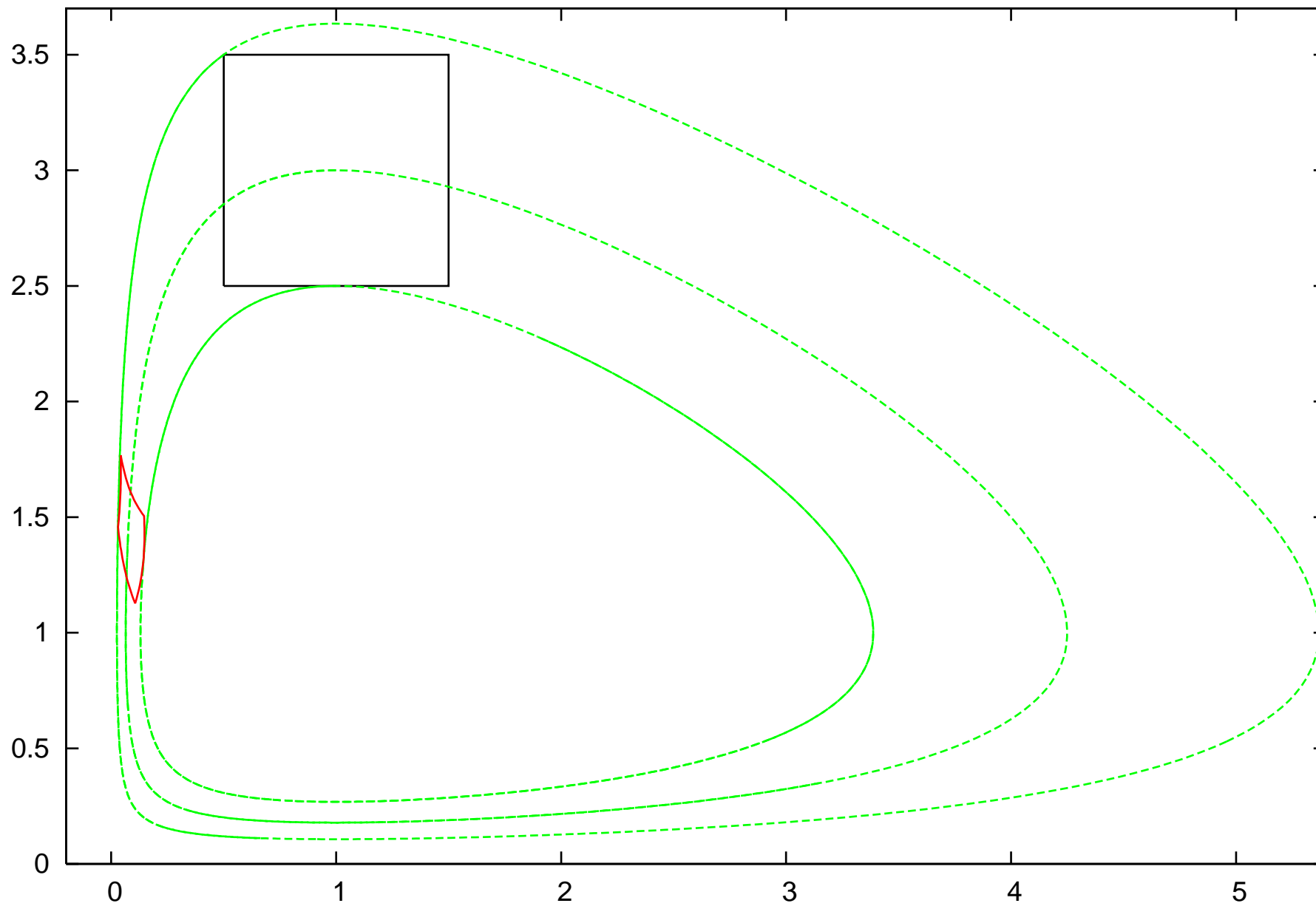
Volterra. IC=(1,3)+-0.5. T= 0.0



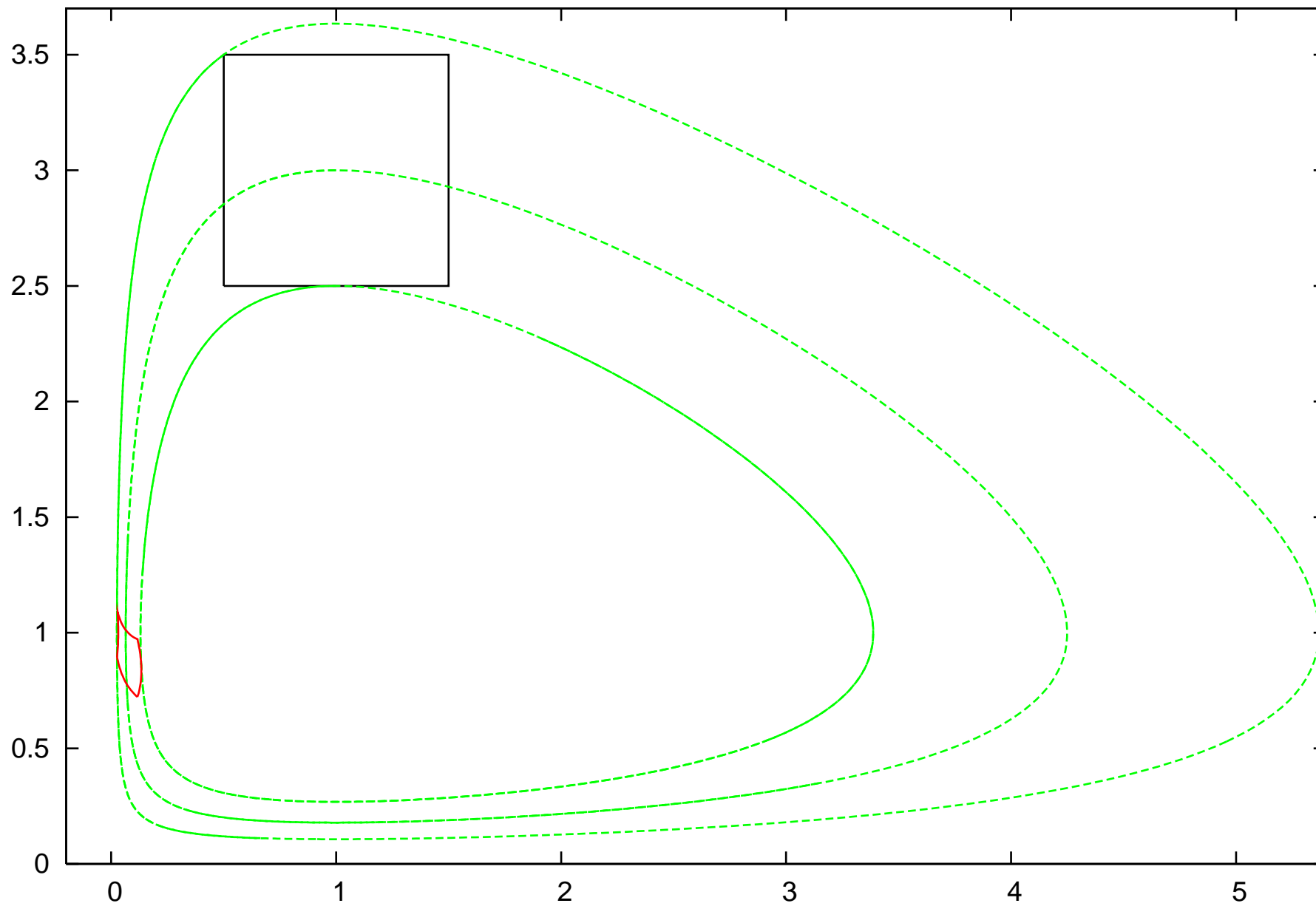
Volterra. IC=(1,3)+-0.5. T= 0.5



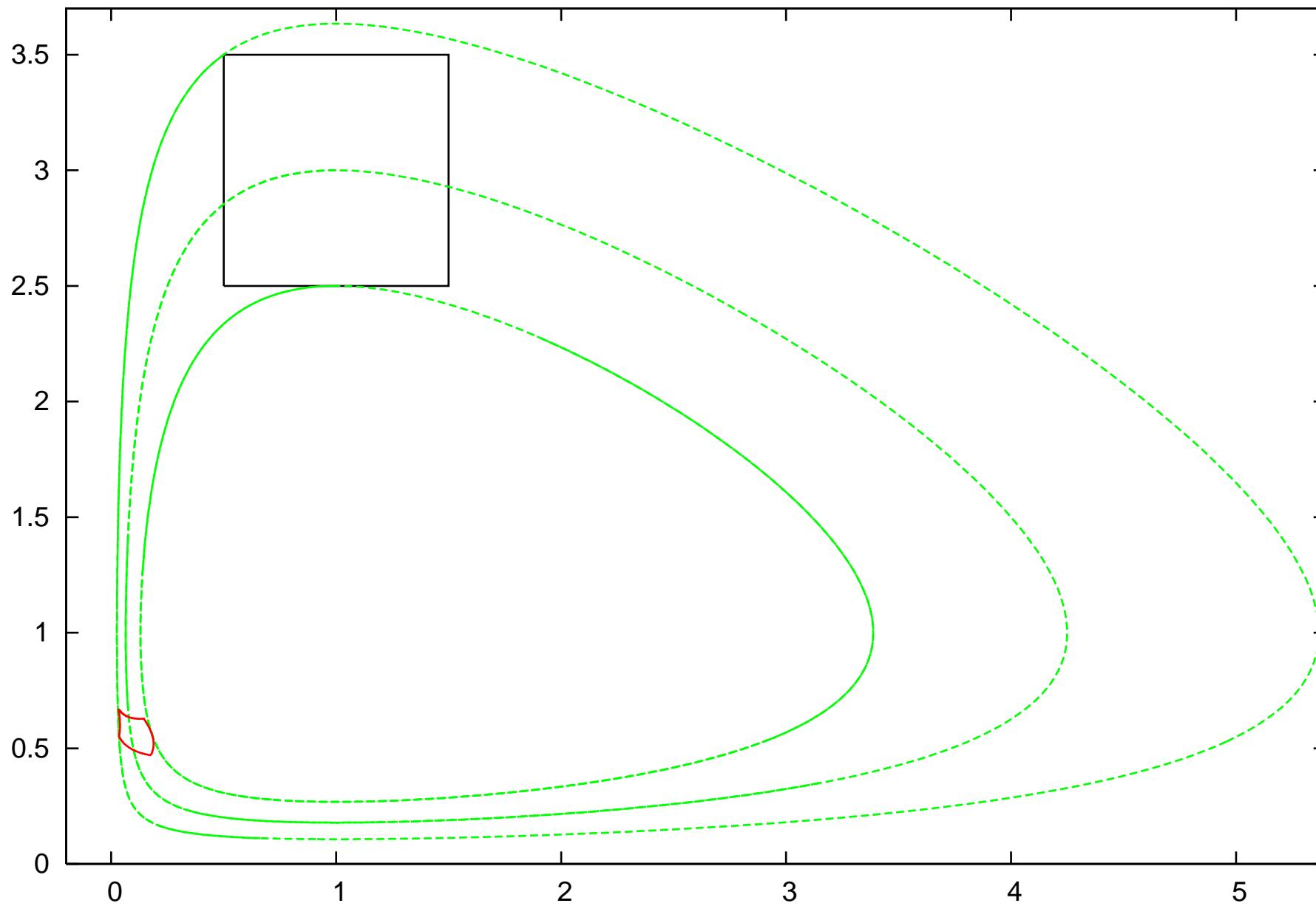
Volterra. IC=(1,3)+-0.5. T= 1.0



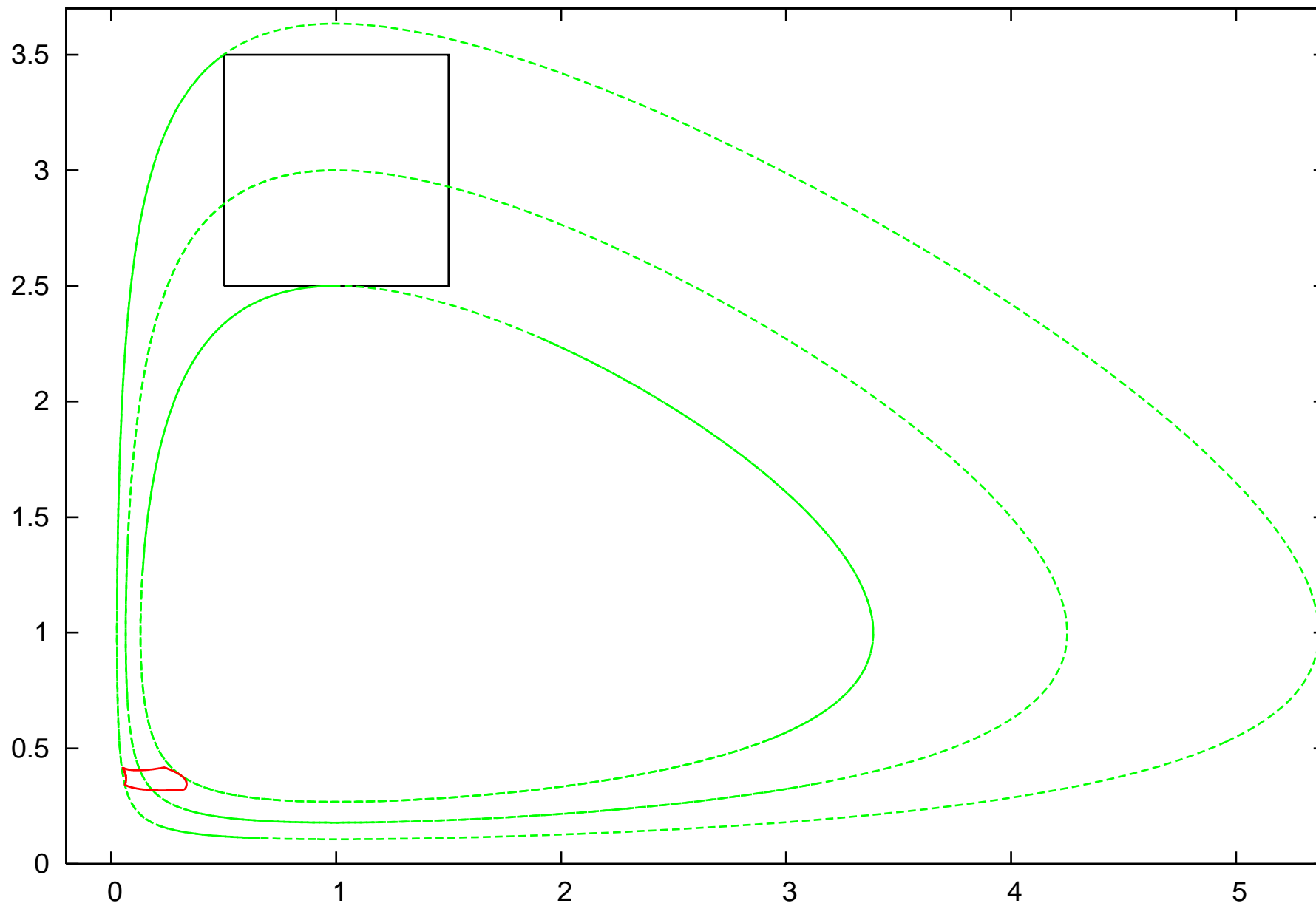
Volterra. IC=(1,3)+-0.5. T= 1.5



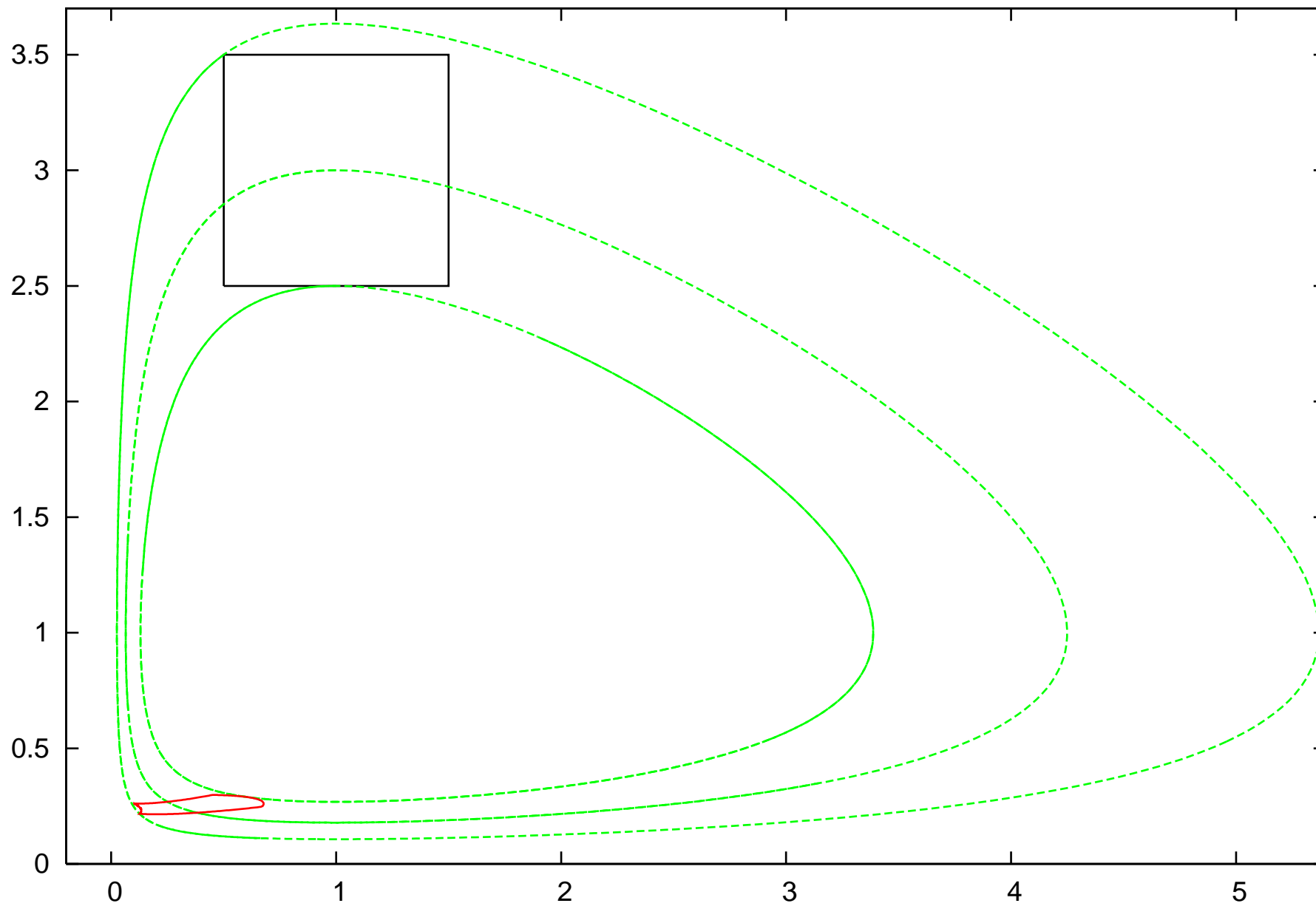
Volterra. IC=(1,3)+-0.5. T= 2.0



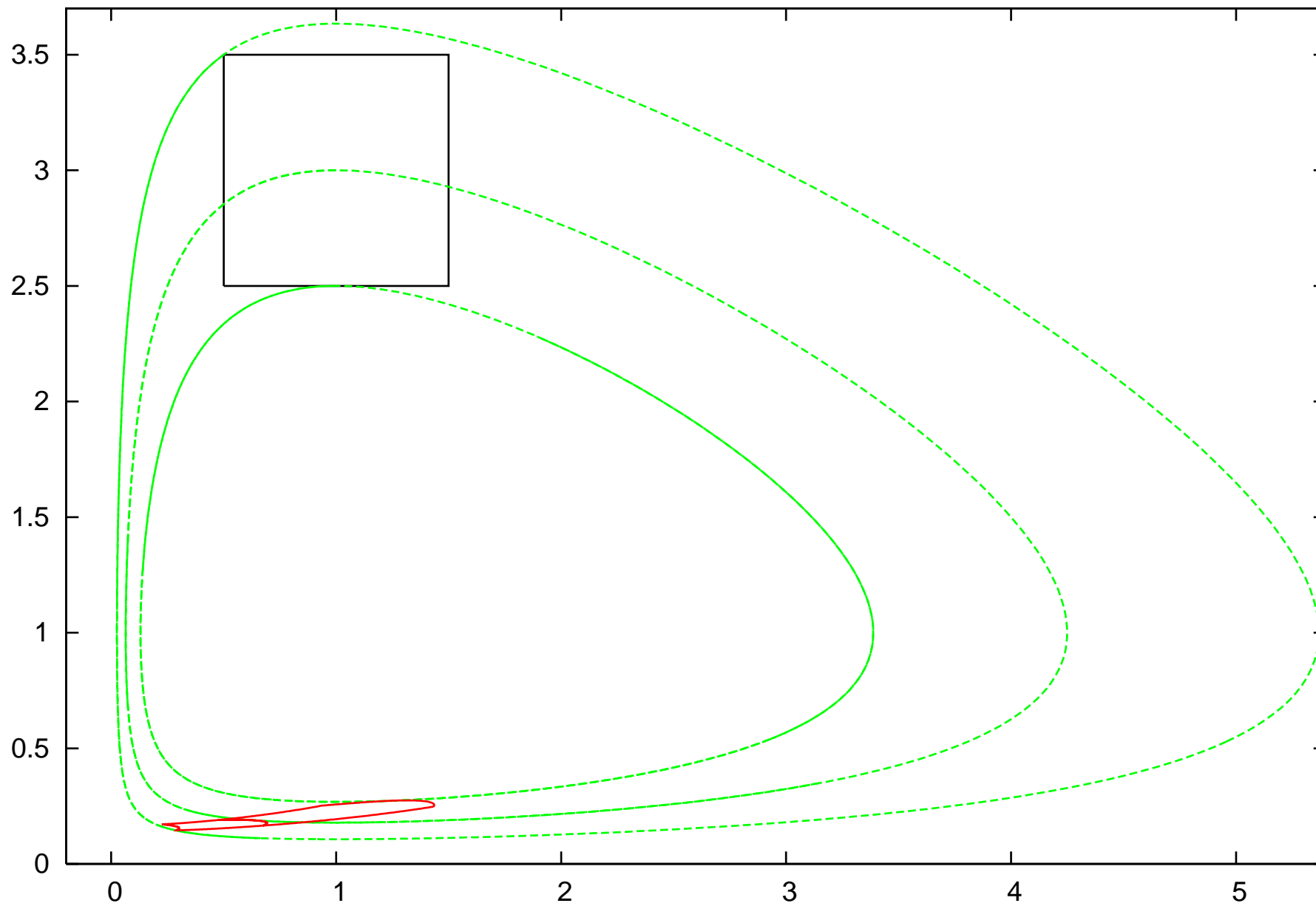
Volterra. IC=(1,3)+-0.5. T= 2.5



