Indentifying Uncertain Behavior of Chemical Systems using Bayesian Inference

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Identifying parametric uncertainty in chemical systems is the key to learn physical information from experimental data. The parametric uncertainty enables model-based stochastic design and control that extends the interpretability and capability of optimization problems. However, most inference methods identifying parametric uncertainty require the explicit likelihood function and a heavy computational cost of sampling, which are infeasible for first-principle based models such as electrochemical reactor models using computational fluid dynamics, density functional theory, and rigorous process model. Here, we propose two Bayesian inference methodologies, adversarial Bayesian inference and hybrid Bayesian inference, for complex first-principle-based models that conquer both high accuracy as the level of state-of-the-art Hamiltonian Monte Carlo and low computational cost as variational inference. We exemplify the methodologies to various chemical systems to verify the performance of the proposed algorithm.