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MULTI-FIDELITY MONTE-CARLO SAMPLING IN MECHANICS

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ABSTRACT

In recent years, the Hamiltonian Monte Carlo (HMC) method has emerged as a state-of-the-art Markov chain Monte Carlo (MCMC) technique that exploits the geometry of the target distribution to generate samples in high dimensional space efficiently. Despite its impressive empirical success and increasing popularity, its wide-scale adoption is still limited due to the high computational cost associated with the gradient calculation. Moreover, the application of this method is simply not possible in scenarios where we cannot compute the gradient of the posterior (for example, with black-box simulators, and with non-differentiable priors). We propose a novel two-stage Hamiltonian Monte Carlo algorithm with a deep learning (DL)-based surrogate model to overcome these challenges. In this two-stage algorithm, the acceptance probability is computed in the first stage via a standard HMC proposal using an inexpensive DL-based surrogate model. The full posterior is evaluated in the second stage using the high fidelity (HF) numerical solver if the proposal is accepted. Splitting the standard HMC algorithm into these two stages allows for the efficient and computationally inexpensive evaluation of the gradient of the posterior using automatic differentiation capabilities of DL-based surrogates (thus retaining advantages of HMC, such as scalability to high dimensions and faster convergence) while producing accurate posterior samples by using HF numerical solvers in the second stage. We demonstrate the effectiveness of this algorithm for linear and nonlinear Bayesian inverse problems for simulated data and a nonlinear hydraulic tomography problem using experimental data, where it outperforms the traditional HMC algorithm in computational and statistical efficiency while retaining similar accuracy.