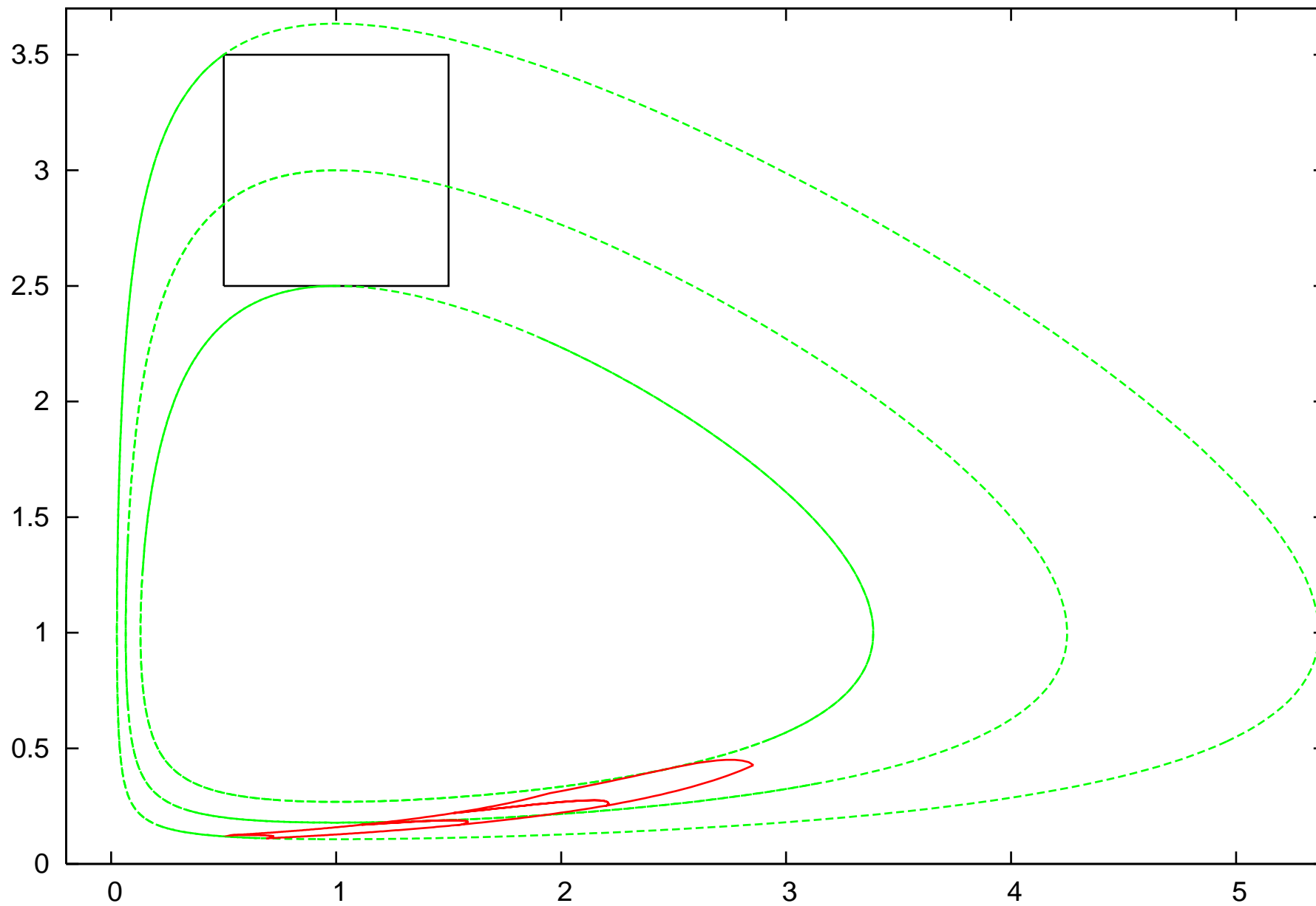
Volterra. IC=(1,3)+-0.5. T= 3.0



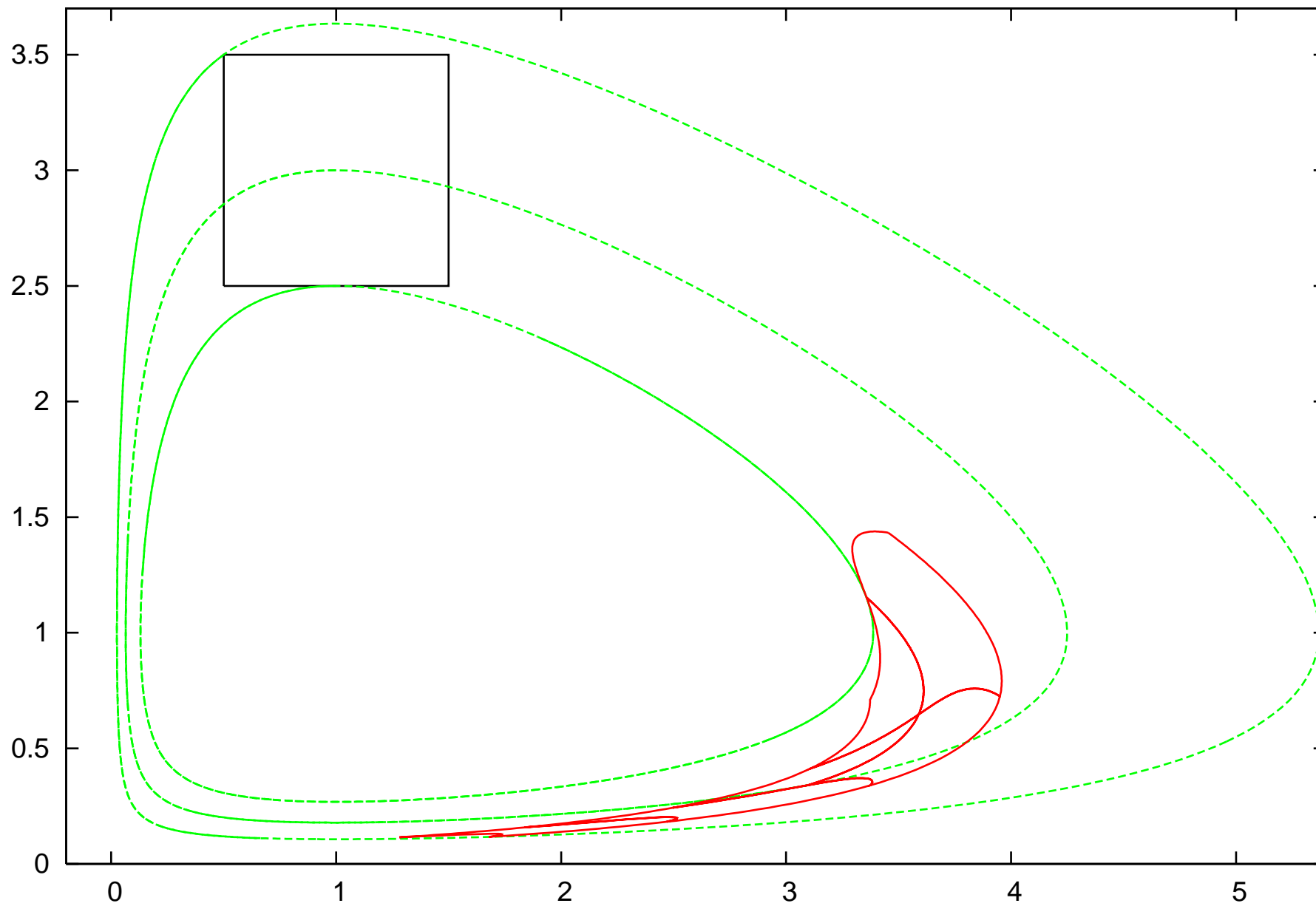
Volterra. IC=(1,3)+-0.5. T= 3.5



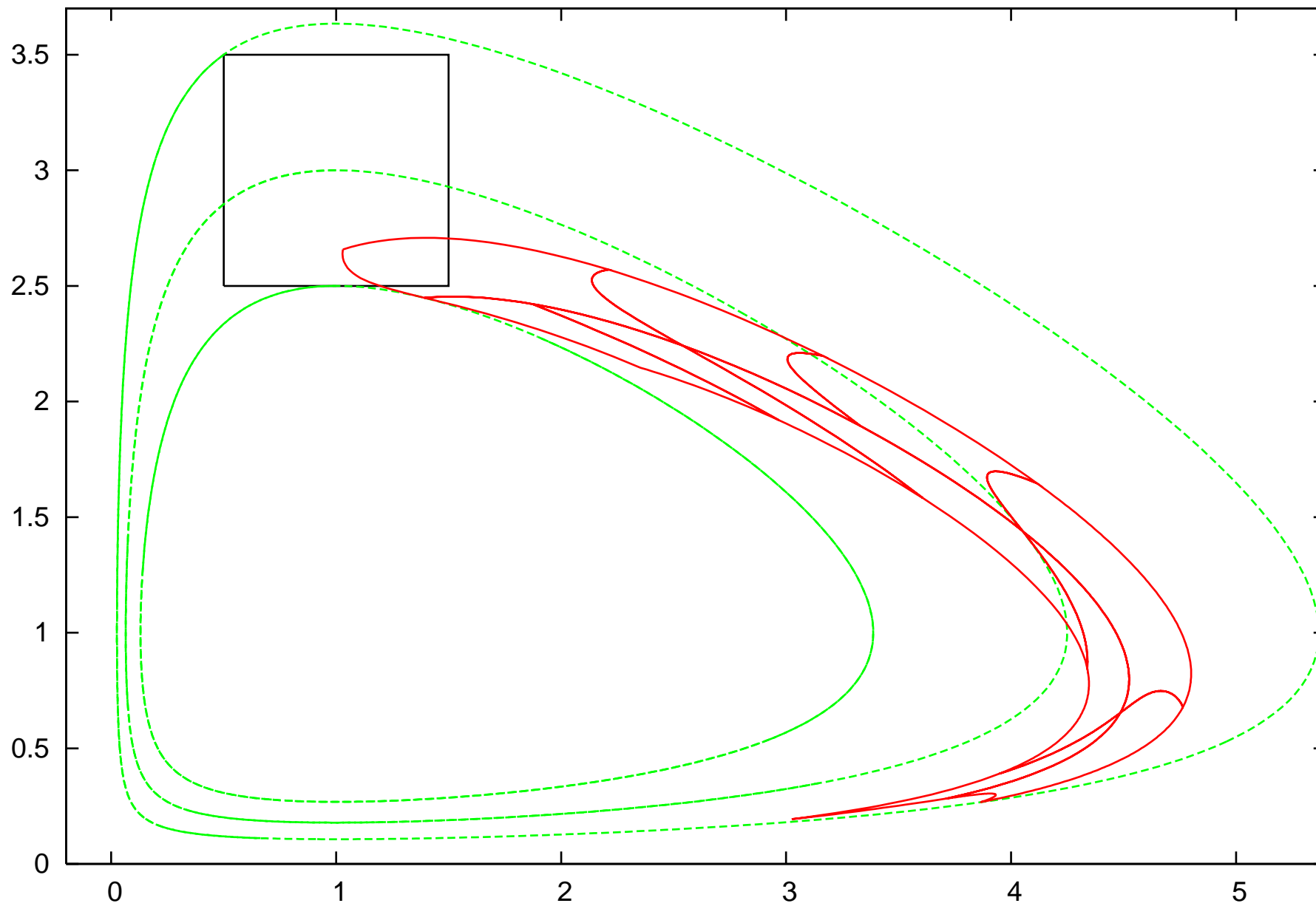
Volterra. IC=(1,3)+-0.5. T= 4.0



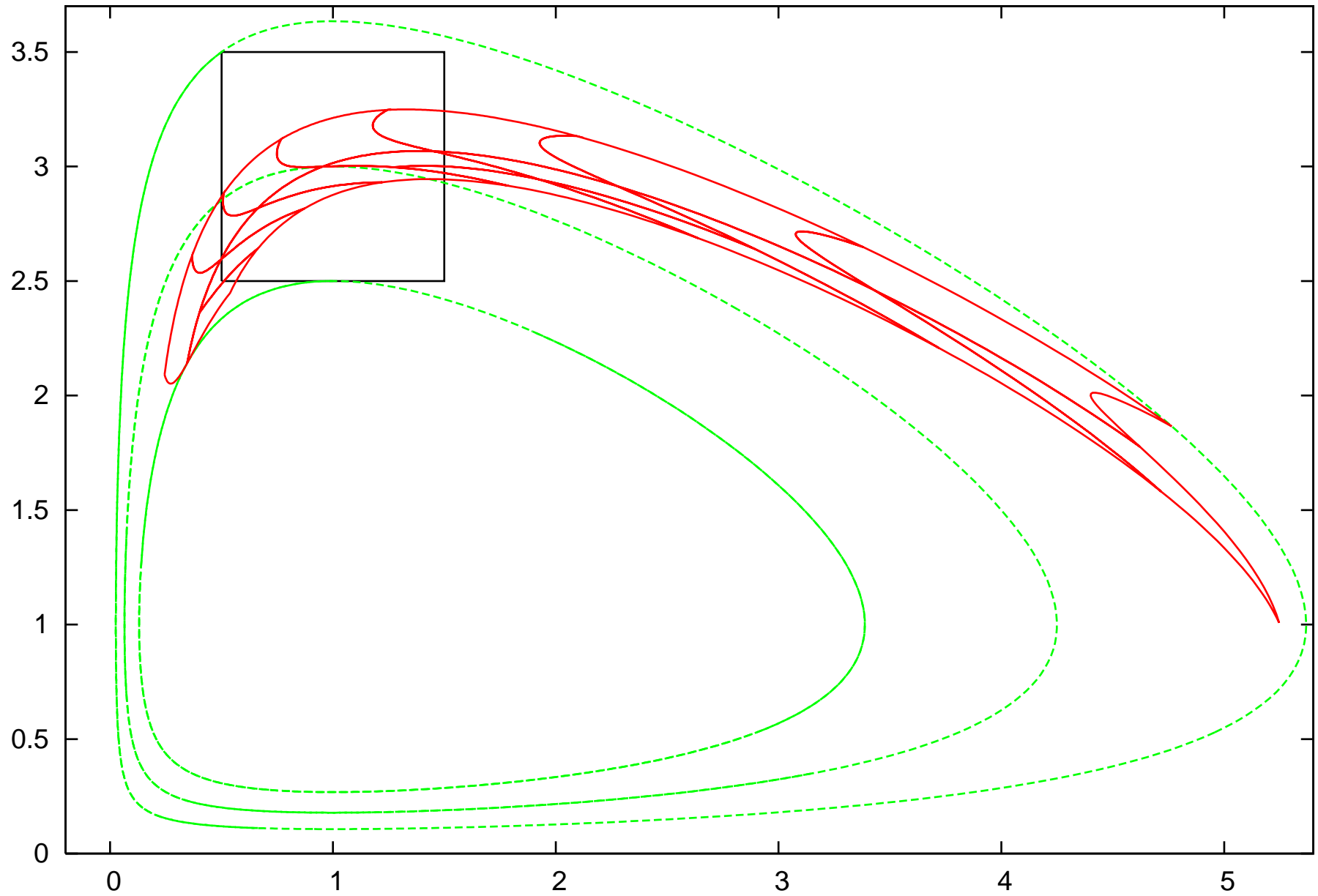
Volterra. IC=(1,3)+-0.5. T= 4.5



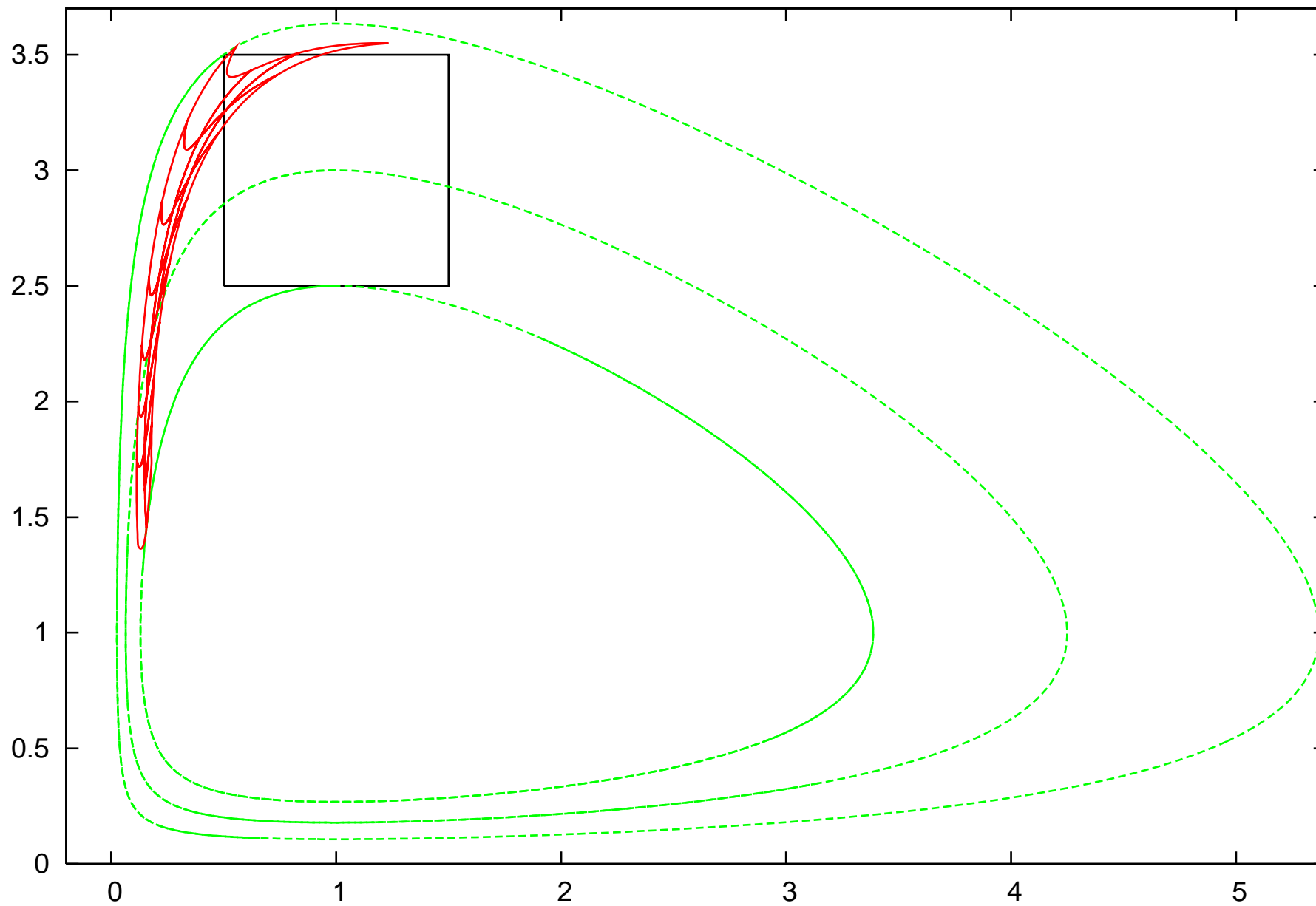
Volterra. IC=(1,3)+0.5. T= 5.0



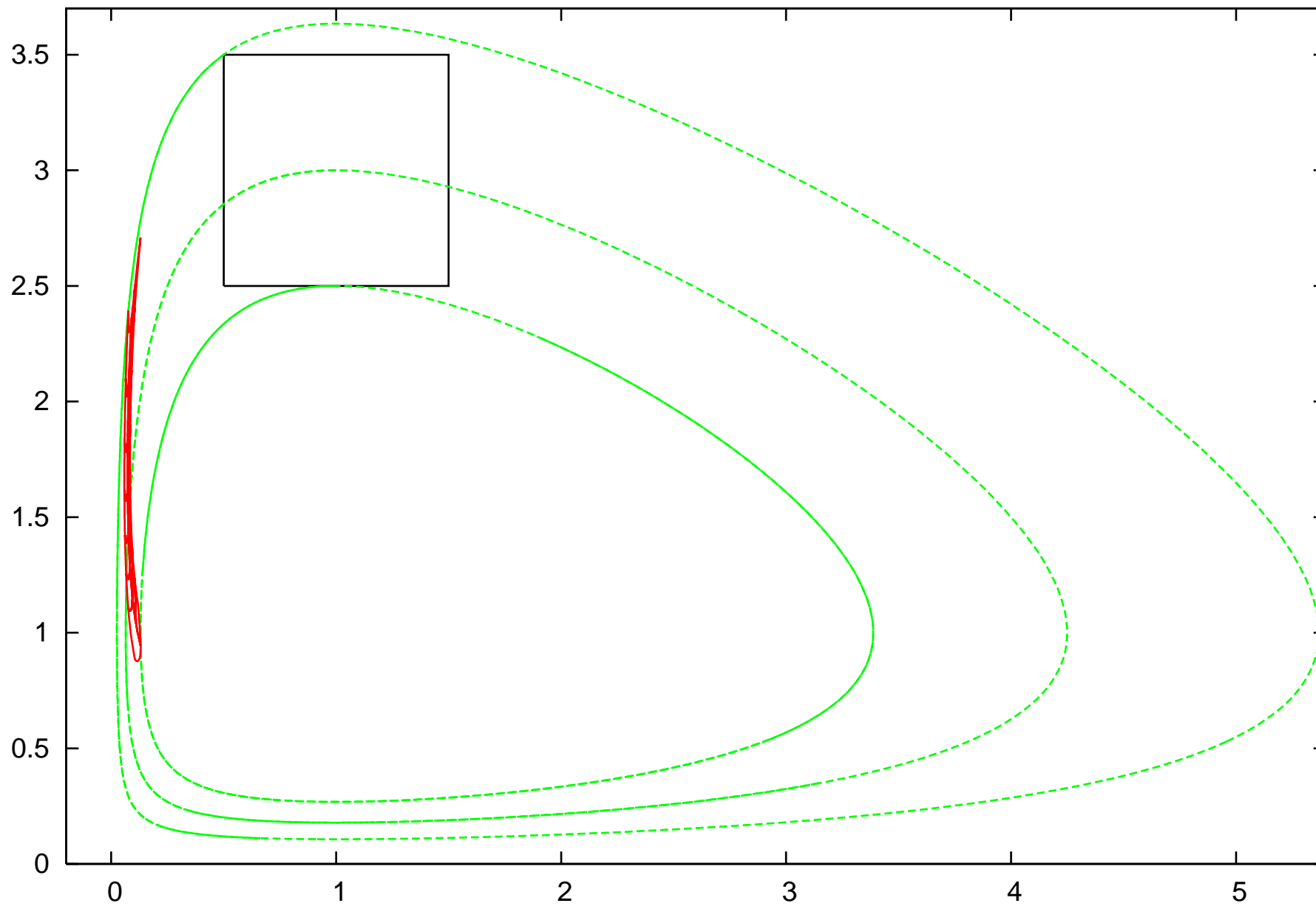
Volterra. IC=(1,3)+0.5. T= 5.5



