Philipp Reiser
philipp.reiser@simtech.uni-stuttgart.de

Bayesian Uncertainty Quantification with Surrogate Models

Surrogate Modelling

- Meta-model/emulator
- Statistical approximation of complex simulation
  - Polynomial Chaos Expansion (PCE)
  - Gaussian Processes (GP)
  - Neural Networks (NN)

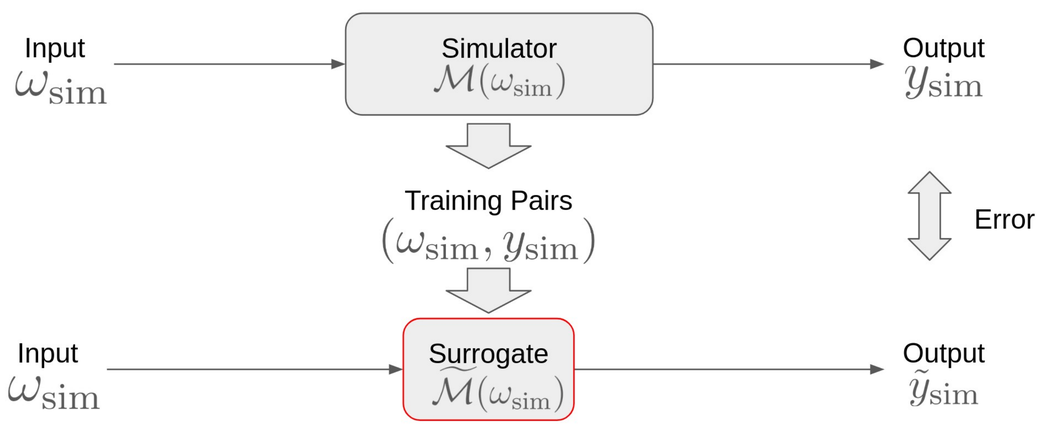


Figure 1. Surrogate Model.

Bayesian Inverse Modelling using Surrogate Models

We use measurement data where y is measurable, but ω not.
Goal: Infer p(ω|y).

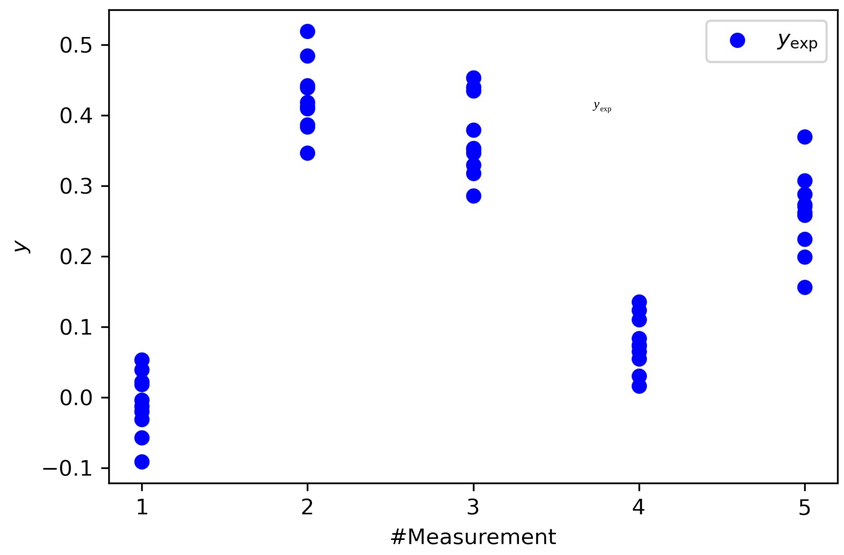


Figure 3. Experimental Data.

