Propagation of Uncertainties in Nonlinear Dynamic Models

Youdong Lin[1], Scott Ferson[2], George F. Corliss[3] and Mark A. Stadtherr[1]

[1]Department of Chemical and Biomolecular Engineering, University of Notre Dame,
Notre Dame, IN, USA

[2]Applied Biomathematics, Setauket, NY, USA

[3]Department of Electrical and Computer Engineering, Marquette University,
Milwaukee, WI, USA

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- Validated Solution of Parametric ODEs
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Problem Statement

- Consider a nonlinear ODE model with uncertain parameters:

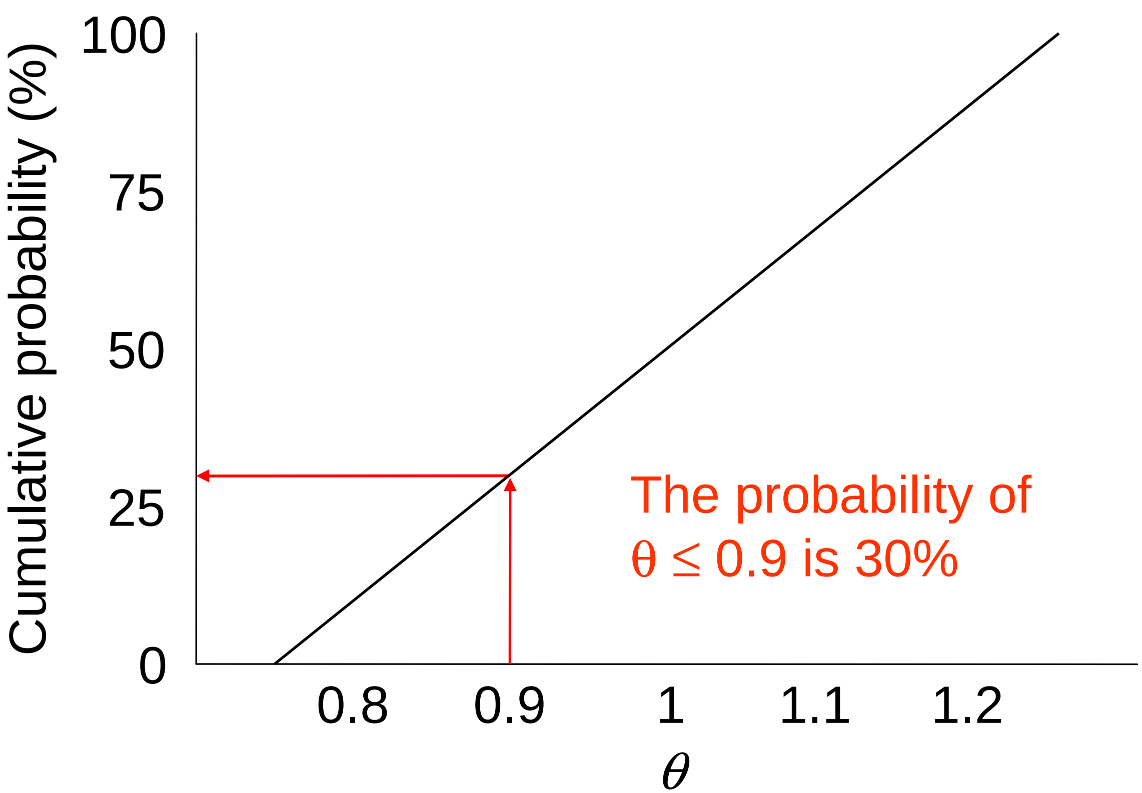
$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta})$$

  where $\boldsymbol{\theta}$ is uncertain

- There is information about the distribution of uncertainties, but the distribution is not known precisely
  - The uncertainty can be represented by a “probability box” (p-box)
- What is the effect of parameter uncertainties on the state vector $\boldsymbol{x}$?
  - Determine bounds on the distribution of state values
  - Represent using p-boxes

