Projecting uncertainty through nonlinear ODEs

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Uncertainty

- Artifactual uncertainty
  - Too few polynomial terms
  - Numerical instability
  - Can be reduced by a better analysis
- Authentic uncertainty
  - Genuine unpredictability due to input uncertainty
  - Cannot be reduced by a better analysis

Uncertainty propagation

- We *want* the predition to ‘break down’ if that’s what should happen
- But we don’t want artifactual uncertainty
  - Wrapping effect
  - Dependence problem
  - Repeated parameters

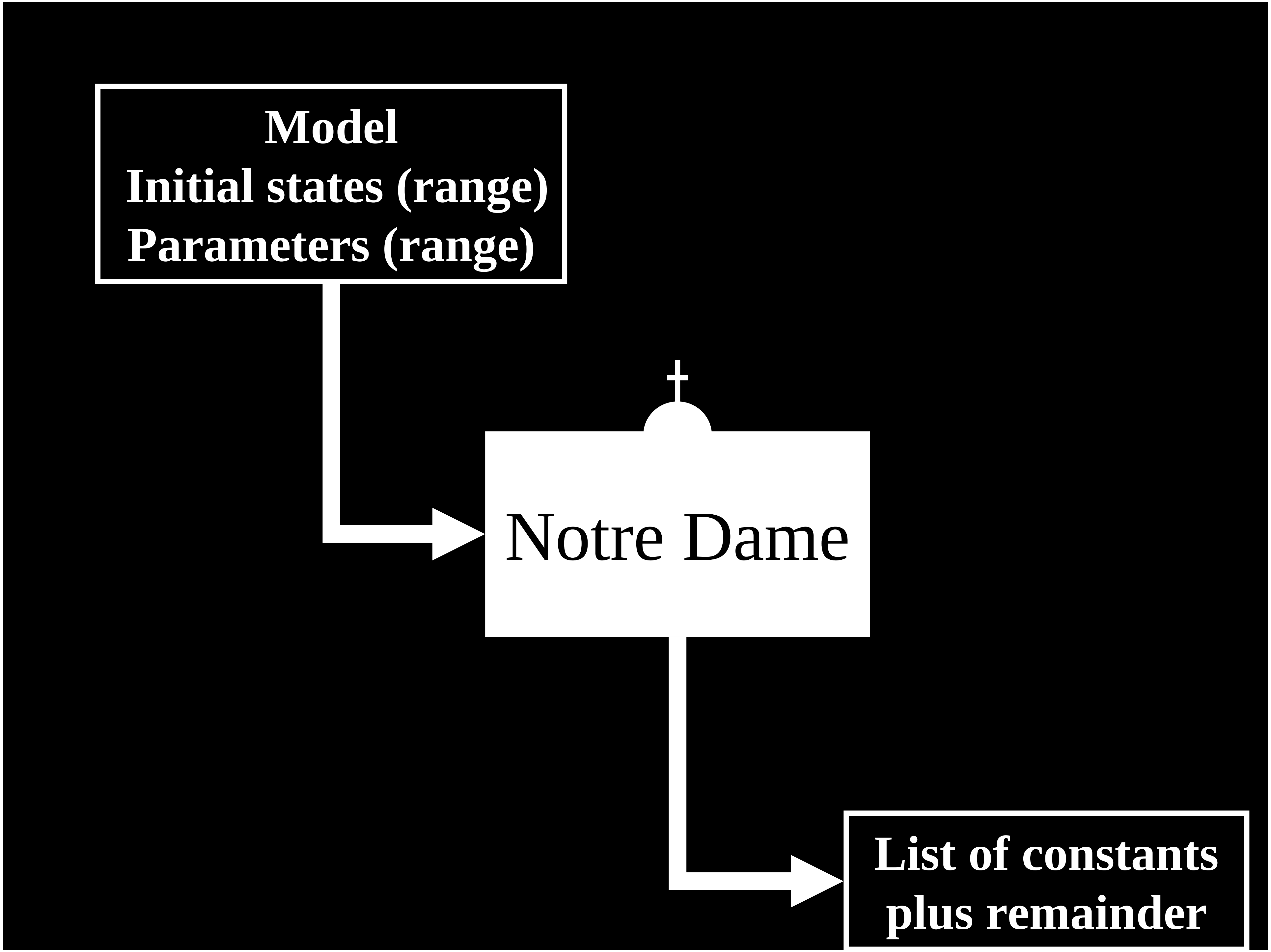
Problem

- Nonlinear ordinary differential equation (ODE)

$$\mathrm{d}\boldsymbol{x}/\mathrm{d}t = f(\boldsymbol{x}, \theta)$$

  with uncertain θ and initial state x_0

- Information about θ and x_0 comes as
  - Interval ranges
  - Probability distribution
  - Something in between


Model
Initial states (range)
Parameters (range)
Notre Dame
List of constants
plus remainder

Inside VSPODE

- Interval Taylor series (à la VNODE)
  - Dependence on time
- Taylor model
  - Dependence of parameters

(Comparable to COSY)

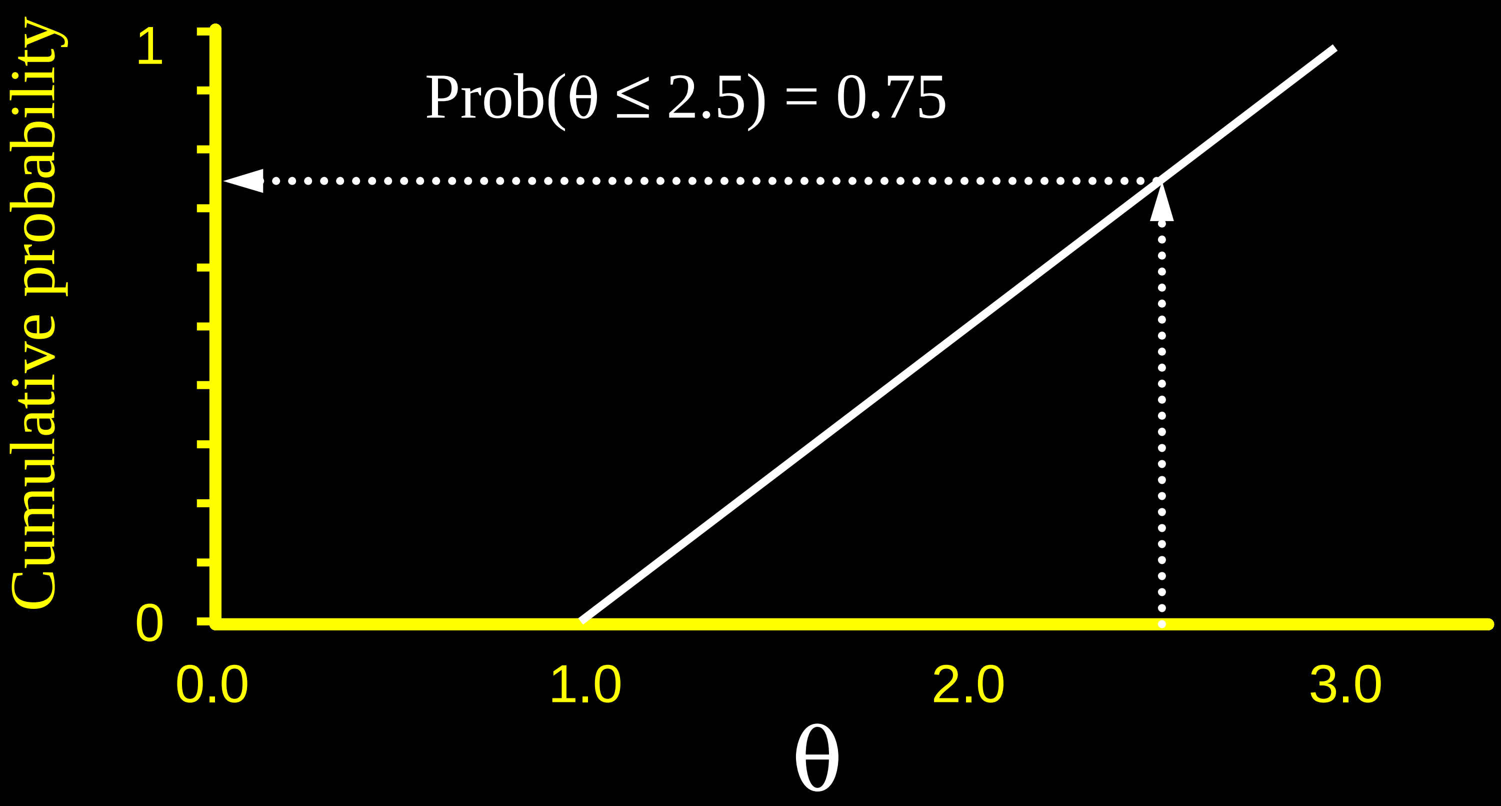
Representing uncertainty

- Cumulative distribution function (CDF)
  - Gives the probability that a random variable is smaller than or equal to any specified value

