



Aalto University  
School of Science

# Simulation Metamodeling with Bayesian Networks

Jouni Pousi, Jirka Poropudas, Mikko Harju and Kai Virtanen

Aalto University

School of Science

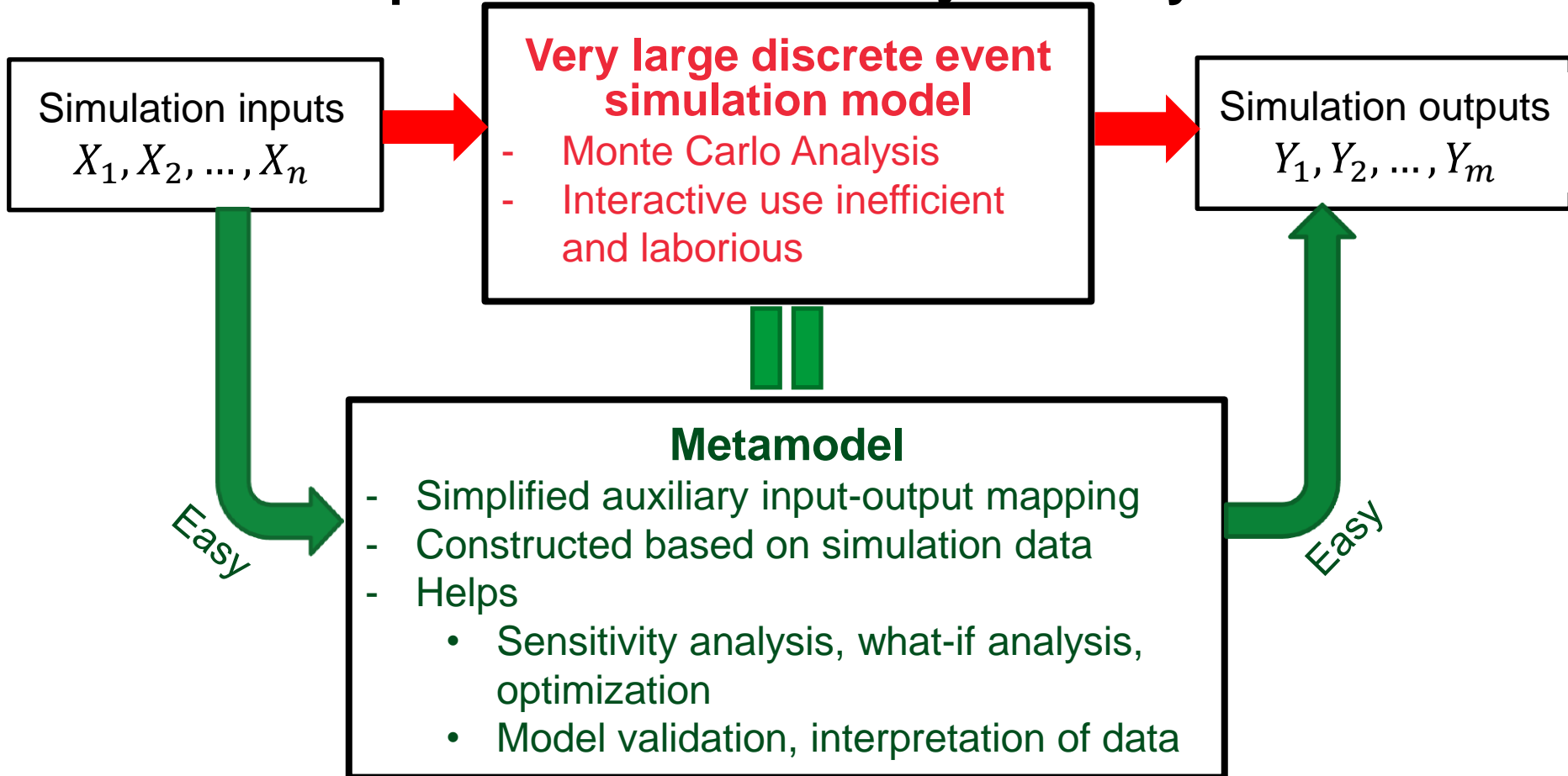
Systems Analysis Laboratory

[sal.aalto.fi](http://sal.aalto.fi)

[mikko.harju@aalto.fi](mailto:mikko.harju@aalto.fi)

# Simulation metamodeling

Complex and stochastic dynamic system



# Increasing the complexity of models increases the need for metamodeling

- Several existing approaches
  - Regression models, kriging models, splines, games, neural networks...
    - Mappings from inputs to **the expected values** of outputs
    - LOSS OF INFORMATION!