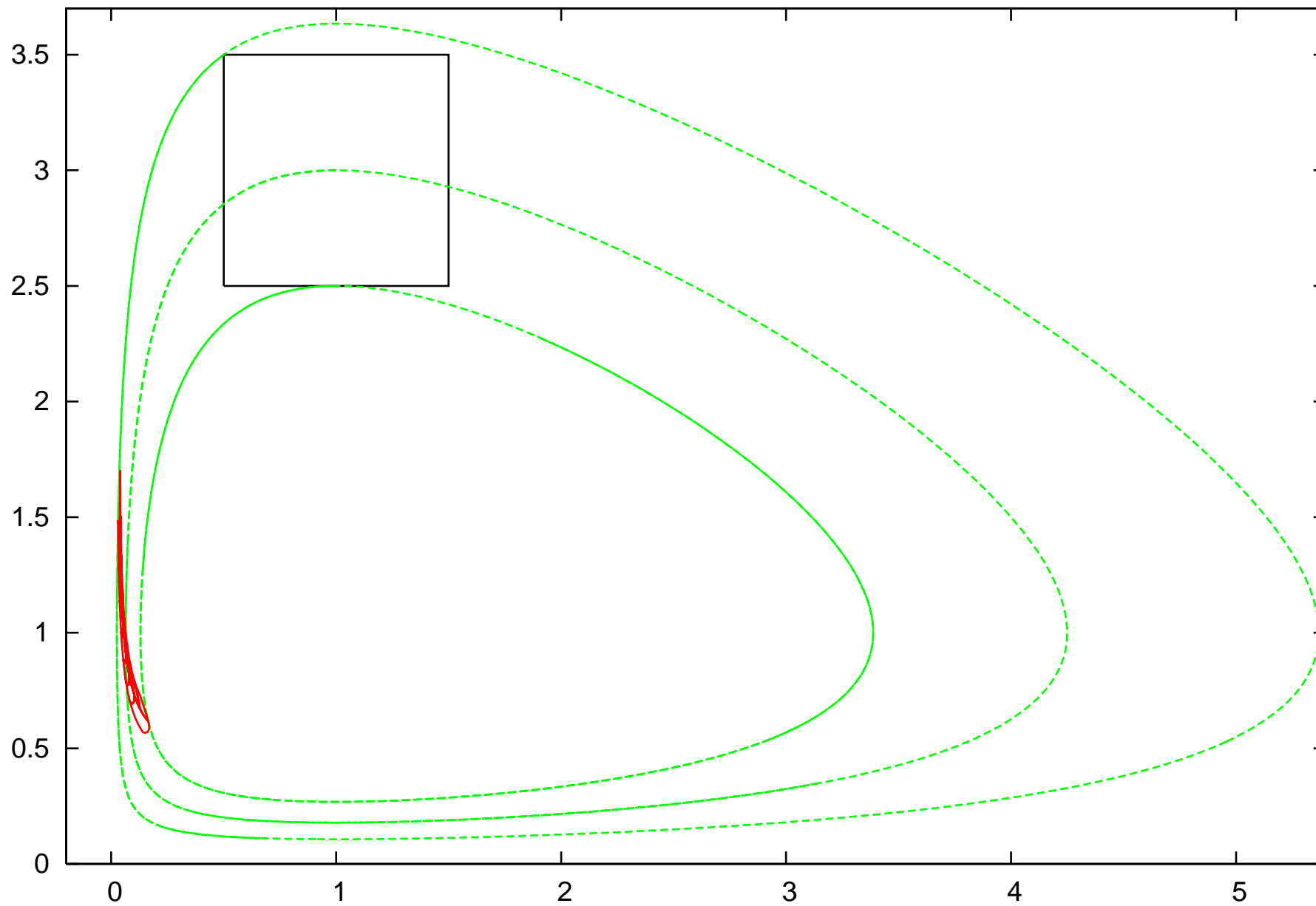
Volterra. IC=(1,3)+-0.5. T= 6.0



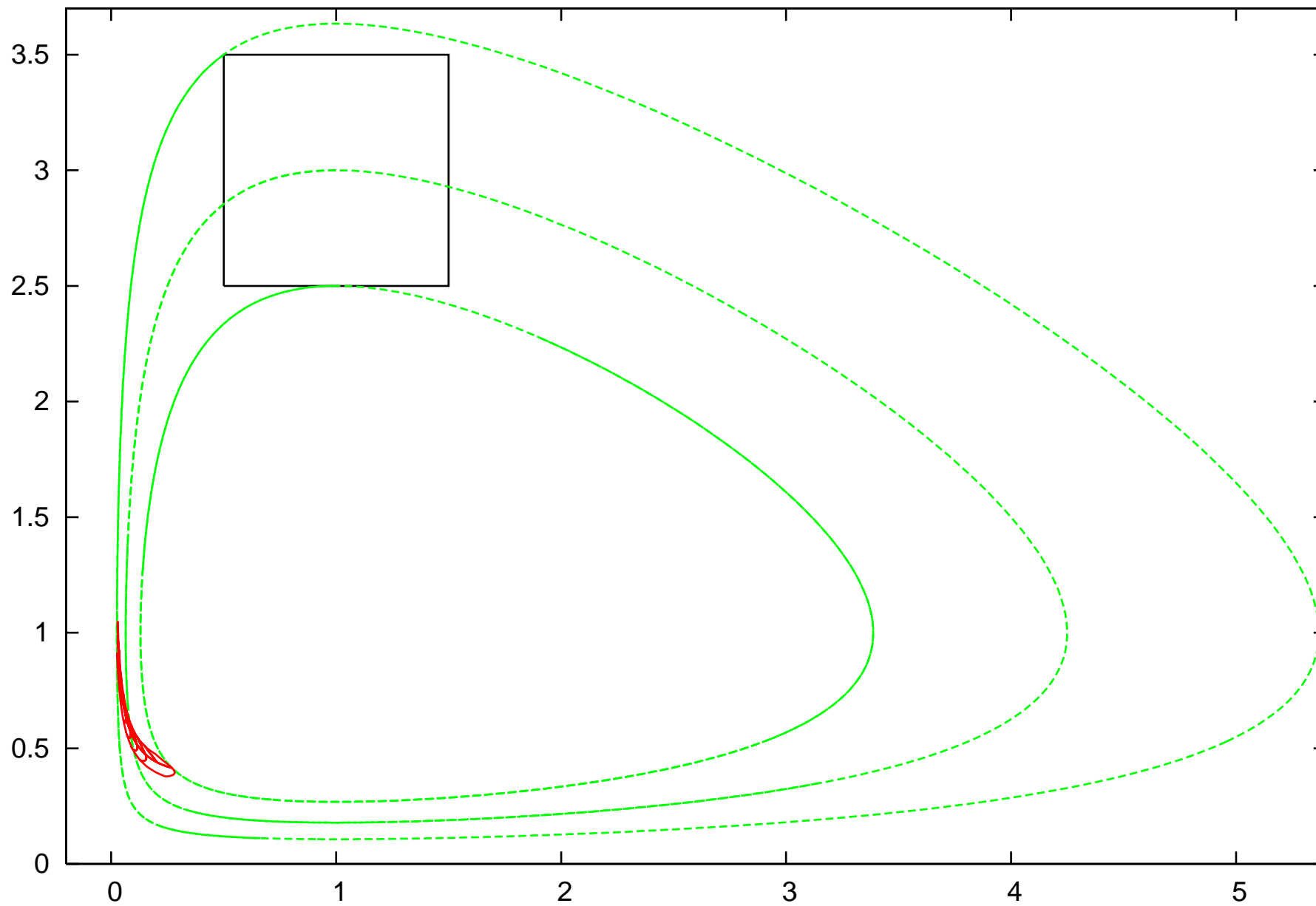
Volterra. IC=(1,3)+-0.5. T= 6.5



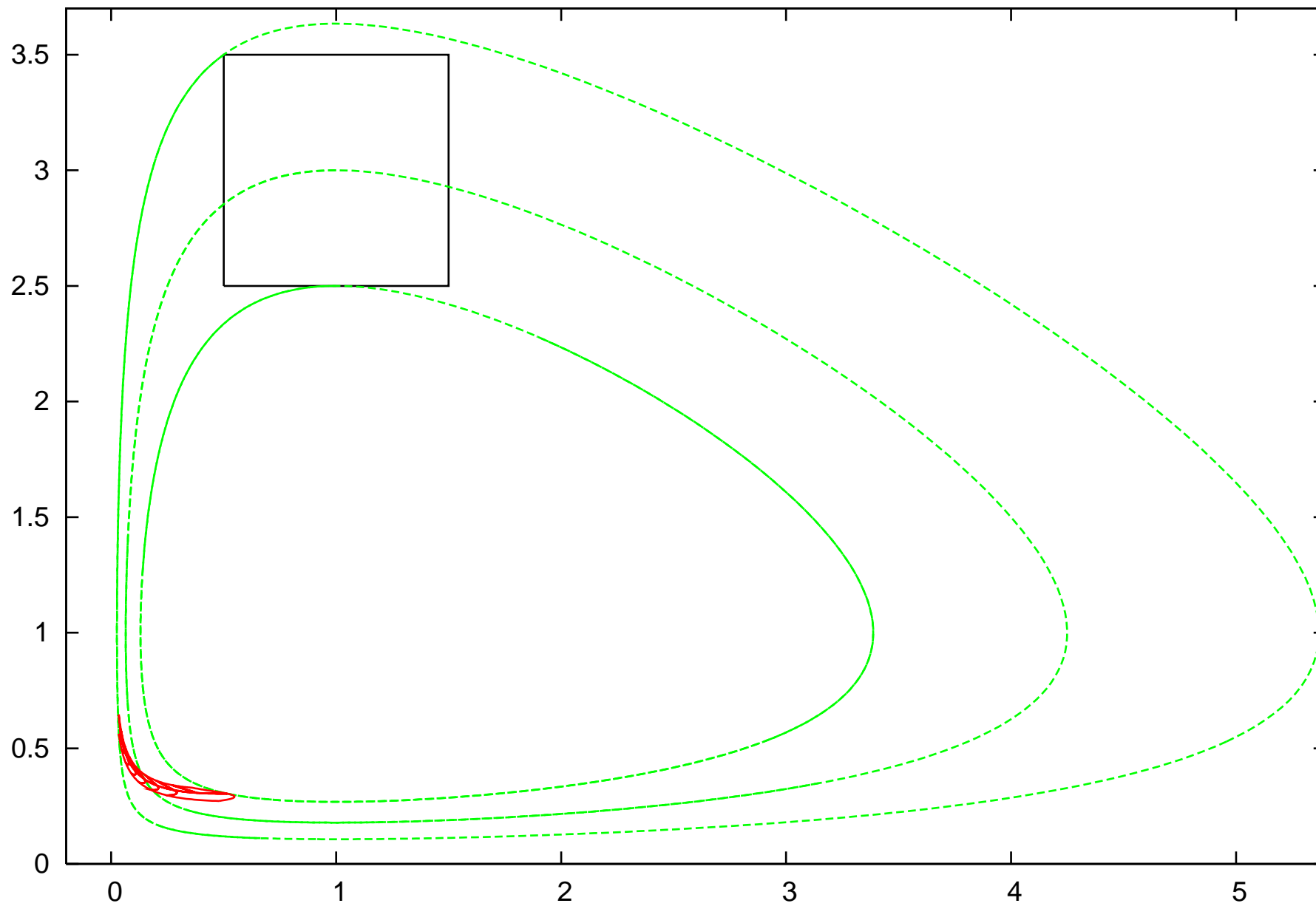
Volterra. IC=(1,3)+-0.5. T= 7.0



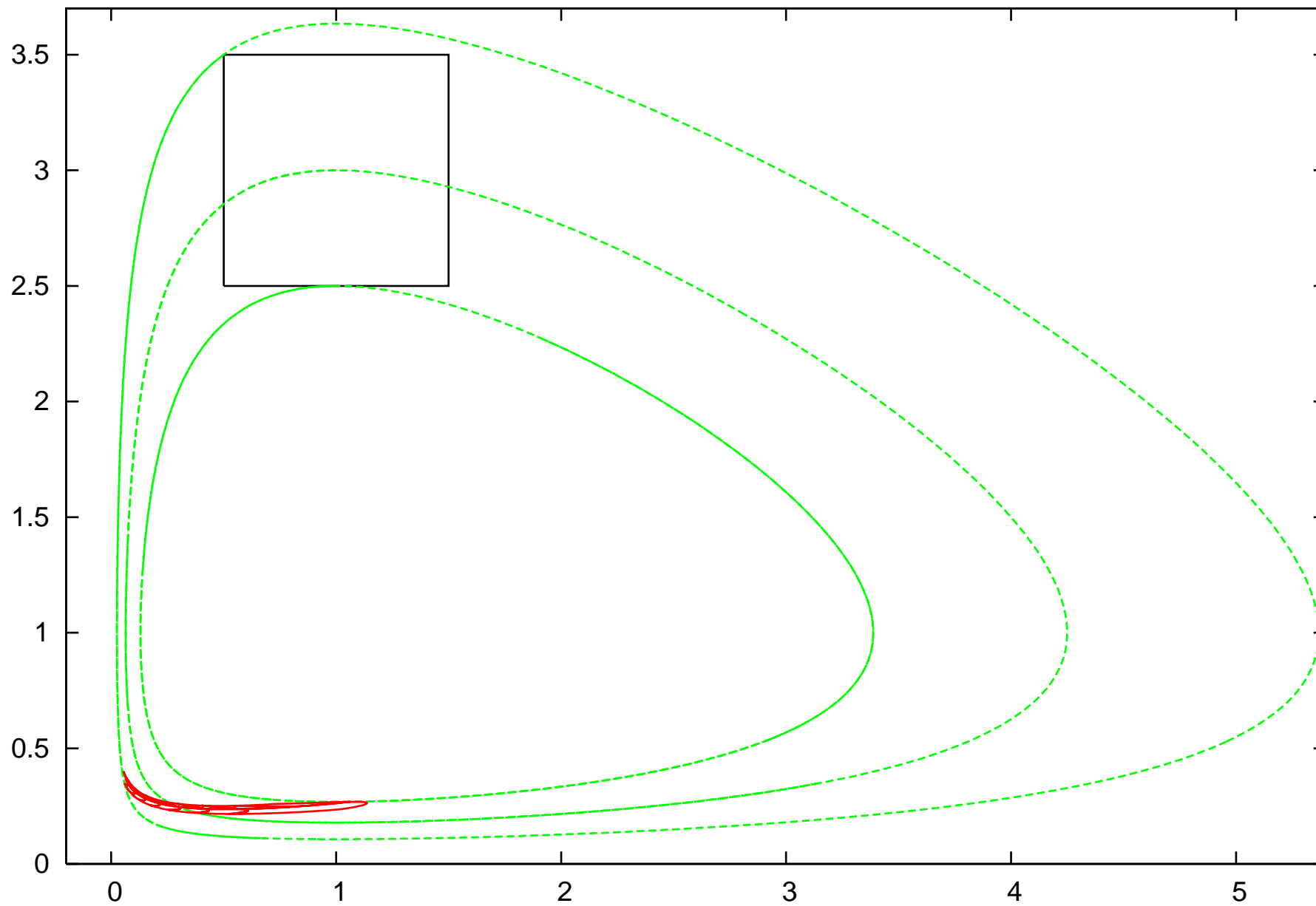
Volterra. IC=(1,3)+-0.5. T= 7.5



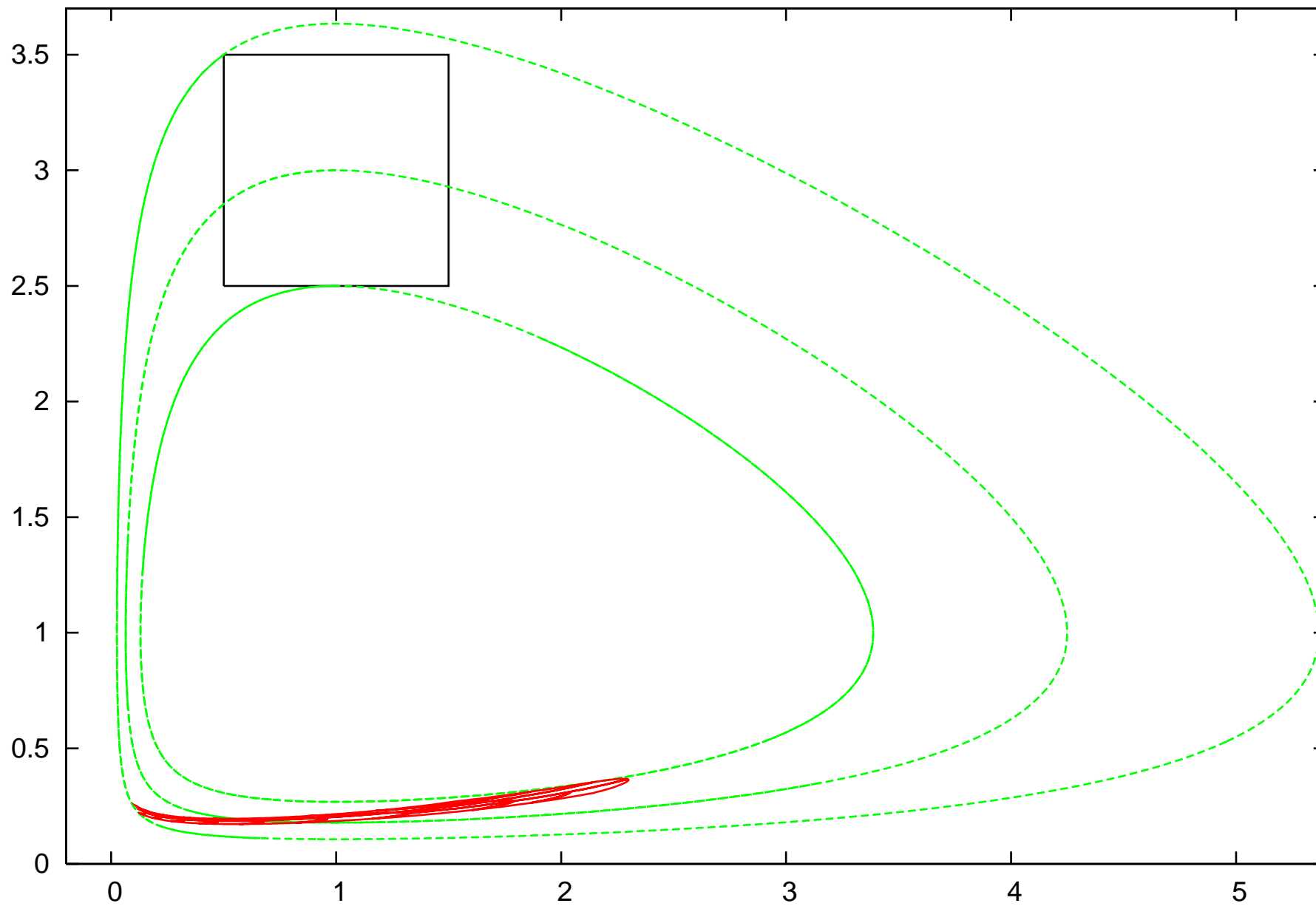
Volterra. IC=(1,3)+-0.5. T= 8.0



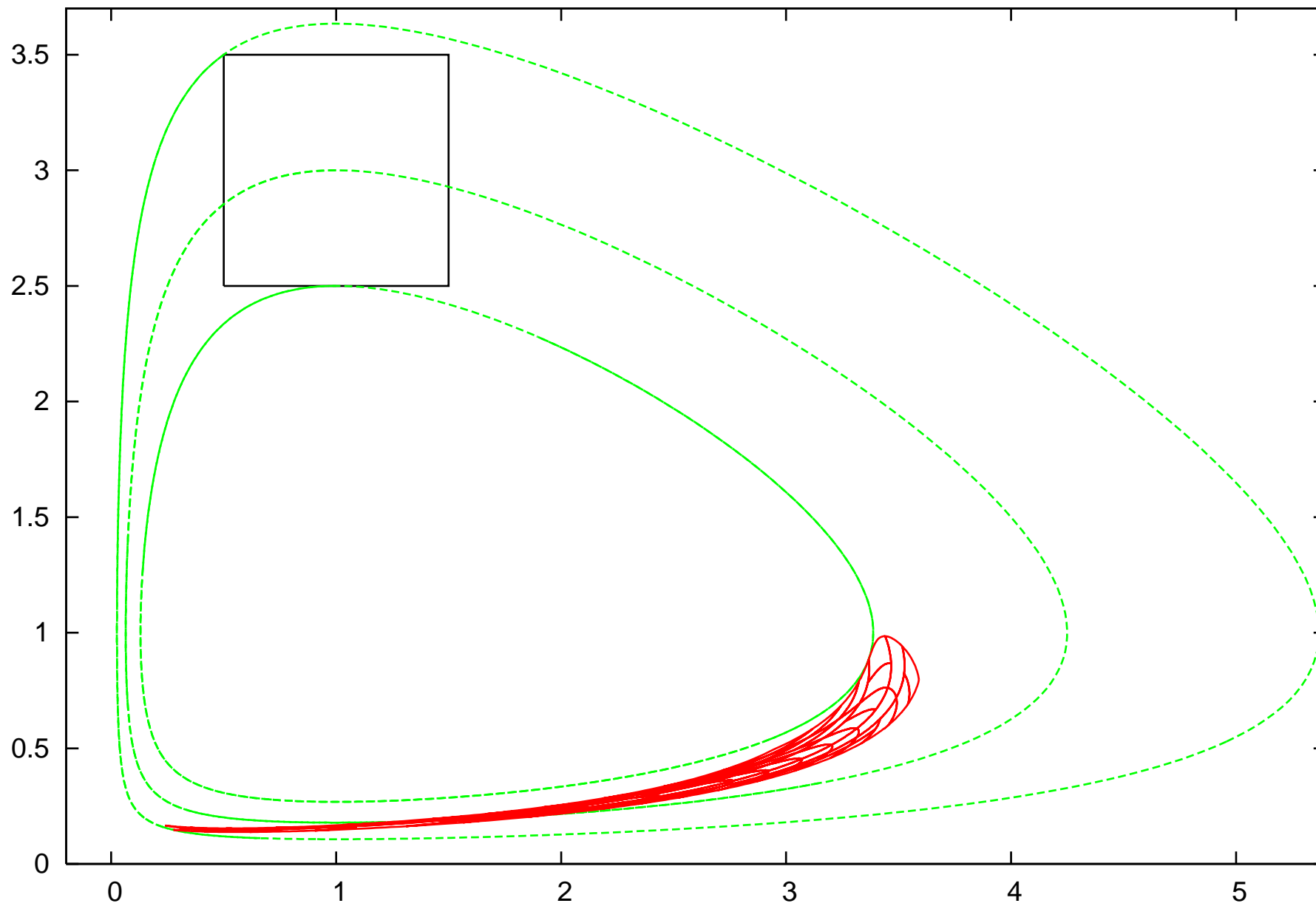
Volterra. IC=(1,3)+-0.5. T= 8.5



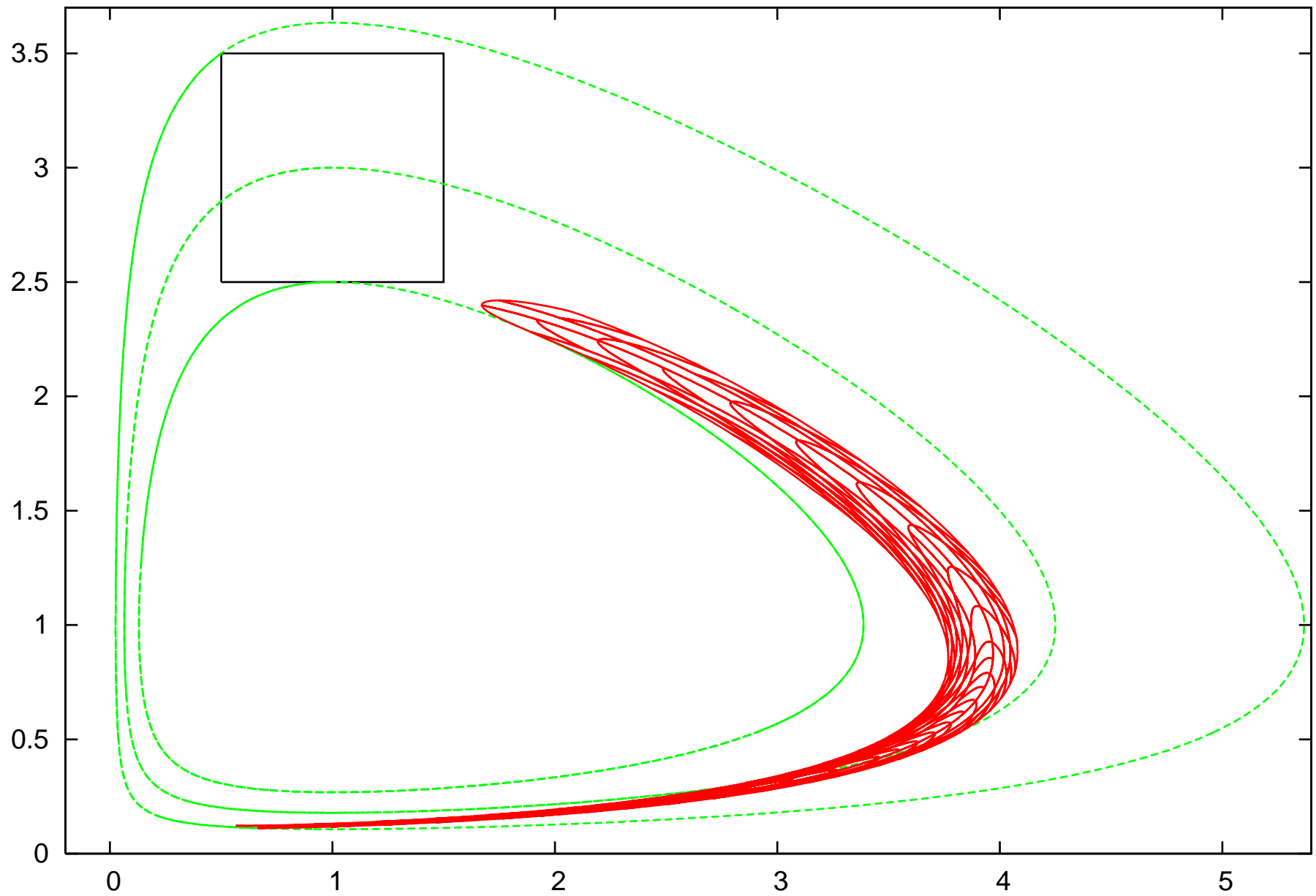