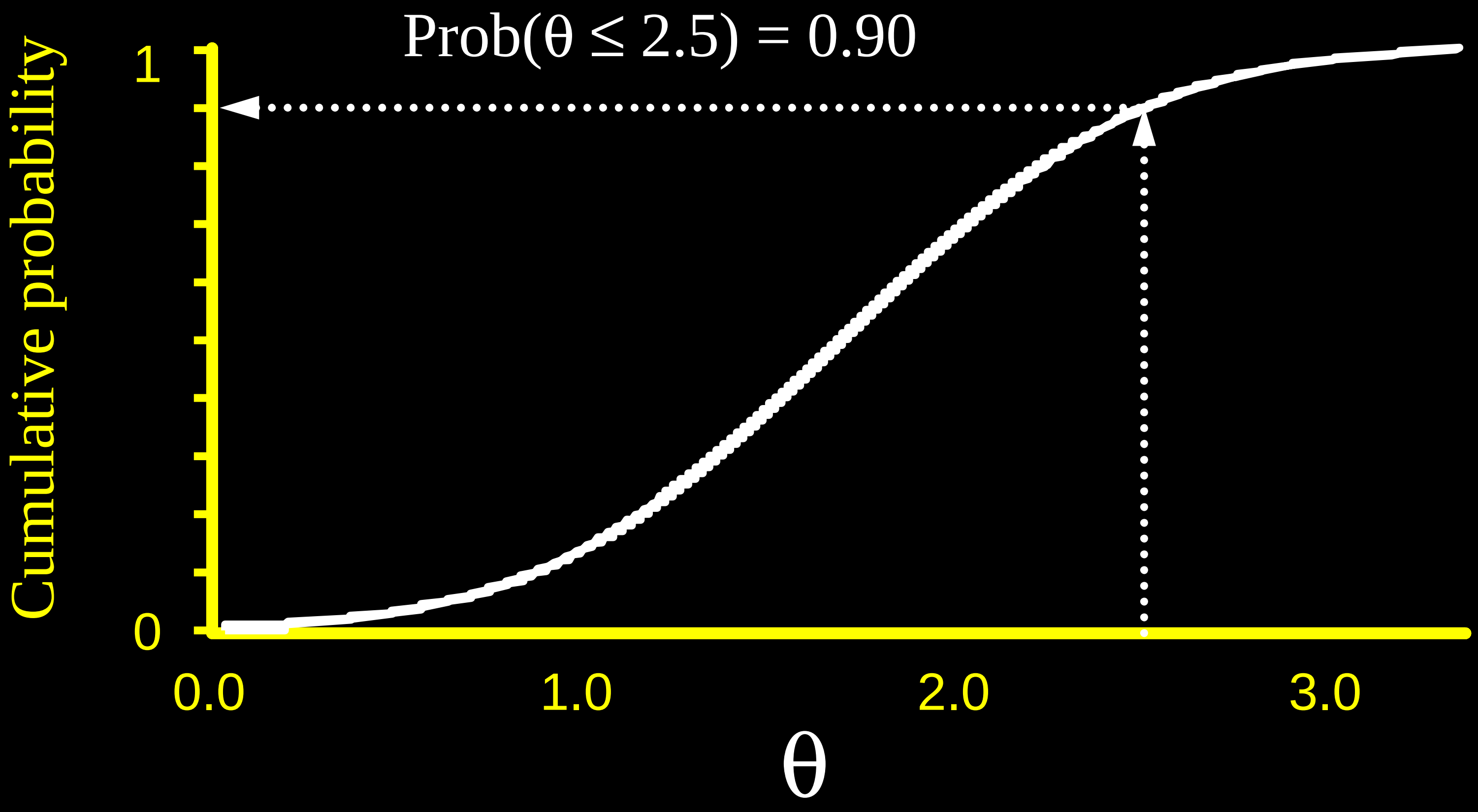
F is the CDF of θ, if $F(z) = \text{Prob}(\theta \leq z)$

