Propagating Uncertainties in Modeling Nonlinear Dynamic Systems

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Overview

- Problem Statement
- Representations of Uncertainty
  - Intervals and Taylor Models
  - Cumulative Probability Functions and P-boxes
- Solution Procedure
- Examples
  - Lotka-Volterra Model
  - Microbial Bioreactor with Haldane Kinetics
  - Three-State Bioreactor
- Concluding Remarks

A Motivating Problem: Lotka-Volterra Model

- Simulate a simple predator-prey model with the ODE system with uncertainty in parameters

$$\frac{dx_1}{dt} = \theta_1 x_1 (1 - x_2)$$

$$\frac{dx_2}{dt} = \theta_2 x_2 (x_1 - 1)$$

over the interval $t = [0, 10]$

- The variables x represent the biomasses of the prey and predator
- The parameters θ affect the growth and death of each species
- The distribution of uncertainties in θ_1 and θ_2 is not entirely unknown

Problem Statement

- We consider the general ODE initial value problem

$$y'(t) = f(y, \theta), \qquad y(t_0) = y_0 \in Y_0, \qquad \theta \in \Theta,$$

where at least one of the initial conditions on state variables y or one of the time-invariant parameters θ is uncertain (contained in Y_0 and/or Θ)

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  - Guaranteed enclosure of solution across all times of interest

  - Ability to see p-box enclosure of state variables y at any time of interest

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- In short, we wish to propagate all knowledge of uncertainty through a dynamic model

Representation of Uncertainty: Intervals

- The most basic way to represent uncertainty in a value is to declare its lower and upper bound
- An real interval is just that, a segment of the real number line $X = [a, b] = \{x \in \mathbb{R} \mid a \leq x \leq b\}$
- An interval vector $\boldsymbol{X} = [X_1, X_2, \ldots X_n]^T$ can be thought of as an n-dimensional rectangle
- We can define basic interval arithmetic using set notation:

$$X \ \mathrm{op}\ Y = \{x \ \mathrm{op}\ y \mid x \in X, y \in Y\}$$

- We can define other elementary interval functions (e.g., $\exp(X)$, $\sin(X)$)

Representation of Uncertainty: Intervals

- An interval extension $F(X)$ encloses $f(x)$ for every $x \in X$:

$$F(X) \supseteq \{f(x) \mid x \in X\}$$

- If the function calls an interval-valued variable more than once, direct substitution may lead to overestimation (the "dependency" problem)

- If the function range is not interval-shaped, the interval enclosure will include the interval as well as other values (the "wrapping effect")

- Repeated applications of such overestimations can quickly lead to the loss of any meaningful interval enclosure

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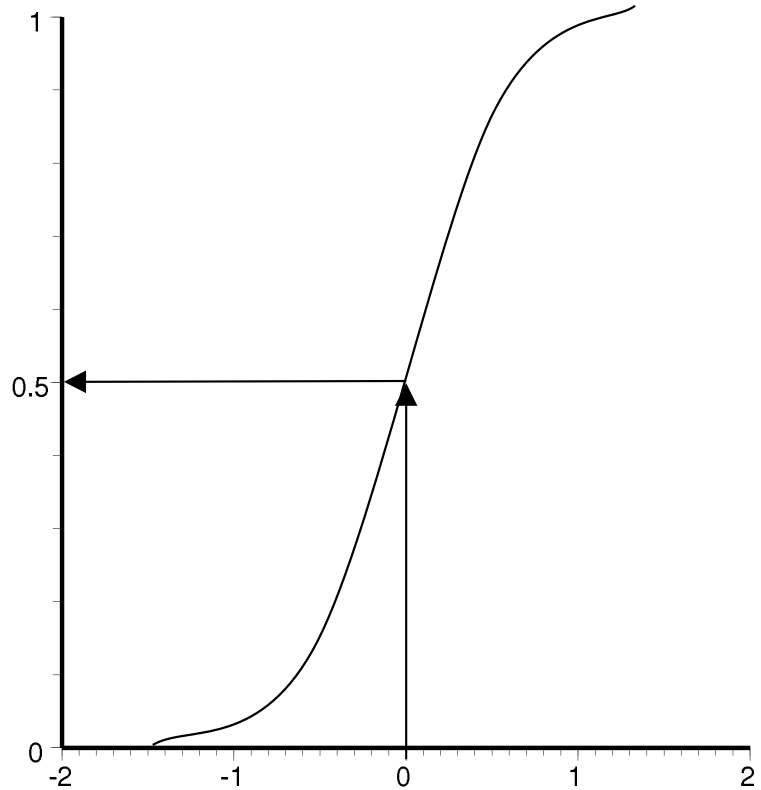
  - Beginning with Taylor models of simple functions (e.g., constant, identity) and using TM operations, one we can compute the TM of a complicated function
- Compared to other methods, the Taylor model often provides sharper bounds for modest and more complicated functions

Representation of Uncertainty: CDF's

- For a quantity x, the cumulative distribution function (CDF) $F(z)$ gives the probability that $x \leq z$
- Example: in the CDF below, $P(x \leq 0) = 0.5$



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- A p-box is the set of all CDFs enclosed by two bounding functions $F(z)$ and $G(z)$:

$$(F, G) = \{H(z) \mid F(z) \geq H(z) \geq G(z) \quad \forall z \in \mathbb{R}\}$$

