Proceedings of the 2020 Winter Simulation Conference
K.-H. Bae, B. Feng, S. Kim, S. Lazarova-Molnar, Z. Zheng, T. Roeder, and R. Thiesing, eds.

A FLEXIBLE PARALLELIZED REVERSIBLE JUMP MARKOV CHAIN MONTE CARLO METHOD

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ABSTRACT

Reversible jump Markov chain Monte Carlo (RJMCMC) is a powerful Bayesian trans-dimensional algorithm for performing model selection while inferring the distribution of model parameters. Despite the general applicability of this trans-dimensional sampler, there remains a question about the degree to which the resulting Markov Chains have converged and can provide accurate samples from the desired stationary distribution. The present work introduces a parallel RJMCMC implementation that aims to increase the accessibility of RJMCMC to practitioners and to help assess the accuracy and convergence of Markov Chains generated from applying RJMCMC to real data.

1 INTRODUCTION

When attempting to describe a system with a model, one is frequently uncertain about the precise model form to use. Theory, experience, or hunches can all play a role in defining a plausible model space to explore. *Model selection* is the name frequently given to this challenging problem, along with the concomitant problem of parametric instantiation of the selected model. Object recognition, image segmentation, and change-point analysis are a few examples where one must evaluate both the model and corresponding, within-model, parameters for a given problem. The *Reversible jump Markov chain Monte Carlo (RJMCMC)* method embodies a trans-dimensional Bayesian framework for estimating a joint posterior distribution over the space of models, and their associated model-parameters (Green 1995; Green et. al 2009) RJMCMC has been used in a diverse range of disciplines such as Statistics/Probability, Computer Science, Engineering and Biology (Sisson 2005). While interest in RJMCMC within the scientific community is expected, what is a bit unexpected is that it is not more widespread in its use, given the impressive theoretical benefits accompanying its application. We believe that this state of affairs is an artifact of a combination of factors that make implementing RJMCMC complicated and create difficulties when interpreting results from RJMCMC analyses.

Despite RJMCMC's provable ability to navigate complex trans-dimensional probability spaces, and subsequently converge to the correct stationary joint posterior distribution, there are currently significant practical impediments to using this method, such as: 1) how to translate the complex mathematical descriptions into reliable code; and 2) how to properly assess convergence and accuracy when applying the method to real data. For example, do the individual model Markov chains contain sufficiently representative samples? Have all the individual competing models received due consideration by the method? To overcome these issues, we present an open source software system, CU-MSDSp (**C**ornell **U**niversity-Model Selection **D**ependent **S**earch in **P**arallel) for implementing RJMCMC in parallel; and in manner that is flexible enough to work well in many different problem contexts.

2 SOFTWARE DESIGN

Our software, approaches the evaluation of the joint posterior distribution of model index and model parameters by, first, independently forming Markov chains to approximate the posterior distribution of model parameters associated with each of the candidate models. These chains are assumed to have suitably converged to their target stationary distribution, and hence, are referred to as *gold standard* chains. Then, these gold standard parameter chains are incorporated into a separate parallel RJMCMC algorithm, to approximate the posterior distribution of model indices. We refer readers to more of the technical details of RJMCMC and similar parallel approaches (Ye et. al 2009;Green 1995; Sisson 2005).

CU-MSDSp is constructed from a mixture of C++, C, Bash, and Python software elements. In particular, it adopts a *single program multiple data (SPMD)* programming model; using *Message Passing Interface (MPI)* for its implementation. The gold standard parameter chains are estimated via calls to Stan *application programming interface (API) for C++* (Carpenter et. al); an open source API that automates Bayesian MCMC sampling. These gold standard chains are then used to approximate the posterior probability of the model given the data. This is realized in parallel using MPI, where processors are responsible for instantiating a Markov chain to estimate the model probabilities. A numerical estimate of each model's parameter posterior distribution is required in order to estimate model selection probabilities via Green's RJMCMC algorithm. Currently, we only implement a Gaussian kernel density estimate, but users have the flexibility to implement kernel densities of their choice. Finally, our software provides automated visualizations which include trace plots for each model's parameter's marginal posterior distributions and the acceptance probability from model selection.

3 DISCUSSION

RJMCMC is a powerful trans-dimensional Bayesian framework that assists in model selection and each model’s associated parameters. We believe that, in spite of RJMCMC’s general applicability, the lack of traction emanates from the complex theoretical basis for the method and difficulty in turning “math into code” for this method. Additionally, RJMCMC appears to suffer from difficulty in gauging convergence. We present software, CU-MSDSp, that address these challenges by approximating posterior distributions for model indices and model parameters separately. This simplification is expected to help researchers better identify when results obtained from RJMCMC have converged and hence, are robust to repeats of analysis. Finally, CU-MSDSp increases computational efficiency through parallelism; enhances user understanding regarding the RJMCMC algorithm, and bolster user confidence concerning convergence properties within RJMCMC characterization of the competing models via the joint model/model parameters posterior distribution.

ACKNOWLEDGEMENTS

The authors would like to acknowledge the support of the Science Mathematics and Research for Transformation (SMART) program as funded by the USD/R&E (Under Secretary of Defense-Research and Engineering) and National Defense Education Program (NDEP)/ BA-1, Basic Research. The same author also thanks the Alfred P. Sloan Foundation’s Minority Ph.D. (MPHD) Program (Award No. 70481).

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