We write: $\theta \sim F$

Example: uniform

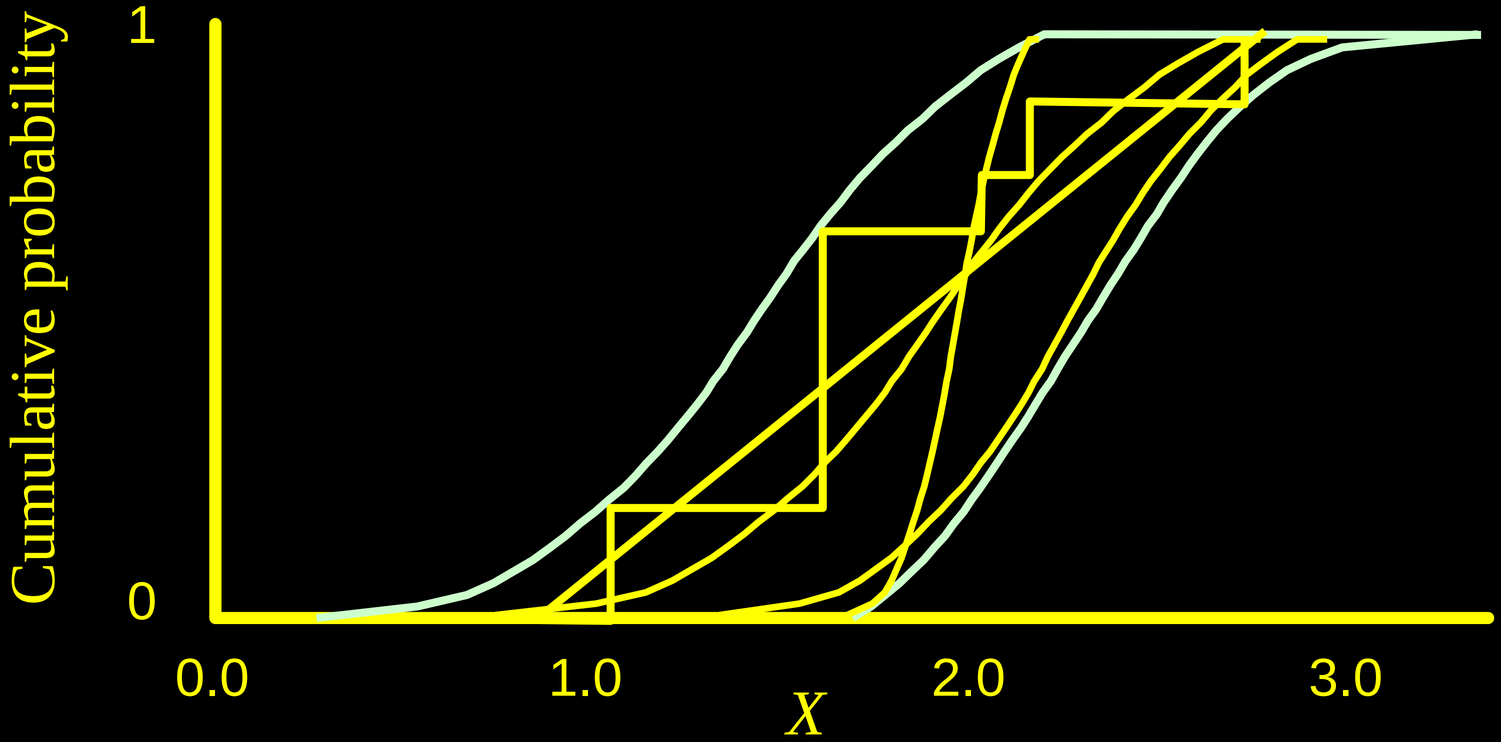


Another example: normal

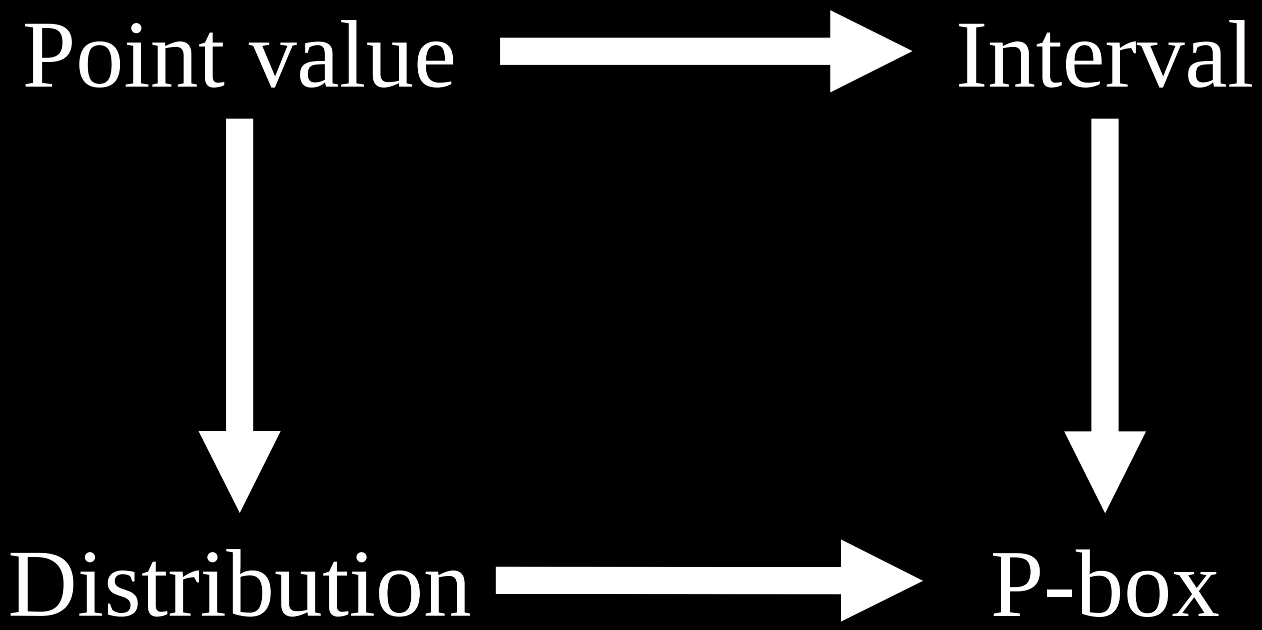


P-box (probability box)

Interval bounds on an CDF



Marriage of two approaches

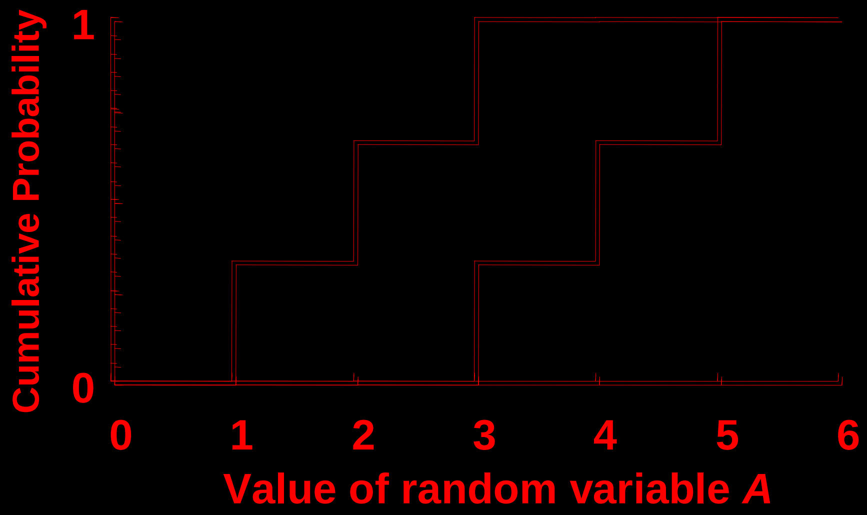


Probability bounds analysis

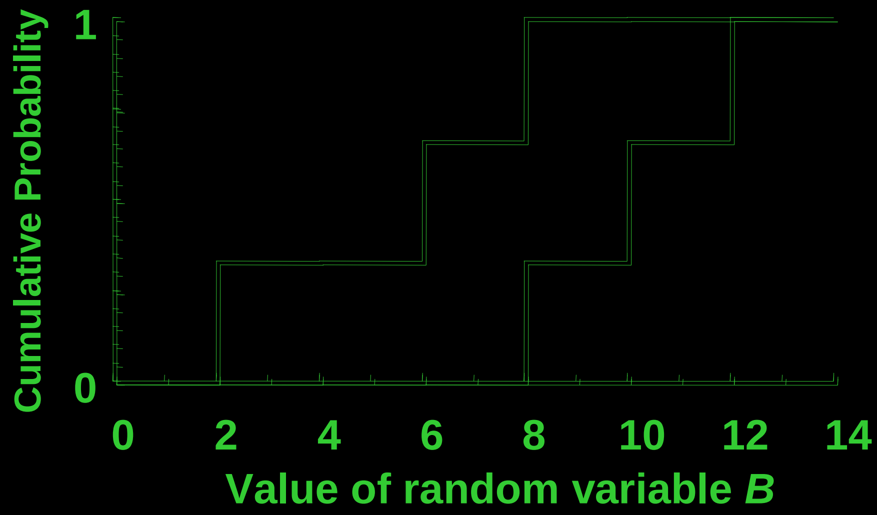
- All standard mathematical operations
  - Arithmetic (+, –, ×, ÷, ^, min, max)
  - Transformations (exp, ln, sin, tan, abs, sqrt, etc.)
  - Other operations (and, or, ≤, envelope, etc.)
- Quicker than Monte Carlo
- Guaranteed (automatically verified)