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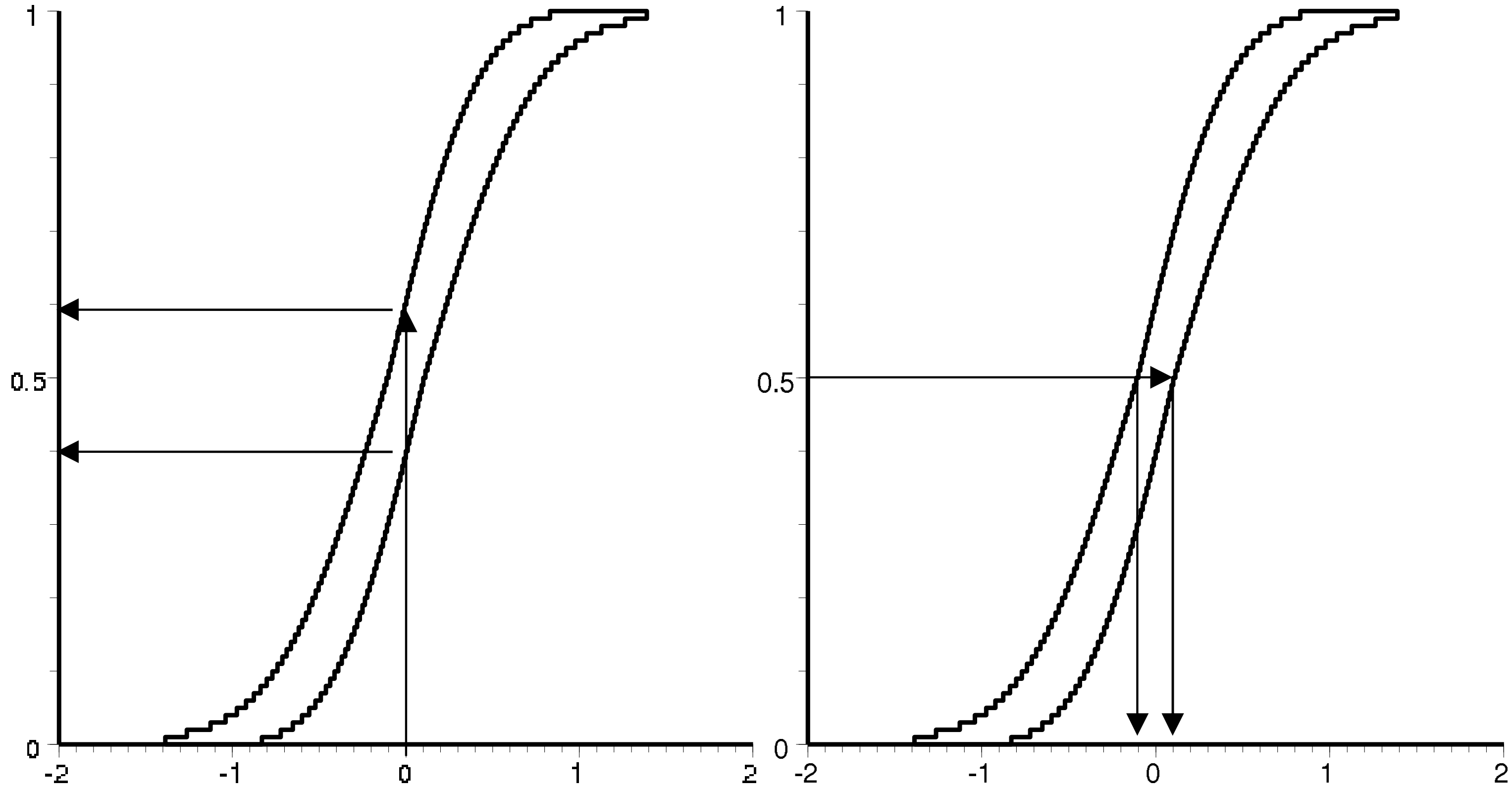
- Arithmetic operations can be defined in a manner analogous to intervals
- P-box operations are implemented in Risk Calc

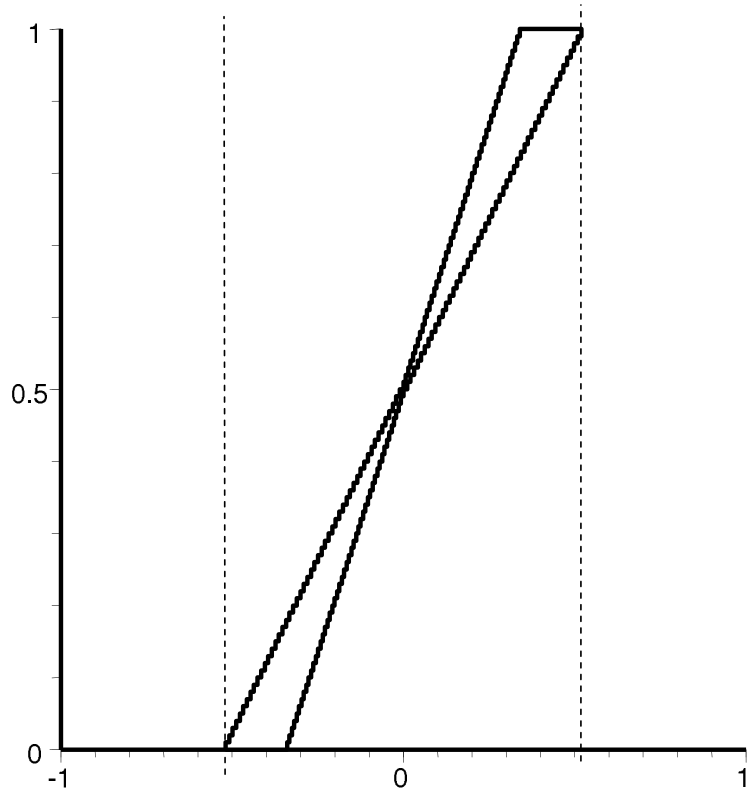
Representation of Uncertainty: P-boxes

- P-boxes provide an interval of probabilities for a corresponding value or an interval of values for a corresponding probability



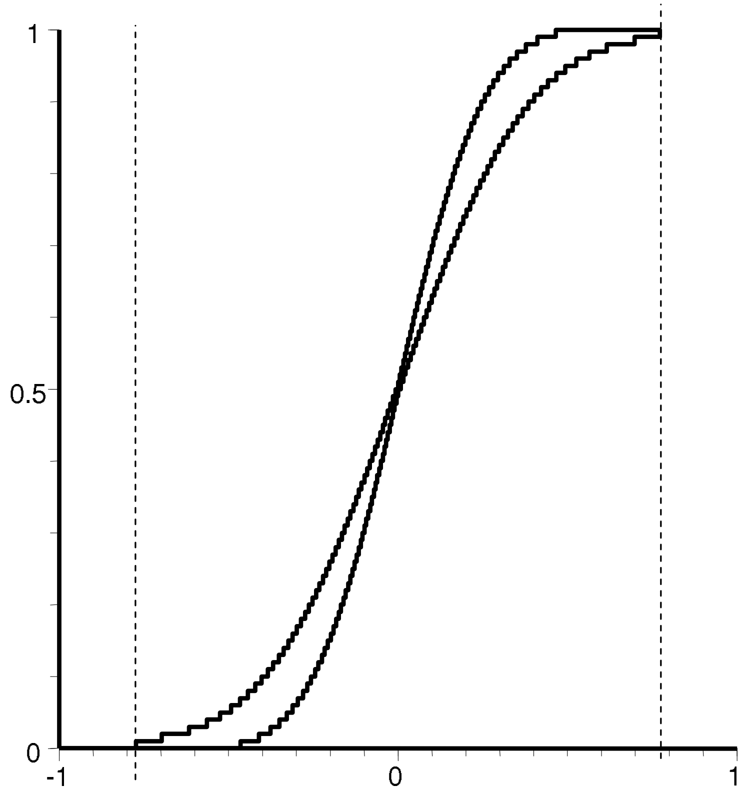
Representation of Uncertainty: P-boxes

- Example of a p-box from a known distribution and uncertain parameter:
  - A "uniform" p-box with bounds obtained from a uniform distribution with fixed mean 0 and interval standard deviation $[0.2, 0.3]$
  - This p-box can be enclosed in the interval $[-0.52, 0.52]$



