

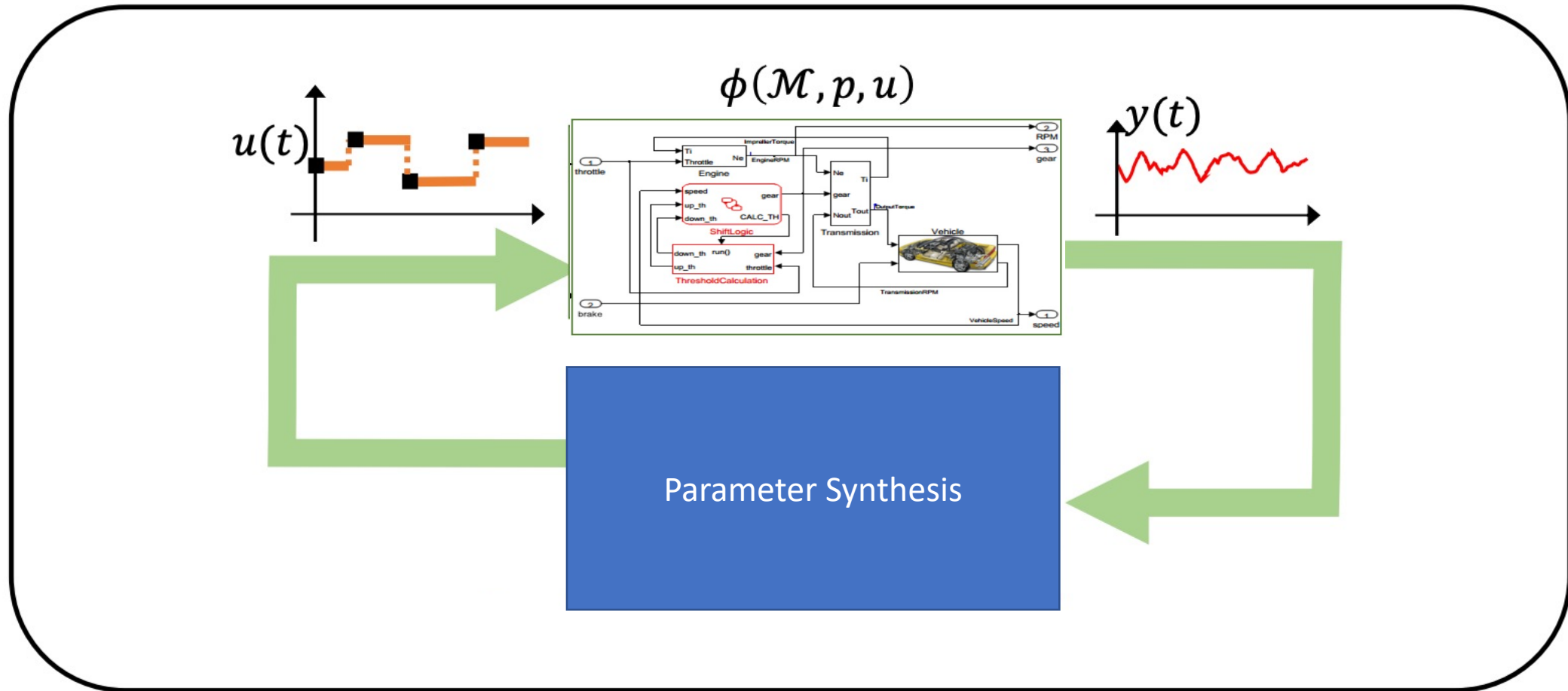
# Cyber-Physical Systems

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Lecture 12\_a: STL applications: parameter synthesis

# Parameter Synthesis



# Parameter Synthesis

## Problem

Given a model, depending on a set of parameters  $\theta \in \Theta$ , and a specification  $\phi$  (STL formula), find the parameter combination  $\theta$  s.t. the system satisfies  $\phi$  as more as possible



## Solution Strategy

- **rephrase** it as a optimisation problem (maximizing  $\rho$ )
- **evaluate** the function to optimise
- **solve** the optimisation problem

# Parametric Chemical Reaction Network (PCRN)

Population CTMC models, i.e. CTMC models in the biochemical reactions style.

## SET OF SPECIES

$\mathcal{S} = \{S_1, \dots, S_n\}$ , i.e. the different agent states.

## STATE SPACE

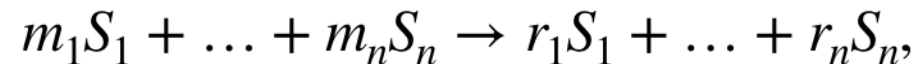
The state space is described by a vector of  $n$  variables

$$\mathbf{X} = (X_{S_1}, \dots, X_{S_n}) \in \mathbb{N},$$

each counting the number of agents (jobs, molecules, ...) of a given kind.

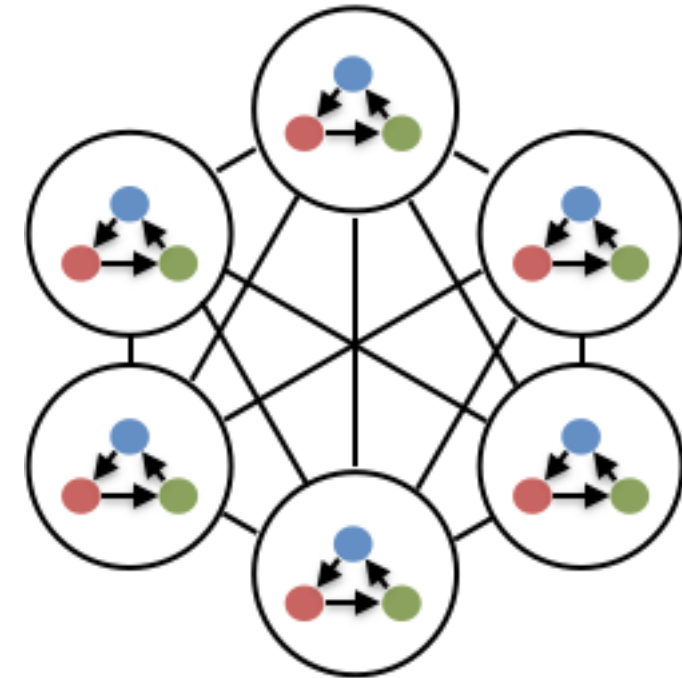
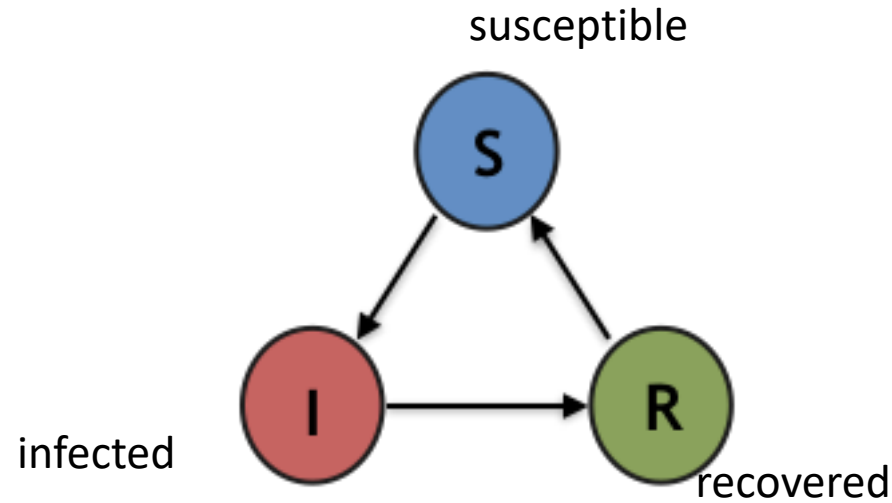
## TRANSITIONS

The dynamics is given by a set of chemical reactions:



with a rate given by a function  $f(\mathbf{X}, \boldsymbol{\theta})$ .