Probability bounds arithmetic

P-box for random variable *A*



P-box for random variable *B*

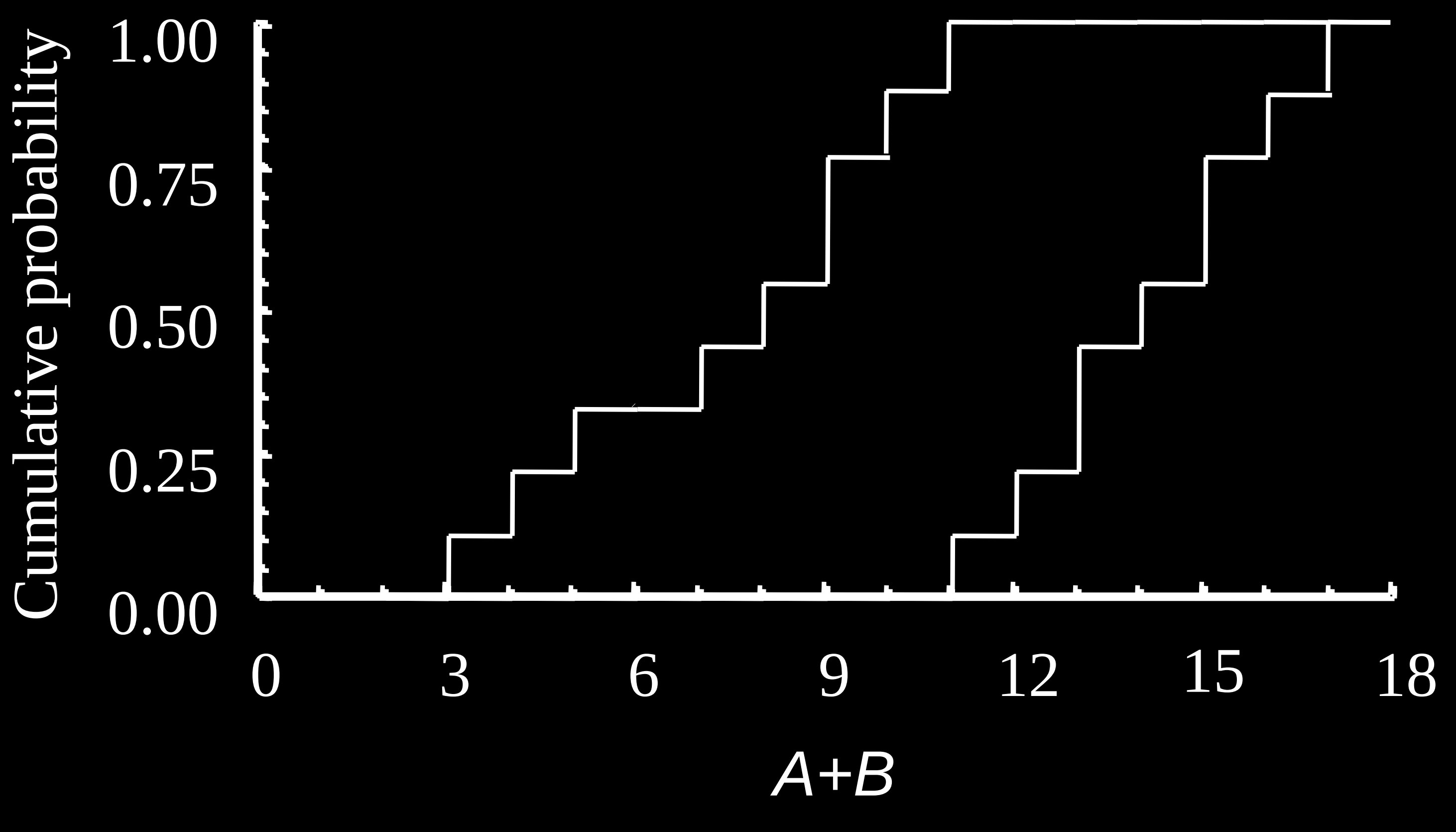


What are the bounds on the distribution of the sum of *A*+*B*?

Cartesian product

$A+B$ independence	$A \in [1,3]$ $p_1 = 1/3$	$A \in [2,4]$ $p_2 = 1/3$	$A \in [3,5]$ $p_3 = 1/3$
$B \in [2,8]$ $q_1 = 1/3$	$A+B \in [3,11]$ prob=1/9	$A+B \in [4,12]$ prob=1/9	$A+B \in [5,13]$ prob=1/9
$B \in [6,10]$ $q_2 = 1/3$	$A+B \in [7,13]$ prob=1/9	$A+B \in [8,14]$ prob=1/9	$A+B \in [9,15]$ prob=1/9
$B \in [8,12]$ $q_3 = 1/3$	$A+B \in [9,15]$ prob=1/9	$A+B \in [10,16]$ prob=1/9	$A+B \in [11,17]$ prob=1/9

A+B under independence



When independence is untenable

Suppose $X \sim F$ and $Y \sim G$. The distribution of $X+Y$ is bounded by

$$\left[\sup_{z=x+y} \max\big(F(x)+G(y)-1,\, 0\big),\ \inf_{z=x+y} \min\big(F(x)+G(y),\, 1\big)\right]$$

whatever the dependence between X and Y

Similar formulas for operations besides addition

Example ODE

$$dx_1/dt = \theta_1 x_1(1 - x_2)$$
$$dx_2/dt = \theta_2 x_2(x_1 - 1)$$

What are the states at $t = 10$?

$$x_0 = (1.2, 1.1)^T$$
$$\theta_1 \in [2.99, 3.01]$$
$$\theta_2 \in [0.99, 1.01]$$

VSPODE

- Constant step size $h = 0.1$, Order of Taylor model $q = 5$,
- Order of interval Taylor series $k = 17$, QR factorization