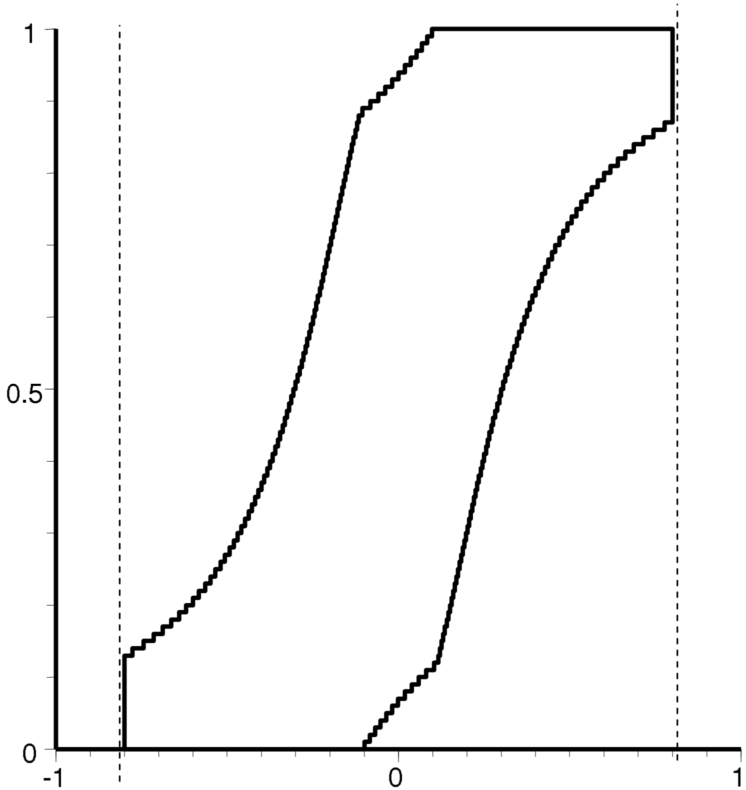
Representation of Uncertainty: P-boxes

- Another example of a p-box from a known distribution / uncertain parameter:
  - A “normal” p-box with bounds obtained from a truncated normal distribution with fixed mean 0 and interval standard deviation $[0.2, 0.3]$
  - This p-box can be enclosed in the interval $[-0.78, 0.78]$



Representation of Uncertainty: P-boxes

- An example of a p-box with unknown distribution and certain parameters:
  - This "mmms" p-box bounds all CDF's with known minimum (-0.8), maximum (0.8), mean (0), and standard deviation (0.3)
  - This p-box can be enclosed in the interval $[-0.8, 0.8]$



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- P-box arithmetic allows for propagation of non-interval (probabilistic) uncertainties in algebraic models
  - There is a need for propagation of probabilistic uncertainties in dynamic models

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  - Compute a p-box enclosure of state variables at specific times

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- Solution procedure
  - Use VSPODE (Lin and Stadtherr, 2007) to compute a Taylor model $T_y(y_0, \theta)$ of the state variables at the desired time
  - Substitute p-boxes for y_0 and θ into $T_y(y_0, \theta)$ and use Risk Calc to compute a p-box enclosure of y

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- To obtain an enclosure at time t_{j+1}, an appropriate time step $h_j = t_{j+1} - t_j$ and *a priori* enclosure $\tilde{Y} \in \tilde{Y}_j^0$ are found to satisfy

$$Y_j + \left(\sum_{i=1}^{k-1} [0, h_j]^i F^{[i]}(Y_j) \right) + [0, h_j]^k F^{[k]}(\tilde{Y}_j^0) \subseteq \tilde{Y}_j^0$$

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- If this condition holds, then there is a unique solution $y(t; t_j, y_j, \theta) \in \tilde{Y}_j$ for all $t \in [t_j, t_{j+1}]$, all $y_j \in Y_j$, and all $\theta \in \Theta$

Solution Procedure

- In the second phase of VSPODE, we obtain a tighter enclosure, so we represent uncertain initial states and parameters using Taylor models T_{y_0} and T_θ, with components

$$T_{y_{i0}} = (m(Y_{i0}) + (y_{i0} - m(Y_{i0})), [0,0]), \quad i = 1, \cdots, m$$

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- This results in a Taylor model $T_{y_{j+1}}$ in terms of the initial states y_0 and parameters θ
- The interval enclosure Y_{j+1} is computed by bounding $T_{y_{j+1}}$ over Y_0 and Θ

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- This process is completed using standard independent p-box arithmetic
  - The computations are done by discretizing the p-box for different probabilities
  - Using an optional procedure known as subinterval reconstitution (SIR), the p-boxes are partitioned in both directions, to reduce what is analogous to the “dependency” effect in intervals, and the resulting p-box has a tighter enclosure

Examples: Lotka-Volterra Model

- Simulate a simple predator-prey model with the ODE system with uncertainty in parameters

$$\frac{dx_1}{dt} = \theta_1 x_1 (1 - x_2), \qquad x_1(0) = 1.2, \qquad \theta_1 \in [2.99, 3.01]$$

