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Quantifying Uncertainty in Surrogate-based Bayesian Inference

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Proper sensitivity and uncertainty analysis for complex Earth and environmental systems models may become computationally prohibitive. Surrogate models can be an alternative to enable such analyses: they are cheap-to-run statistical approximations to the simulation results of the original expensive model. Several approaches to surrogate modelling exist, all with their own challenges and uncertainties. It is crucial to correctly propagate the uncertainties related to surrogate modelling to predictions, inference and derived quantities in order to draw the right conclusions from using the surrogate model.

While the uncertainty in surrogate model parameters due to limited training data (expensive simulation runs) is often accounted for, what is typically ignored is the approximation error due to the surrogate's structure (bias in reproducing the original model predictions). Reasons are that such a full uncertainty analysis is computationally costly even for surrogates (or limited to oversimplified analytic cases), and that a comprehensive framework for uncertainty propagation with surrogate models was missing.

With this contribution, we propose a fully Bayesian approach to surrogate modelling, uncertainty propagation, parameter inference, and uncertainty validation. We illustrate the utility of our approach with two synthetic case studies of parameter inference and validate our inferred posterior distributions by simulation-based calibration. For Bayesian inference, the correct propagation of surrogate uncertainty is especially relevant, because failing to account for it may lead to biased and/or overconfident parameter estimates and will spoil further interpretation in the physics' context or application of the expensive simulation model.

Consistent and comprehensive uncertainty propagation in surrogate models enables more reliable approximation of expensive simulations and will therefore be useful in various fields of applications, such as surface or subsurface hydrology, fluid dynamics, or soil hydraulics.