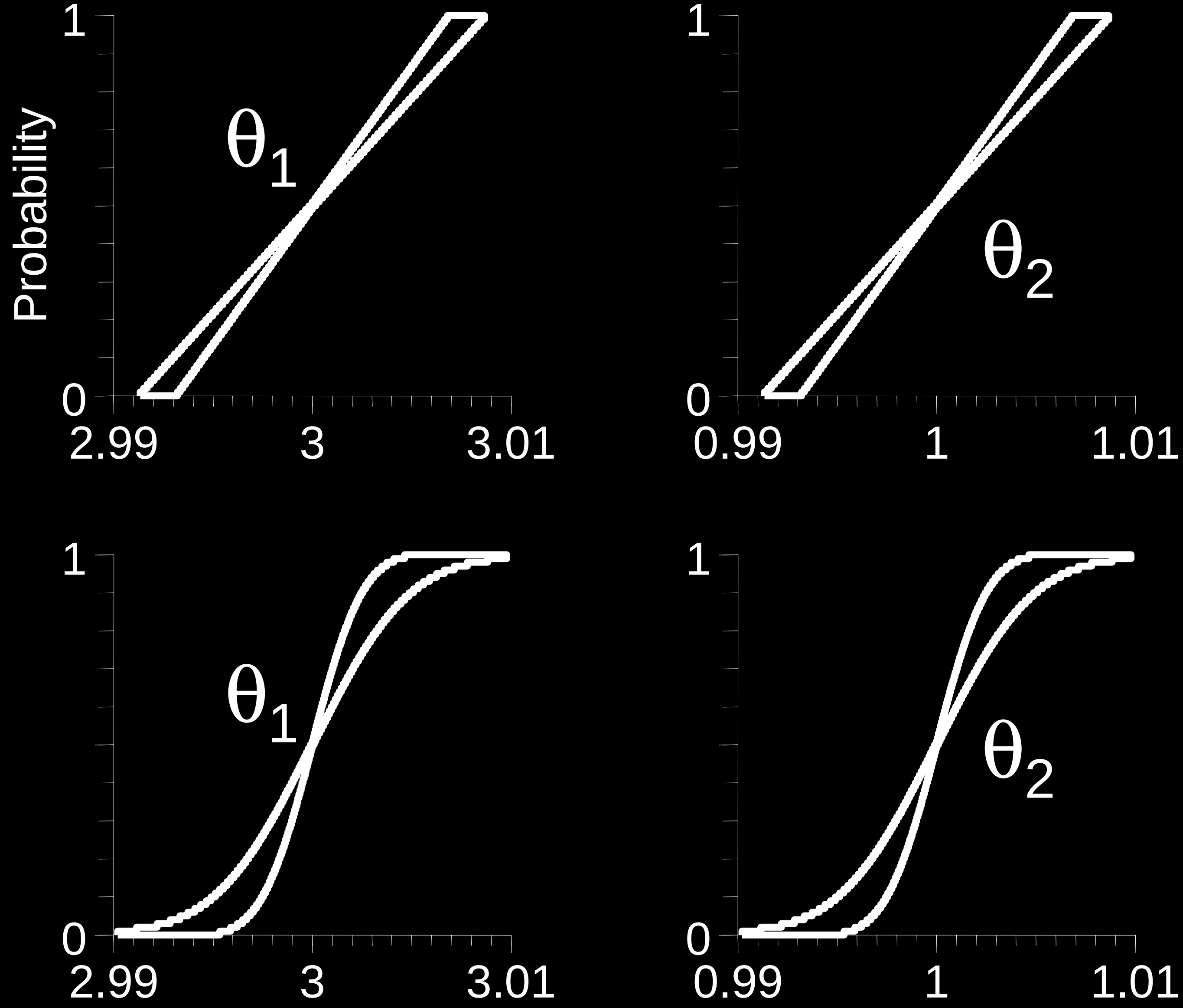
Calculation of X_1

$$
\begin{aligned}
&1.916037656181642 \times \theta_1^{0} \times \theta_2^{1} \; + \; 0.689979149231081 \times \theta_1^{1} \times \theta_2^{0} \; + \\
&-4.690741189299572 \times \theta_1^{0} \times \theta_2^{2} \; + \; -2.275734193378134 \times \theta_1^{1} \times \theta_2^{1} \; + \\
&-0.450416914564394 \times \theta_1^{2} \times \theta_2^{0} \; + \; -29.788252573360062 \times \theta_1^{0} \times \theta_2^{3} \; + \\
&-35.200757076497972 \times \theta_1^{1} \times \theta_2^{2} \; + \; -12.401600707197074 \times \theta_1^{2} \times \theta_2^{1} \; + \\
&-1.349694561113611 \times \theta_1^{3} \times \theta_2^{0} \; + \; 6.062509834147210 \times \theta_1^{0} \times \theta_2^{4} \; + \\
&-29.503128650484253 \times \theta_1^{1} \times \theta_2^{3} \; + \; -25.744336555602068 \times \theta_1^{2} \times \theta_2^{2} \; + \\
&-5.563350070358247 \times \theta_1^{3} \times \theta_2^{1} \; + \; -0.222000132892585 \times \theta_1^{4} \times \theta_2^{0} \; + \\
&218.607042326120308 \times \theta_1^{0} \times \theta_2^{5} \; + \; 390.260443722081675 \times \theta_1^{1} \times \theta_2^{4} \; + \\
&256.315067368131281 \times \theta_1^{2} \times \theta_2^{3} \; + \; 86.029720297509172 \times \theta_1^{3} \times \theta_2^{2} \; + \\
&15.322357274648443 \times \theta_1^{4} \times \theta_2^{1} \; + \; 1.094676837431721 \times \theta_1^{5} \times \theta_2^{0} \; + \\
&[\, 1.147753762081105\,8, \; 1.1477539164945061 \,]
\end{aligned}
$$

where θ's are centered forms of the parameters; $\theta_1 = \mathrm{\theta}_1 - 3$, $\theta_2 = \mathrm{\theta}_2 - 1$