# Example: SIR epidemic model



infection:  $S + I \rightarrow 2I$

recover:  $I \rightarrow R$

loss of immunity:  $R \rightarrow S$

$$f_i(\mathbf{X}, \boldsymbol{\theta}) = k_i X_S X_I$$

$$f_r(\mathbf{X}, \boldsymbol{\theta}) = k_r X_I$$

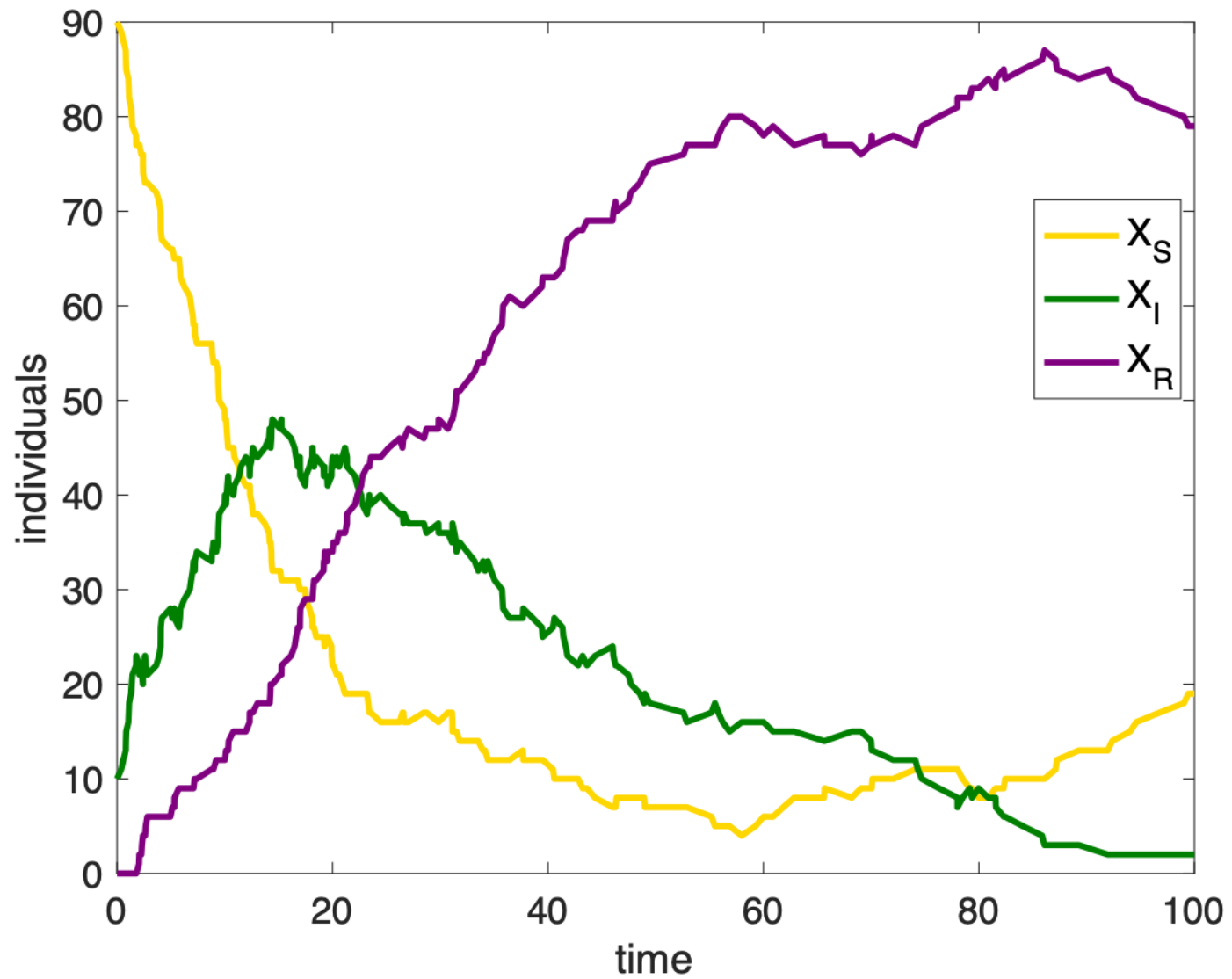
$$f_l(\mathbf{X}, \boldsymbol{\theta}) = k_l X_R$$

State vector:  $\mathbf{X} = (X_S, X_I, X_R)$

Vector of parameters:  $\boldsymbol{\theta} = (k_i, k_r, k_l)$

$$\mathcal{M}_{\boldsymbol{\theta}}$$

# Example: SIRS epidemic model



# Stochastic Semantics

## SATISFACTION PROBABILITY(Boolean Semantics)

$$P(\varphi) = \mathbb{P}\{I_\varphi(X) = 1\} := P\{\vec{x} \in Path^{\mathcal{M}} \mid \mathcal{X}(\vec{x}, 0, \varphi) = 1\}$$

