The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5 – 9 June 2022, Oslo, Norway

Hyper-differential sensitivity analysis with respect to model discrepancy

Joseph Hart[1] and Bart van Bloemen Waanders[2]

[1] Optimization and Uncertainty Quantification, Sandia National Laboratories,
P.O. Box 5800, Albuquerque, NM 87123-1320, joshart@sandia.gov
[2] Optimization and Uncertainty Quantification, Sandia National Laboratories,
P.O. Box 5800, Albuquerque, NM 87123-1320, bartv@sandia.gov

Key Words: *Post optimality sensitivity analysis, PDE-constrained optimization*

Model discrepancy is ubiquitous in computational models for physical systems. The most common scenario is to derive partial differential equations (PDEs) from first principles physics but make simplifying assumptions to produce tractable expressions for the governing equations or closure models. Further, in many applications these PDEs are still too computationally intensive for use in many query analysis. This necessitates reduced order models which lessen the computational burden at the expense of model fidelity.

An end goal in many applications is solving an optimization problem constrained by the approximate model to design the system or calibrate parameters. This article considers the sensitivity of such optimization problems with respect to model discrepancy. We introduce a general representation of the model discrepancy, which is a function of the optimization variable, and apply post optimality sensitivity analysis to derive an expression for the sensitivity of the optimal solution with respect to it. A computationally efficient algorithm is presented which combines the model discretization, post optimality sensitivity operator, adjoint-based derivatives, and a randomized generalized singular value decomposition algorithm to enable scalable computation of the sensitivity of the optimal solution with respect to model discrepancy. Kronecker product structure in the underlying linear algebra and infrastructure investment in optimization formulation is exploited to yield a general-purpose algorithm which is computationally efficient and portable across applications.

The key problem specific components in our framework are the user's choice of weighting matrices which impose soft physics constraints, and the option to constrain the model discrepancy using sparse high-fidelity data. By leveraging the weighting matrices and high-fidelity data, we formulate a computationally efficient algorithm to characterize uncertainty through a probabilistic analysis of the solution of the optimization problem.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. SAND2021-14715 A.