Verified Probability Bounds Analysis Around Bifurcations in an Ecosystem Model

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Overview

- Overall project — Rigorous propagation of uncertainty in nonlinear models of ecological dynamics
  - Interval uncertainty (upper and lower bounds only)
  - Probability box (p-box) uncertainty (upper and lower bounds on the cumulative distribution function)
- Ecological models
  - May be considerable uncertainty in parameters and/or models
  - Nonlinear dynamics provides a rich variety of possible behaviors
  - Collaboration with Notre Dame Ecology Program — Experimental and modeling studies of new chemicals in aquatic ecosystems

Overview (cont'd)

- Earlier work — Rigorous propagation of interval and p-box uncertainties in ecological models can be done using verified integration and Taylor models (Enszer et al., 2009)
- Today's presentation — Consider cases for which multiple Taylor models (over different parameter subdomains) may be needed
  - State bounds diverge due to accumulation of overestimation errors (dependency, wrapping)
  - Divergence of state bounds is a feature of the model
    - Bifurcation enclosed by parameter interval
    - Separatrix enclosed by initial state interval
  - How to do arithmetic with p-boxes split over multiple subdomains and multiple Taylor models

Example 1: Aquatic Food Web Model

- Consider the aquatic food web model (Kulacki et al., 2008) consisting of the species Chlamydomonas, Daphnia, and Zebra Mussels

$$\frac{dC}{dt} = C\left[r_C\left(1 - \frac{C}{K_C}\right) - \frac{a_{CD}D}{b_D + C} - a_{CZ}Z\right]$$

$$\frac{dD}{dt} = D\left[\frac{a_{DC}C}{b_D + C}\left(1 - \frac{D}{K_D}\right) - d_D\right]$$

$$\frac{dZ}{dt} = Z\left[a_{ZC}C - d_Z\right]$$

- Values of the growth rate r_C and the interaction parameter a_{CD} are uncertain

Example 1: Aquatic Food Web Model

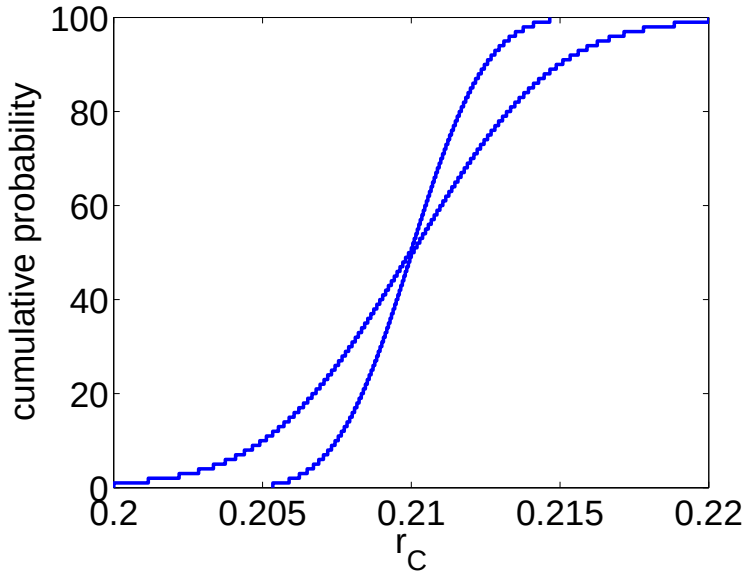
- Parameters and initial conditions:

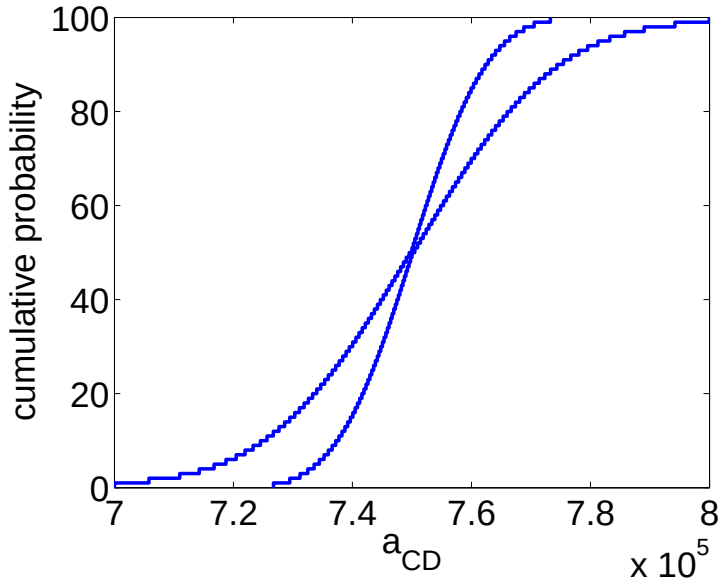
	Value	Units		Value	Units
b_D	8.82×10^6	indv			
K_C	5.15×10^{17}	indv	a_{ZC}	3.78×10^{-8}	day^{-1}
a_{CZ}	7.47×10^{-11}	day^{-1}	a_{DC}	0.125	day^{-1}
d_D	0.016	day^{-1}	d_Z	0.001	day^{-1}
K_D	3.25×10^{10}	indv	$C(0)$	5.15×10^{16}	indv
$D(0)$	1.25×10^9	indv	$Z(0)$	8.9×10^8	indv
r_C	$[0.40, 0.45]$	day^{-1}	a_{CD}	$[4.0, 5.0] \times 10^6$	day^{-1}

- Relatively large uncertainties: 12.5% for r_C and 25% for a_{CD}

Example 1: Aquatic Food Web Model

- P-box representation of uncertain parameters





- Cumulative probability functions for the uncertain parameters are bounded by truncated normal distributions

General Problem Statement

- Consider initial value problem (IVP) for nonlinear ODE problem,

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{f}(\boldsymbol{y}, \boldsymbol{\theta}), \qquad \boldsymbol{y}(t_0) = \boldsymbol{y}_0 \in \boldsymbol{Y}_0, \qquad \boldsymbol{\theta} \in \boldsymbol{\Theta},$$

  in which at least one of the initial states in $\boldsymbol{y}_0$ or one of the time-invariant parameters in $\boldsymbol{\theta}$ is uncertain (contained in $\boldsymbol{Y}_0$ and/or $\boldsymbol{\Theta}$)

- There is information about the distribution of the uncertainty that can be represented by p-boxes

- Goal 1: Obtain a rigorous, verified enclosure of all possible solutions to this uncertain, parametric IVP to a time horizon t_{f} of interest

- Goal 2: Obtain rigorous, verified bounds (p-boxes) on the probability distribution of the states at times of interest