Probabilistic Model for 1-step procedure using the surrogate model

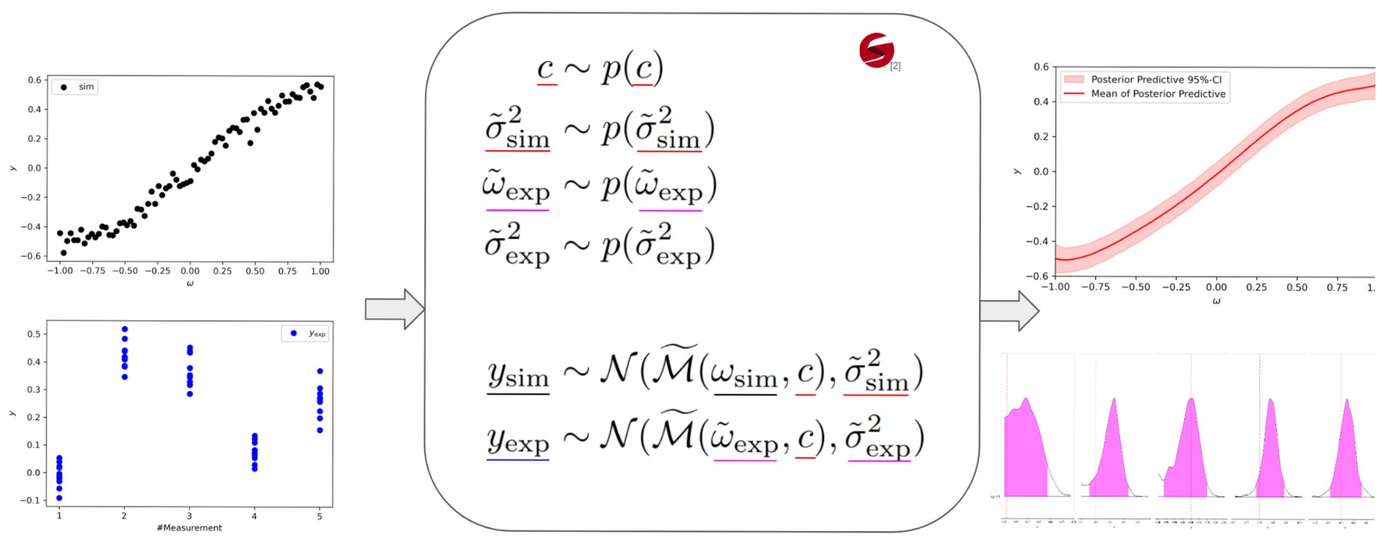


Figure 4. 1-step procedure.

Polynomial Chaos Expansion

Surrogate approximation of true model (PCE)

$$\mathcal{M}(x,t,\omega) \approx \widetilde{\mathcal{M}}(x,t,\omega) = \sum_{i=0}^{d} c_i(x,t)\psi_i(\omega),$$

The probabilistic model for Bayesian PCE:

$$\begin{aligned} c &\sim p(c) \\ \tilde{\sigma}^2_{\text{sim}} &\sim p(\tilde{\sigma}^2_{\text{sim}}) \\ y_{\text{sim}} &\sim \mathcal{N}(\widetilde{\mathcal{M}}(\omega_{\text{sim}}, c), \tilde{\sigma}^2_{\text{sim}}) \end{aligned}$$

