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Bayesian Neural Networks for Surrogate-based Optimization in Aerodynamic Shape Optimization

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Abstract

This paper explores the integration of Bayesian Neural Networks (BNNs) within Surrogate-Based Optimization (SBO) for aerodynamic shape optimization (ASO). SBO is a robust framework for optimizing computationally expensive black-box functions, leveraging surrogate models to approximate the objective function and guide iterative evaluations. Gaussian Process Regression (GPR), traditionally a cornerstone of SBO, provides uncertainty-aware predictions but struggles with scalability and high-dimensional data. To address these limitations, we propose BNNs as an alternative surrogate model due to their flexibility and ability to model uncertainty through a Bayesian framework.

BNNs extend traditional artificial neural networks by treating weights and biases as random variables, yielding probabilistic predictions. The posterior distribution over the model parameters is inferred using Bayes' theorem. Despite their theoretical appeal, exact posterior inference in BNNs is computationally prohibitive. This work employs variational inference (VI), in the form of Monte Carlo Dropout (MCD) and infinite-width BNN to approximate the posterior efficiently, and compares it to classical Hamiltonian Monte Carlo (HMC) methods.

The methodology is benchmarked on synthetic test problems and extended to an ASO problem. On synthetic test problems, BNNs demonstrate competitive performance compared to GPR while showcasing superior scalability. The application to ASO is examined using the RAE2822 airfoil parameterized by Hicks-Henne bump functions in unconstrained drag minimization using RANS simulations under transonic conditions. Here, BNNs achieve faster improvement compared to GPR.

Results reveal that BNNs outperform GPR in low-data regimes typical in SBO. These findings underscore the promise of BNNs in complex optimization tasks, particularly when computational efficiency and uncertainty modeling are paramount.

Keywords: bayesian optimization, bayesian neural networks, surrogate-based optimization, aerodynamic shape optimization,