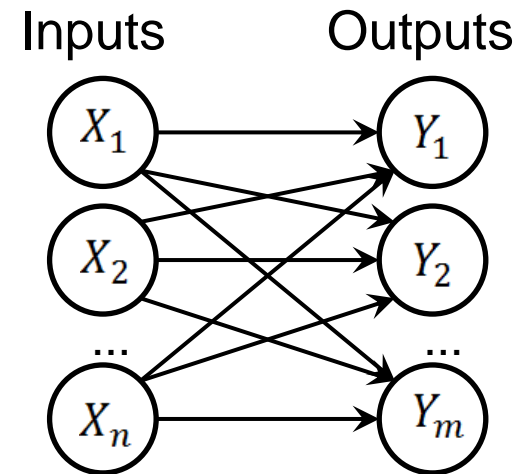
## New features allowed by Bayesian networks

Joint probability distribution of all inputs and outputs

→

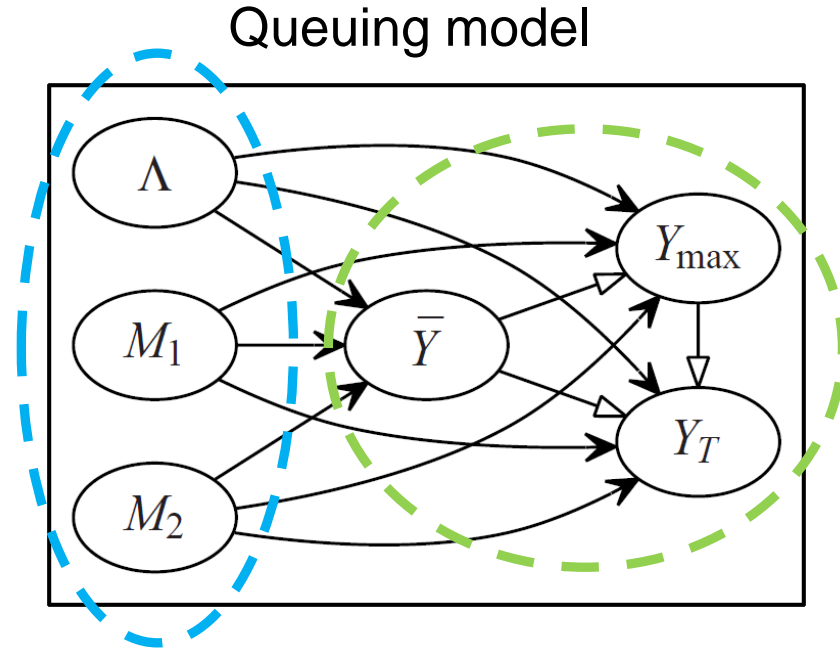
”Mappings between input and output distributions”

- Probabilistic dependencies between variables, in particular between outputs
- Efficient calculation of conditional probability distributions → Versatile what-if analyses



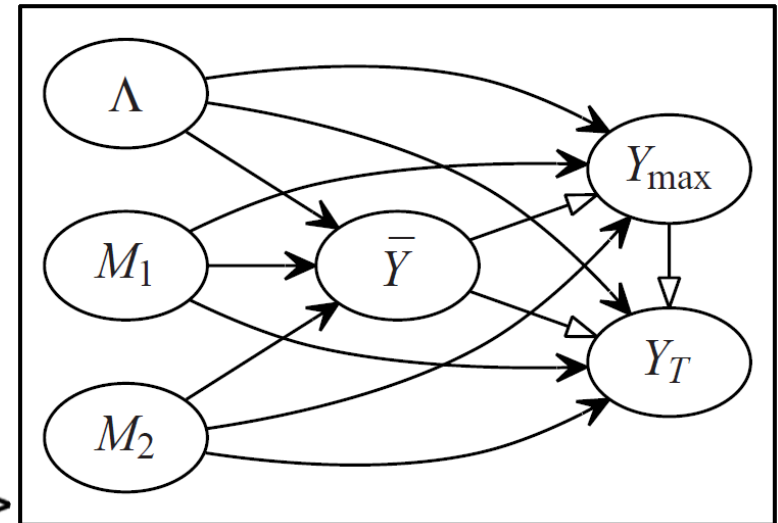
# Bayesian networks (BNs) as simulation metamodels

- Joint probability distribution of random variables
- Simulation **inputs** and **outputs**
  - Nodes
  - Discrete random variables
- Dependencies
  - Arcs
  - Conditional probabilities
- Available algorithms
  - Calculation of conditional probability distributions
  - Construction of BNs (sparse networks more efficient)