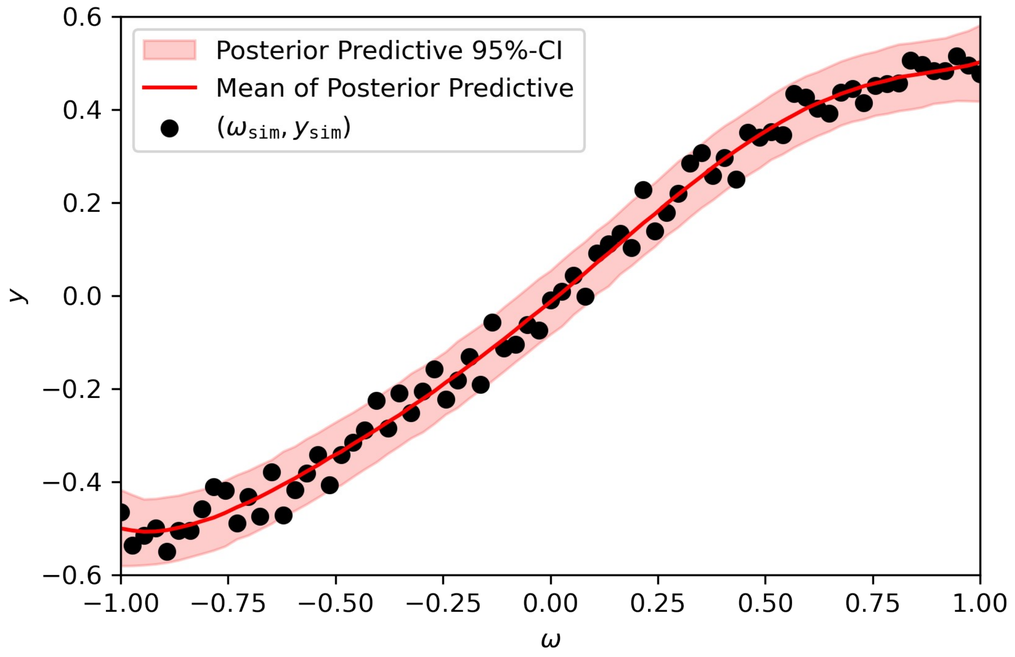
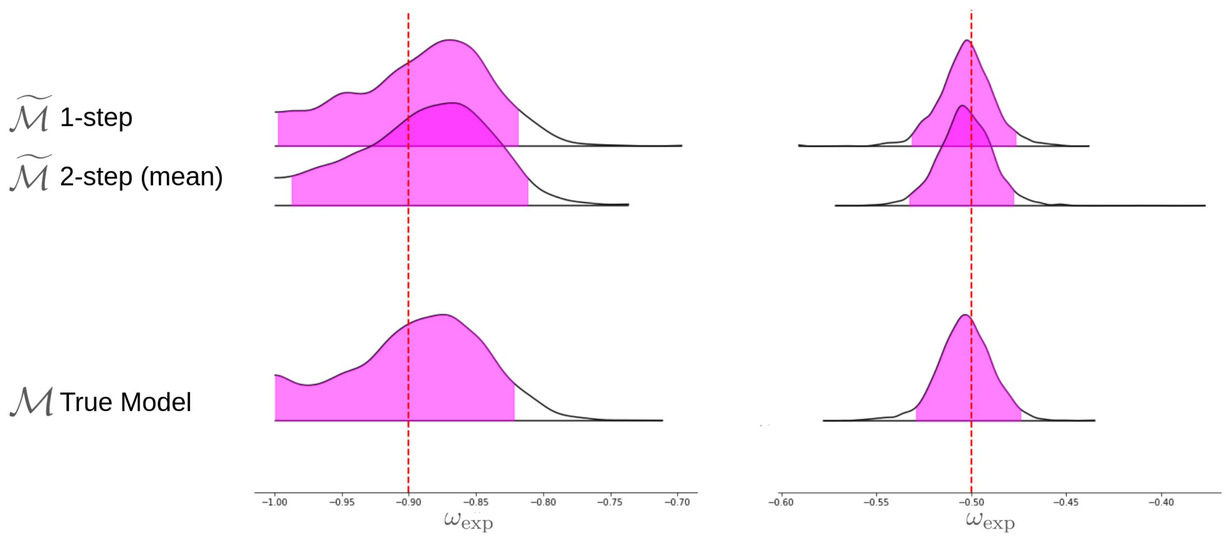


Figure 2. Posterior Preidictive of PCE.

Results



Tools & Methods

- Stan
- Python
- R

Future Applications

- Multidimensional Input
- ODEs/PDEs
- Complex Biological Systems
- Chemical Master Equation (CME)

References

[1] Paul-Christian Bürkner et al. The sparse Polynomial Chaos expansion: a fully Bayesian approach with joint priors on the coefficients and global selection of terms. arXiv e-prints, page arXiv:2204.06043, April 2022.
[2] Bob Carpenter et al. Stan: A probabilistic programming language. Journal of Statistical Software, 76(1), 2017
[3] Norbert Wiener. The Homogeneous Chaos. American Journal of Mathematics, 60(4):897–936, 1938.