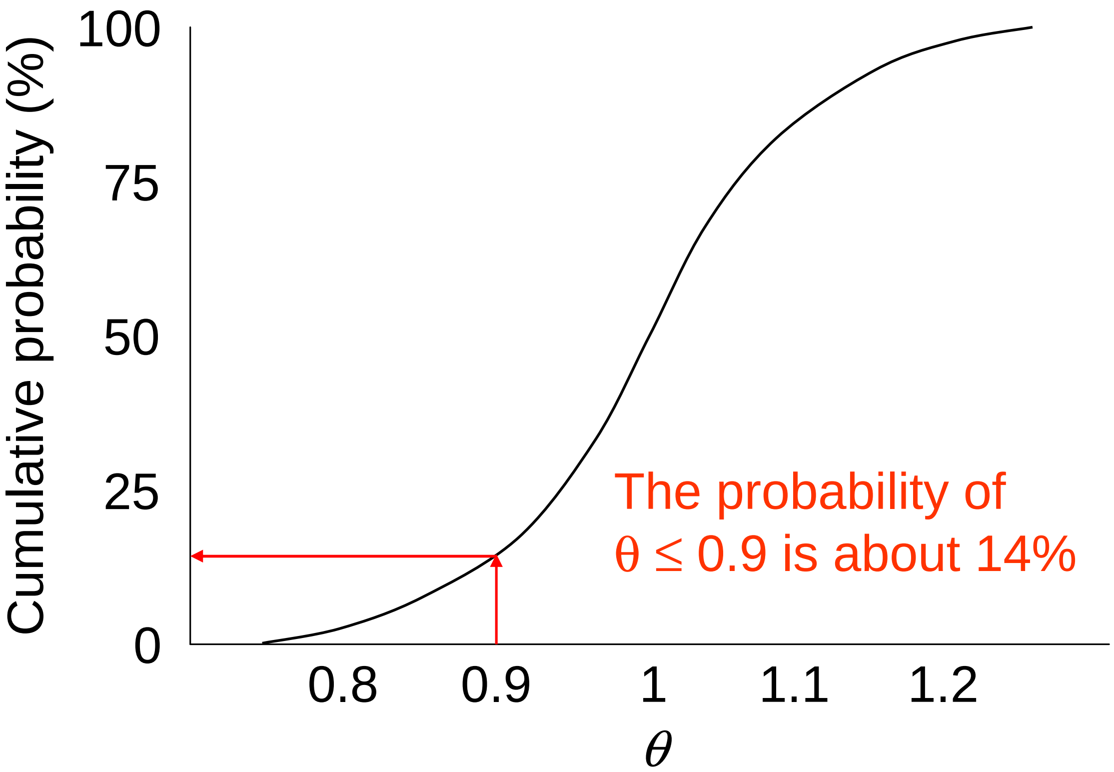
Representing Uncertainties: CDFs

- For a quantity θ, the CDF (cumulative distribution function) $F(x)$ gives the probability that $\theta \leq x$
- Example: CDF of a uniform distribution on $\theta \in [0.75, 1.25]$



Representing Uncertainties: CDFs

- Example: CDF of a normal distribution on $\theta \in [0.75, 1.25]$



Representing Uncertainties: P-Boxes

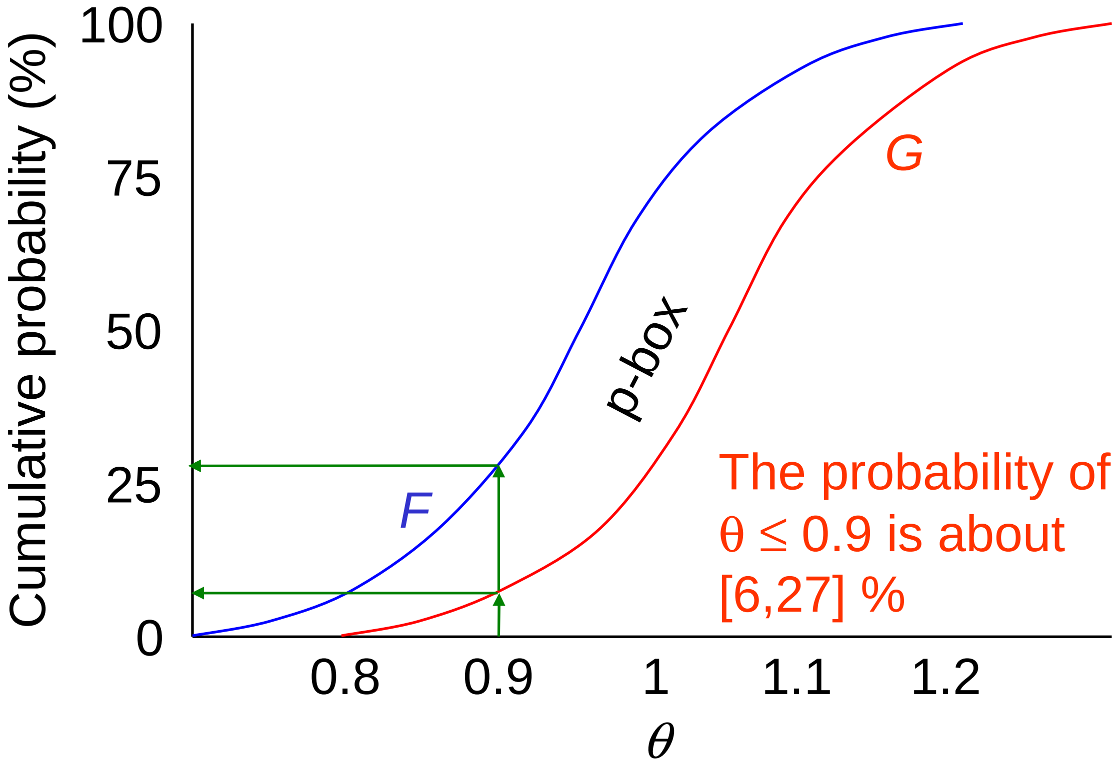
- A p-box bounds the uncertainty about a probability distribution in the same way that an ordinary interval bounds the uncertainty about a number (Ferson, 2002)
- A p-box H is the set of all CDFs enclosed by the bounding CDFs $F(x)$ and $G(x)$:

