Semi-supervised Invertible DeepONets for Bayesian Inverse Problems

S. Kaltenbach[1], P. Perdikaris[2], and P.-S. Koutsourelakis[1,3]

[1]*Professorship of Data-driven Materials Modeling, School of Engineering and Design, Technical University Munich, Munich*
[2]*Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia*
[3]*Munich Data Science Institute (MDSI - Core Member), www.mdsi.tum.de*

Deep Operator Networks (DeepONets) [2] offer a powerful, data-driven tool for solving parametric PDEs by learning operators, i.e. maps between infinite-dimensional function spaces. Recently proposed physics-informed versions have made use of governing law residuals in the loss function in order to significantly reduce requirements for expensive, labeled training data (i.e. input-output pairs), as well as to improve predictive accuracy under extrapolative conditions [3]. In this work, we employ physics-informed DeepONets in the context of high-dimensional, Bayesian inverse problems. Traditional solution strategies necessitate an enormous, and frequently infeasible, number of forward model solves, as well as the computation of parametric derivatives. In order to enable efficient solutions, we extend DeepONets by employing a realNVP architecture [1] which yields an invertible and differentiable map between the parametric input and the branch net output. This allows us to construct accurate approximations of the full posterior which can be readily adapted irrespective of the number of observations and the magnitude of the observation noise. As a result, no additional forward solves are required, nor is there any need for costly sampling procedures. We demonstrate the efficacy and accuracy of the proposed methodology in the context of inverse problems based on a reaction-diffusion and a Darcy-flow equation.

References

[1] L. Dinh, J. Sohl-Dickstein, and S. Bengio. Density estimation using real NVP. *ICLR*, 2017.

[2] L. Lu, P. Jin, G. Pang, Z. Zhang, and G. E. Karniadakis. Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators. *Nature Machine Intelligence*, 3(3):218–229, 2021.

[3] S. Wang, H. Wang, and P. Perdikaris. Learning the solution operator of parametric partial differential equations with physics-informed DeepONets. *Science advances*, 7(40):eabi8605, 2021.