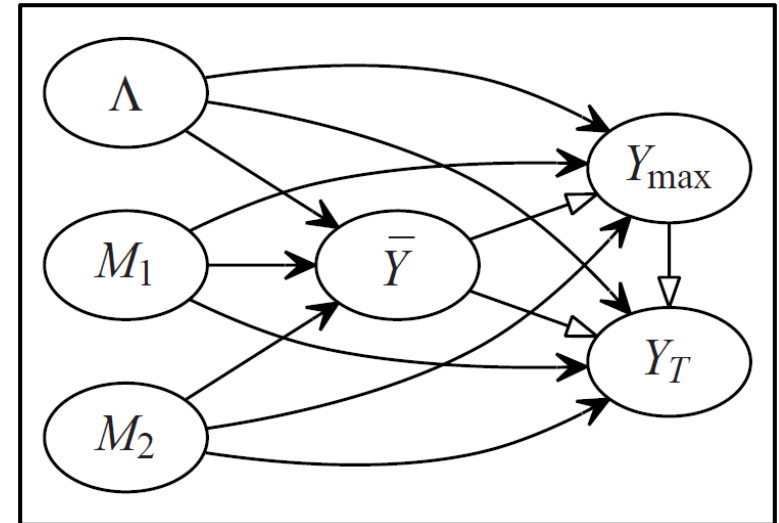
# Construction of BN Metamodels

- 1) Selection of variables
  - Simulation inputs and outputs
- 2) Collection of simulation data
  - All feasible input combinations simulated
- 3) Determination of network structure
  - Initial structure:  $\longrightarrow$
  - Dependencies found in data:  $\longrightarrow$
- 4) Estimation of probabilities
  - Conditional probability distributions for outputs
  - Input uncertainty
- + ) Validation



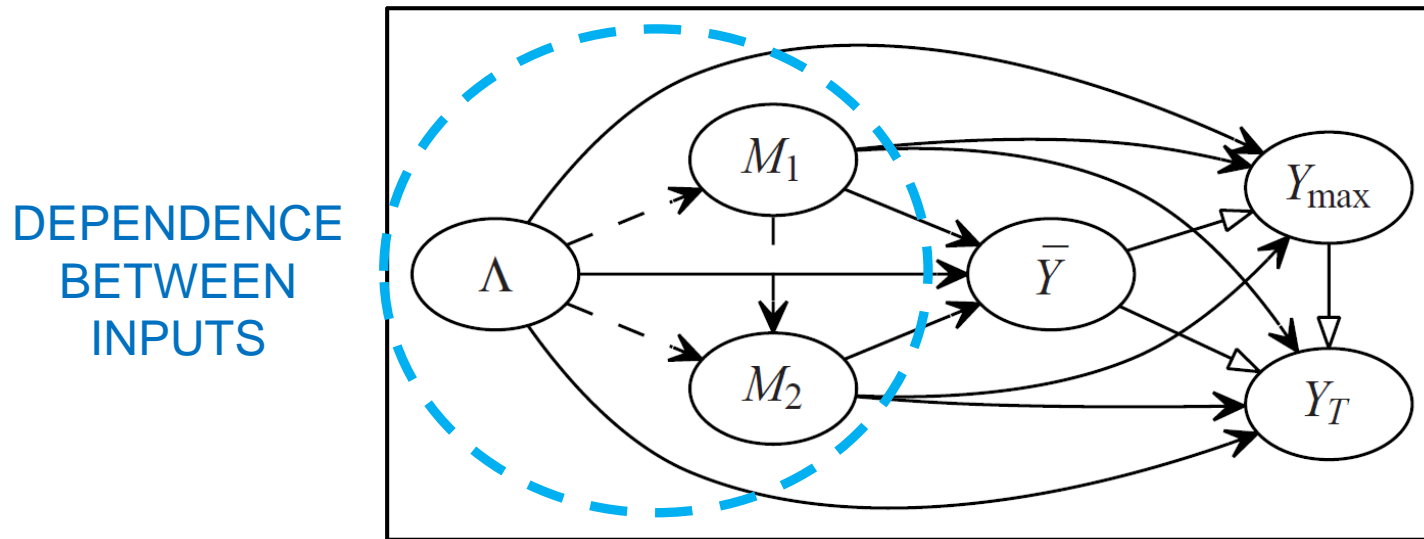
# Utilization of BN Metamodels

- What-if analysis
  - Values of some variables fixed → Conditional probability distributions for other variables updated
- Applications of what-if analyses
  - Dependence between inputs and outputs
  - Effect of input uncertainty on outputs
  - Dependence between outputs
  - Inverse reasoning