Solution Procedure – Goal 1

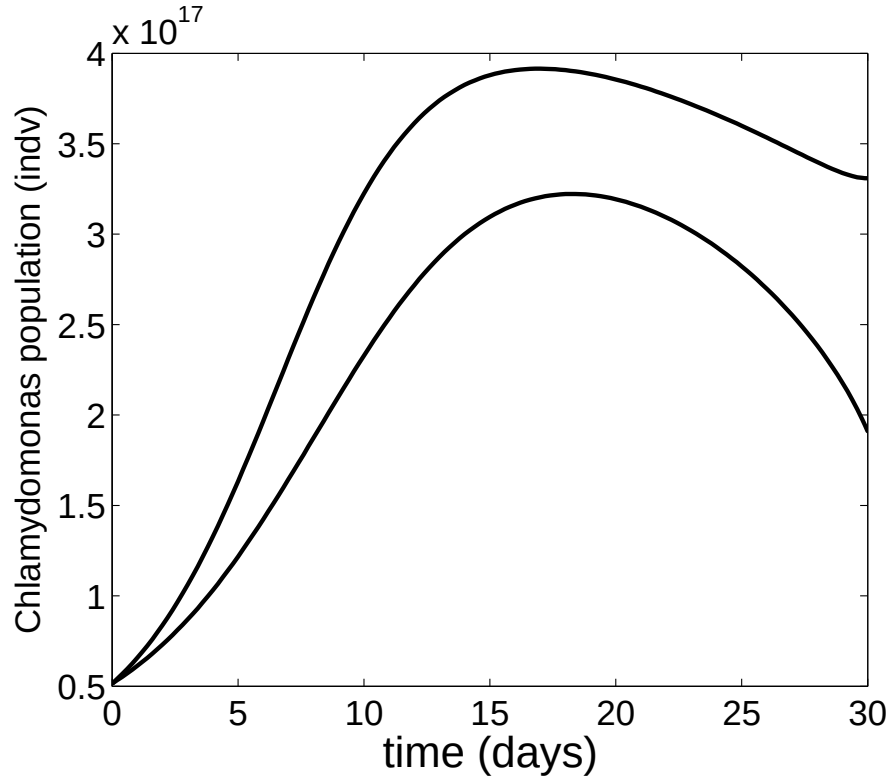
- Goal 1: Obtain a rigorous, verified enclosure of all possible solutions to this uncertain, parameter IVP over a time horizon of interest
- Use a method for verified (validated) solution of IVP
  - Guarantees there exists a unique solution $\boldsymbol{y}(t)$ for interval $t \in [t_0, t_\mathrm{f}]$, for each $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ and $\boldsymbol{y}_0 \in \boldsymbol{Y}_0$
  - At time step j, computes an interval $\boldsymbol{Y}_j$ that encloses all solutions $\boldsymbol{y}_j$ of the ODE system at t_j for $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ and $\boldsymbol{y}_0 \in \boldsymbol{Y}_0$
- Tools are available – AWA, VNODE, COSY VI, ValEncIA-IVP, VSPODE, etc.

Summary of VSPODE

- Use interval Taylor series to represent dependence on time
- Use Taylor model $\boldsymbol{T}_{\boldsymbol{y}_j} = \boldsymbol{T}_{\boldsymbol{y}_j}(\boldsymbol{y}_0, \boldsymbol{\theta})$ to represent dependence on the initial states $\boldsymbol{y}_0$ and parameters $\boldsymbol{\theta}$; consists of
  - A real-valued polynomial function of $\boldsymbol{y}_0$ and $\boldsymbol{\theta}$
  - A parallelepiped remainder bound
- Assuming $\boldsymbol{Y}_j$ is known, then
  - Phase 1: Compute a coarse enclosure $\widetilde{\boldsymbol{Y}}_j$ and prove existence and uniqueness using fixed point iteration with Picard operator and high-order interval Taylor series (as in VNODE)
  - Phase 2: Refine the coarse enclosure to obtain $\boldsymbol{Y}_{j+1}$ using Taylor models in terms of the uncertain parameters and initial states
- Implemented by Lin and Stadtherr (2007)

Example 1: Aquatic Food Web Model

- VSPODE enclosure of Chlamy population C over $t \in [0, 30]$ based on interval uncertainties in r_C and a_{CD}



- Bounds diverge past $t = 30$
- To extend integration time, can use some bisection strategy, e.g. bisect the parameter intervals

Solution Procedure – Goal 2

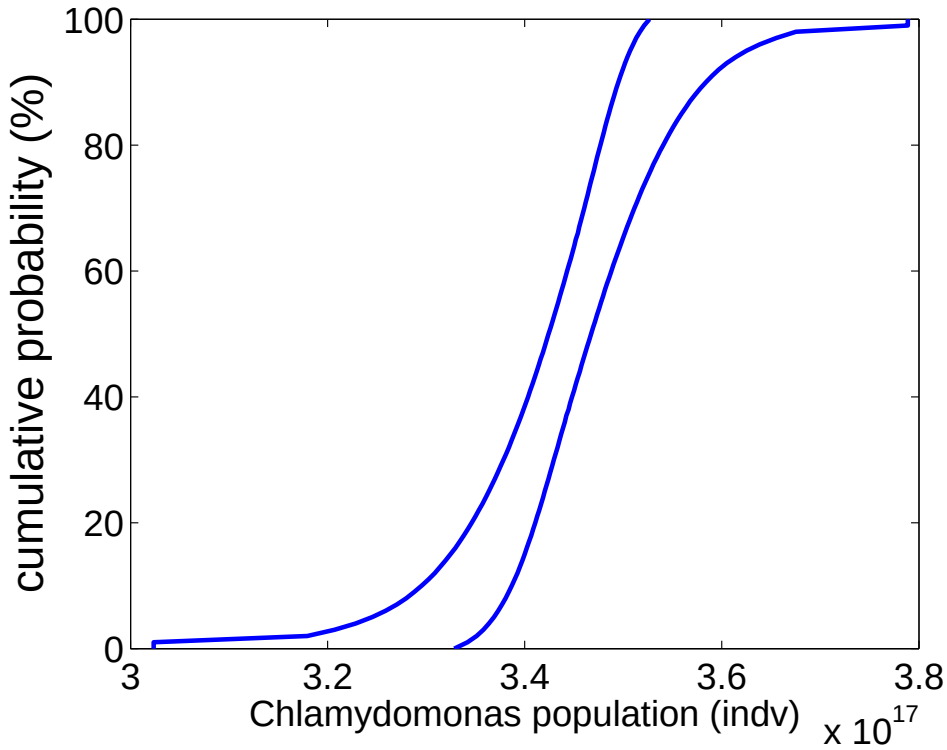
- Goal 2: Obtain rigorous, verified bounds (p-boxes) on the probability distribution of the states at times of interest
- For a time of interest t_j (end of j-th time step), VSPODE has computed a Taylor model representation $\boldsymbol{T}_{\boldsymbol{y}_j} = \boldsymbol{T}_{\boldsymbol{y}_j}(\boldsymbol{y}_0, \boldsymbol{\theta})$ of the state variables as a function of the initial states $\boldsymbol{y}_0$ and parameters $\boldsymbol{\theta}$
- This Taylor model is valid for all $\boldsymbol{y}_0 \in \boldsymbol{Y}_0$ and $\boldsymbol{\theta} \in \boldsymbol{\Theta}$
- Substitute distributions (p-boxes) for $\boldsymbol{y}_0$ and $\boldsymbol{\theta}$ into $\boldsymbol{T}_{\boldsymbol{y}_j} = \boldsymbol{T}_{\boldsymbol{y}_j}(\boldsymbol{y}_0, \boldsymbol{\theta})$ and use p-box arithmetic to compute p-boxes of state variables $\boldsymbol{y}_j = \boldsymbol{y}(t_j)$

P-box Arithmetic on a Taylor Model (TM)

- For p-box arithmetic, the p-boxes are typically discretized into a set of intervals corresponding to different probability levels
- Each interval is then substituted into the TM $\boldsymbol{T}_{\boldsymbol{y}_j}$ and interval arithmetic is used to evaluate the TM
- The results of each interval TM evaluation are collected and assembled into a final p-box for $\boldsymbol{y}_j$
- Because interval arithmetic is used, there are dependency and wrapping issues that can result in overestimation
- If regular interval arithmetic results in too much overestimation, then for each interval used to represent the p-box, subdivide it, evaluate the TM over each subinterval and take the union of the results (subinterval reconstitution) (Ferson and Hajagos, 2004)
- Then the (tighter) results of the interval TM evaluations are collected into the output p-box