Volterra. IC=(1,3)+-0.5. T= 9.0



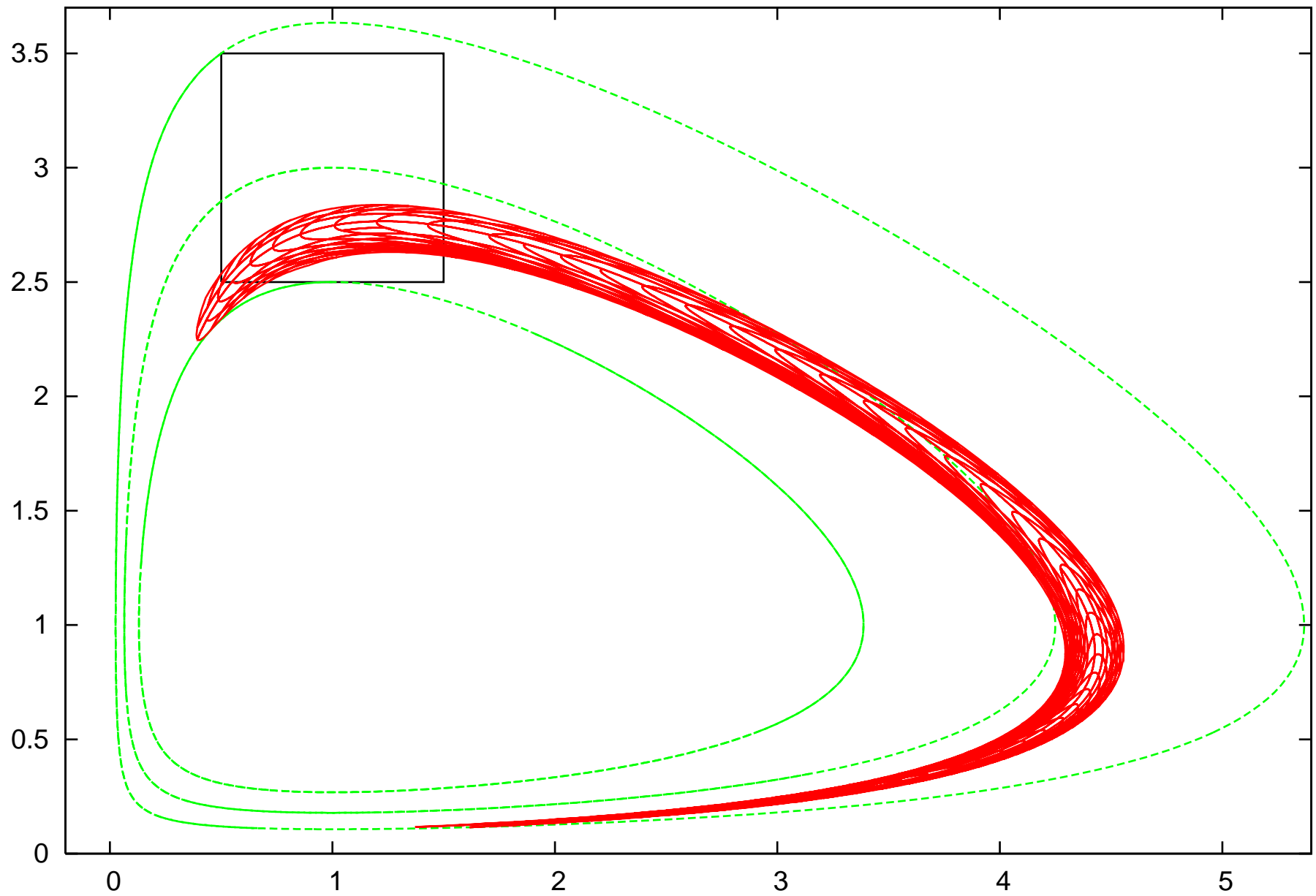
Volterra. IC=(1,3)+-0.5. T= 9.5



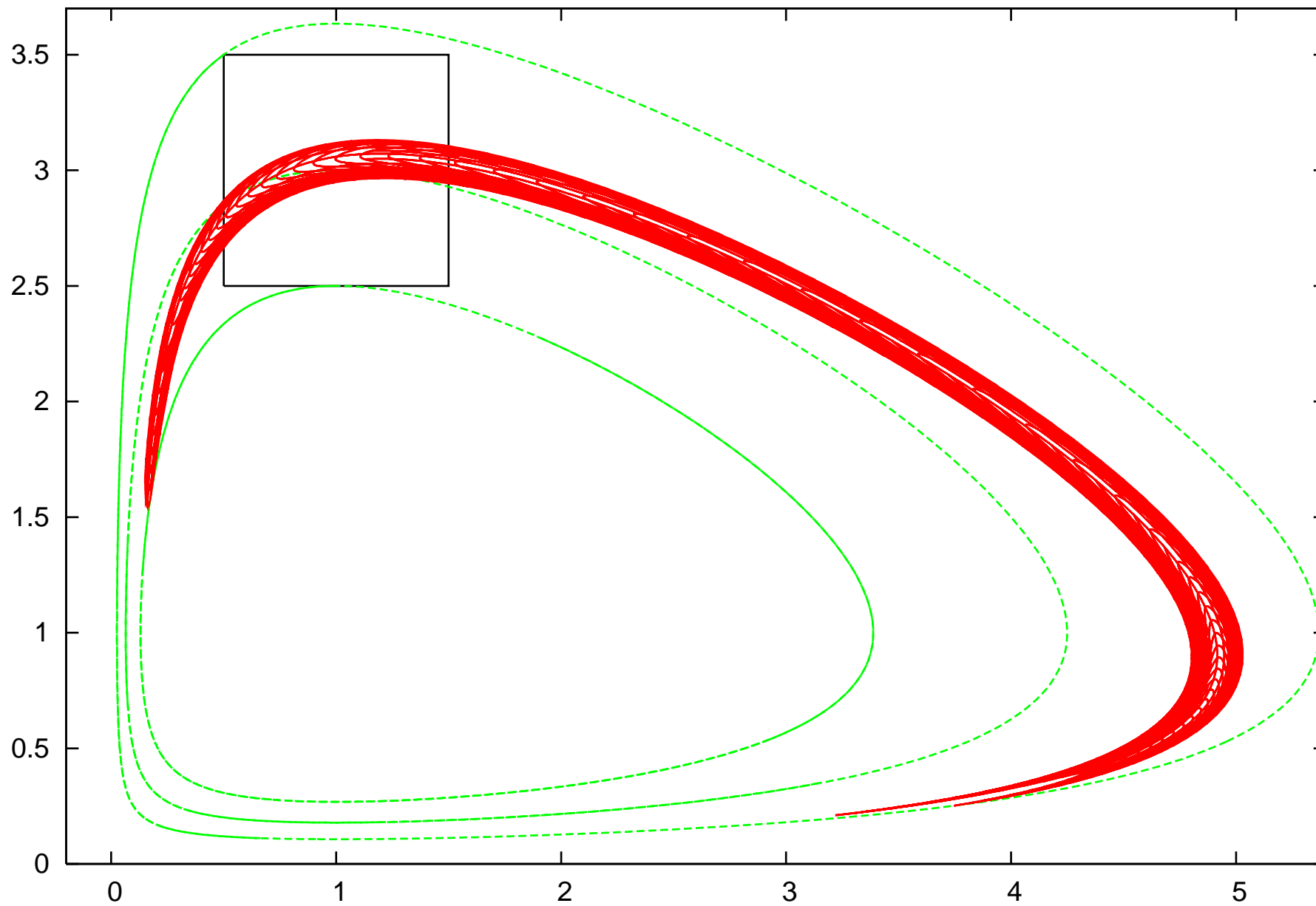
Volterra. IC=(1,3)+-0.5. T=10.0



Volterra. IC=(1,3)+-0.5. T=10.5



Volterra. IC=(1,3)+-0.5. T=11.0



The Milano-Michigan ESA Project

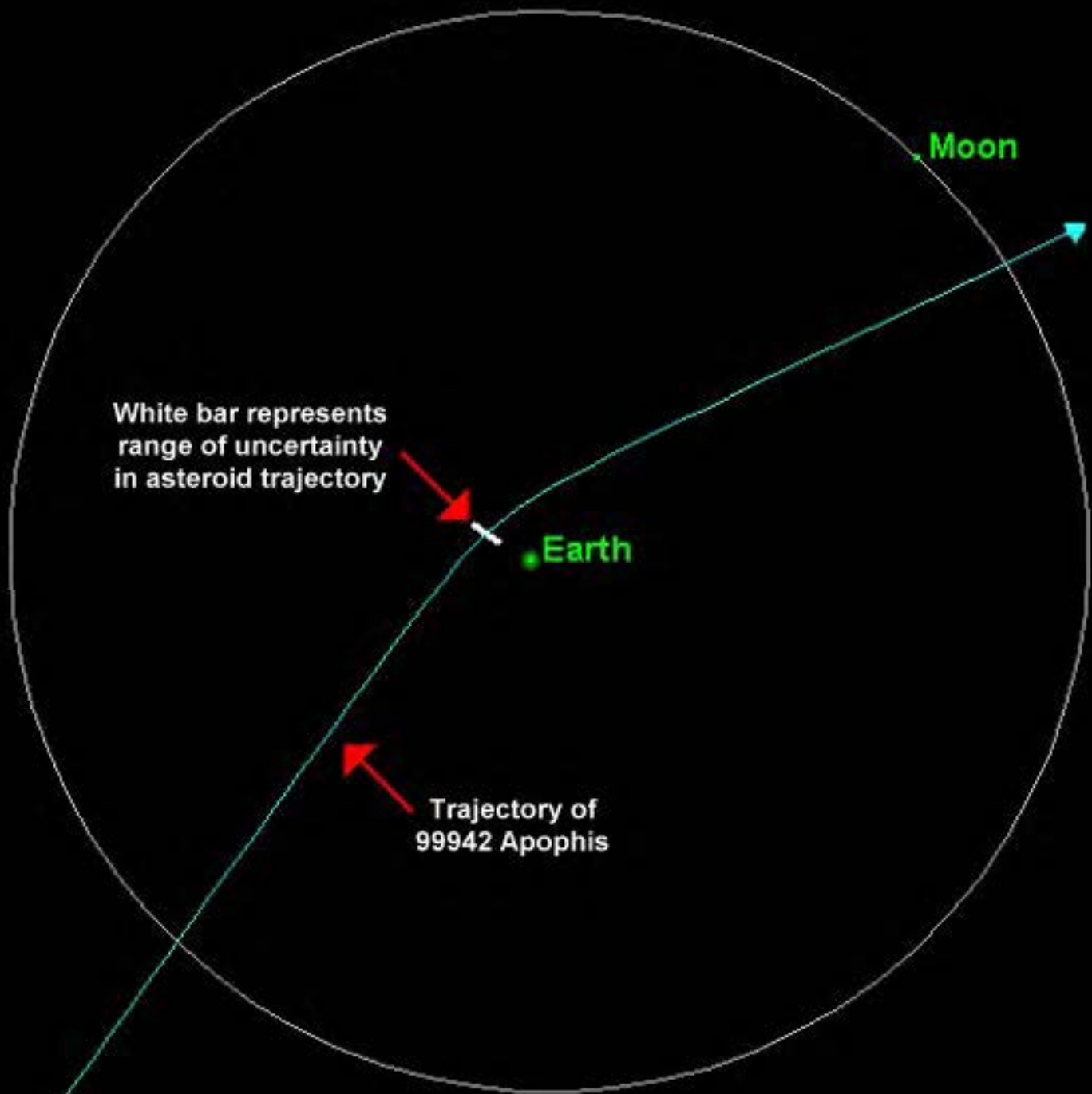
A Collaboration of the Istituto Aerospaziale at Politecnico di Milano and Michigan State University. Currently funded by the European Space Agency to