# Example: Queuing model

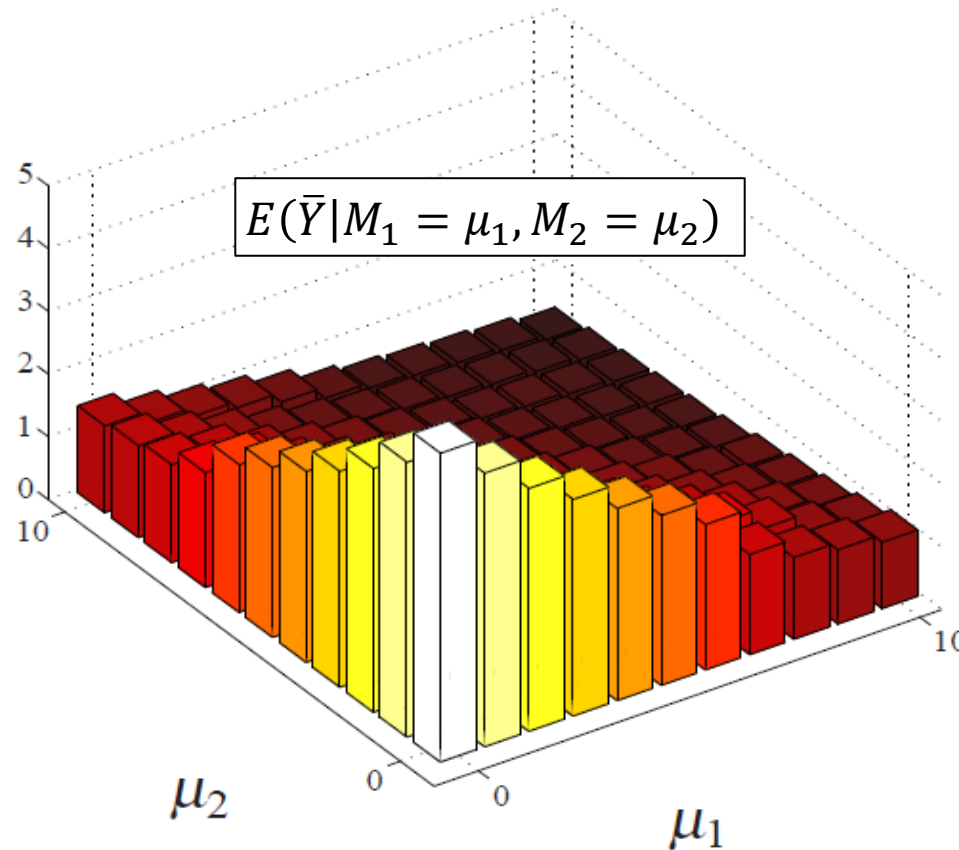
Single queue with Poisson arrivals and two servers with exponential service times



- Simulation inputs:  $\Lambda, M_1, M_2$  (Arrival intensity; Service intensities)
- Simulation outputs:  $\bar{Y}, Y_{max}, Y_T$  (Average and maximum number of customers; Number of customers at the end of simulation)

# Dependence between Inputs and Outputs

- Studied by calculating conditional probability distributions of outputs for fixed values of inputs



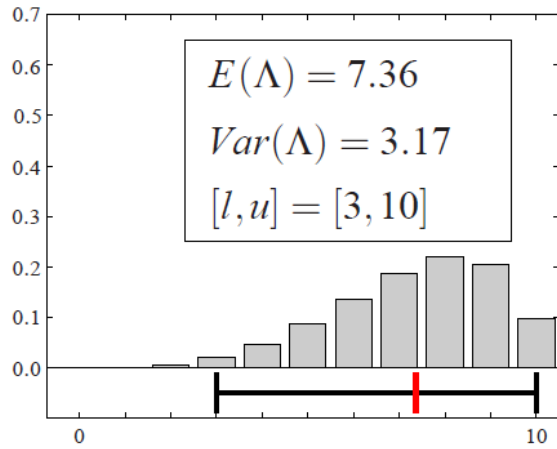
**Only the conditional expected value is presented**



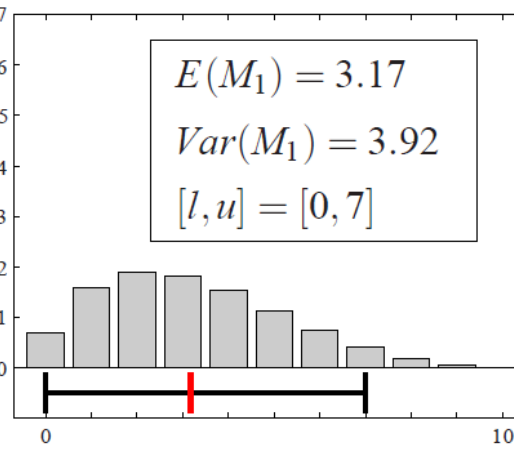
# Effect of Input Uncertainty...