Example 1: Aquatic Food Web Model

- P-box enclosure of probability distribution for C at time $t = 15$, based on p-boxes for r_C and a_{CD}



- For beyond $t = 30$, need to bisect the parameter intervals

- Need for p-box arithmetic on multiple Taylor models

Example 2: Tritrophic Rosenzweig-MacArthur (RM) Model

- Model of food chain with three trophic levels - basal (prey), predator, and superpredator
- Logistic prey growth
- Holling type II (hyperbolic) predator (and superpredator) response functions

$$\frac{dx_1}{dt} = x_1 \left[r(1 - \frac{x_1}{K}) - \frac{a_2 x_2}{b_2 + x_1} \right]$$

$$\frac{dx_2}{dt} = x_2 \left[e_2 \frac{a_2 x_1}{b_2 + x_1} - \frac{a_3 x_3}{b_3 + x_2} - d_2 \right]$$

$$\frac{dx_3}{dt} = x_3 \left[e_3 \frac{a_3 x_2}{b_3 + x_2} - d_3 \right]$$

Example 2: Tritrophic RM Model

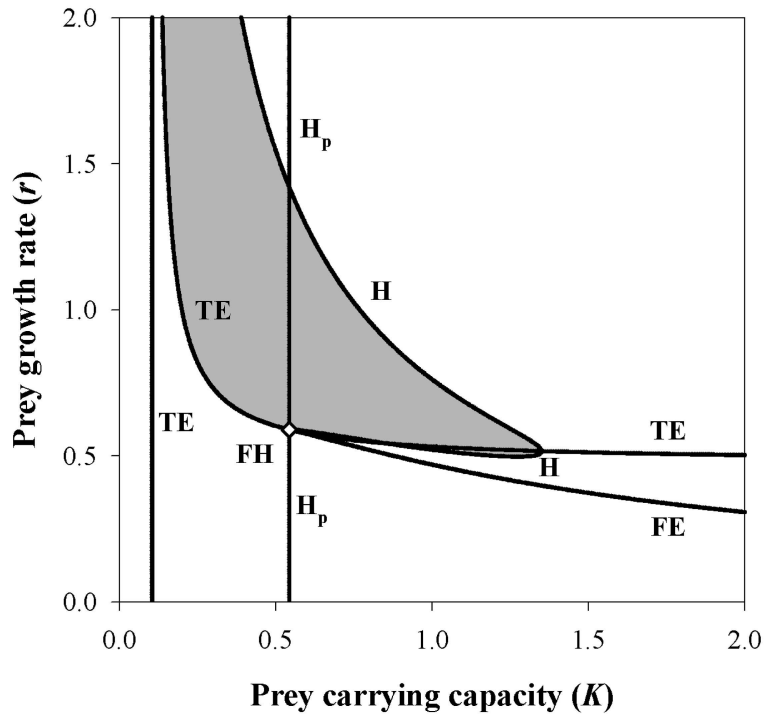
- Fixed parameters (Gragnani et al., 1998)

	Value		Value
a_2	$5/3$	a_3	0.05
b_2	$1/3$	b_3	0.5
e_2	1	e_3	1
d_2	0.4	d_3	0.01

- Initial condition $\boldsymbol{x}_0$ and/or parameters r (prey growth rate) and K (prey carrying capacity) are uncertain

- This system exhibits a rich variety of dynamical behaviors

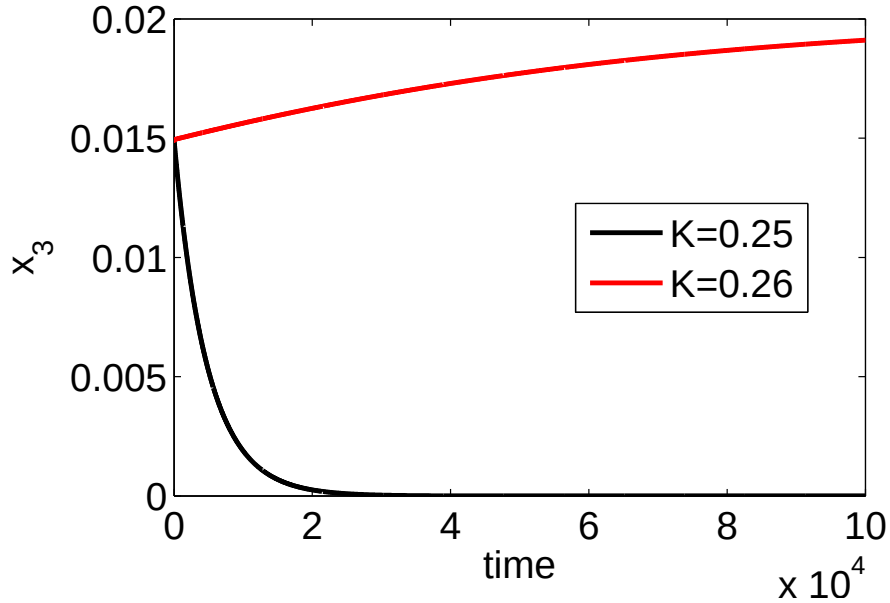
Example 2: Tritrophic RM Model



- This two-parameter bifurcation diagram shows bifurcations of equilibrium (E) only (TE = transcritical; FE = fold; H = Hopf; H_p = planar Hopf)
- There are also bifurcations of cycles
- This diagram was computed rigorously using an interval method (Gwaltney et al., 2007)

Example 2: Tritrophic RM Model

- Consider $r = 0.8$, $\boldsymbol{x}_0 = (0.10, 0.10, 0.015)$, with $K \in [0.25, 0.26]$ containing a transcritical bifurcation.



- Equilibrium (steady-state) value for x_3 is zero for part of the K interval and nonzero for the other part; the states with zero and nonzero x_3 collide at the bifurcation point $\Longrightarrow$ Divergence of state bounds is a feature of the model

- How will VSPODE perform in this situation? Is bisection of parameter interval useful?

Example 3: Model of Two Competitors

- Model of two species who compete for the same resources

$$\frac{dx_1}{dt} = r_1 x_1 \left[1 - \frac{x_1 + \alpha_1 x_2}{K_1} \right]$$

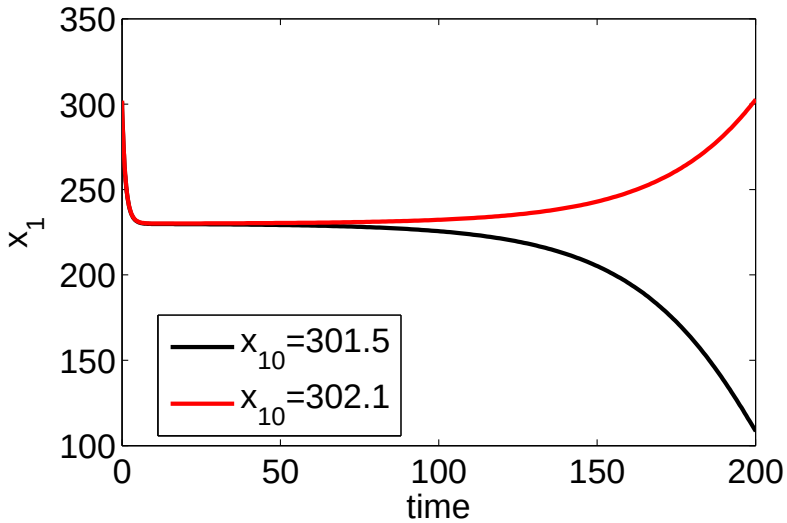
$$\frac{dx_2}{dt} = r_2 x_2 \left[1 - \frac{x_2 + \alpha_2 x_1}{K_2} \right]$$

