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:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
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<tbody>
<tr>
<td>$b_D$</td>
<td>$8.82 \times 10^6$</td>
<td>indv</td>
<td>$K_C$</td>
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<td></td>
<td></td>
<td></td>
<td>$a_{ZC}$</td>
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<td>$a_{CZ}$</td>
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<td>$d_Z$</td>
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<td>$K_D$</td>
<td>$3.25 \times 10^{10}$</td>
<td>indv</td>
<td>$C(0)$</td>
<td>$5.15 \times 10^{16}$</td>
<td>indv</td>
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<td>$D(0)$</td>
<td>$1.25 \times 10^9$</td>
<td>indv</td>
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<td>$8.9 \times 10^8$</td>
<td>indv</td>
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<tr>
<td>$r_C$</td>
<td>[0.40, 0.45]</td>
<td>day$^{-1}$</td>
<td>$a_{CD}$</td>
<td>$[4.0, 5.0] \times 10^6$</td>
<td>day$^{-1}$</td>
</tr>
</tbody>
</table>

- 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,

\[ \frac{dy}{dt} = f(y, \theta), \quad y(t_0) = y_0 \in Y_0, \quad \theta \in \Theta, \]

in which at least one of the initial states in \( y_0 \) or one of the time-invariant parameters in \( \theta \) is uncertain (contained in \( Y_0 \) and/or \( \Theta \))

- 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 \( y(t) \) for interval \( t \in [t_0, t_f] \), for each \( \theta \in \Theta \) and \( y_0 \in Y_0 \)
  
  – At time step \( j \), computes an interval \( Y_j \) that encloses all solutions \( y_j \) of the ODE system at \( t_j \) for \( \theta \in \Theta \) and \( y_0 \in Y_0 \)

• 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 $T_{y_j} = T_{y_j}(y_0, \theta)$ to represent dependence on the initial states $y_0$ and parameters $\theta$; consists of
  - A real-valued polynomial function of $y_0$ and $\theta$
  - A parallelepiped remainder bound
- Assuming $Y_j$ is known, then
  - Phase 1: Compute a coarse enclosure $\tilde{Y}_j$ 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 $Y_{j+1}$ 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 $T_{y_j} = T_{y_j}(y_0, \theta)$ of the state variables as a function of the initial states $y_0$ and parameters $\theta$

• This Taylor model is valid for all $y_0 \in Y_0$ and $\theta \in \Theta$

• Substitute distributions (p-boxes) for $y_0$ and $\theta$ into $T_{y_j} = T_{y_j}(y_0, \theta)$ and use p-box arithmetic to compute p-boxes of state variables $y_j = y(t_j)$
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 $T_{y_j}$ 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 $y_j$.

- 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

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

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

\[
\frac{dx_3}{dt} = x_3 \left[ e_3 \frac{a_3 x_2}{b_3 + x_2} - d_3 \right]
\]
Example 2: Tritrophic RM Model

• Fixed parameters (Gragnani et al., 1998)

<table>
<thead>
<tr>
<th></th>
<th>Value</th>
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<th>Value</th>
</tr>
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<td>$b_3$</td>
<td>0.5</td>
</tr>
<tr>
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<td>1</td>
<td>$e_3$</td>
<td>1</td>
</tr>
<tr>
<td>$d_2$</td>
<td>0.4</td>
<td>$d_3$</td>
<td>0.01</td>
</tr>
</tbody>
</table>

• Initial condition $x_0$ 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 \( r = 0.8, x_0 = (0.10, 0.10, 0.015) \), 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 \( \frac{\partial f}{\partial x_3} \), which indicates 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

<table>
<thead>
<tr>
<th></th>
<th>Value</th>
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<th>Value</th>
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<tbody>
<tr>
<td>( r_1 )</td>
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<td>( r_2 )</td>
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<tr>
<td>( \alpha_1 )</td>
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<tr>
<td>( K_1 )</td>
<td>560</td>
<td>( K_2 )</td>
<td>202</td>
</tr>
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<td>( x_{10} )</td>
<td>[301.5, 302.1]</td>
<td>( x_{20} )</td>
<td>130</td>
</tr>
</tbody>
</table>
Example 3: Model of Two Competitors

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

- For part of the \( x_0 \) 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 \( x_2 = 0 \) \( \implies \) 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

- 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: $r = 0.8$, $K \in [0.25, 0.26]$, $x_0 = (0.10, 0.10, 0.02)$
- 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 $\alpha$ at $t = 175$ (no bisection)
Example 3: Model of Two Competitors

- Probability distributions (p-boxes) for $x$ 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