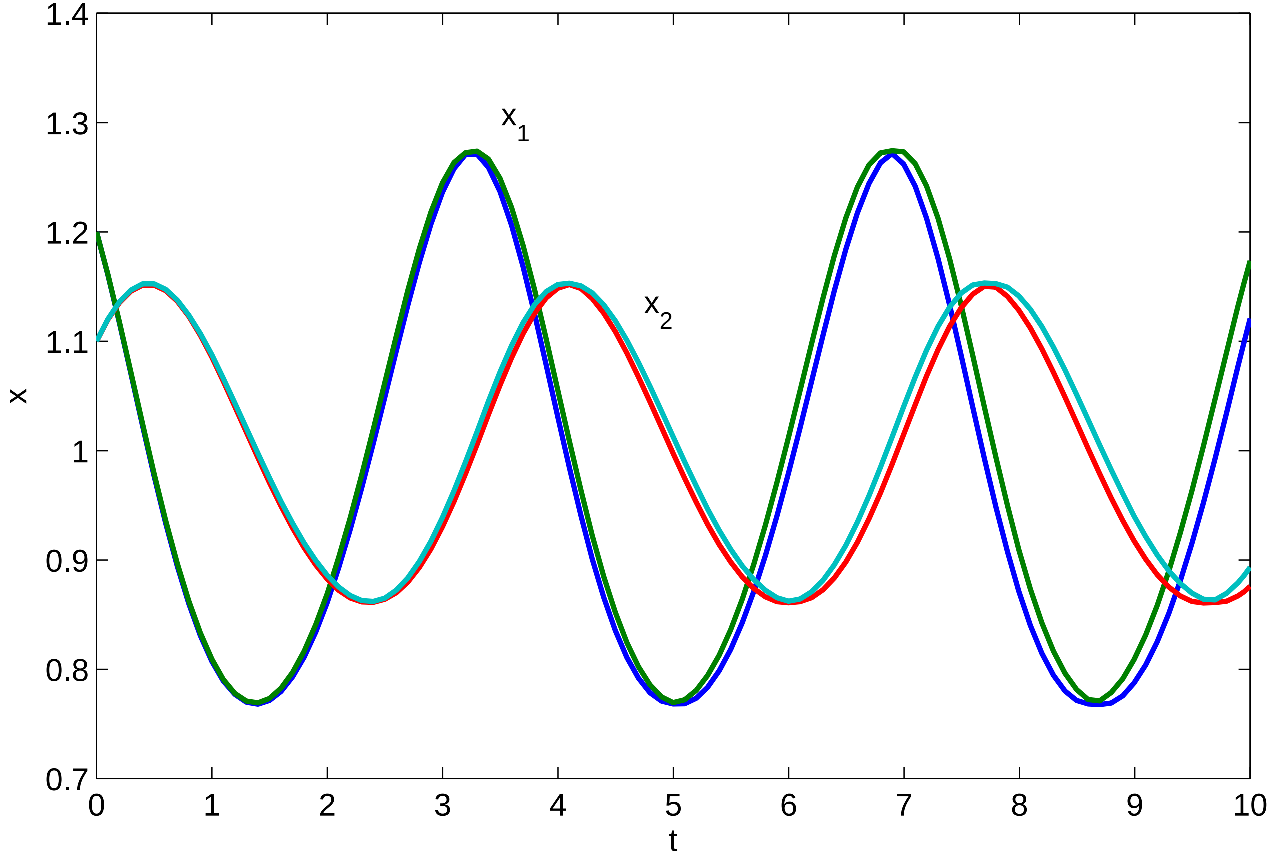
$$\frac{dx_2}{dt} = \theta_2 x_2 (x_1 - 1), \qquad x_2(0) = 1.1, \qquad \theta_2 \in [0.99, 1.01]$$

  over the interval $t = [0, 10]$

- The variables x represent the biomasses of the prey and predator
- The parameters θ affect the growth and death of each species
- The distribution of uncertainties in θ_1 and θ_2 is described by uniform p-boxes with means equal to the interval midpoints and standard deviations in $[0.0050, 0.0057]$

Example: Lotka-Volterra Model

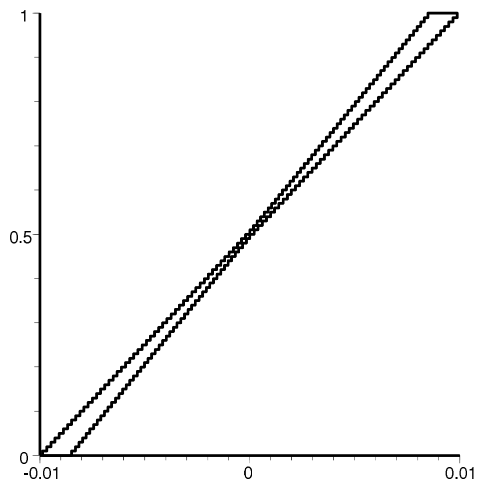
- VSPODE enclosure of variable trajectory over $[0, 10]$ based on interval uncertainty



Example: Lotka-Volterra Model

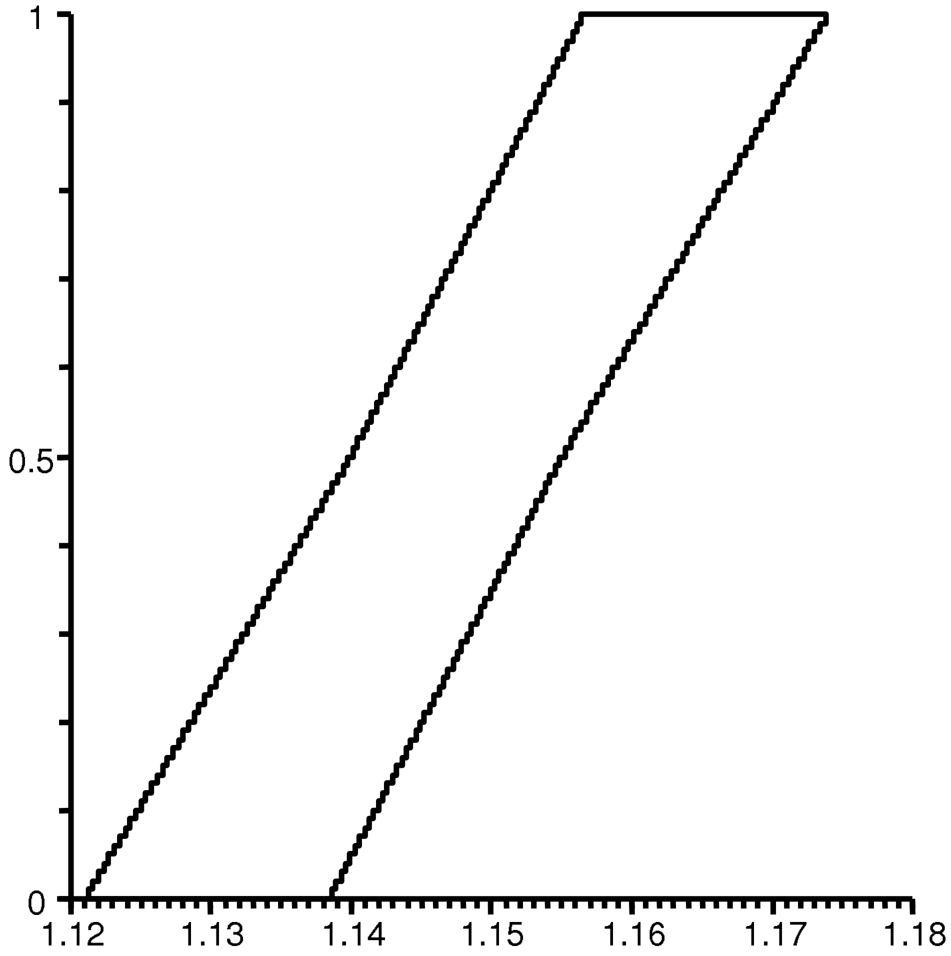
- P-box inputs into Taylor model at time $t = 10$