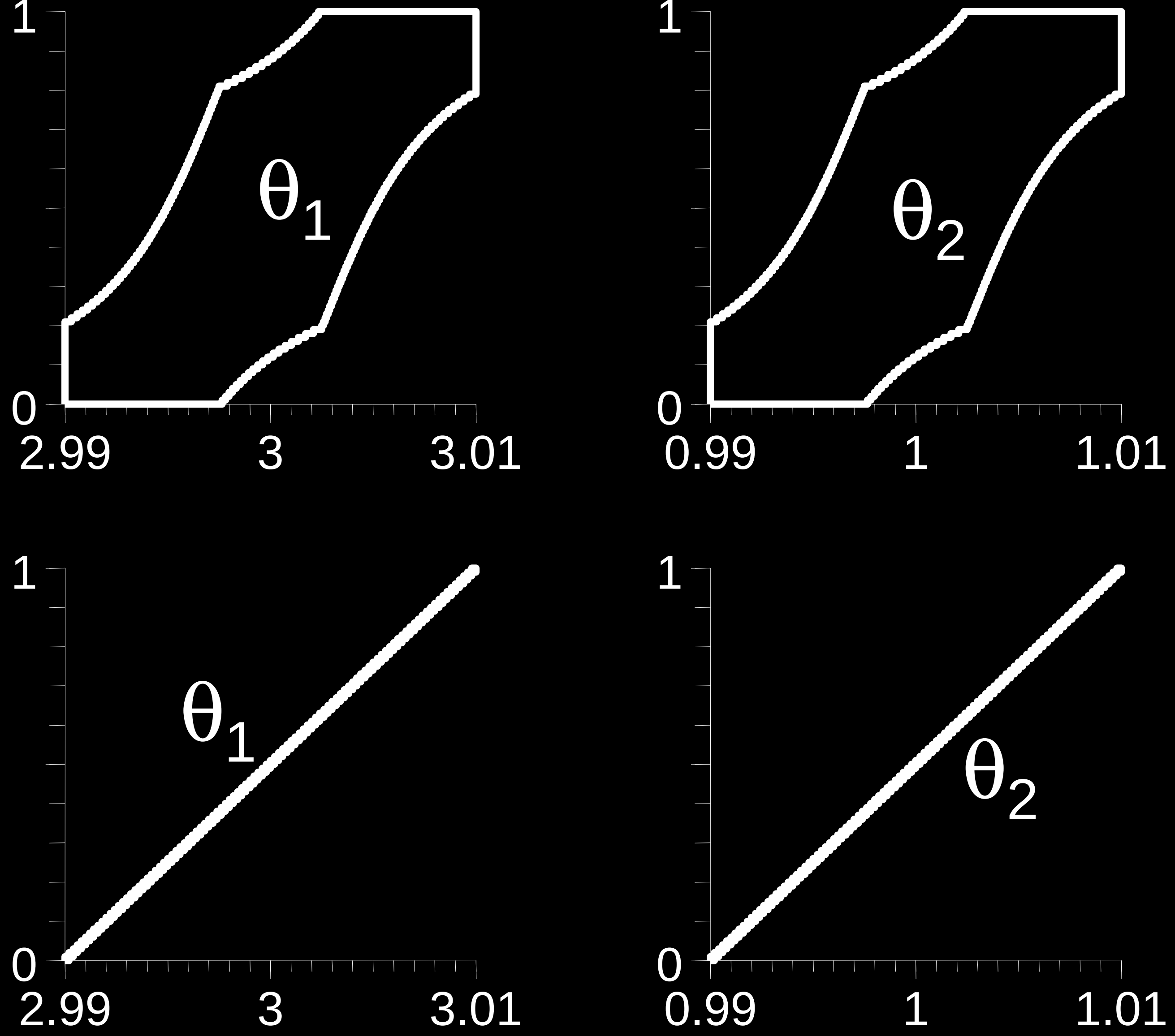
uniform

normal



min, max,
mean, var

precise



Calculation of X_1

$1.916037656181642 \times \theta_1^{0} \times \theta_2^{1}$ + $0.689979149231081 \times \theta_1^{1} \times \theta_2^{0}$ +
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$218.607042326120308 \times \theta_1^{0} \times \theta_2^{5}$ + $390.260443722081675 \times \theta_1^{1} \times \theta_2^{4}$ +
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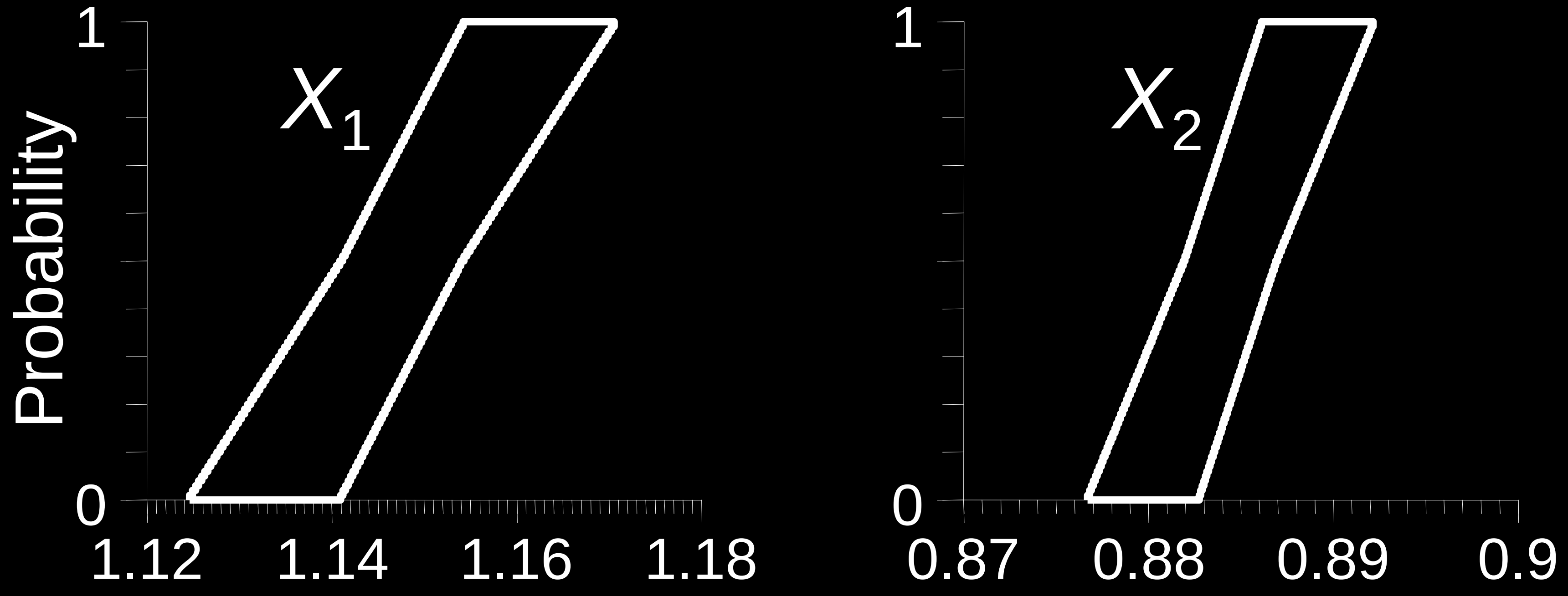
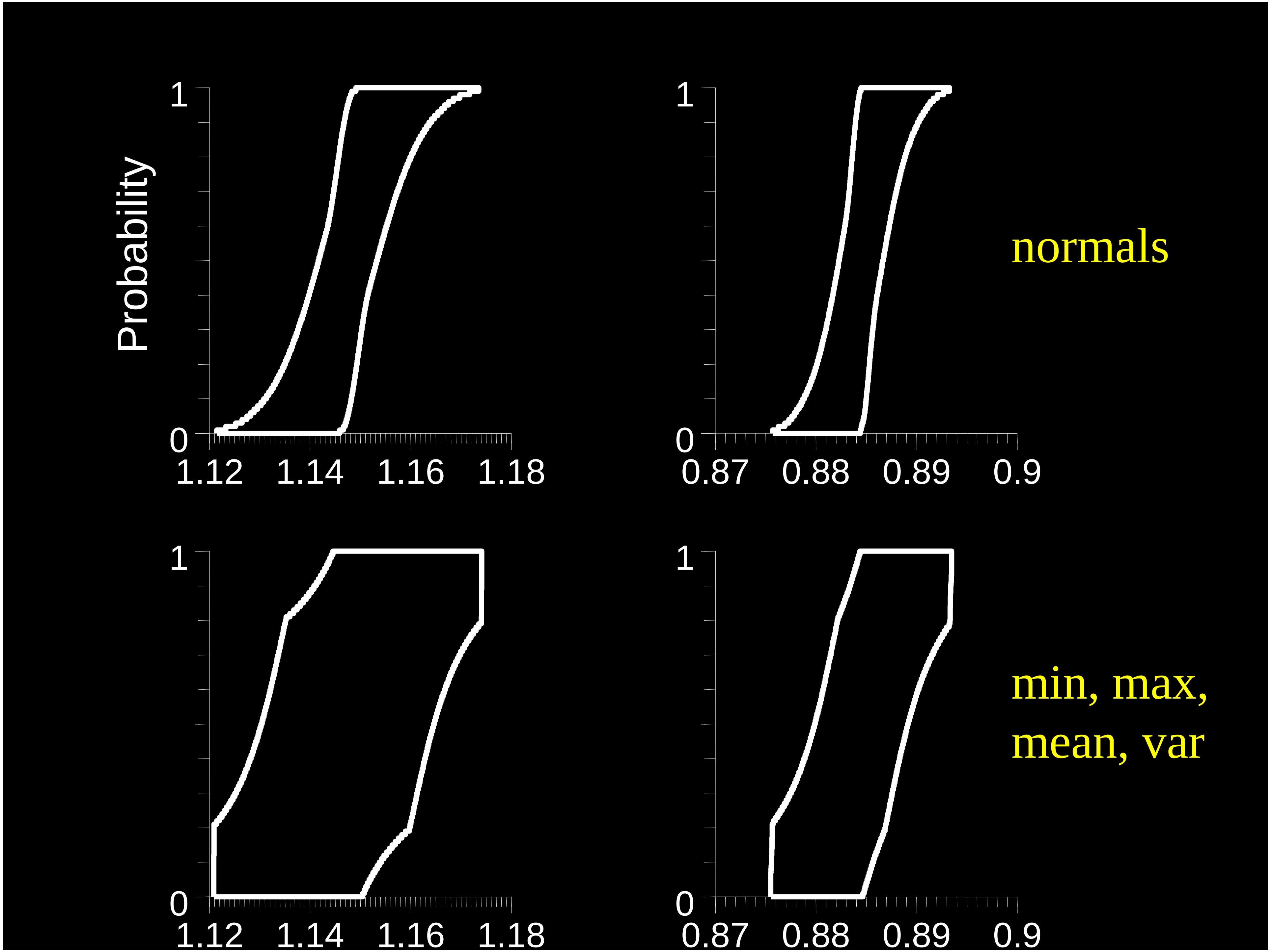
$15.322357274648443 \times \theta_1^{4} \times \theta_2^{1}$ + $1.094676837431721 \times \theta_1^{5} \times \theta_2^{0}$ +
[1.1477537620811058, 1.1477539164945061]

where θ's are centered forms of the parameters; $\theta_1 = \theta_1 - 3$, $\theta_2 = \theta_2 - 1$

Results for uniform p-boxes




Probability
1
0
1.12
1.14
1.16
1.18
0.87
0.88
0.89
0.9
normals
min, max,
mean, var