$$H = \{H(x) \mid G(x) \leq H(x) \leq F(x), \forall x \in \Re\}$$

- P-boxes may arise from:
  - Parametric distributions with uncertain parameters (e.g., mean, SD)
  - Imprecise knowledge of the shape of the CDF: Use bounds consistent with the available empirical information
- Arithmetic operations can be done on p-boxes
  - Analogous to interval arithmetic
  - Implemented in Risk Calc (Ferson, 2002)

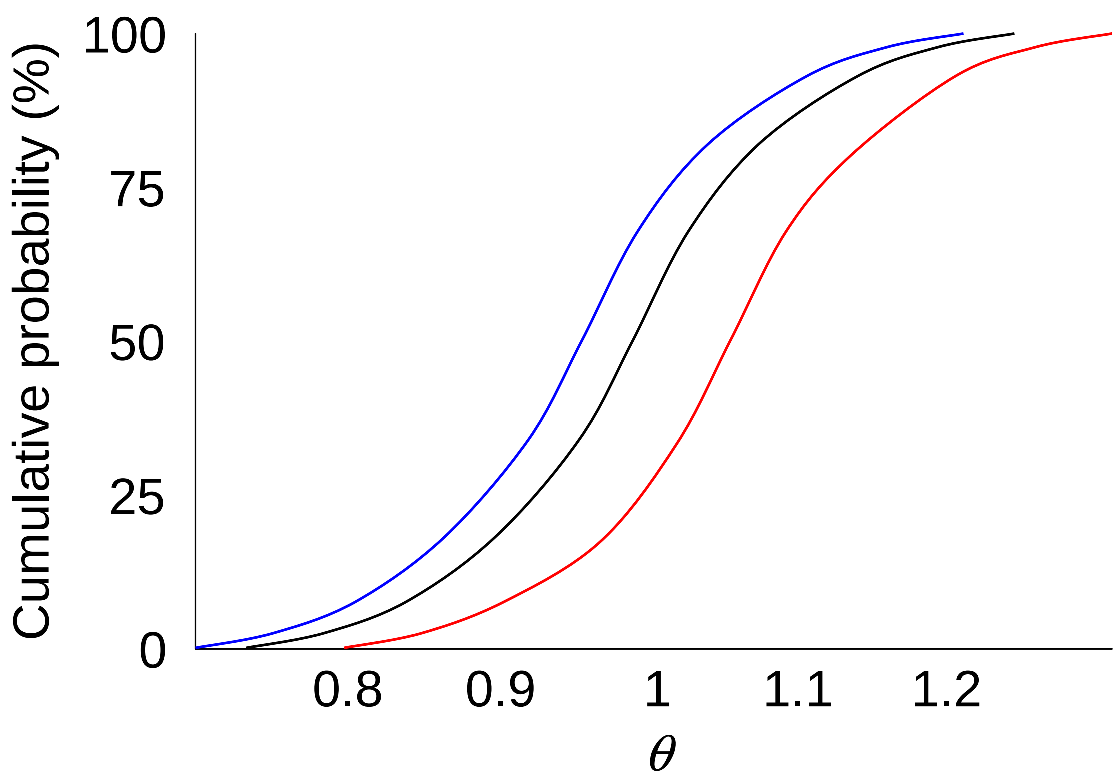
Representing Uncertainties: P-Boxes

- Example: A p-box bounded by normal distributions F and G



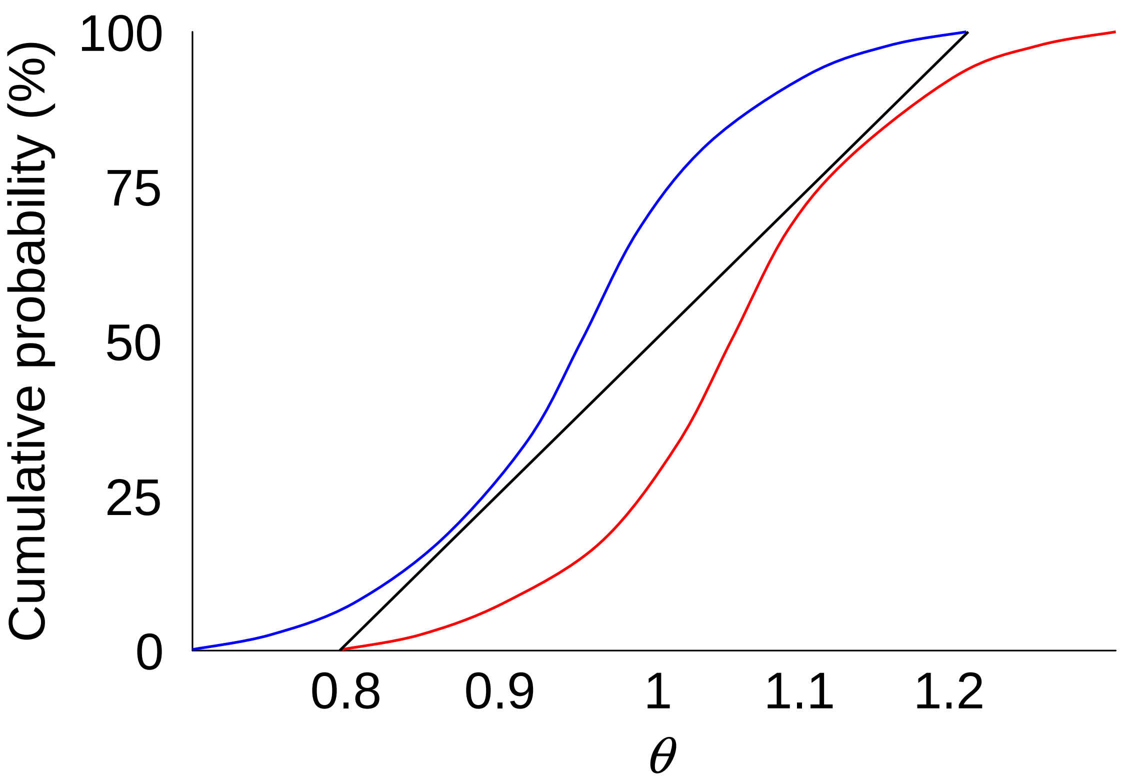
Representing Uncertainties: P-Boxes

- Example: This p-box can contain another normal CDF



Representing Uncertainties: P-Boxes

- Example: Or, this p-box can contain a uniform CDF



Propagating Uncertainties

- Goal:
  - Given p-boxes for the parameters in a nonlinear ODE model
  - Determine p-boxes for the state variables at specified values of time
- Tools:
  - Taylor models
  - Validating solver for parametric ODEs (VSPODE)

Taylor Models

- Taylor Model $T_f = (p_f, R_f)$: Bounds the range of $f(\boldsymbol{x})$ over an interval $\boldsymbol{X}$ using a q-th order Taylor polynomial p_f and an interval remainder bound R_f
- Could obtain T_f using a truncated Taylor series

$$p_f = \sum_{i=0}^{q} \frac{1}{i!} \left[(\boldsymbol{x} - \boldsymbol{x}_0) \cdot \bigtriangledown \right]^i f(\boldsymbol{x}_0)$$

