**Title:** Information fusion and machine learning for sensitivity analysis using physics knowledge and experimental data

**Abstract**

Sensitivity analysis is often performed using computational models of the physical phenomena; such models could be physics-based or data-driven, and the sensitivity estimate is affected by the accuracy and uncertainty of the physics model. If the physics-based computational model is expensive, an inexpensive surrogate model is built and used to compute the Sobol’ indices in variance-based sensitivity analysis (also referred to as global sensitivity analysis, or GSA) since many input-output samples are required for such computation; and the surrogate model introduces further approximation in the sensitivity estimate. This paper considers GSA for situations where both a physics-based model and a small number of experimental observations are available, and investigates strategies to effectively combine the two sources of information in order to maximize the accuracy and minimize the uncertainty of the sensitivity estimate. Physics-informed and hybrid machine learning strategies are proposed to achieve these objectives. Two machine learning (ML) techniques are considered, namely, deep neural networks (DNN) and Gaussian process (GP) modeling, and two strategies for incorporating physics knowledge within these ML techniques are investigated, namely: (i) incorporating loss functions in the ML models to enforce physics constraints, and (ii) pre-training and updating the ML model using simulation data and experimental data respectively. Four different models are built for each type (DNN and GP), and the uncertainties in these models are also included in the Sobol’ indices computation. The DNN-based models, since they have many degrees of freedom in terms of model parameters, are found to result in more consistent sensitivity computation results with much smaller prediction bounds when compared to GP-based models. The proposed methods are illustrated for an additive manufacturing example.

**Introduction**

Elaborate each sentence in the abstract to a paragraph, and add literature references.

1. Effect of model accuracy on sensitivity estimate; Effect of model uncertainty on sensitivity estimate (Gratie et al); prior and posterior sensitivities reported in many papers
2. Sensitivity analysis is done with surrogate models when physics model is expensive
3. Data-driven models, neural networks, degrees of freedom
4. Computational efficiency of NN models in sensitivity analysis
5. Model uncertainty
   1. GP model
   2. NN and DNN models (MC dropout)
   3. Model discrepancy estimation – two ways (Bayesian, GP-based)
6. Physics-informed ML
7. Novel contributions of this paper
   1. Two strategies for PIML, and their combinations 🡪 fusion of physics knowledge and experimental data
   2. Application to DNN and GP
   3. Inclusion of model uncertainty in GSA
8. Outline of the rest of the paper

Background (with mathematical details)

1. Sobol’ indices
2. GP
3. DNN
4. Model discrepancy, Bayesian estimation
5. Auxiliary variable approach

Proposed methodology (with mathematical details)

1. Two PIML strategies
2. Implementation in GP
3. Implementation in DNN
4. Model uncertainty quantification in GP and DNN
5. Sobol’ indices computation with model uncertainty

Numerical example

1. Description of the example
2. Very brief description of physics model, inputs and outputs
3. Description of experimental data
4. DNN models (4 of them)
5. GP models (4 of them)
6. Physics model discrepancy (for comparison with PIML results)
   1. using GP
   2. using Bayesian
7. Numerical results and discussions
   1. Comparison of results of different ML models to sensitivity results from the physics model
   2. Comparison of GP vs. DNN results
   3. Comparison of results with and without model uncertainty (for GP and DNN)

Conclusion

1. Brief summary of accomplished work
2. Insights learned
3. Future needs

References