



Sensitivity Analysis and Active Subspace Construction for Surrogate Models Employed for Bayesian Inference

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For many complex models, the computational cost of high-fidelity codes precludes their direct use for Bayesian inference and uncertainty propagation. For example, the considered neutronics and nuclear thermal hydraulics codes can take hours for a single run. Furthermore, models often have tens to thousands of inputs – comprised of parameters, initial conditions, or boundary conditions – many of which are nonidentifiable or noninfluential in the sense that they are not uniquely determined by measured responses. In this presentation, we will discuss techniques to isolate influential inputs and construct surrogate models for Bayesian inference and uncertainty propagation.

As detailed in [1, 5], global sensitivity analysis is commonly employed to isolate subsets of influential parameters. Since parameter distributions are not typically known *a priori*, one often assumes that parameters are independent and uniformly distributed. However, we will demonstrate for a problem arising in quantum-informed continuum modeling for ferroelectric materials that this can yield incorrect conclusions for correlated parameter sets.

Alternatively, one can employ QR or SVD analysis to construct active subspaces comprised of linear combinations of parameters [2, 6]. We will motivate this analysis by considering gradient-based techniques but focus primarily on gradient-free active subspace techniques for codes that do not have adjoint capabilities [3]. We illustrate these techniques for a neutronics code having approximately 5000 inputs.

Finally, by employing activity scores to rank parameter sensitivity, we will demonstrate the manner in which Bayesian inference using surrogate models constructed on active subspaces can be used to construct posterior densities for nonidentifiable physical parameter sets [4]. We illustrate these techniques for an elliptic PDE having 91 input parameters and a closure relation employed in a two-phase nuclear thermal hydraulic code.

References

- [1] F. Campolongo, J. Cariboni, and A. Saltelli. An effective screening design for sensitivity analysis of large models. *Environmental Modelling and Software*, 22:1509–1518, 2007.
- [2] P. G. Constantine. *Active Subspaces: Emerging Ideas for Dimension Reduction in Parameter Studies*. SIAM, Philadelphia, PA, 2015.
- [3] A. Lewis, R. C. Smith, and B. Williams. Gradient-free active subspace construction using Morris screening elementary effects. *Computers and Mathematics with Applications*, 72:1603–1615, 2016.
- [4] A. Lewis, R. C. Smith, and B. Williams. Bayesian model calibration on active subspaces. *Proceedings of the 2017 American Control Conference*, Paper 978-1-5090-5994-2, 2017.
- [5] R. C. Smith. *Uncertainty Quantification: Theory, Implementation, and Applications*. SIAM, Philadelphia, PA, 2014.
- [6] M. Stoyanov and C. G. Webster. A gradient-based sampling approach for dimension reduction of partial differential equations with stochastic coefficients. *International Journal for Uncertainty Quantification*, 5(1):49–72, 2015.