where  $I_\varphi(X)$  is a Bernoulli random variable

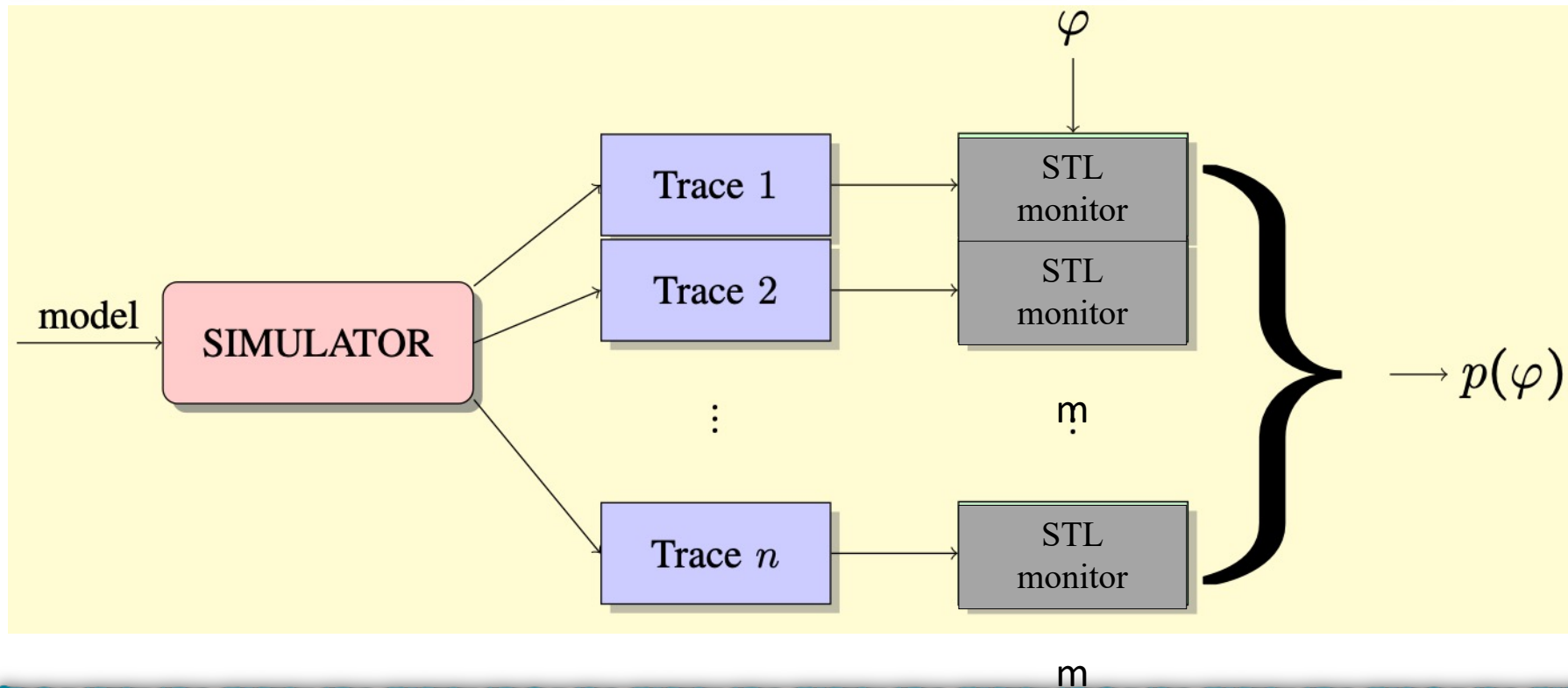
## AVERAGE ROBUSTNESS(Quantitative Semantics)

$$\mathbb{P}\{R_\varphi(X) \in [a, b]\} := P\{\vec{x} \in Path^{\mathcal{M}} \mid \rho(\vec{x}, 0, \varphi) \in [a, b]\}$$

where  $R_\varphi(X)$  is a measurable function

# Statistical Model Checking (SMC)

The probability satisfaction can be estimated as an average of the truth values  $T_i$  of the formula  $\varphi$  over many sample trajectories.

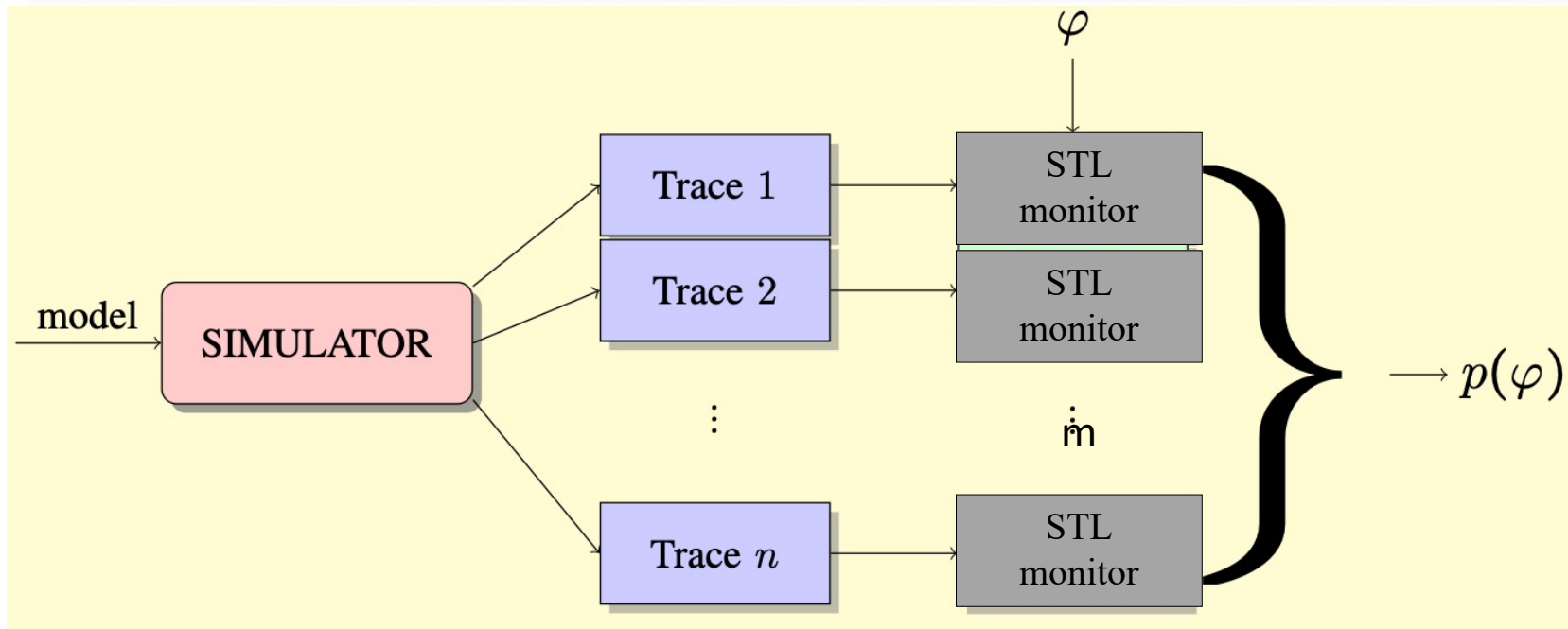


**Bayesian SMC** uses the fact the satisfaction probability of a formula given a model is a number in  $[0, 1]$ , and prior distributions on numbers between  $[0, 1]$  exist (Beta distribution)}



# Statistical Model Checking

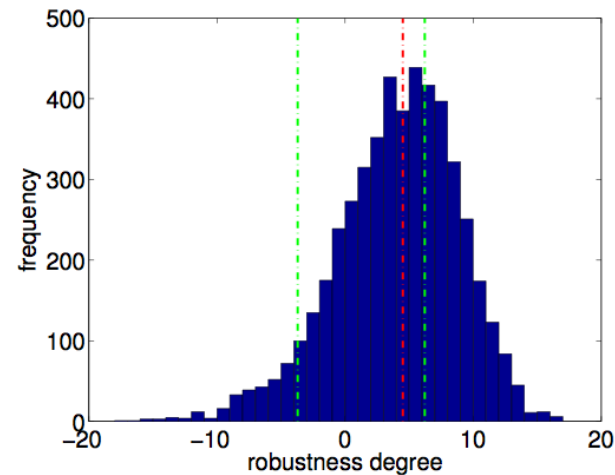
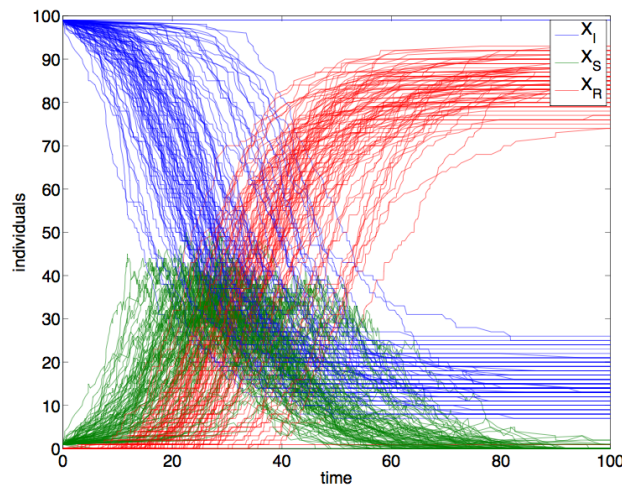
- **Statistical Model Checking:**  $p_\phi$  can be estimated as an average of the truth values  $T_i$  of the formula  $\phi$  over many sample trajectories.
- **Bayesian SMC** specifying (Beta) priors  $prob\{p_\phi\}$  and estimating a posteriori  $prob\{p_\phi | T_i\}$  using Bayes' theorem and the fact that  $prob\{T_i | p_\phi\}$  is Bernoulli.