- Inputs considered as dependent random variables
  - "Prior uncertainty" assessed by subject matter expert

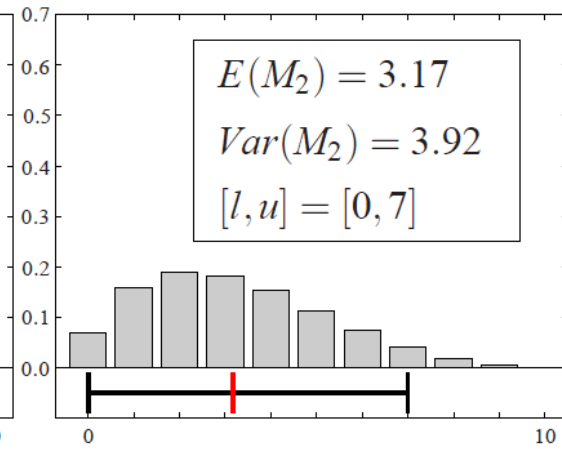
MARGINAL DISTRIBUTIONS



(a)  $P(\Lambda = \lambda)$ .

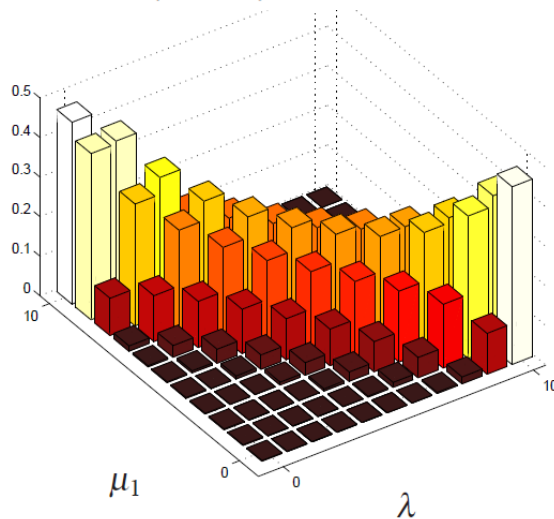


(b)  $P(M_1 = \mu_1)$ .

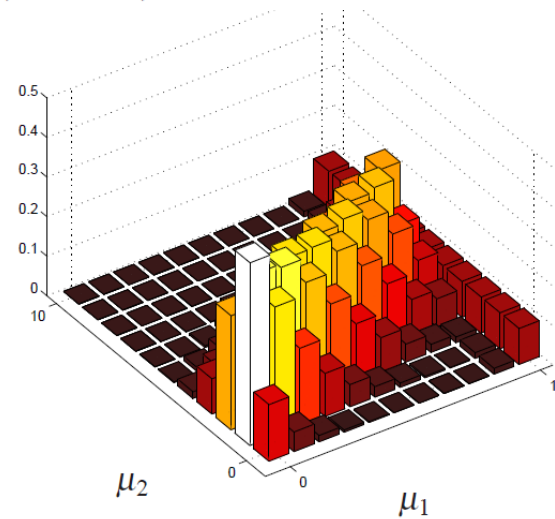


(c)  $P(M_2 = \mu_2)$ .