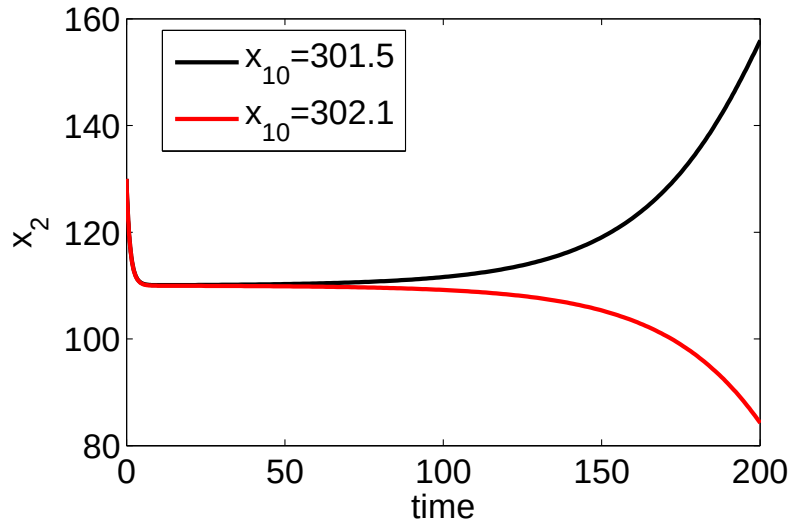
- Parameters and initial conditions

	Value		Value
r_1	1	r_2	0.6
α_1	3	α_2	0.4
K_1	560	K_2	202
x_{10}	$[301.5, 302.1]$	x_{20}	130

Example 3: Model of Two Competitors

- $x_{10} \in [301.5, 302.1]$ contains a separatrix





- For part of the $\boldsymbol{x}_0$ interval, trajectories go to an equilibrium state with $x_1 = 0$ and $x_2 \neq 0$, and in the other part trajectories go to an equilibrium state with $x_1 \neq 0$ and $x_2 = 0 \Longrightarrow$ Divergence of state bounds a feature of the model

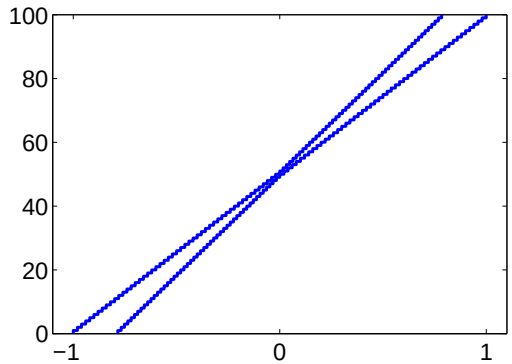
- How will VSPODE perform in this situation? Is bisection of initial state interval useful?

P-box Arithmetic on Multiple Taylor Models

- If parameter and/or initial state interval is bisected, then for the time of interest t_j, VSPODE has computed multiple Taylor model representations $T_{y_j,i}$, one for each subinterval i of the uncertain quantities
- Each Taylor model $T_{y_j,i}$ is only valid over its corresponding subinterval, and each TM has its own expansion point (midpoint of subinterval)
- P-boxes must be reformulated for input to the multiple Taylor models

P-box Arithmetic on Multiple Taylor Models

- Preparation of p-box for a bisected parameter interval (original width = 2) for input to Taylor model on each parameter subdomain



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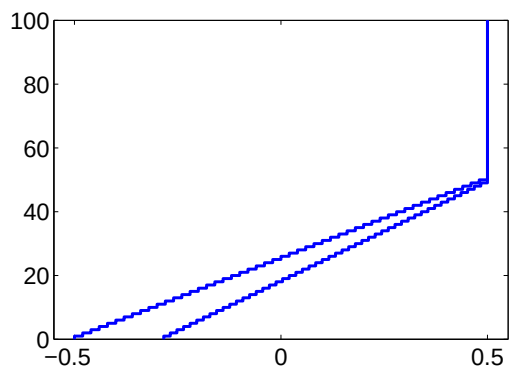
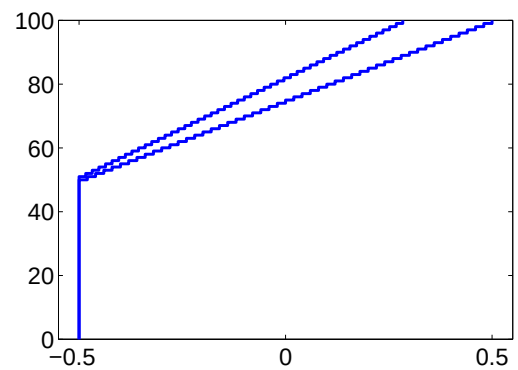




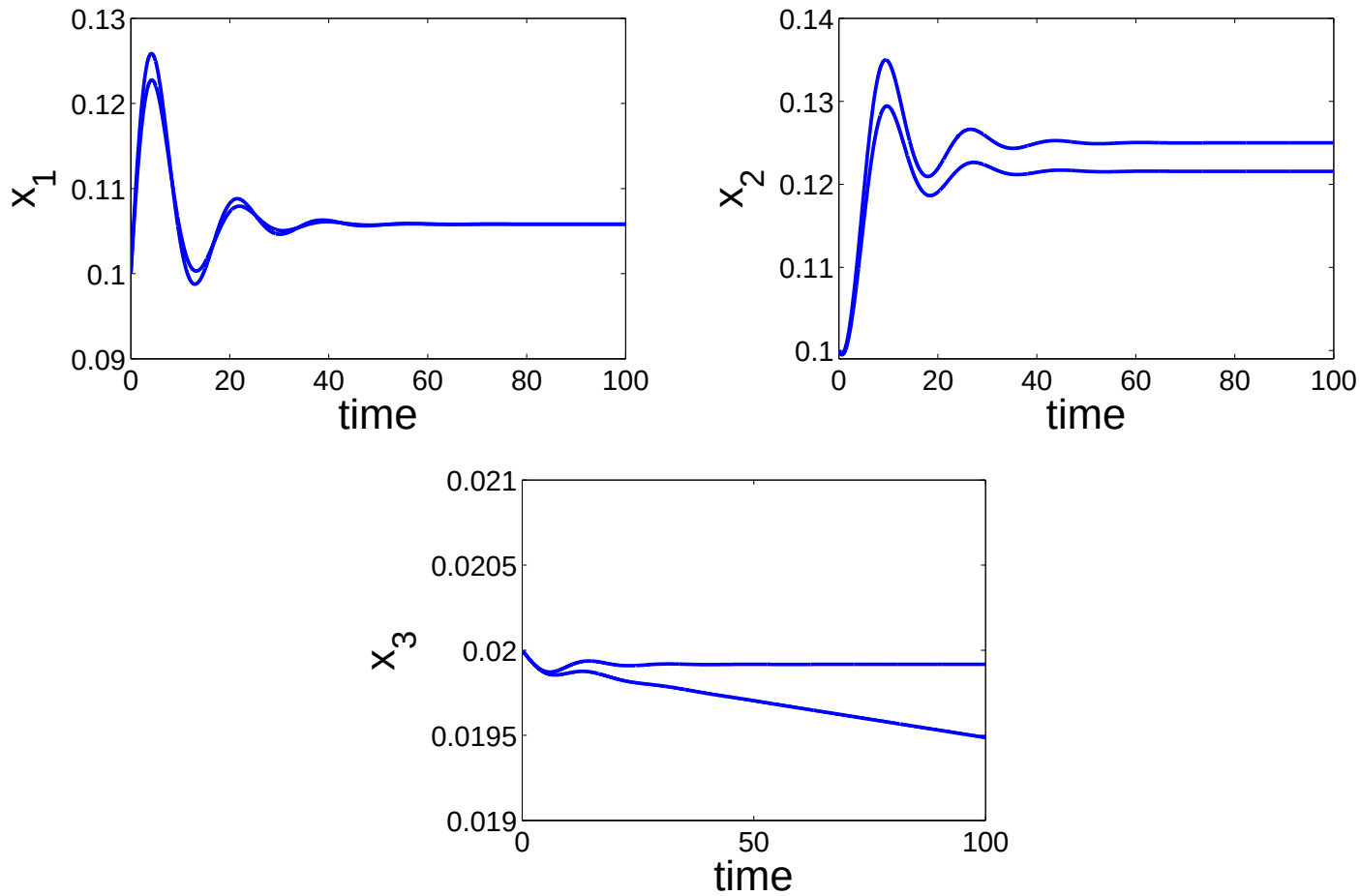
- Parameter values relative to expansion point for TM (here interval midpoint)