# Parameter Synthesis via Robustness Maximisation

## Robustness Distribution

$$\mathbb{P}(R_\varphi(\mathbf{X}) \in [a, b]) = \mathbb{P}(\mathbf{X} \in \{\mathbf{x} \in \mathcal{D} \mid \rho(\varphi, \mathbf{x}, 0) \in [a, b]\})$$



## Indicators

$$\mathbb{E}(R_\varphi)$$

(the average robustness degree)

$$\mathbb{E}(R_\varphi \mid R_\varphi > 0) \quad \text{and} \quad \mathbb{E}(R_\varphi \mid R_\varphi < 0)$$

(the conditional averages)

# Parameter Synthesis

## Problem

Find the parameter configuration that maximizes  $E[R_\phi](\theta)$ , of which we have few **costly** and **noisy** evaluations.



## Methodology

1. Sample  $\{(\theta_{(i)}, y_{(i)}), i = 1, \dots, n\}$
2. Emulate (**GP Regression**):  $E[R_\phi] \sim \text{GP}(\mu, k)$
3. Optimize the emulation via **GP-UCB algorithm**, new  $\theta_{(n+1)}$

# Gaussian Process Regression

Gaussian Processes can be used for Bayesian prediction and classification tasks.

Idea: put a **GP prior** on functions; condition on **observed data (training set)**  $(x_i, y_i)$ ; we compute a **posterior** distribution on functions; make **predictions**.

**Latent function:**  $f$ , GP ; **Noise model:**  $p(y_i|f(x_i))$

**Prediction** (latent function  $f^*$  at  $x^*$ )

$$p(f^*|\mathbf{y}) \propto \int d\mathbf{f}(\mathbf{x}) p(f^*, \mathbf{f}(\mathbf{x})) p(\mathbf{y}|\mathbf{f}(\mathbf{x}))$$

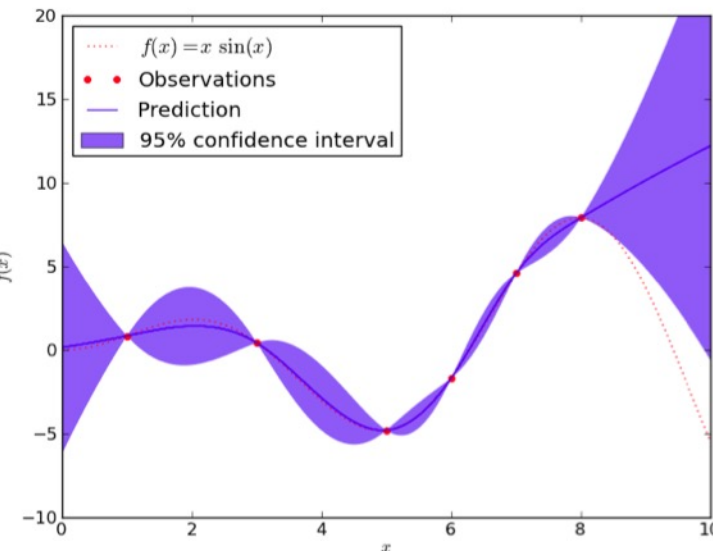
Under Gaussian noise  $y(\mathbf{x}) = f(\mathbf{x}) + \varepsilon$ ,  $\varepsilon \sim \mathcal{N}(0, \sigma^2)$  predictions have an analytic expression.

$$\begin{bmatrix} \mathbf{y} \\ \mathbf{f}_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} K(X, X) + \sigma_n^2 I & K(X, X_*) \\ K(X_*, X) & K(X_*, X_*) \end{bmatrix}\right)$$

$\mathbf{f}_*|X, \mathbf{y}, X_* \sim \mathcal{N}(\bar{\mathbf{f}}_*, \text{cov}(\mathbf{f}_*))$ , where

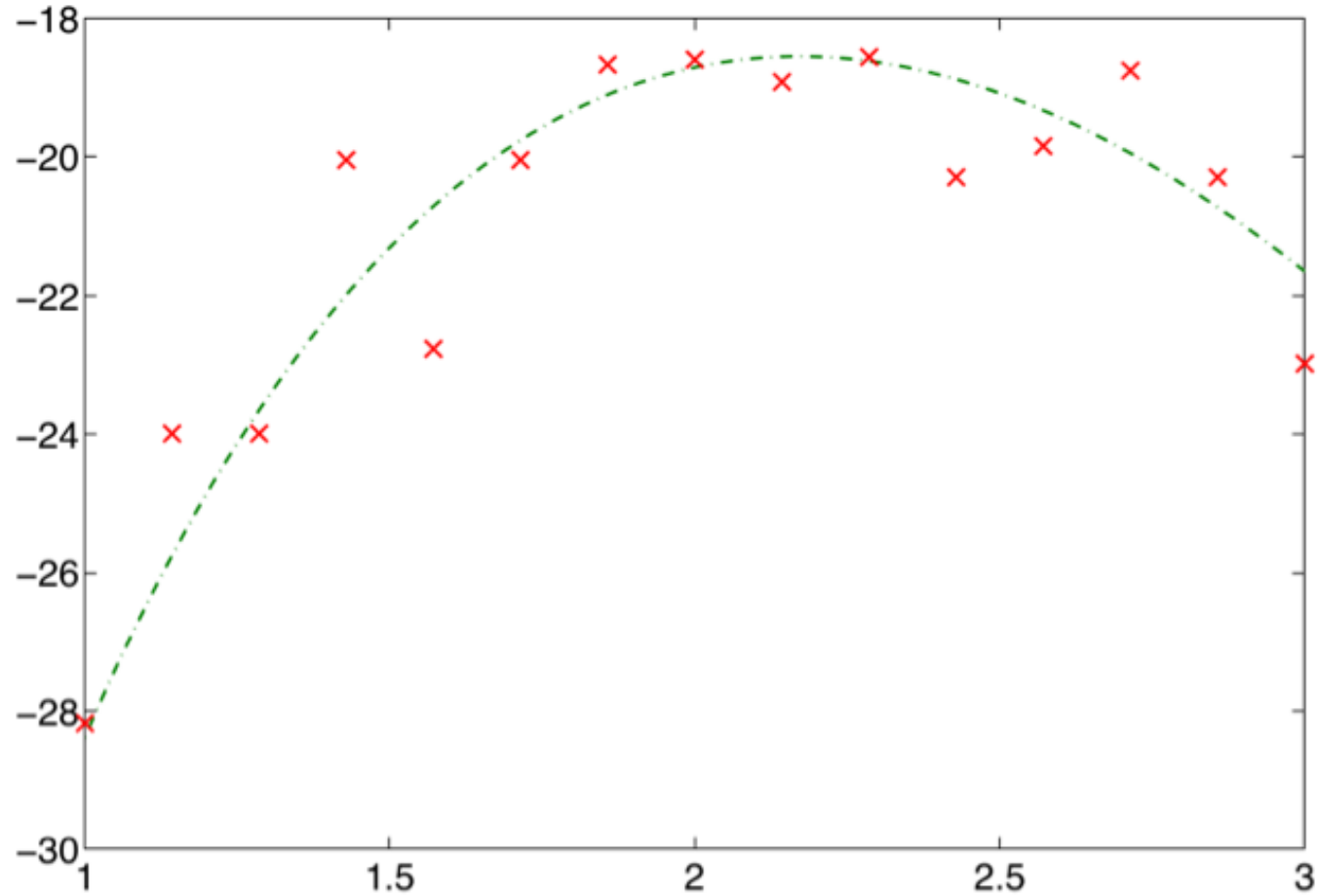
$$\bar{\mathbf{f}}_* \triangleq \mathbb{E}[\mathbf{f}_*|X, \mathbf{y}, X_*] = K(X_*, X)[K(X, X) + \sigma_n^2 I]^{-1} \mathbf{y},$$