Still repetitions of uncertainties

$$\begin{aligned}
&1.916037656181642 \times \theta_1^{0} \times \theta_2^{1} \ + & &0.689979149231081 \times \theta_1^{1} \times \theta_2^{0} \ + \\
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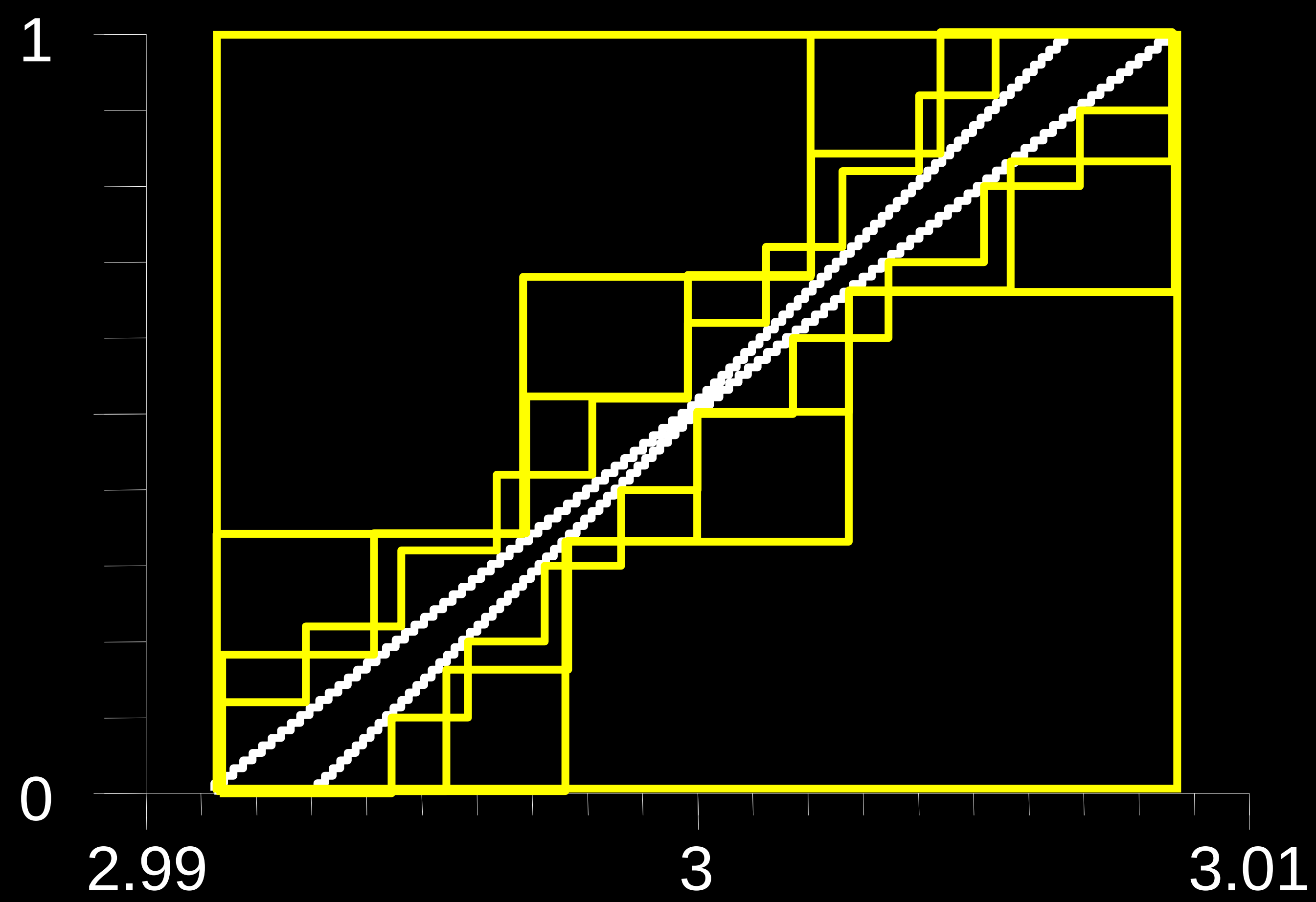
&15.322357274648443 \times \theta_1^{4} \times \theta_2^{1} \ + & &1.094676837431721 \times \theta_1^{5} \times \theta_2^{0} \ +
\end{aligned}$$

[1.1477537620811058, 1.1477539164945061]

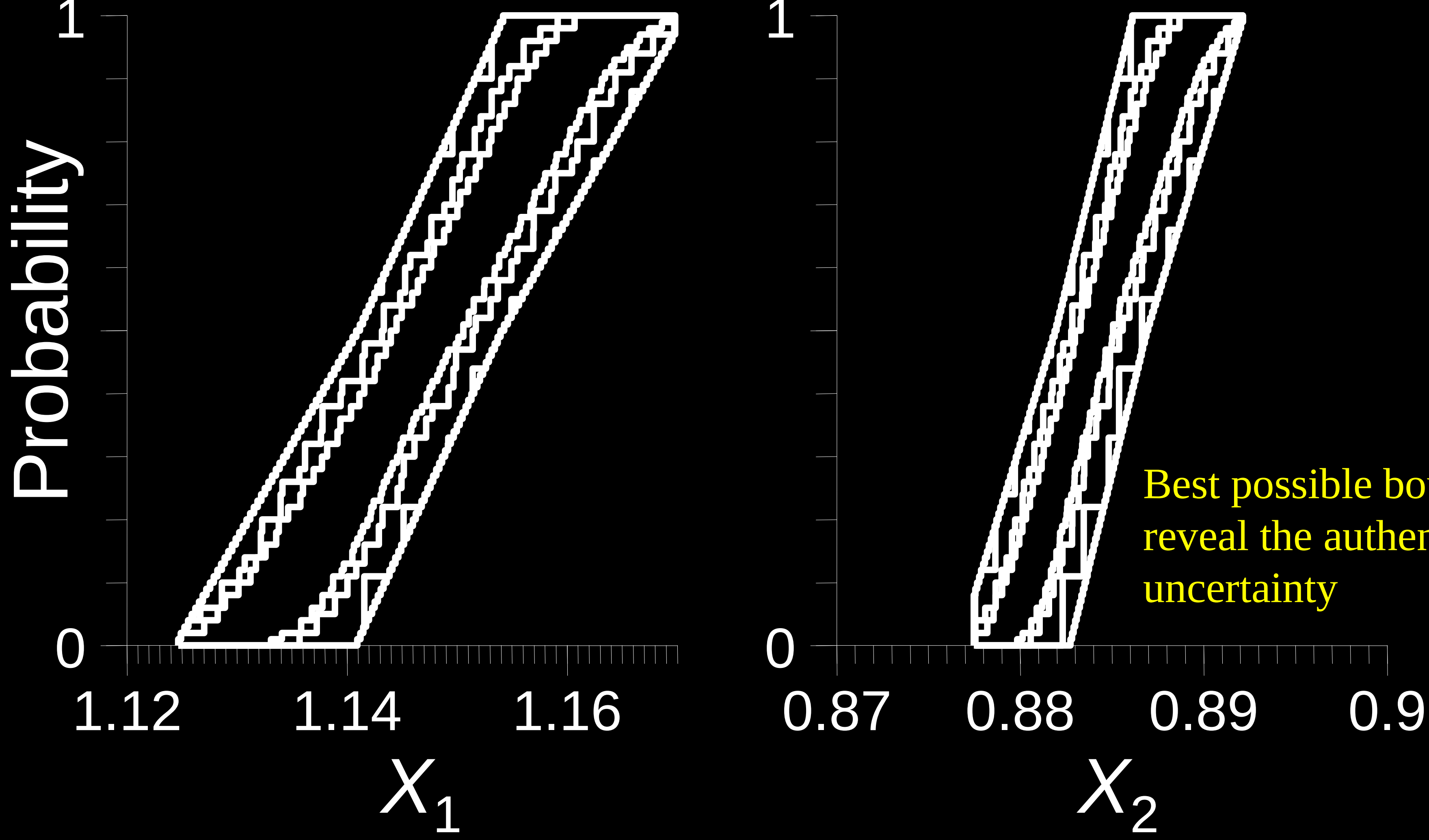
Subinterval reconstitution

- Subinterval reconstitution (SIR)
  - Partition the inputs into subintervals
  - Apply the function to each subinterval
  - Form the union of the results
- Still rigorous, but often tighter
  - The finer the partition, the tighter the union
  - Many strategies for partitioning
- Apply to *each cell* in the Cartesian product