P-box Arithmetic on Multiple Taylor Models

- An additional complication is that when the p-boxes are discretized into intervals for p-box arithmetic, there are two possibilities
  - The interval is completely contained in a single subdomain, so it is evaluated only on its single corresponding TM
  - The interval is not contained in a single subdomain, so it must be evaluated on multiple TMs and the union of the result used
- Ultimately, the results of all the TM evaluations are collected and a single output p-box is constructed

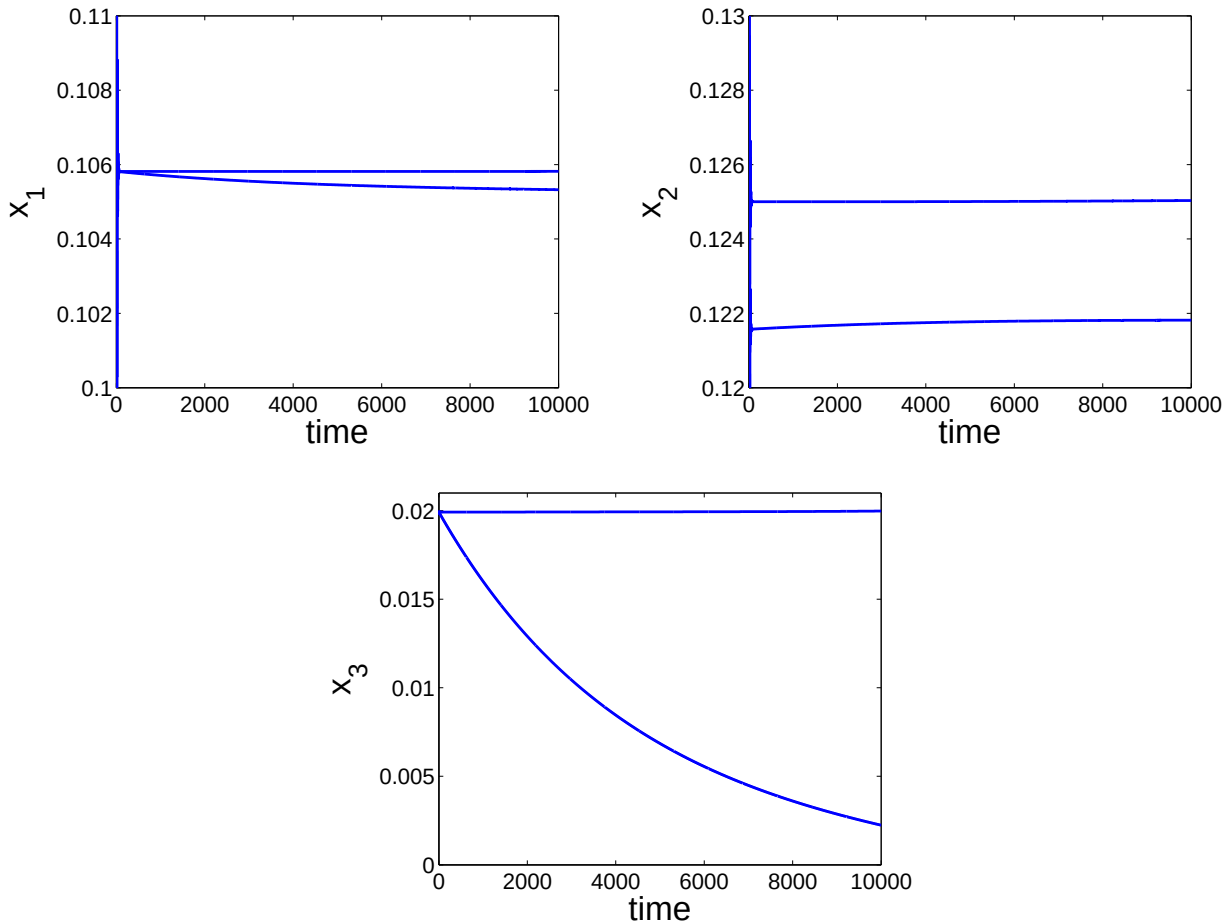
Example 2: Tritrophic RM Model

- Revisit the RM model with transcritical bifurcation: $r = 0.8$, $K \in [0.25, 0.26]$, $\boldsymbol{x}_0 = (0.10, 0.10, 0.02)$
- VSPODE enclosures of $x_1(t)$, $x_2(t)$, and $x_3(t)$ over $t = [0, 100]$



Example 2: Tritrophic RM Model

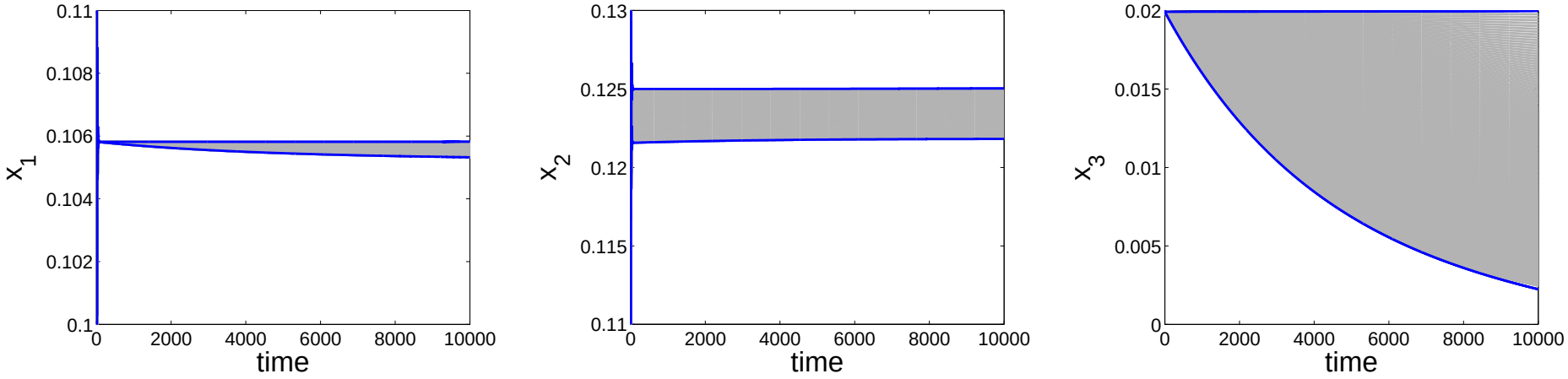
- VSPODE enclosures of $x_1(t)$, $x_2(t)$, and $x_3(t)$ over $t = [0, 10000]$



- How tight are these bounds?