$$\text{cov}(\mathbf{f}_*) = K(X_*, X_*) - K(X_*, X)[K(X, X) + \sigma_n^2 I]^{-1} K(X, X_*)$$



# (1) Sample

Collection of the **training set**  $\{(\theta^{(i)}, y^{(i)}), i = 1, \dots, m\}$  for parameters values  $\theta$ .

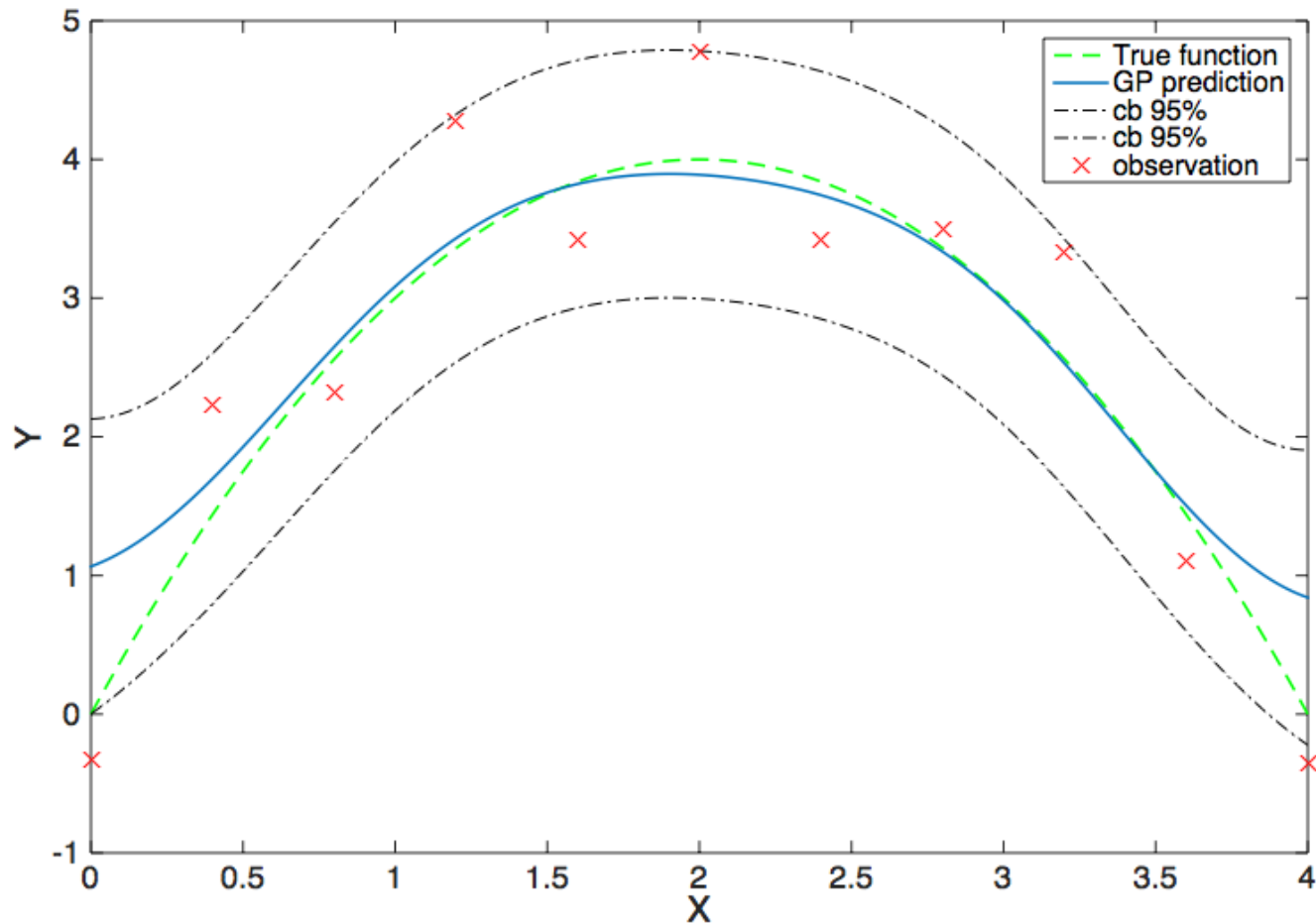


## (2) The GP Regression

We have noisy **observations**  $y$  of the function value distributed around an unknown **true value**  $f(\theta)$  with spherical Gaussian noise