CONDITIONAL DISTRIBUTIONS

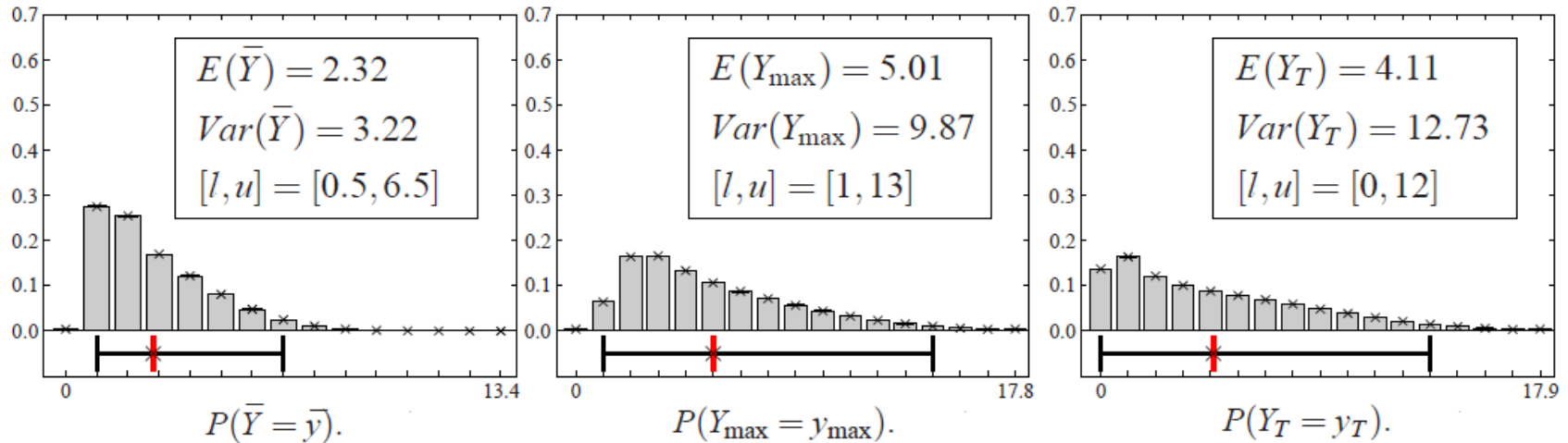


(a)  $P(M_1 = \mu_1 | \Lambda = \lambda)$ .



(b)  $P(M_2 = \mu_2 | \Lambda = 8, M_1 = \mu_1)$ .

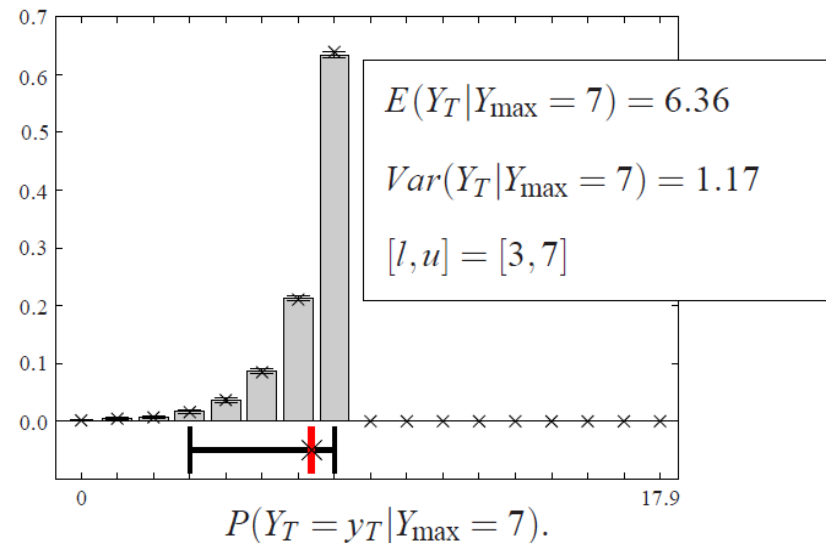
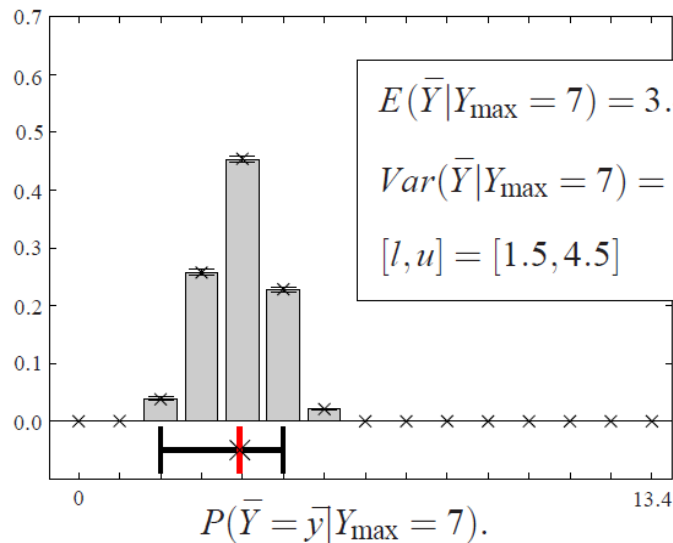
# ... on Distributions of Outputs



- Probability distributions include the effect of input uncertainty
- Enables calculation of descriptive statistics such as expected values, variances, and quantiles