Example 2: Tritrophic RM Model

- Comparison of VSPODE bounds to Monte Carlo simulations

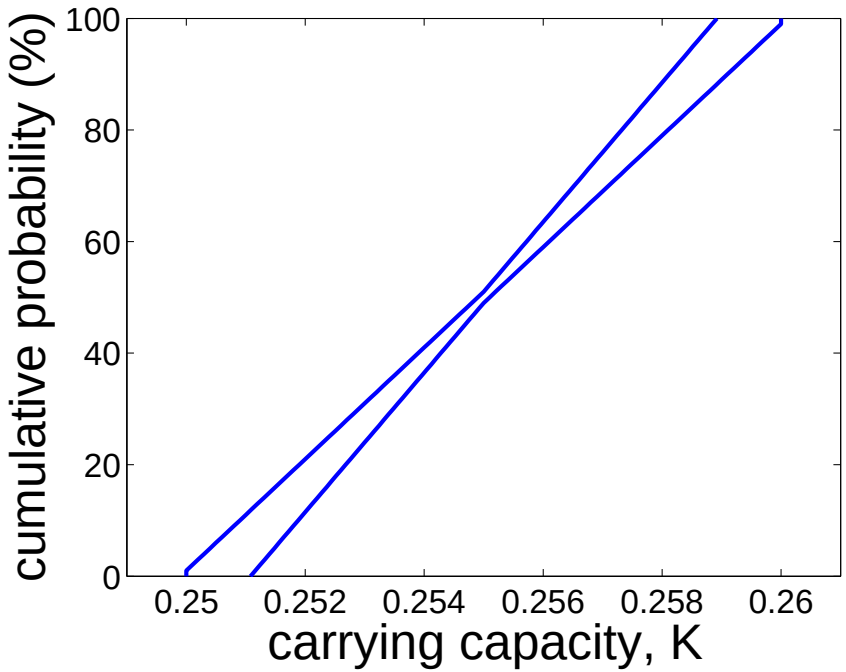


- VSPODE bounds with parameter bisection are the same: No need for bisection

- Knowledge of bifurcation will help avoid unnecessary bisections

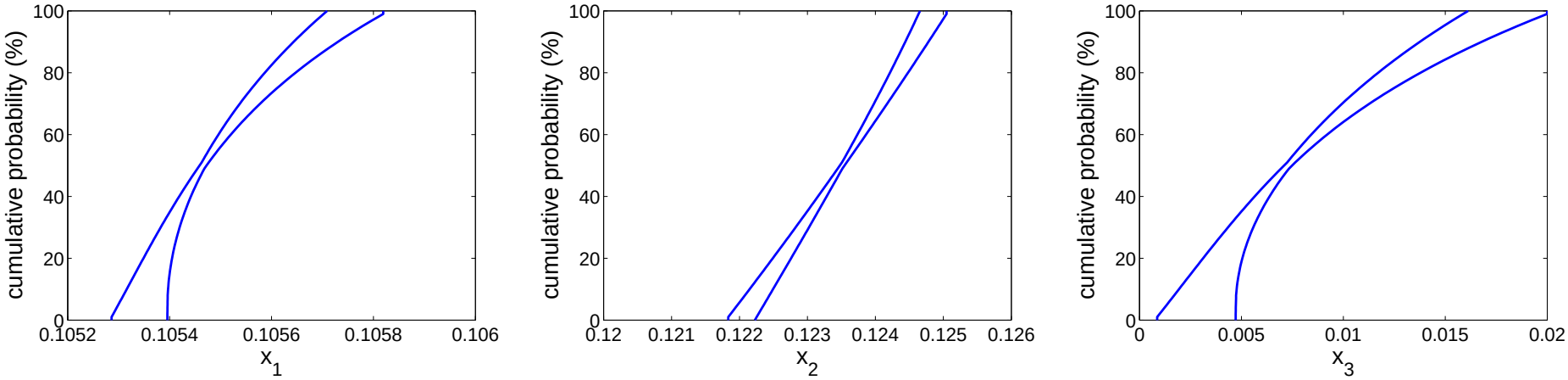
Example 2: Tritrophic RM Model

- P-box representation of uncertain parameter K



Example 2: Tritrophic RM Model

- Probability distributions (p-boxes) for $\boldsymbol{x}$ at $t = 10000$

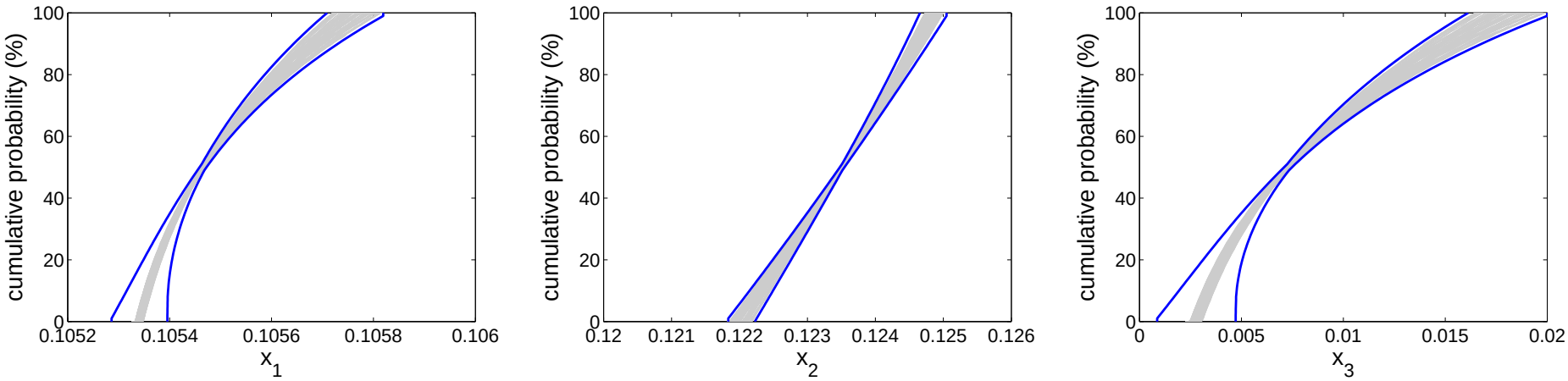


- Same results with or without bisection (at midpoint or at bifurcation)

- Validates new procedure for p-box arithmetic over multiple Taylor models

Example 2: Tritrophic RM Model

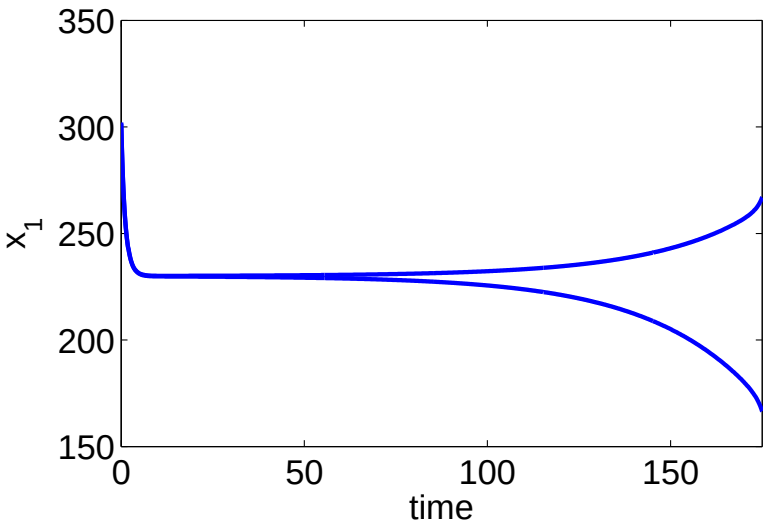
- Comparison with Monte Carlo simulations: 100 simulations, each with a uniform probability distributions for K sampled from the input p-box, with each simulation consisting of 10000 trials