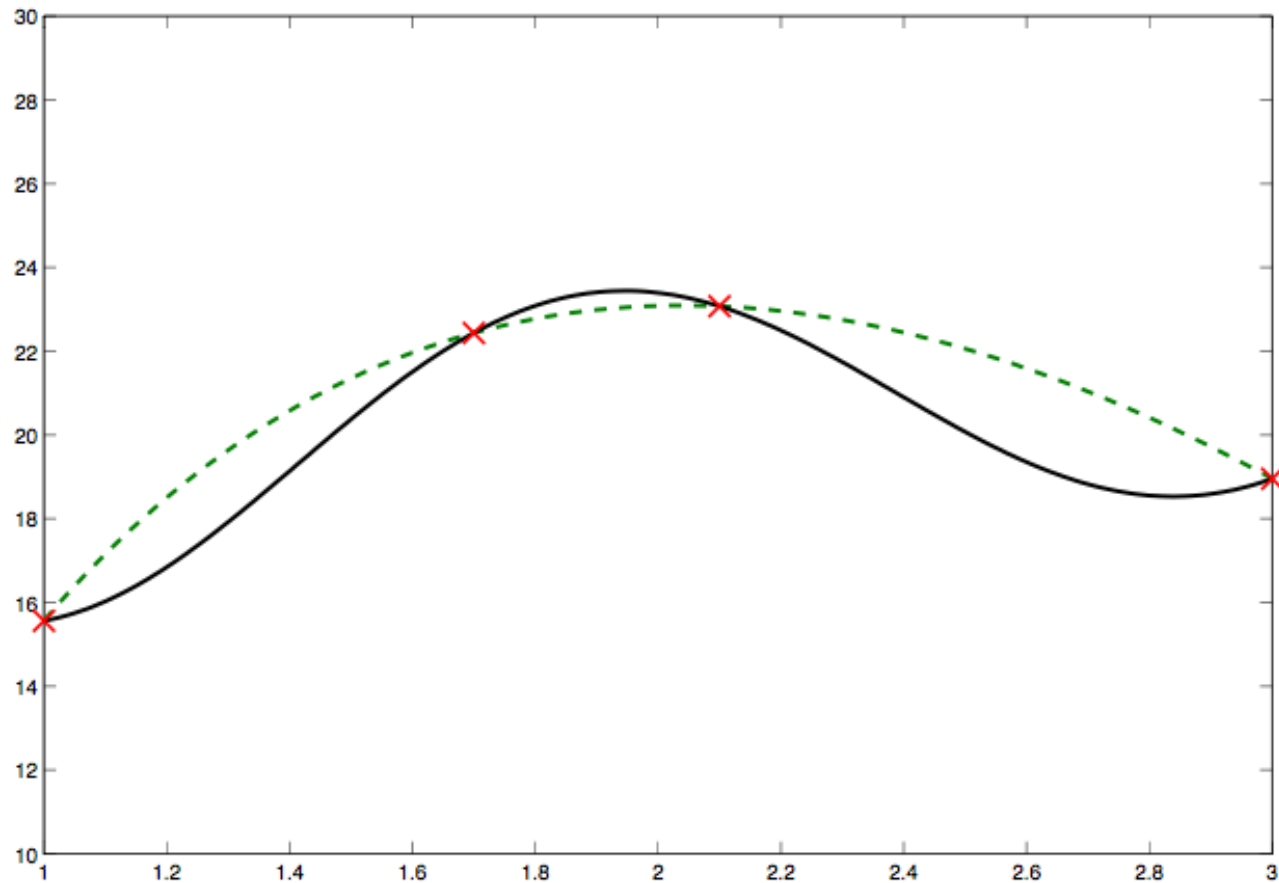
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### (3) The GP-UCB Algorithm

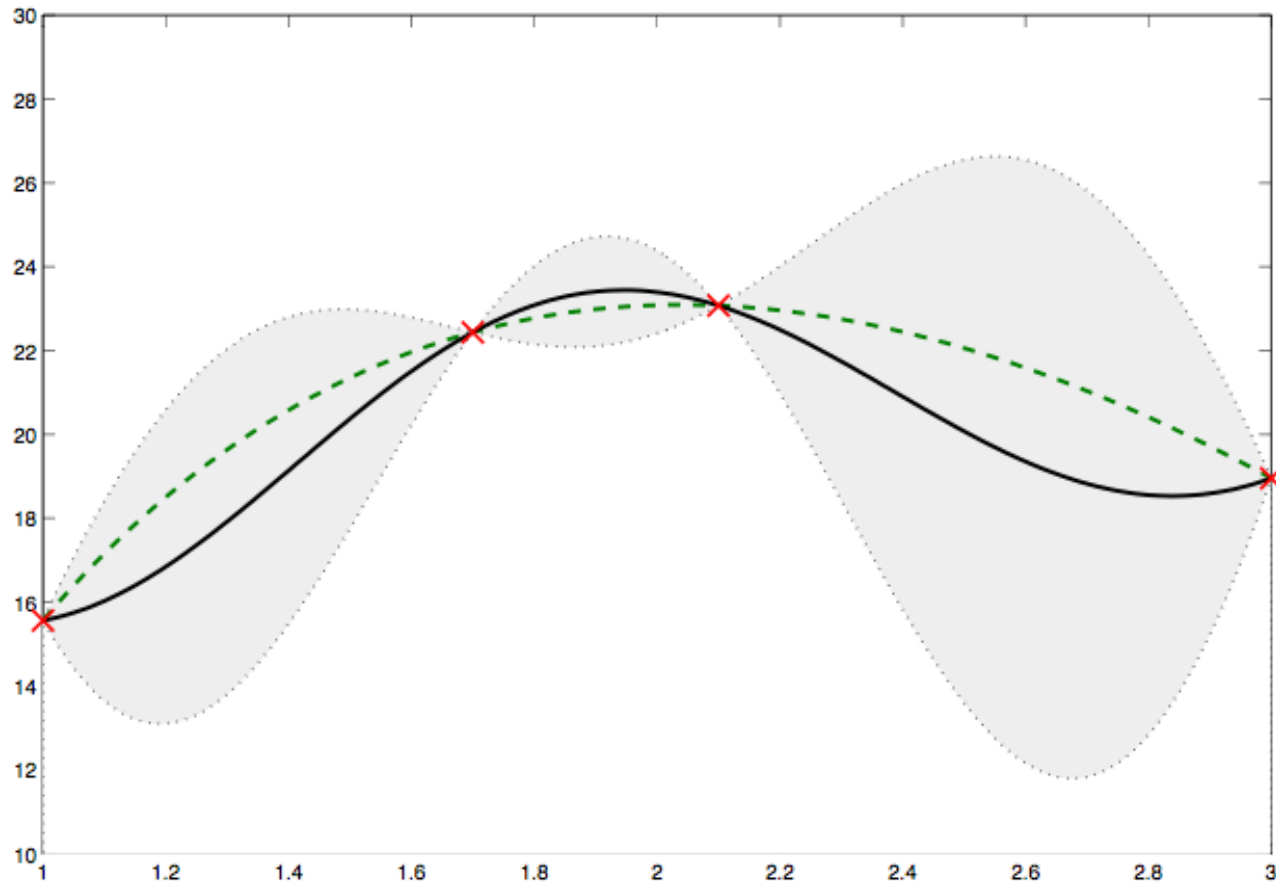
Balance Exploration and Exploitation: we maximise the **95% upper quantile of the distribution**:  $\theta_{t+1} = \operatorname{argmax}_{\theta} [\mu^*(\theta) + \beta_t \sqrt{k^*(\theta, \theta)}]$





