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Approximate Bayesian Computation by Subset Simulation using hierarchical state-space models

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ABSTRACT

A new multi-level Markov Chain Monte Carlo algorithm for Approximate Bayesian Computation, ABC-SubSim, has recently appeared that exploits the Subset Simulation method for efficient rare-event simulation. ABC-SubSim adaptively creates a nested decreasing sequence of data-approximating regions in the output space that correspond to increasingly closer approximations of the observed output vector in this output space. At each level, multiple samples of the model parameter vector are generated by a component-wise Metropolis algorithm so that the predicted output corresponding to each parameter value falls in the current data-approximating region. Theoretically, if continued to the limit, the sequence of data-approximating regions would converge on to the observed output vector and the approximate posterior distributions, which are conditional on the data-approximation region, would become exact, but this is not practically feasible. In this paper we study the performance of the ABC-SubSim algorithm for Bayesian updating of the parameters of dynamical systems using a general hierarchical state-space model. We note that the ABC methodology gives an approximate posterior distribution that actually corresponds to an exact posterior where a uniformly distributed combined measurement and modeling error is added. We also note that ABC algorithms have a problem with learning the uncertain error variances in a stochastic state-space model and so we treat them as nuisance parameters and analytically integrate them out of the posterior distribution. In addition, the statistical efficiency of the original ABC-SubSim algorithm is improved by developing a novel strategy to regulate the proposal variance for the component-wise Metropolis algorithm at each level. We demonstrate that *Self-regulated ABC-SubSim* is well suited for Bayesian system identification by first applying it successfully to model updating of a two degree-of-freedom linear structure for three cases: globally, locally and un-identifiable model classes, and then to model updating of a two degree-of-freedom non-linear structure with Duffing nonlinearities in its interstory force-deflection relationship.
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1. Introduction

In the Bayesian updating framework, the likelihood function of a model parameter vector expresses the probability of getting measured data based on a particular stochastic predictive model, and it is essential since the data affects the posterior through it via Bayes' theorem. However, for some complex models, e.g., hidden Markov models or dynamic state-

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space models, an analytical formula for the likelihood function might be difficult, or even impossible to establish. Approximate Bayesian Computation (ABC) was conceived to bypass the explicit evaluation of the likelihood function [1,2] by sampling from a posterior probability distribution conditional on model predicted outputs that are acceptably close under some metric in the output space to the observed data vector, rather than using this observed data vector directly in Bayes' theorem. Thus, an approximate likelihood function is defined for use in Bayes' theorem to be the probability that the predicted output corresponding to a value of the model parameter vector falls in the data-approximating region of the observed data vector where the accuracy of the approximation is determined by a tolerance level ε on the chosen metric. Theoretically, when $\varepsilon \to 0$, this algorithm gives draws from the exact posterior distribution, but this cannot be accomplished in practice. Furthermore, when the data vector is in a high-dimensional output space, a summary statistics vector $\eta(\bullet)$, which is a function of the observed or predicted output vector, may be introduced to project the predicted output and data onto a low-dimensional space for a "weaker" comparison.

The ABC method can be utilized for any model for which forward simulation is available and it broadens the realm of models for which Bayesian statistical inference can be applied. It has gained popularity over the last decade, as can be observed by the increasing range of applications to complex model updating or inverse problems, e.g., dynamical systems [3,4], biological sciences [5,6] and ecology [7], amongst many others. Numerous new ABC methods have been proposed over the last decade or so with the goal of improving the approximation accuracy and computational efficiency, e.g., ABC-MCMC [8–10], ABC-PRC [11,12], ABC-SMC [4,13,14] and ABC-PMC [15] and, very recently, ABC-SubSim [16].

For a good approximation of the posterior distribution in the ABC approach, we want the tolerance parameter ε to be sufficiently small so that only the predicted outputs falling in a close neighborhood centered on the observed data vector are accepted. However, this leads to a problem of rare-event simulation and so if Monte Carlo simulation is used, the model output must be computed for a huge number of candidate samples in order to produce an acceptable sample size in the specified data-approximating region. The computational cost can be reduced by using Markov Chain Monte Carlo (MCMC) sampling directly, but it is still not very efficient due to difficulty in initializing the chain and in achieving fast convergence in order to sample from the stationary distribution.

To improve the efficiency of ABC, Chiachio et al. [16] recently proposed a new algorithm, named ABC-SubSim, by incorporating the Subset Simulation technique [17] into the ABC algorithm. In Subset Simulation, rare-event simulation is converted into sampling from a sequence of nested subsets that correspond to large conditional probabilities. This is automatically accomplished by ABC-SubSim adaptively selecting a sequence of intermediate tolerance parameters ε that control the conditional probabilities at each level. In this way, ABC-SubSim automatically creates a nested decreasing sequence of regions in the output space that corresponds to increasingly closer approximations of the observed data vector. As the procedure continues, the sequence of data-approximating regions becomes more concentrated around the actual data vector so that a good approximation of the posterior distribution is achieved.

Subset Simulation uses a MCMC algorithm with a relatively small number of samples to explore the conditional distributions over the model parameter space and no burn-in period is needed to converge to its stationary distribution at each level, that is, it exhibits "perfect sampling" [18,19]. In the original Subset Simulation technique [17], a modified Metropolis algorithm (MMA) was proposed to generate a candidate sample vector in a component-wise manner, i.e., using a sequence of univariate proposal PDFs to avoid the small acceptance rate of the original Metropolis sampler in high dimensions. It is found that the choice of the spread (e.g., variance) of the local proposal distribution is very important for enhancing computational efficiency but not the choice of the distribution type. A large variance may reduce the acceptance rate and lead to more repeated MCMC samples, while a small variance may result in a high acceptance rate, but still produce high correlation of the MCMC samples because the chain moves very slowly through the support of the posterior distribution. Based on previous studies of adaptive proposal PDFs for MCMC algorithms [19,20], we introduce a novel self-regulating strategy to find the optimal variance for the proposal distributions in Subset Simulation, which is one of the important contributions of this paper.

Wilkinson [21] showed that a standard ABC posterior gives an exact posterior distribution for a new model in which the summary statistics are assumed to be corrupted with a uniform additive error term. In this paper, we show that formulating the dynamic problem in terms of a general hierarchical stochastic state-space model enables us to extend Wilkinson's interpretation for ABC posterior distributions that use the entire measured output signal, not just summary statistics. For this hierarchical stochastic model, the basic ABC approximation with an infinity norm as the metric in output space can be interpreted as performing exact Bayesian updating with independent uniformly-distributed combined measurement and modeling errors.[1] This interpretation provides a theoretical foundation which allows the accuracy of the ABC approximation to be judged and also helps to understand the effect of the metric and tolerance ε on the quality of the ABC approximation of the evidence.

Another important contribution is that we uncover and fix a problem that ABC algorithms have with learning the variances for Gaussian prediction errors in a stochastic state-space model: these variances are suppressed by the original ABC algorithm as the tolerance level ε decreases. This is due to the fact that the formulation of the stochastic state-space model has built-in state and output prediction errors such that a sample of the model prediction of the system output includes a realization of these error signals. For high-dimensional data vectors, the probability of exactly matching the actual measured

[1] This can be generalized to any norm on the output space, although in general the errors will be dependent.

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