Toward Reliable Operator Learning: Uncertainty-Aware Prediction and Physics-Guided Correction

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Abstract: Operator learning is a core task in scientific machine learning (SciML) for learning mappings between input and output fields. Among the most widely used architectures, the Deep Operator Network (DeepONet) has been successfully applied to learning and inferring complex physical systems. However, the classical DeepONet formulation requires fixed sensor numbers and locations, lacks built-in mechanisms for uncertainty quantification (UQ), and may suffer from model misspecification in practical applications. To address these challenges, we first propose UQ-SONet, a permutation-invariant operator learning framework with integrated UQ. UQ-SONet incorporates a set-transformer embedding to handle sparse observations with variable sensor locations and employs a conditional variational autoencoder (cVAE) to approximate the conditional distribution of the solution operator. By minimizing the negative evidence lower bound (ELBO), UQ-SONet provides principled uncertainty estimation while maintaining predictive accuracy. We further develop a data–physics fusion correction framework to mitigate biases induced by imperfect physical models, enabling reliable operator learning under model discrepancies. Numerical experiments demonstrate the robustness and effectiveness of the proposed frameworks.