Quantity	Taylor Model	P-box
θ_1	$3 + [-0.01, 0.01]$	$3+$uniform(mean$=0$, s.d. $\in [0.050, 0.057]$)
θ_2	$1 + [-0.01, 0.01]$	$1+$uniform(mean$=0$, s.d. $\in [0.050, 0.057]$)



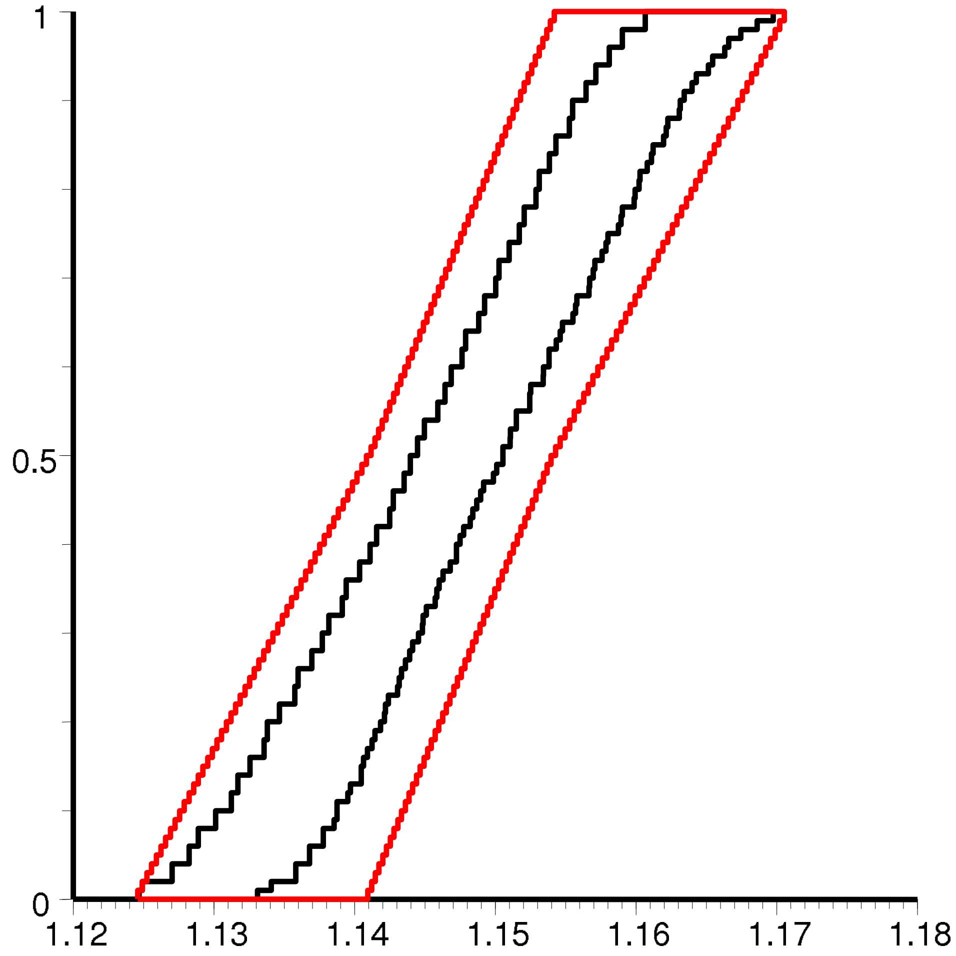
Example: Lotka-Volterra Model

- P-box enclosure of variable x_1 at time $t = 10$ computed with Risk Calc, using Taylor model from VSPODE



Example: Lotka-Volterra Model

- P-box enclosure (using SIR with 100 partitions) of variable x_1 at time $t = 10$



Example: Microbial Bioreactor with Haldane Kinetics

- ODE model of cells with biomass X consuming substrate with mass S

$$\frac{dX}{dt} = (\mu - \alpha D)X$$

$$\frac{dS}{dt} = D(S_f - S) - k\mu X$$

- The growth rate μ is given by

$$\mu = \frac{\mu_{max} S}{K_S + S + K_I S^2}$$

Example: Microbial Bioreactor with Haldane Kinetics

- Parameter and initial condition values

	Value	Units		Value	Units
α	0.5		μ_{max}	$[1.15, 1.25]$	day^{-1}
k	10.53	(g S)/(g X)	K_S	$[6.8, 7.2]$	(g S)/L
D	0.36	day^{-1}	K_I	$[0.0025, 0.01]$	L /(g S)
S_f	5.7	(g S)/L	X_0	$[0.794, 0.864]$	(g X)/L
S_0	0.80	(g S)/L			

- Integrate over the time interval $[0, 10]$
- These interval values in both initial conditions and parameters are the maximums and minimums of the p-boxes that describe the uncertainties
  - P-boxes are mmms distributions with means at the midpoint of the interval and standard deviations one-tenth the width of the interval