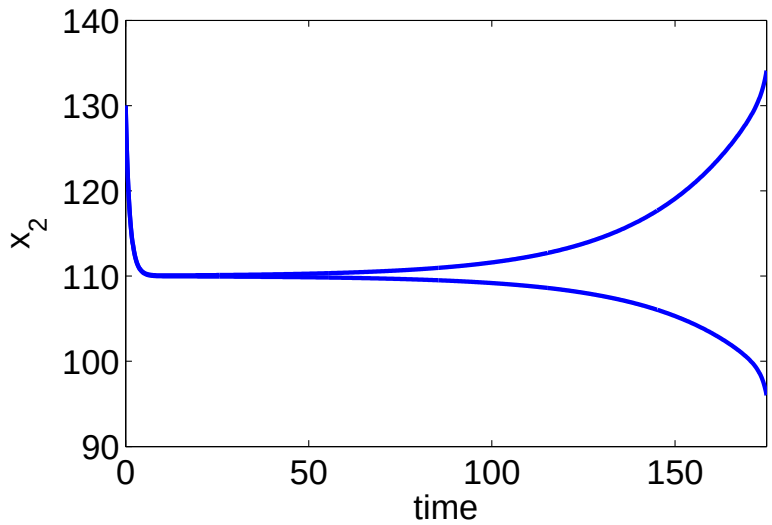


- Additional resolution in p-box arithmetic at lower probability levels is needed
- The second-order (nested) Monte Carlo simulation is computationally expensive

Example 3: Model of Two Competitors

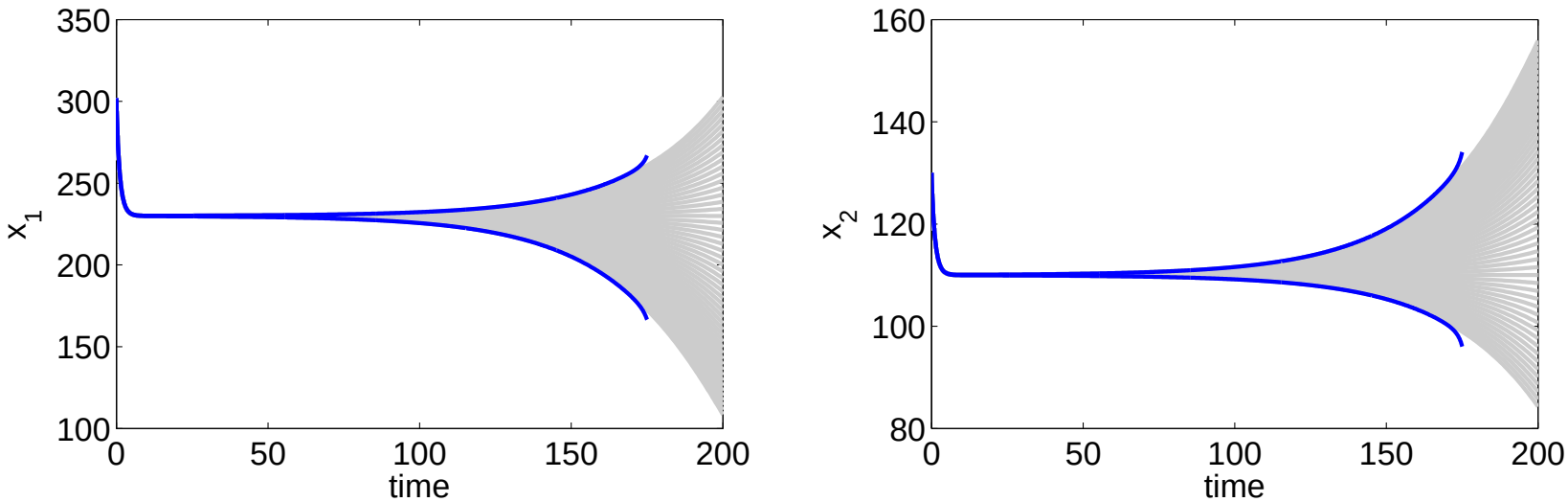
- Revisit the two-competitors model with separatrix: $x_{10} \in [301.5, 302.1]$
- VSPODE enclosures of $x_1(t)$ and $x_2(t)$ over $t = [0, 175]$