$$R_f = \frac{1}{(q+1)!} \left[(\boldsymbol{x} - \boldsymbol{x}_0) \cdot \bigtriangledown \right]^{q+1} F \left[\boldsymbol{x}_0 + (\boldsymbol{x} - \boldsymbol{x}_0)\zeta \right]$$

where,

$$\boldsymbol{x}_0 \in \boldsymbol{X}; \quad \zeta = [0, 1]$$

$$[\boldsymbol{g} \cdot \bigtriangledown]^k = \sum_{\substack{j_1 + \cdots + j_m = k \\ 0 \le j_1, \cdots, j_m \le k}} \frac{k!}{j_1! \cdots j_m!} g_1^{j_1} \cdots g_m^{j_m} \frac{\partial^k}{\partial x_1^{j_1} \cdots \partial x_m^{j_m}}$$

- Can also compute Taylor models by using Taylor model operations
- Taylor models often yield sharper bounds than interval arithmetic, for modest to complicated functional dependencies

Validated Solution for Parametric ODEs

- Consider the IVP for the parametric ODE system

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta}), \quad \boldsymbol{x}(t_0) = \boldsymbol{x}_0 \in \boldsymbol{X}_0, \quad \boldsymbol{\theta} \in \boldsymbol{\Theta}$$

  where $\boldsymbol{X}_0$ and $\boldsymbol{\Theta}$ represent interval bounds on the uncertainties in the initial states and parameters, respectively

- Validated methods:
  - Guarantee there exists a unique solution $\boldsymbol{x}$ in the interval $[t_0, t_f]$, for each $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ and $\boldsymbol{x}_0 \in \boldsymbol{X}_0$
  - Compute an interval $\boldsymbol{X}_j$ that encloses all solutions of the ODE system at t_j for $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ and $\boldsymbol{x}_0 \in \boldsymbol{X}_0$

- Tools are available – AWA, VNODE, COSY VI, VSPODE, etc.