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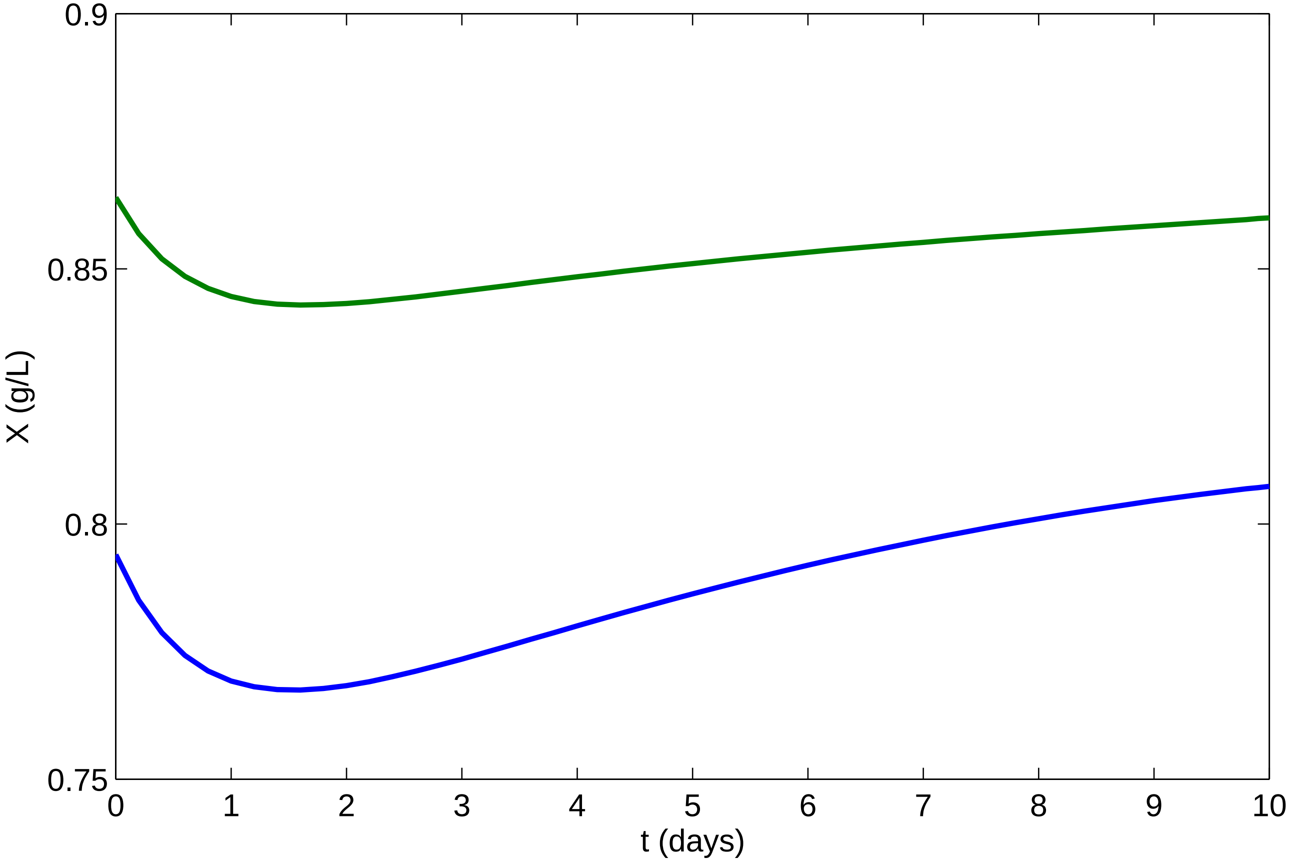
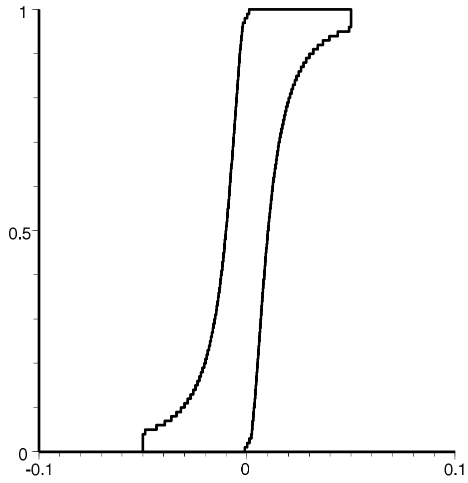
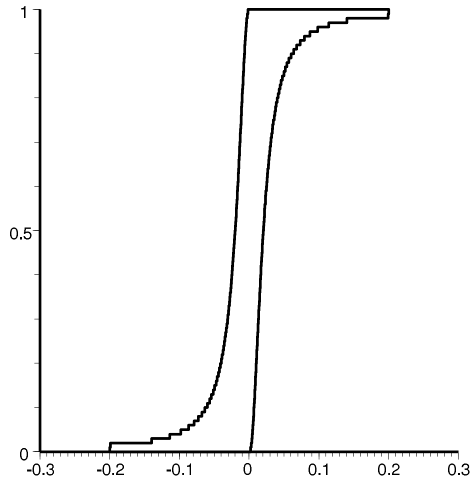


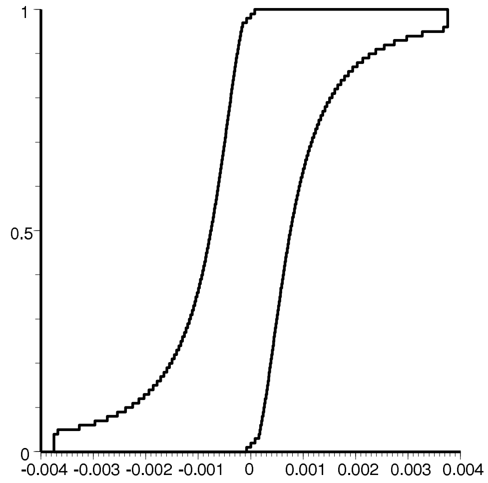
Example: Microbial Bioreactor with Haldane Kinetics

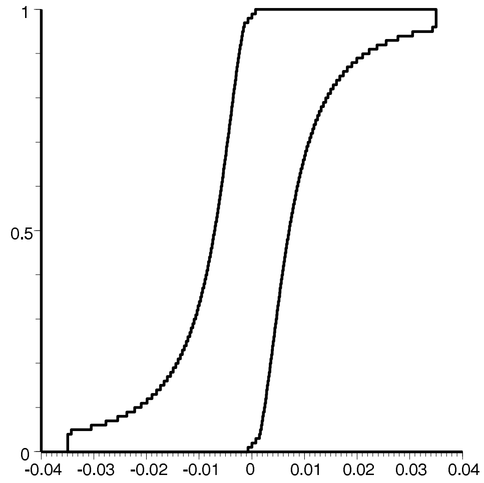
- P-box inputs into Taylor model at time $t = 10$

Quantity	Taylor Model	P-box
μ_{max}	$1.2 + [-0.05, 0.05]$	mmms(mean$=0$, s.d.$=0.01$)
K_S	$7 + [-0.2, 0.2]$	mmms(mean$=0$, s.d.$=0.04$)
K_I	$0.00625 + [-0.00375, 0.00375]$	mmms(mean$=0$, s.d.$=0.00075$)
X_0	$0.829 + [-0.035, 0.035]$	mmms(mean$=0$, s.d.$=0.007$)



