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Probabilistic DiffusionNet as a PDE surrogate endowed with mechanistic uncertainty quantification

Geometric deep learning models are being adopted across science and engineering to estimate large-scale PDE solutions for varying boundary conditions. While accurate uncertainty quantification (UQ) is essential for better decision-making for a variety of downstream tasks like optimisation and control, these models rarely produce efficient and effective UQ. Moreover, most UQ methods focus on constructing distributions on point-wise parameters to elicit uncertainty, and so fail to exploit the useful inductive biases of geometric model architectures. To address this challenge, we propose a probabilistic modification of the DiffusionNet architecture, widely used in surface learning tasks, by introducing latent random variables that are derived from a stochastic reformulation of the underlying mechanism — the diffusion process. We demonstrate that approximate Bayesian treatment of these mechanistic latent variables yields superior UQ performance on standard datasets without sacrificing predictive performance compared to other prevalent models and UQ methods, while enjoying a lower computational cost and interpretability.

AI keywords

DiffusionNet, Variational Inference, PDE surrogate, Neural Operators, Geometric Deep Learning

Primary author: GHOSH, Sanmitra

Co-authors: Dr LEAHY, James-Michael (PhysicsX); Dr HUSSAIN, Aamal (PhysicsX); Mr DJERMANI, Bachir (PhysicsX); MICHAELIDES, Michalis (PhysicsX)

Presenter: GHOSH, Sanmitra

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