New Method for Parametric ODEs

- Use interval Taylor series to represent dependence on time
- Use Taylor models to represent dependence on uncertain quantities (parameters and initial states)
- Assuming $\boldsymbol{X}_j$ is known, then
  - Phase 1: Compute a coarse enclosure $\widetilde{\boldsymbol{X}}_j$ and prove existence and uniqueness using fixed pointed iteration with Picard operator and high-order interval Taylor series
  - Phase 2: Refine the coarse enclosure to obtain $\boldsymbol{X}_{j+1}$ using Taylor models in terms of the uncertain parameters and initial states
- Implemented in VSPODE (Validating Solver for Parametric ODEs, Lin and Stadtherr, 2006)

VSPODE Example

- Lotka-Volterra problem

$$\dot{y}_1 = \theta_1 y_1 (1 - y_2)$$

$$\dot{y}_2 = \theta_2 y_2 (y_1 - 1)$$

$$\boldsymbol{y}_0 = (1.2, 1.1)^{\mathrm{T}}$$

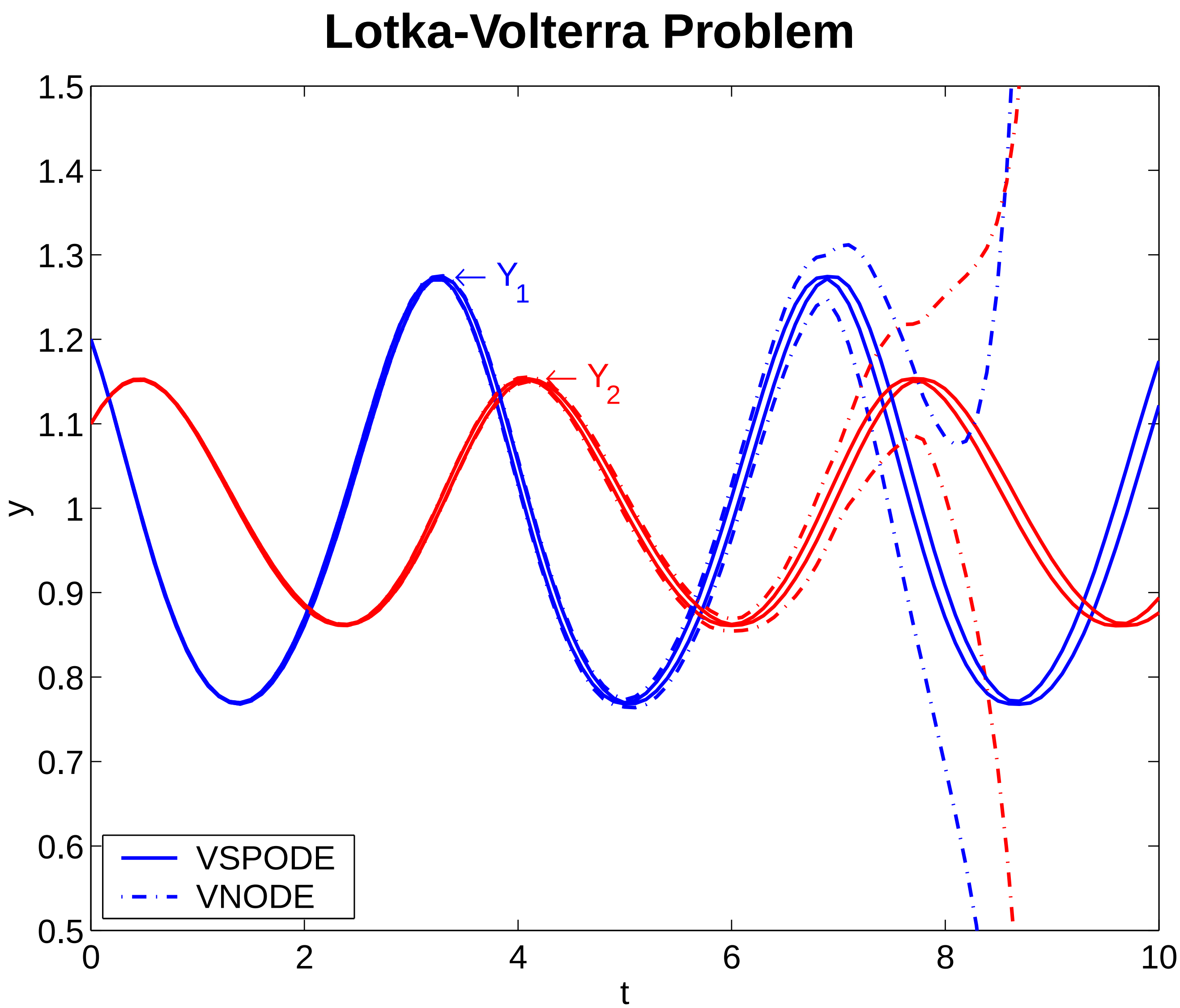
$$\theta_1 \in [2.99, 3.01]$$

$$\theta_2 \in [0.99, 1.01]$$

- Integrate from $t_0 = 0$ to $t_N = 10$

- Compare to results obtained using the popular VNODE solver (Nedialkov, 1999)

- Constant step size of $h = 0.1$ used in both VSPODE and VNODE.



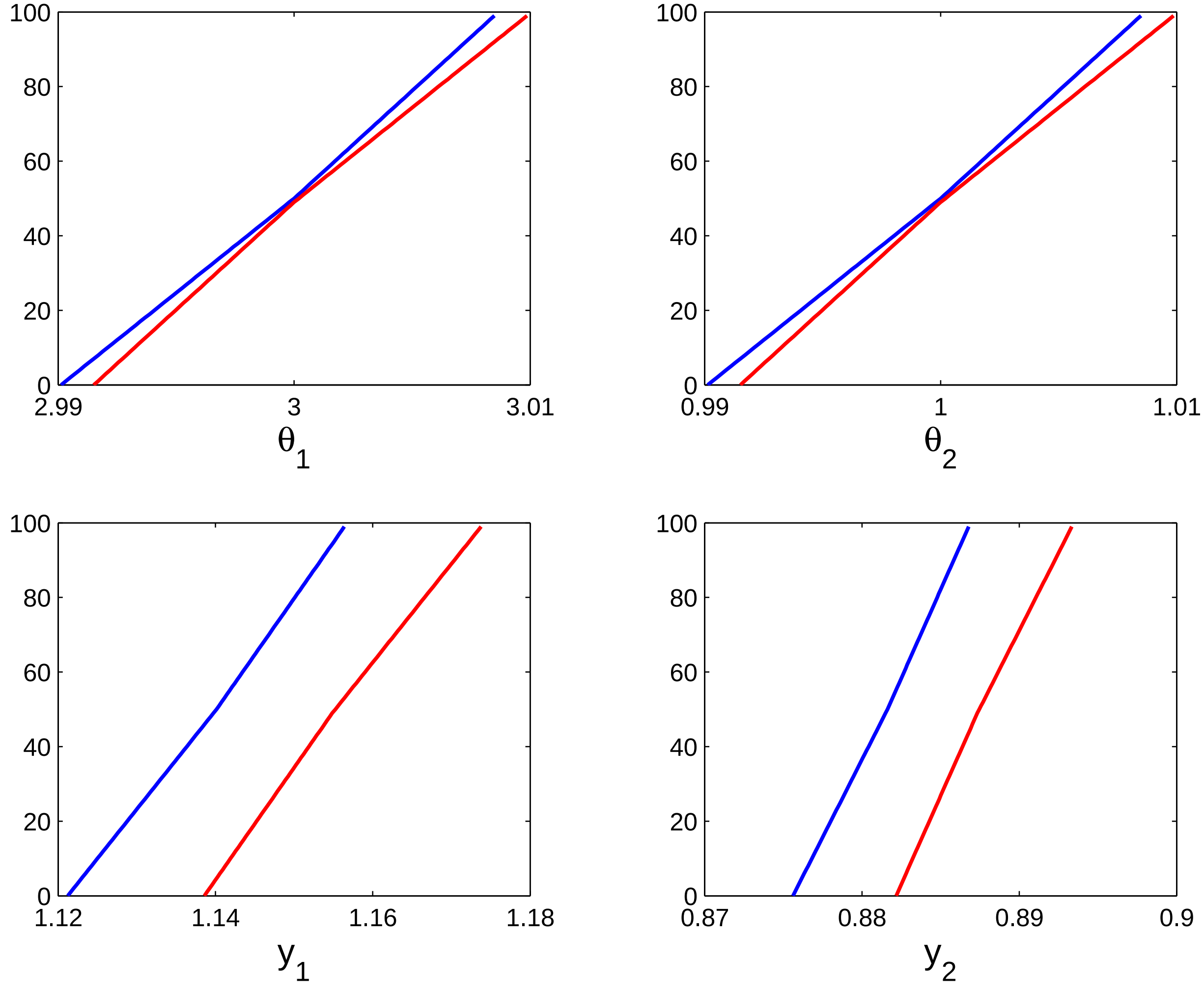
(Eventual breakdown of VSPODE at $t = 31.8$)