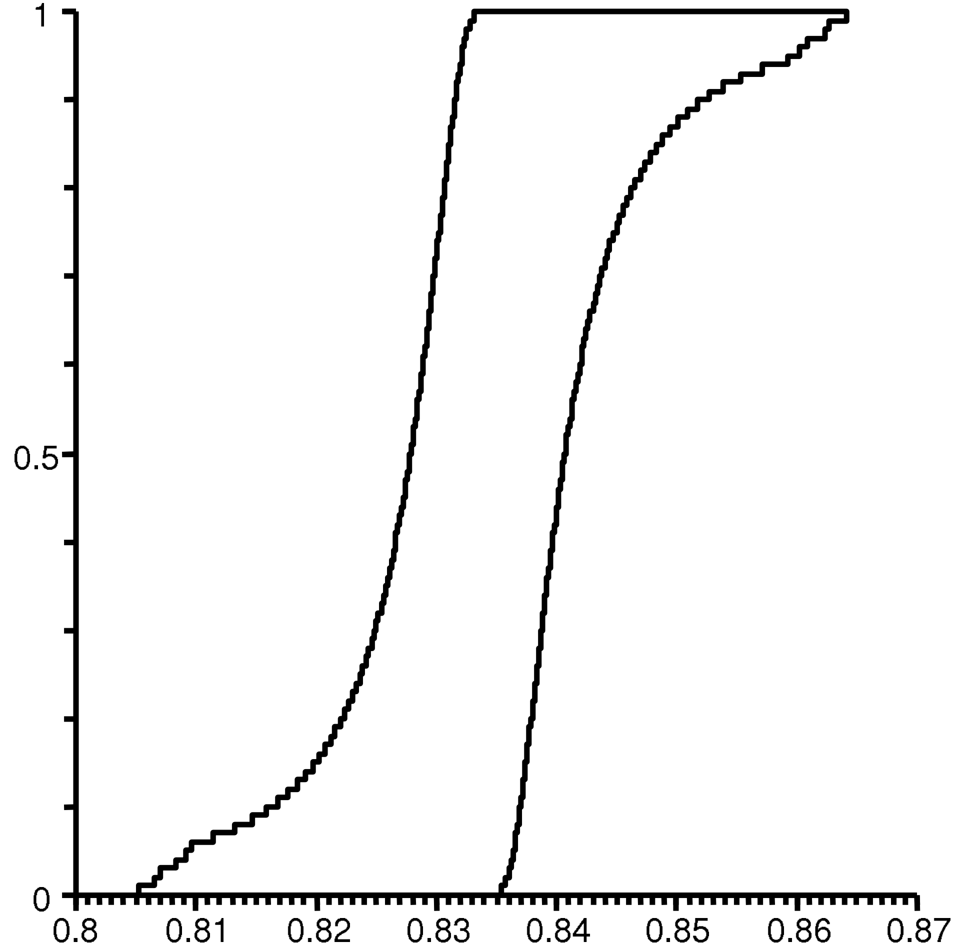






Example: Microbial Bioreactor with Haldane Kinetics

- P-box enclosure of variable X across $[0, 10]$ computed with Risk Calc using Taylor model from VSPODE



Example: Three-State Bioreactor

- Consider cells of biomass x_1 that consume substrate of mass x_2 and create product of mass x_3

$$\frac{dx_1}{dt} = (\mu - D)x_1$$

$$\frac{dx_2}{dt} = D(x_{2f} - x_2) - \frac{\mu x_1}{Y}$$

$$\frac{dx_3}{dt} = -Dx_3 + (\alpha\mu + \beta)x_1,$$

where the growth rate is a function of both substrate and product concentrations

$$\mu = \frac{\mu_{max}\left[1 - (x_3/x_{3m})\right] x_2}{k_s + x_2}$$

Example: Three-State Bioreactor

- Real-valued parameters and initial conditions

	Value	Units		Value	Units
x_{20}	5	g/L	x_{30}	15	g/L
Y	0.4	g/g	β	0.2	hr^{-1}
D	0.202	hr^{-1}	α	2.2	g/g
x_{3m}	50	g/L	x_{3f}	20	g/L

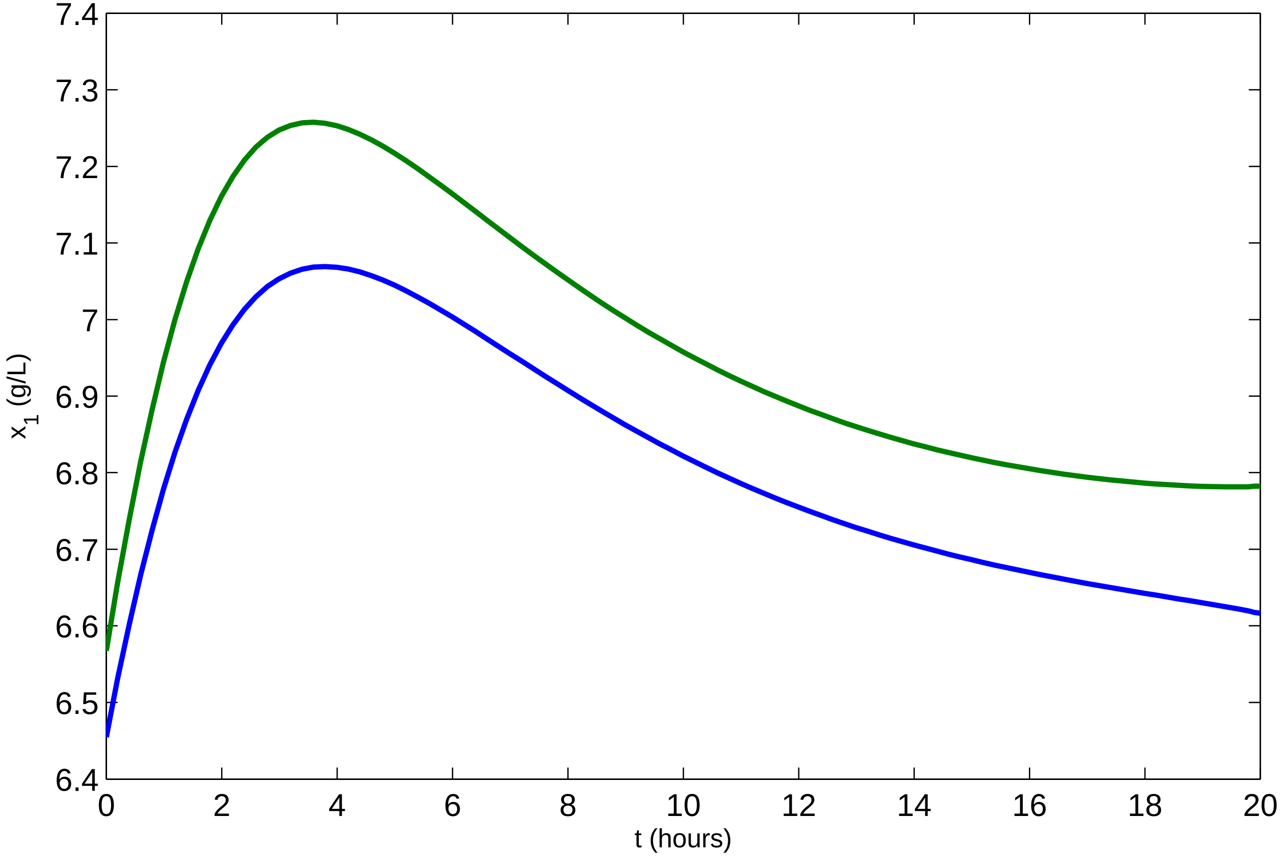
Example: Three-State Bioreactor

- Uncertain parameters and initial conditions

Quantity	Interval	Units	Taylor Model
x_{10}	$[6.4549, 6.5676]$	g/L	$6.51125 + [-0.05635, 0.05635]$
μ_{max}	$[0.46, 0.47]$	g/(g hr)	$0.465 + [-0.005, 0.005]$
k_s	$[1.03, 1.1]$	g/L	$1.065 + [-0.035, 0.035]$

