Robust Uncertainty Quantification for multitask Bayesian neural networks: application to inverse problems in Computational Fluid Dynamics and reactive flows

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While Computational Fluid Dynamics and Direct Numerical Simulation methods have proven themselves to be powerful predictive approaches in a variety of research fields, including computational biology and geosciences, the question of accurately calibrating the PDE model parameters driving the dynamics remains a significant challenge.

In particular, the study of reactive flows in pore-scale porous media requires estimating mineral reactivities and kinetic parameters, often plagued by wide discrepancies that introduce modeling uncertainties. Besides, pore-scale modeling of reactive flows is based on X-ray microtomography experiments, prone to image artefacts such as noise and unresolved morphological features, adding further imaging uncertainties [3].

To enhance the reliability of direct numerical modeling and calibration, we tackle the challenges posed by these two types of uncertainties by developing a deep learning methodology that integrates robust uncertainty quantification [1]. We present an efficient data-assimilation framework based on a Bayesian Physics-Informed Neural Networks (BPINNs) formulation of multi-objective inverse problems involving the PDE constraints and data fidelity as tasks.

We establish a new strategy of automatic task balancing and introduce an adaptive weighting of the target distribution in this Bayesian context by leveraging gradient information of the various objectives [1]. The automatic and adaptive weighting ensures unbiased uncertainty quantification, efficient exploration of the optimal Pareto front, enhanced stability and convergence compared to conventional formulations. Finally, this approach allows us to simultaneously and robustly tackle the direct problem, with a surrogate PDE model, and the inverse problem of determining unknown parameters with probabilistic uncertainty.

After demonstrating the effectiveness of this framework on various benchmarks, we showcase its applications in CFD for flow reconstruction in stenosed arteries, considering unknown noise on the data. We also explore CFD inverse problems in stenosed arteries, targeting the estimation of Reynold number ranges and pressure latent field recovery (without data available). Finally, we address pore-scale reactive inverse problems, combining imaging and modeling uncertainties to capture both unresolved morphological features and reliability ranges on the reactive parameters [2].

[1] S. Perez, S. Maddu, I. F. Sbalzarini and P. Poncet, Adaptive weighting of Bayesian physics informed neural networks for multitask and multiscale forward and inverse problems, *Journal of Computational Physics*, 2023, 491, pp.112342 (https://doi.org/10.1016/j.jcp.2023.112342)

[2] S. Perez and P. Poncet, Auto-weighted Bayesian Physics-Informed Neural Networks and robust estimations for multitask inverse problems in pore-scale imaging of dissolution, *arXiv preprint*, 2023 (https://doi.org/10.48550/arXiv.2308.12864)

[3] S. Perez, P. Moonen and P. Poncet, On the Deviation of Computed Permeability Induced by Unresolved Morphological Features of the Pore Space, *Transport in Porous Media*, 2022, 141, pp.151-184 (https://doi.org/10.1007/s11242-021-01713-z)