Discretizations



Contraction from SIR

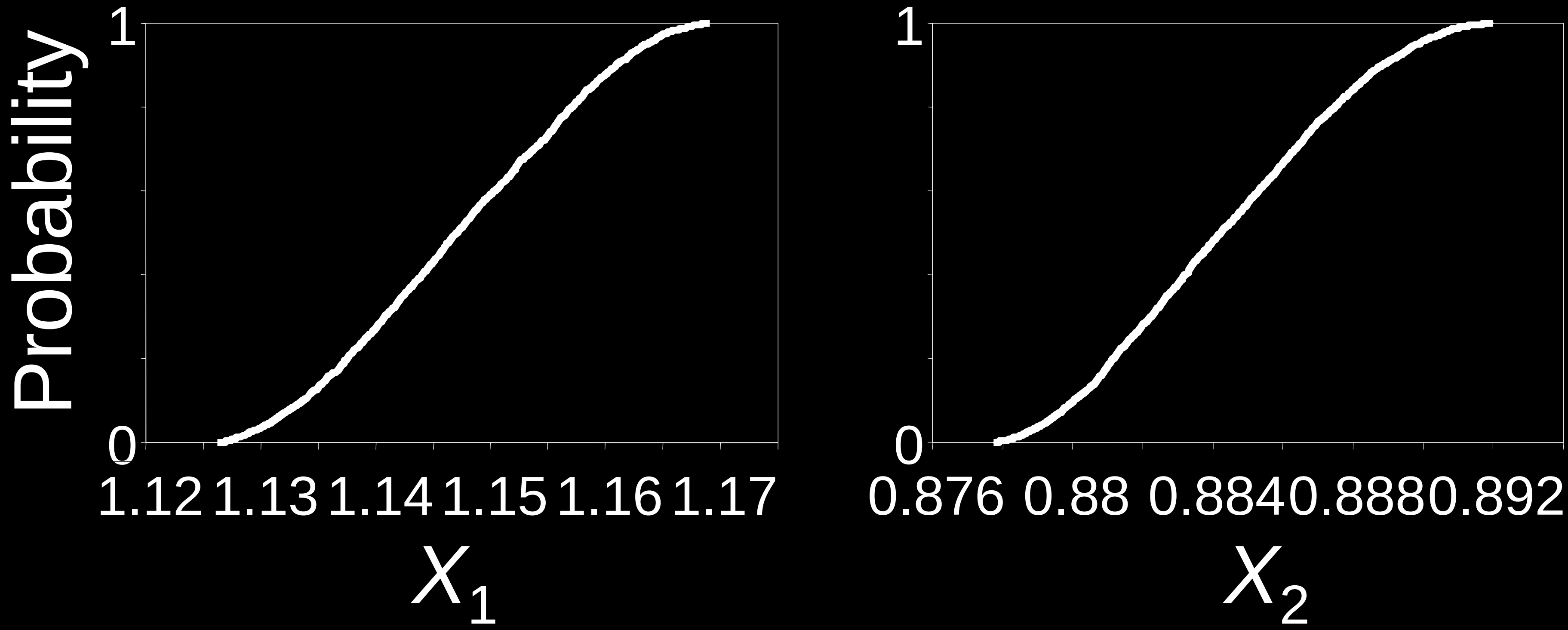


Best possible bounds reveal the authentic uncertainty

Precise distributions

- Uniform distributions (iid)
- Can be estimated with Monte Carlo simulation
  - 5000 replications
- Result is a p-box even though inputs are precise

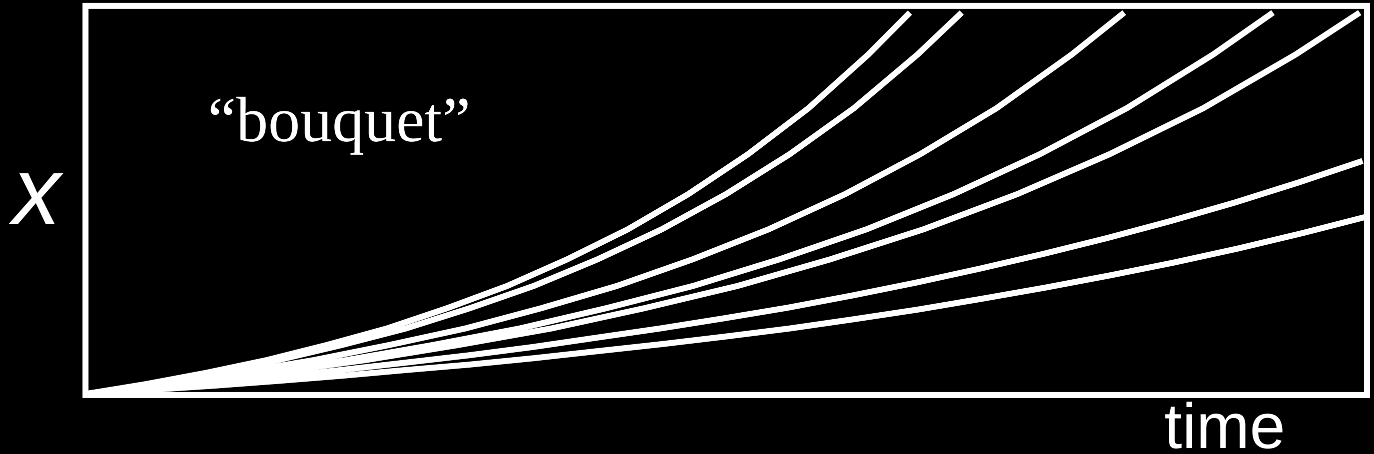
Results are (narrow) p-boxes

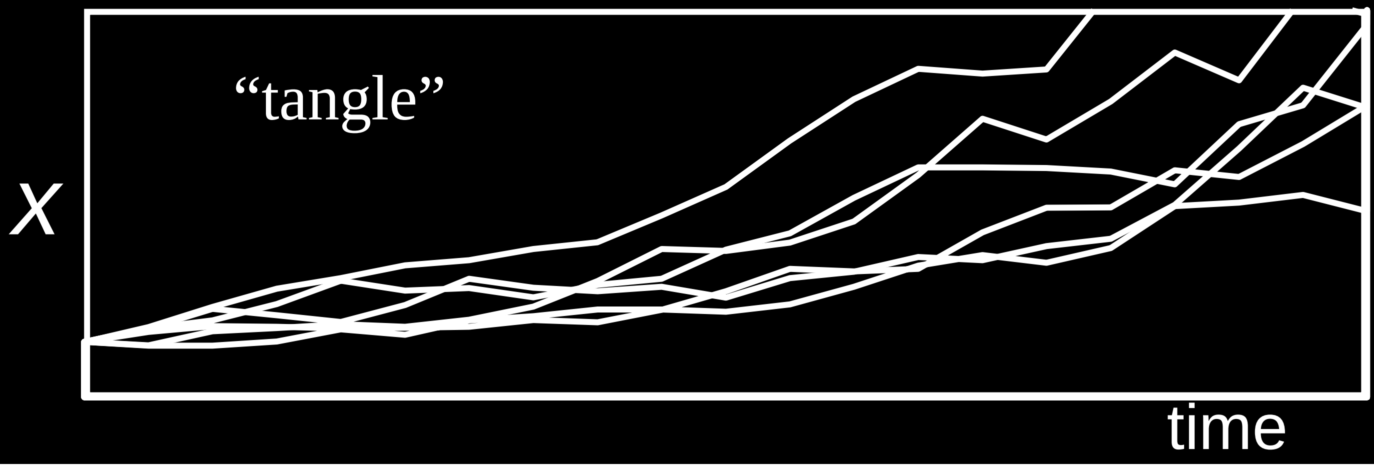


Not automatically verified

- *Monte Carlo cannot yield validated results*
  - Though can be checked by repeating simulation
- Validated results can be achieved by modeling inputs with (narrow) p-boxes and applying probability bounds analysis
- Converges to narrow p-boxes obtained from infinitely many Monte Carlo replications

What are these distributions?





Conclusions

- VSPODE is useful for bounding solutions of parametric nonlinear ODEs
- P-boxes and Risk Calc software are useful when distributions are known imprecisely
- Together, they rigorously propagate uncertainty through a nonlinear ODE

{ Intervals, Distributions, P-boxes } { Initial states, Parameters }

To do

- Subinterval reconstitution accounts for the remaining repeated quantities
- Integrate it more intimately into VSPODE
  - Customize Taylor models for each cell
- Generalize to stochastic case (“tangle”) when inputs are given as intervals or p-boxes

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More information

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