Quantifying Uncertainty in Surrogate-based Bayesian Inference

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Surrogate models are statistical approximations for highly complex simulations. In this context, it is crucial to propagate the uncertainty due to limited simulations and due to the approximation error of the surrogate model to predictions and subsequent decision-relevant quantities. However, quantifying the uncertainty of surrogates is usually limited to the use of special analytic cases [1] or is otherwise very computationally expensive.

We propose a scalable, fully Bayesian approach to surrogate modelling and uncertainty propagation using probabilistic programming languages [2]. We will also present a method for Bayesian inference with surrogate models, where we propagate the uncertainty to the unknown input given measurement output. To evaluate the calibration of our inferred posterior distributions, we introduce an adapted version of Simulation-Based Calibration (SBC) [3] that handles non-identifiable models and multiple posterior modes.

Finally, we validate our Bayesian inference on several case studies with varying complexity ranging from easy-to-visualize one-dimensional models to high-dimensional and complex models. Uncertainty propagation in surrogate models enables more reliable and safe approximation of expensive simulations and will therefore be useful in various fields of applications, such as systems biology, molecular dynamics, or fluid dynamics.

References

[1] Ranftl, Sascha and von der Linden, Wolfgang. Bayesian Surrogate Analysis and Uncertainty Propagation. 2021 *Physical Sciences Forum*

[2] Carpenter, Bob and Gelman, Andrew and Hoffman, Matthew D. and Lee, Daniel and Goodrich, Ben and Betancourt, Michael and Brubaker, Marcus and Guo, Jiqiang and Li, Peter and Riddell, Allen. 2017. Stan: A Probabilistic Programming Language. *Journal of Statistical Software* pp. 1–32.

[3] Modrák, Martin and Moon, Angie H. and Kim, Shinyoung and Bürkner, Paul and Huurre, Niko and Faltejsková, Kateřina and Gelman, Andrew and Vehtari, Aki. 2022. Simulation-Based Calibration Checking for Bayesian Computation: The Choice of Test Quantities Shapes Sensitivity