Propagating Uncertainties

- For a specified time t_j, VSPODE computes a Taylor model of the states, in terms of the uncertain parameters $\boldsymbol{\theta}$ — this Taylor model is valid for all $\boldsymbol{\theta} \in \boldsymbol{\Theta}$
- Substitute the p-boxes for the parameters into the Taylor model and perform p-box arithmetic using Risk Calc
- The results are p-boxes for the state variables at time t_j
- The results are conservative – the true distribution of the states will be enclosed
- Example: Lotka-Volterra problem, $\theta_1 \in [2.99, 3.01]$, $\theta_2 \in [0.99, 1.01]$, $t_j = 10$
- Three different parameter distributions will be considered

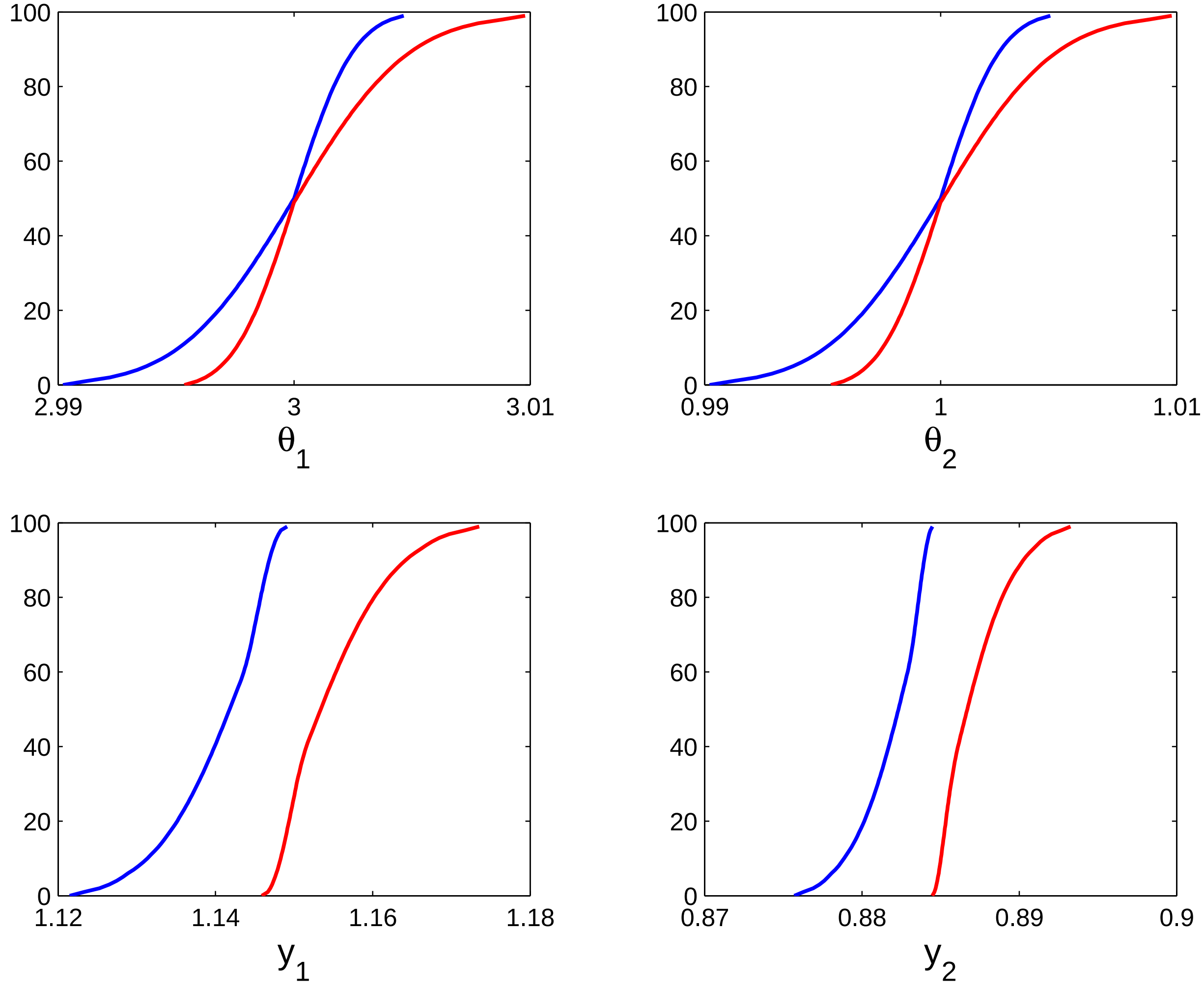
Uniform distribution with known mean and interval SD

θ_1: mean = 3, SD = [0.005, 0.0057] θ_2: mean = 1, SD = [0.005, 0.0057]