Example: Three-State Bioreactor

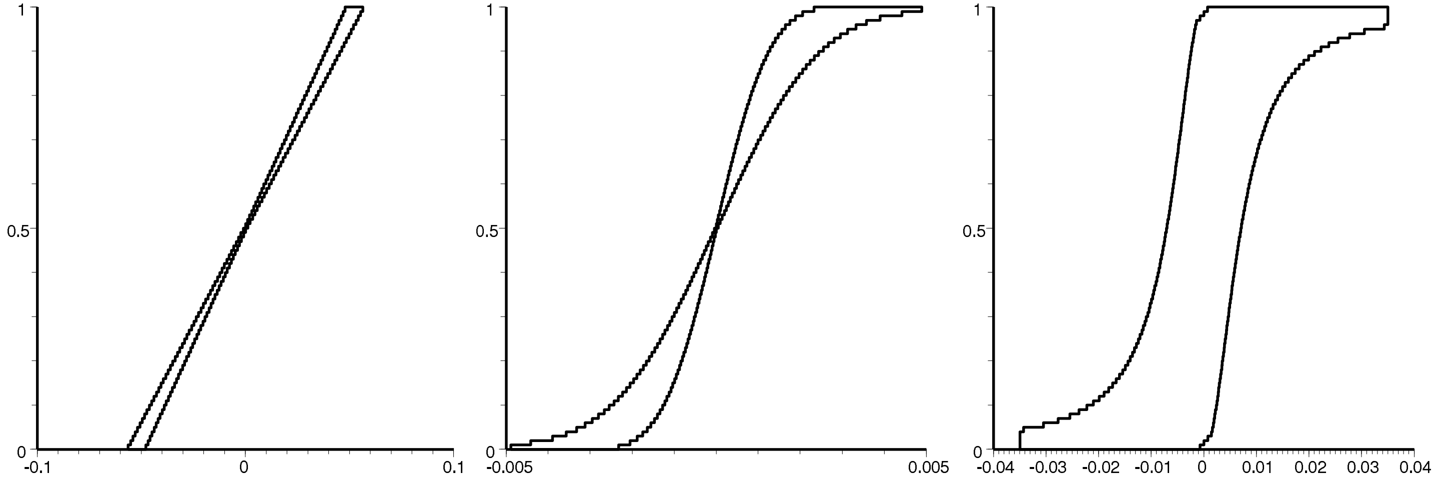
- VSPODE enclosure of trajectory of x_1 over $[0, 20]$ based on interval uncertainty



Example: Three-State Bioreactor

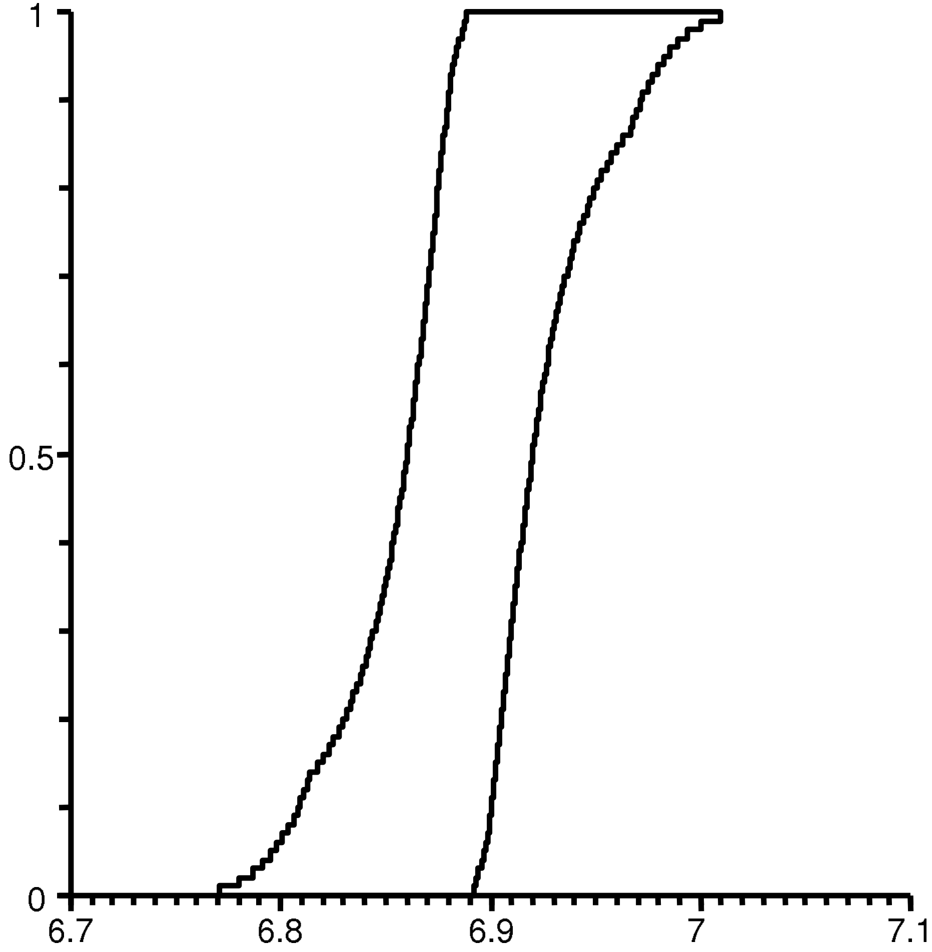
- Uncertain parameters and initial conditions

Quantity	P-box
x_{10}	$6.51125+$uniform(mean$=0$, s.d.$=[0.02817, 0.032533]$)
μ_{max}	$0.465+$normal(mean$=0$, s.d.$=[0.0282, 0.0325]$)
k_s	$1.065+$mmms(max$=0.035$, min$=0.035$, mean$=0$, s.d.$=0.007$)



Example: Three-State Bioreactor

- P-box enclosure of variable x_1 at $t = 10$ computed with Risk Calc using Taylor model from VSPODE



Concluding Remarks

- VSPODE (Lin and Stadtherr, 2007) is a powerful tool to propagate interval uncertainties through nonlinear ODEs
- By using Taylor models from VSPODE and p-box arithmetic from Risk Calc, we can propagate probabilistic uncertainties (represented by p-boxes) through nonlinear ODE models
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