Example 3: Model of Two Competitors

- Comparison with Monte Carlo simulation over $t = [0, 175]$

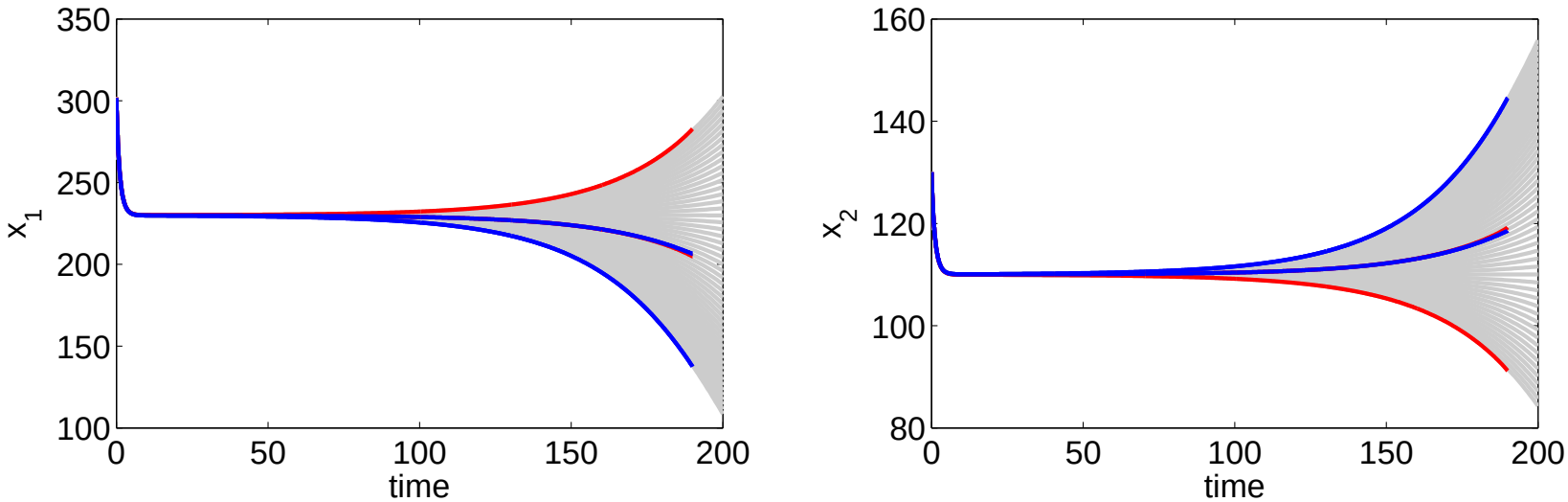


- Begin to see overestimation errors near $t = 175$

- Try bisecting initial state interval

Example 3: Model of Two Competitors

- Comparison with Monte Carlo simulation over $t = [0, 190]$

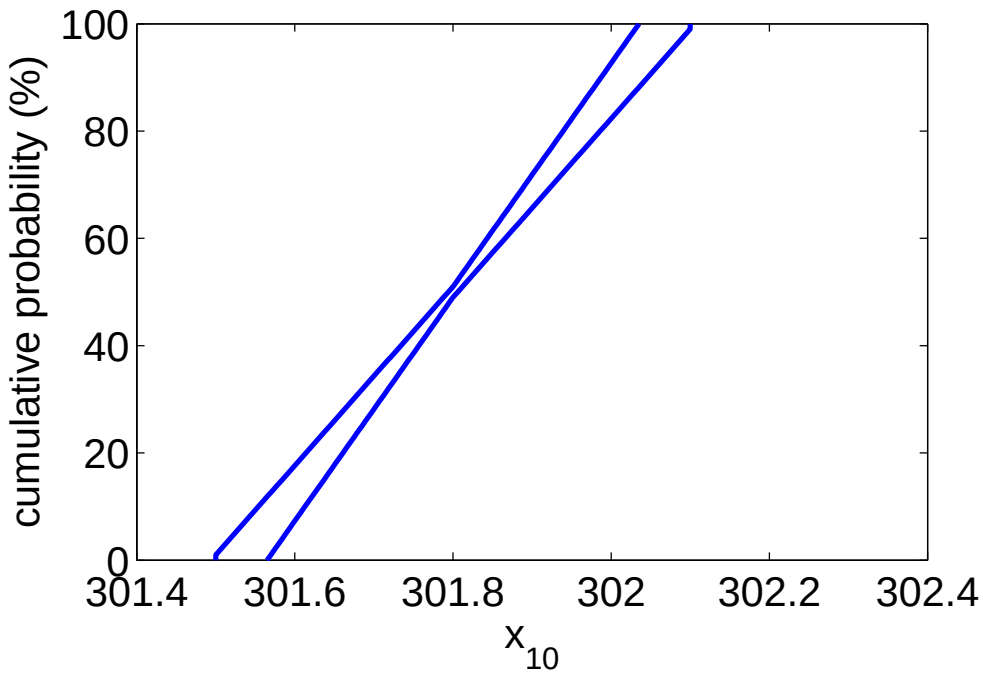


- Subinterval (red) containing the separatrix is beginning to show overestimation errors

- As expected, bisection helps address overestimation errors; additional bisections are needed

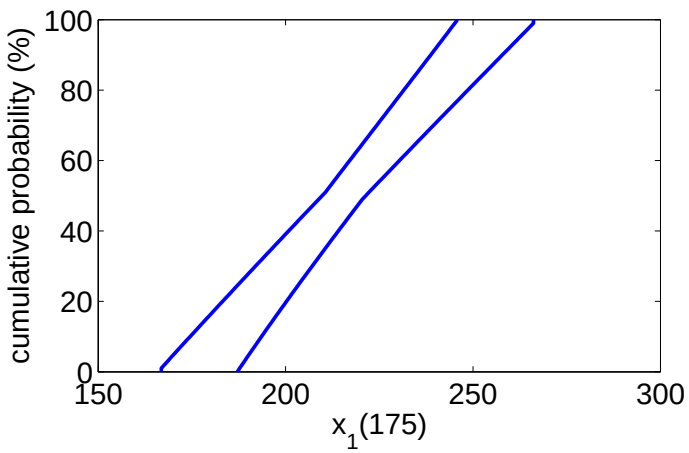
Example 3: Model of Two Competitors

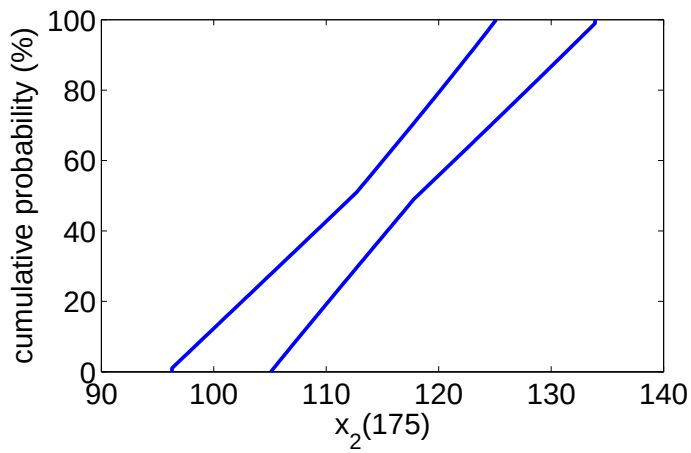
- P-box representation of uncertain initial condition x_{10}



Example 3: Model of Two Competitors

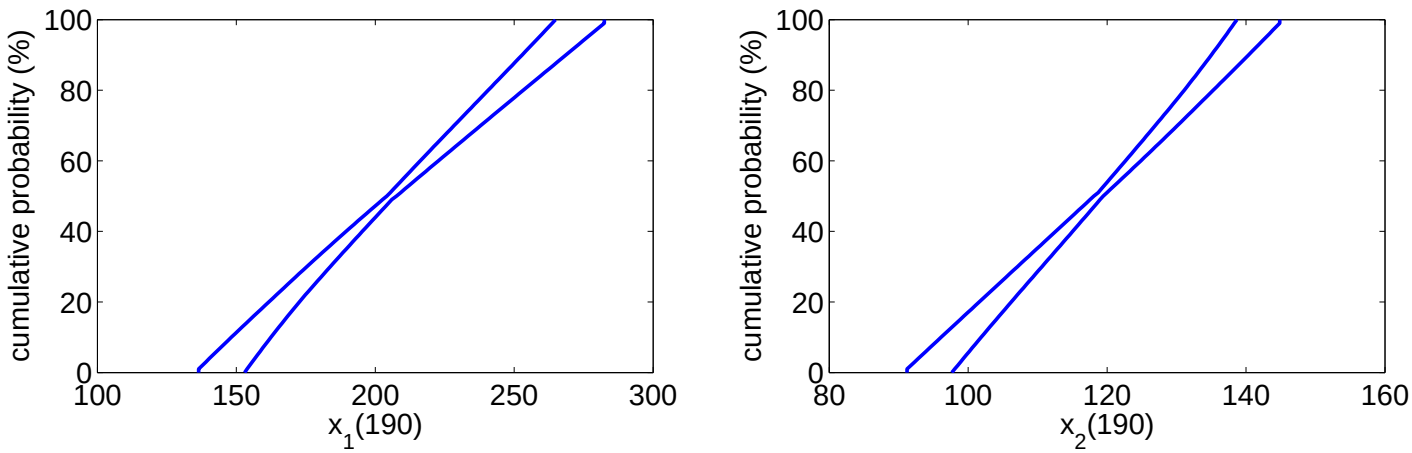
- Probability distributions (p-boxes) for $\boldsymbol{x}$ at $t = 175$ (no bisection)





Example 3: Model of Two Competitors

- Probability distributions (p-boxes) for $\boldsymbol{x}$ at $t = 190$ (with bisection)



- Overestimation errors were reduced

Concluding Remarks

- Behavior of a verified integrator around a bifurcation or separatrix may look like overestimation error
  - Knowledge of bifurcation or separatrix location is helpful
  - Bisection strategies may not help, unless there is overestimation error to reduce
- A procedure was developed for arithmetic with p-boxes split over multiple subdomains and multiple Taylor models
  - Useful in cases where bisection strategies are needed to reduce overestimation error