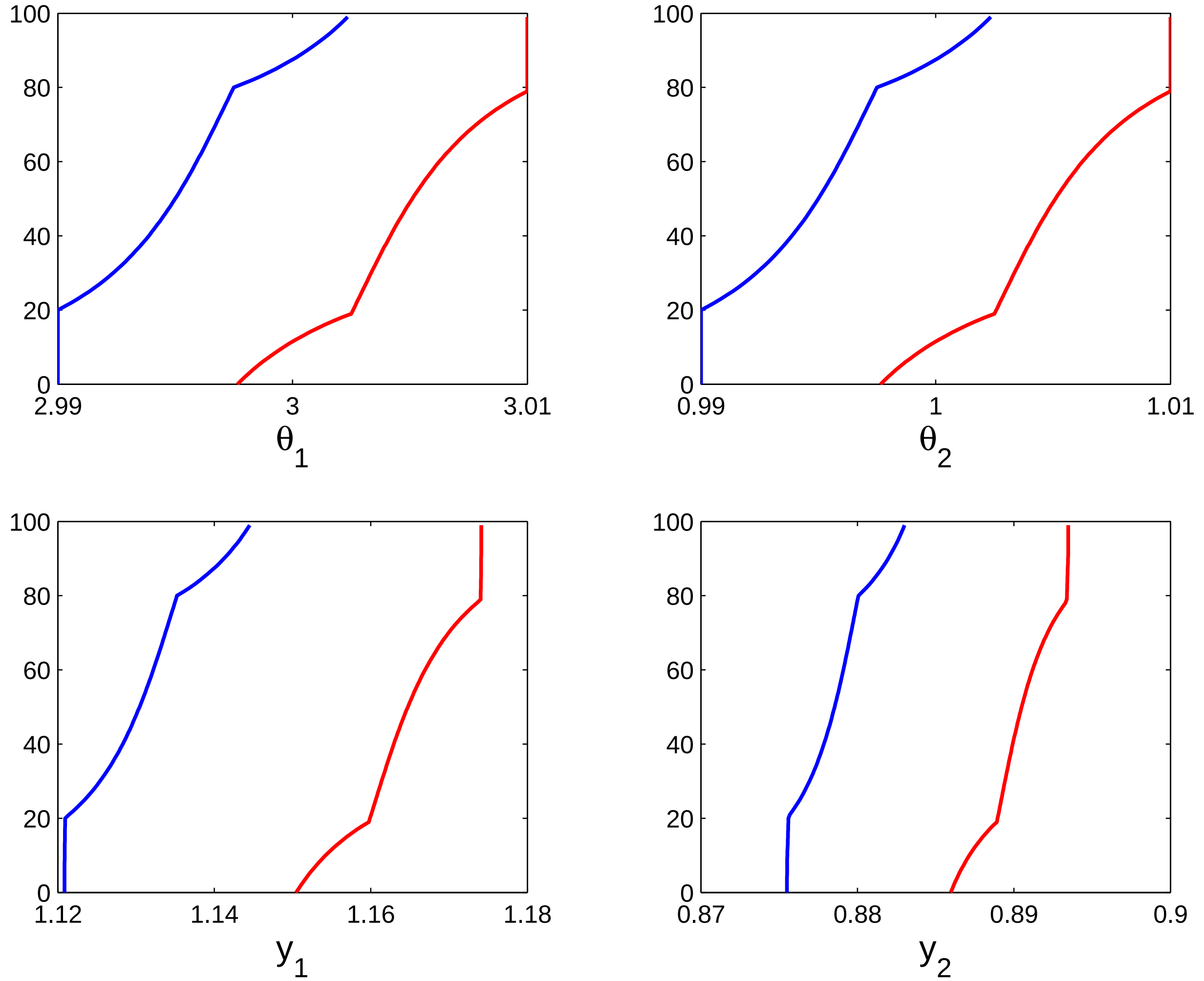
Normal distribution with known mean and interval SD

θ_1: mean = 3, SD = [0.002, 0.0038] θ_2: mean = 1, SD = [0.002, 0.0038]



Distribution with known minimum, maximum, mean and SD

$$\theta_1 \in \text{mmms}(2.99, 3.01, 3, 0.005); \quad \theta_2 \in \text{mmms}(0.99, 1.01, 1, 0.005)$$



Concluding Remarks

- P-boxes and p-box arithmetic (Risk Calc) are useful when probability distributions are known imprecisely
- VSPODE is a useful tool for bounding the solutions of parametric nonlinear ODEs
- Using VSPODE and Risk Calc, it is possible to rigorously propagate uncertainties through a nonlinear ODE model
- The p-boxes for the state variables can be tightened using subinterval reconstitution
- Acknowledgement: U. S. Department of Energy