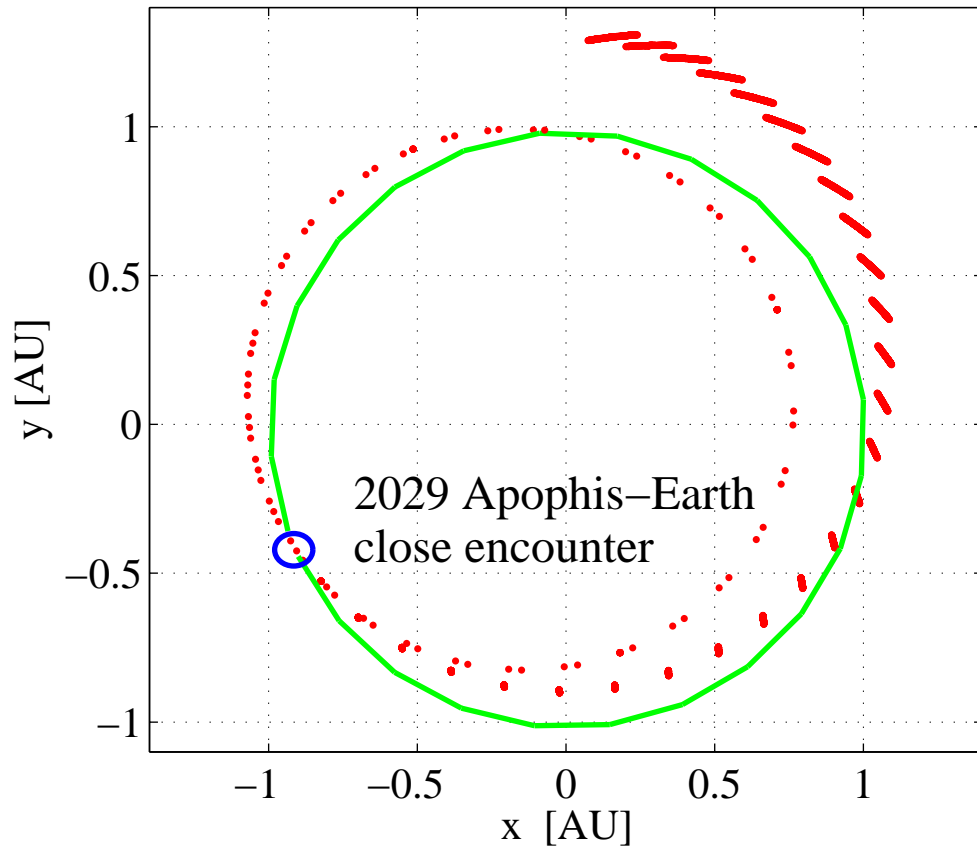
- Develop a verified integrator for solar system dynamics in a complete model of the solar system
- Includes influences of all planets, major asteroids, general relativity, etc
- Analyze its behavior and abilities
- Apply the integrator to study the dynamics of the Near-Earth Asteroid (99942) Apophis

Near Earth Asteroid (99942) Apophis

- A Near-Earth Asteroid discovered in 2004
- Eccentric orbit between the orbits of Venus and Mars
- Apophis will have a first near collision with Earth on **Friday, April 13, 2029**
- Apophis will have another near (???) collision with Earth on (Monday), **April 13, 2036**
- The near collision in 2029 very significantly alters Apophis' orbit

The small uncertainties of Apophis' current orbit parameters, amplified by the influence of the near collision in 2029, makes predictions for 2036 **very difficult**.





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--> Further observations have excluded a deadly collision with Earth :-)

Work in Progress

- Improvement of the Taylor model arithmetic package in COSY to allow arbitrarily high precision Taylor model computations.
 - All the preparation work has been completed.
 - The final system integration work is in progress.
 - Upon the completion, COSY-VI and COSY-GO will be adjusted for utilizing it.
- Improvement of COSY-VI
 - Various schemes to conduct Poincare projections
 - Computations in parallel environment
- Improvement of COSY-GO
 - Utilizing Genetic Algorithm based non-rigorous global optimizers for better cut-off tests
 - * Such an optimizer has been implemented in COSY.
The system integration work has to be done.

TAYLOR MODELS 2017

ISLAMORADA, FLORIDA KEYS DEC 11-14

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Photo: View from
Meeting Room



