Title: End-to-End Uncertainty Quantification in Multiscale Models via Bayesian Active Learning

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Abstract Text:

Powered by growing computing resources and informed by more data, multi-scale computer simulation is playing an increasing role in engineering and science applications. A key barrier to its reliable adoption is the variability in the simulated predictions that has become increasingly driven by data used to inform the model. This raises an emerging need for end-to-end uncertainty quantification (UQ): to measure the variability in simulated predictions (forward UQ), we must first infer the uncertainty within the data-driven model elements (inverse UQ).

One critical technical barrier to end-to-end UQ is how an approximation (surrogate) of the simulation output can be constructed when the computational cost of a simulation denies direct Markov-chain Monte Carlo (MCMC) runs. In this presentation we describe our recent effort in cast surrogate modeling as a machine-learning problem, in which the training data are virtually infinite (in a continuous space) but expensive to obtain (incurring model evaluations). We highlight our concept and developments in “active surrogate modeling” which, during the construction of the surrogate, will actively search the optimal training points (samples) at which to query the model. This high-dimensional active search is further embedded into a low-dimensional latent space through probabilistic generative modeling. Finally, we present surrogate-accelerated MCMC algorithms that utilize the surrogate to theoretically accelerate the convergence of MCMC sampling. We demonstrate the efficacy of these developments in the application context of patient-specific cardiac modeling. These developments are highly novel at several aspects. In the area of surrogate modeling, this is the first-time active learning concepts are introduced to intelligently realize a locally-focused approximation. In the general area of active learning, this is the first integration of generative modeling to realize active learning over a high-dimensional continuous space.