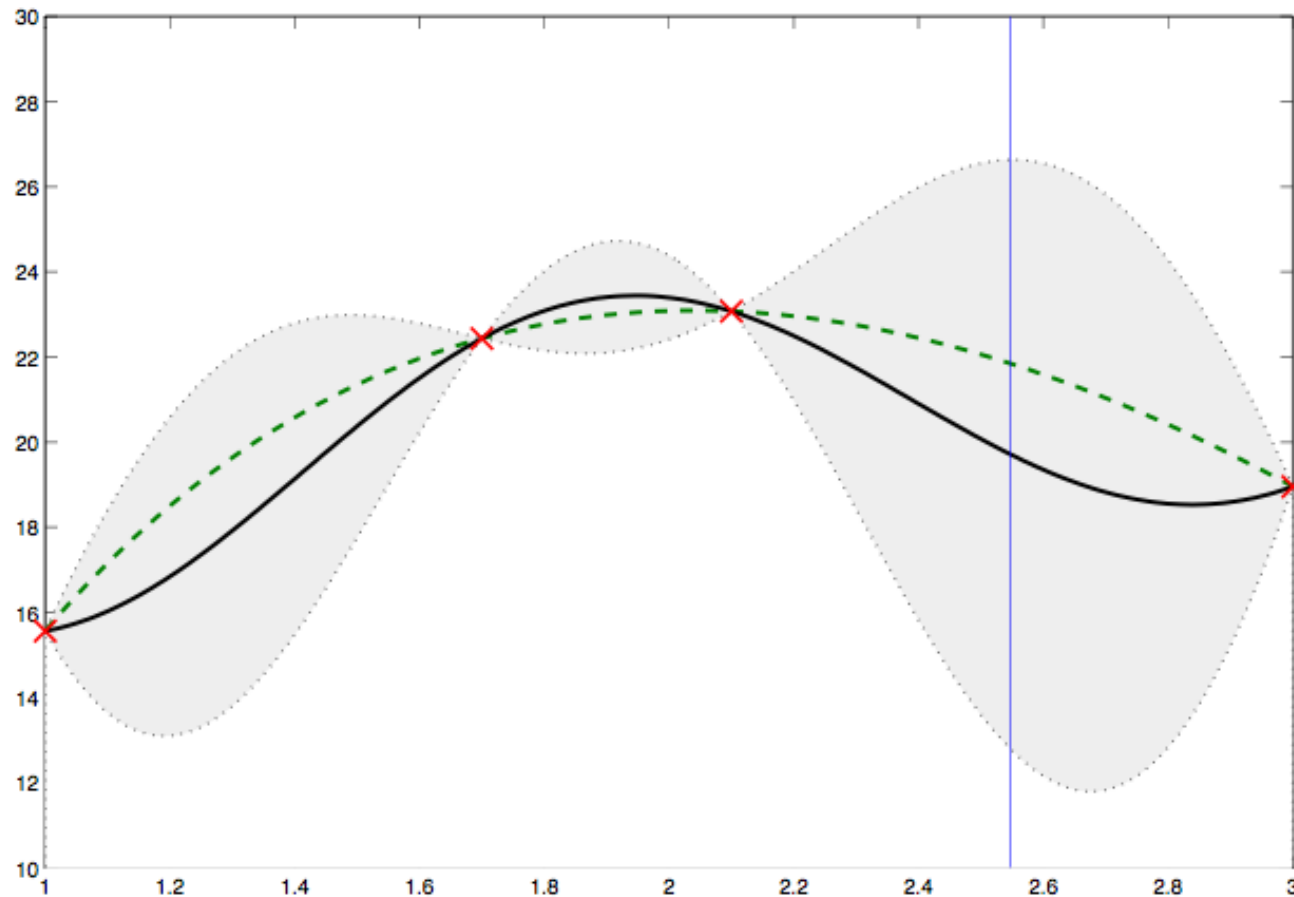
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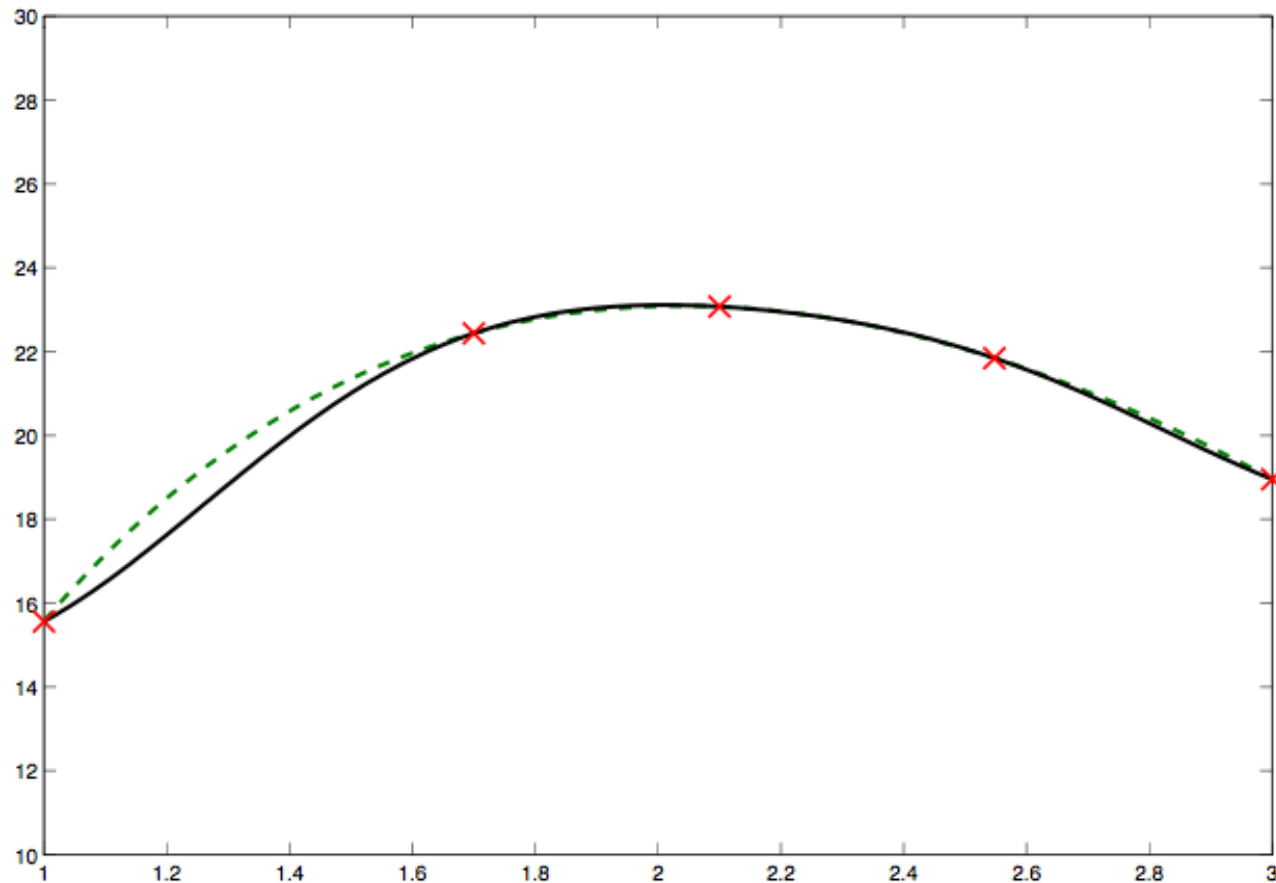
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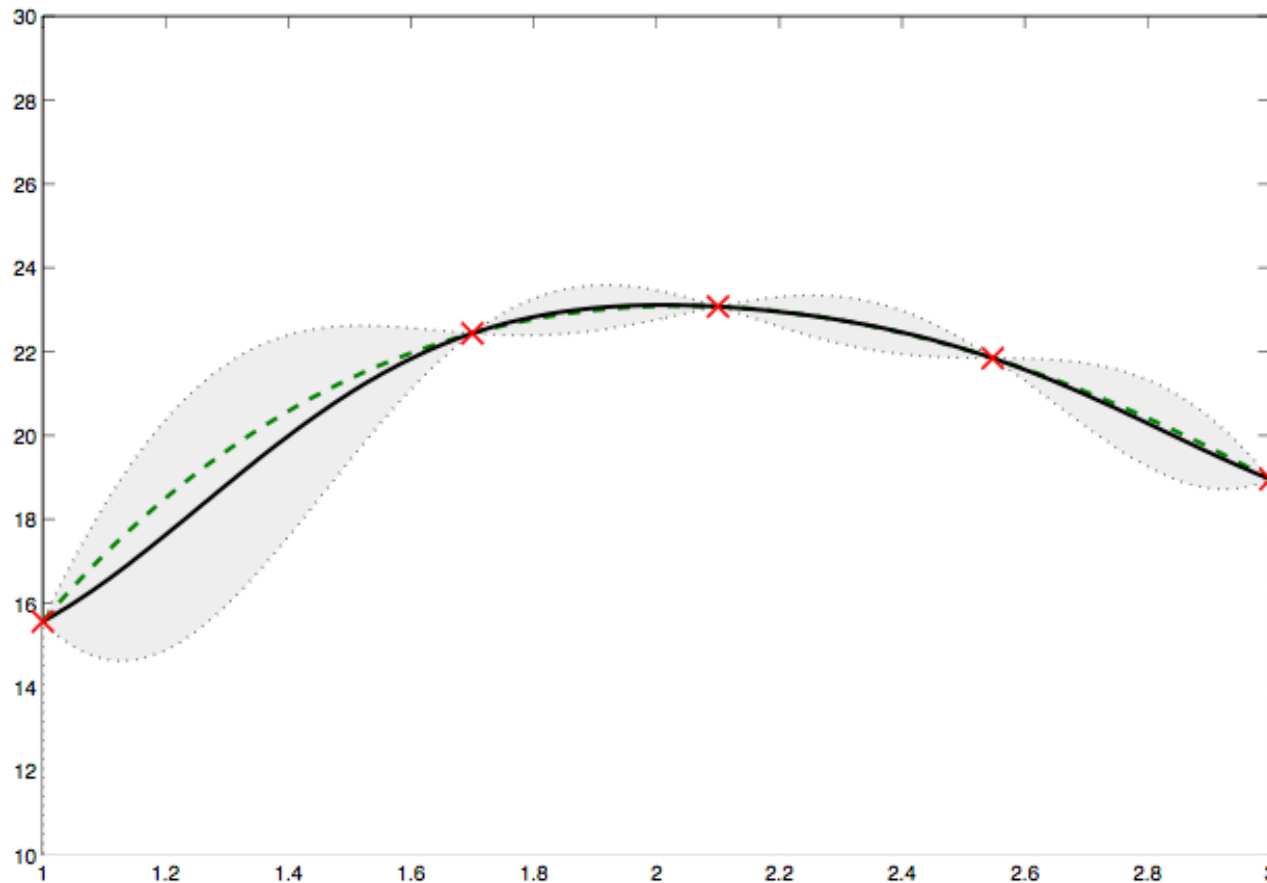
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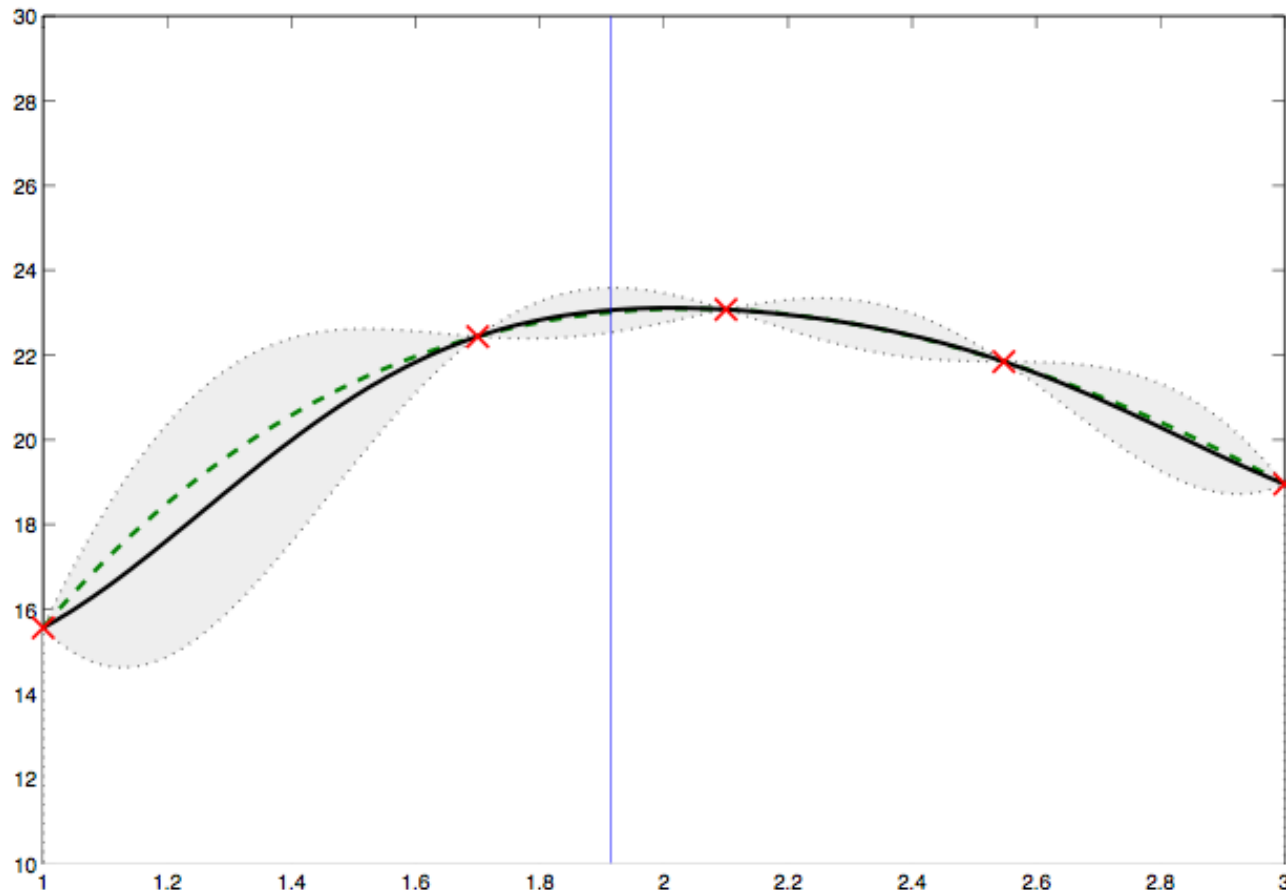
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# Bibliography

## Parameter Synthesis:

- ▶ Ezio Bartocci, Luca Bortolussi, Laura Nenzi, Guido Sanguinetti, System design of stochastic models using robustness of temporal properties. *Theor. Comput. Sci.* 587: 3-25 (2015)
- ▶ Bortolussi L., Silveti S. (2018) *Bayesian Statistical Parameter Synthesis for Linear Temporal Properties of Stochastic Models*. TACAS 2018. LNCS, vol 10806. Springer, Cham