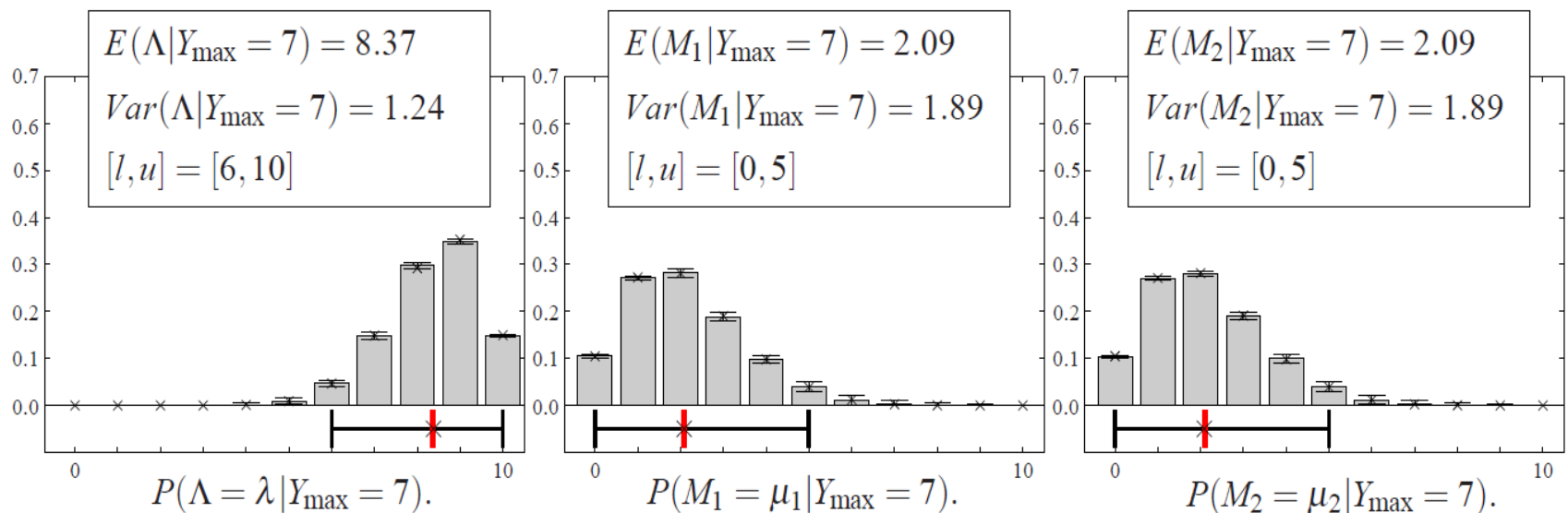
# Dependence between Outputs

- Studied by calculating conditional probability distributions for fixed values of outputs (for example:  $Y_{max} = 7$ )



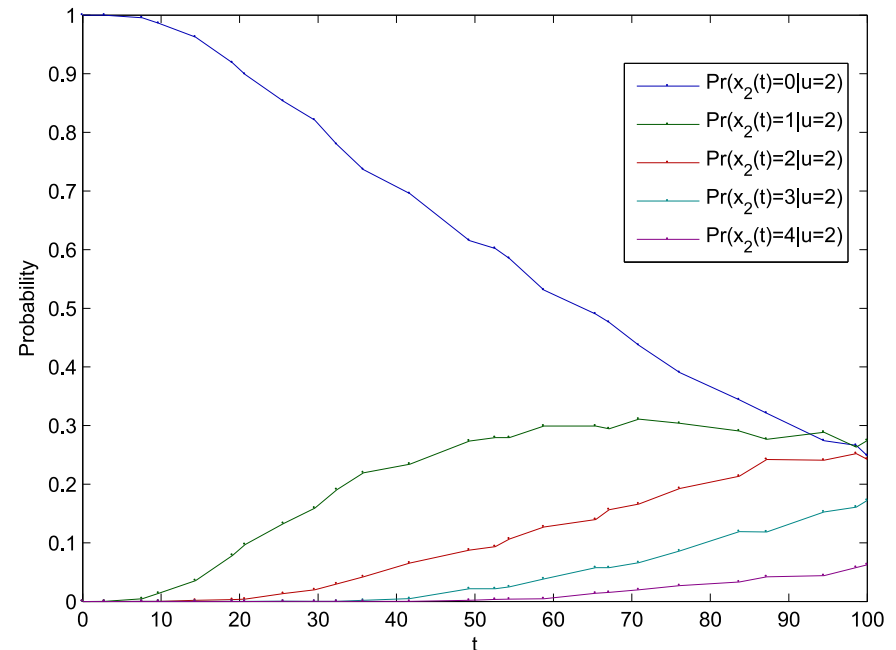
# Inverse reasoning

- Probability distributions of inputs updated conditional on fixed values of outputs (for example:  $Y_{max} = 7$ )
  - "Posterior uncertainty" (cf. "prior uncertainty" related to inputs)



