APPROXIMATE BAYESIAN MODEL CALIBRATION WITH SUMMARY STATISTICS

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ABSTRACT

Uncertainty quantification (UQ) in computational models relies on probabilistic characterization of uncertain model inputs and parameters, which is effectually arrived at by the solution of a Bayesian inference problem given available data on model output observables. This talk will address specific challenges in this context related to missing data. In many practical situations, actual data is simply not available, and one is limited to available, *e.g.* published, processed data summaries, in the form of statistics, such as nominal values and conditional/marginal bounds, on model parameters, or functions thereof. One strategy to deal with this challenge relies on maximum entropy (MaxEnt) methods, which are useful for inference employing constraints. I will describe the basics of our computational implementation of the MaxEnt principle, employing approximate Bayesian computation (ABC) methods, to enable inference of uncertain parameters given available summary statistics [1]. These statistics define a constraint on the data, conditioned on all available information. The method samples the joint posterior on both data and parameters using a nested pair of Markov chains, enabling subsequent marginalization to arrive at the parameter posterior of interest. I will present illustrations of the performance of this construction in model application problems, including combustion chemistry [2,3,4], and materials modeling [5]. While ABC methods have been useful in the emerging landscape of UQ in machine learning models of physical systems, the above outlined challenges have yet to be dealt with in this context. This MaxEnt-ABC construction, with necessary targeted approximations, may indeed be useful when accounting for uncertainty in the training of neural network models of physical systems.

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