Uncertainty Quantification and Automatic Task Balancing of Bayesian Physics Informed Neural Networks for Inverse Problems in Reactive Flows

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We present an efficient data-assimilation framework based on deep learning and integrating robust uncertainty quantification to address pore-scale reactive inverse problems, targeting both imaging data and physics-based constraints. This approach lies in a Bayesian Physics-Informed Neural Networks (BPINNs) formulation of multi-objective inverse problems involving the PDE constraints as tasks, for which we introduce a new method of automatic task balancing. This strategy establishes an adaptive weighting of the target distribution in a Bayesian context and ensures unbiased uncertainty quantification through an automatic weighting of the tasks in multi-objective problems.

Task balancing is directly achieved by leveraging gradient information of the various objectives within the BPINNs framework, maintaining efficient computational costs. Our approach benefits from improved convergence and stability in contrast to conventional formulations, and eliminates the need for manual adjustment of critical weighting parameters. The adjusted weights also bring information on the task un-certainties and thus improve the reliability of the noise-related and model adequacy estimates.

After demonstrating the effectiveness of this framework on data assimilation problems of various complexities, we apply it to pore-scale imaging of reactive inverse problems in porous media, to capture morphological uncertainties on the micro-porosity field and reliability ranges on the kinetic parameters.

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