# Dynamic Bayesian networks (DBNs) as simulation metamodels

- Time-dependent state variables of the simulation model
- Key time instants treated precisely - approximations used for other time instants
- Allows for a broader range of analyses
  - Time evolution of probability distributions
- Construction and utilization more demanding
  - DBN metamodeling tool

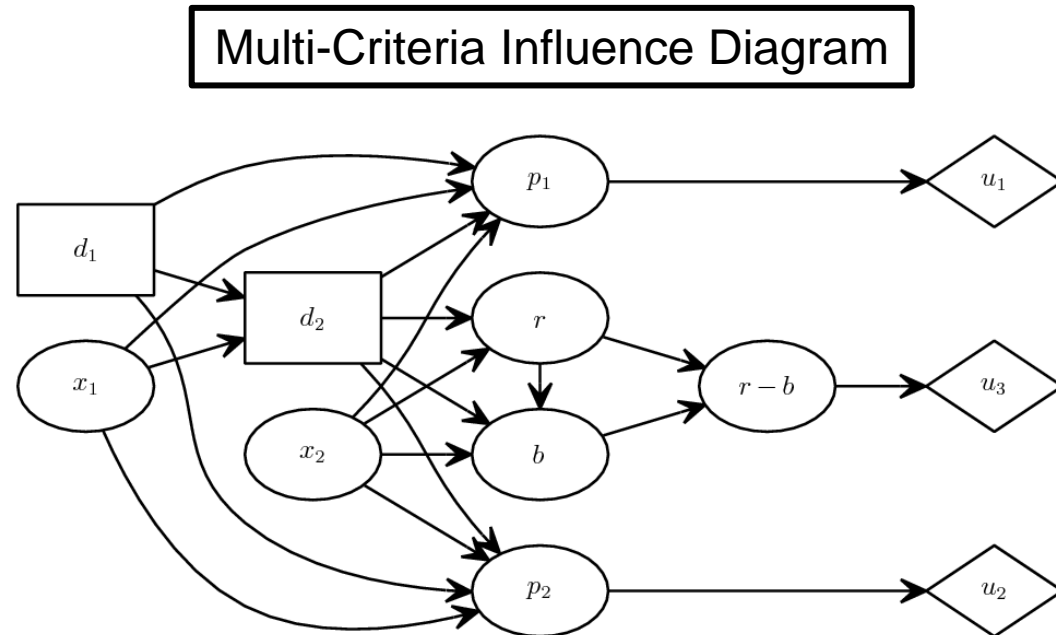


# Conclusion

- Simulation metamodeling benefits from BNs
  - Complete representation of probability distributions
    - No loss of information
      - cf. existing metamodels representing only expected values
  - New analysis capabilities
    - For example, input uncertainty and inverse reasoning
  - Available software with readily implemented algorithms
- Limitations
  - Construction necessitates large simulation data sets
  - Continuous variables have to be discretized

# Future research

- BN metamodeling
  - Continuous variables
    - Discretization
    - Interpolation
  - Sequential sampling
- Multi-criteria influence diagrams
  - Tool for decision support



# References

- Friedman, L. W. 1996. *The simulation metamodel*. Norwell, MA: Kluwer Academic Publishers.
- Harju, M. 2013. *Automated Construction of Dynamic Bayesian Networks in Simulation Metamodeling*, Doctoral dissertation, Aalto University School of Science.
- Henderson, S. G. 2003. Input model uncertainty: why do we care and what should we do about it?, *Winter Simulation Conference 2003*.
- Kleijnen, J. P. C. 2008. *Design and analysis of simulation experiments*. New York, NY: Springer-Verlag.
- Jensen, F. V., and T. D. Nielsen. 2007. *Bayesian networks and decision graphs*. New York, NY: Springer-Verlag.
- Neapolitan, R. E. 2004. *Learning Bayesian Networks*. Upper Saddle River, NJ: Prentice Hall.
- Poropudas, J., and K. Virtanen. 2007. Analyzing air combat simulation results with dynamic Bayesian networks, *Winter Simulation Conference 2007*.
- Poropudas, J., and K. Virtanen. 2009. Influence diagrams in analysis of discrete event simulation data, *Winter Simulation Conference 2009*.
- Poropudas, J., and K. Virtanen. 2011. Simulation metamodeling with dynamic Bayesian networks, *European Journal of Operational Research*.
- Poropudas, J. 2011. *Bayesian networks, Influence Diagrams, and Games in Simulation Metamodeling*, Doctoral dissertation, Aalto University School of Science.
- Pousi, J., Poropudas, J., Harju, M., and K. Virtanen. 2013. Simulation metamodeling with Bayesian networks, *Journal of Simulation*, to appear.