Note: this cover letter was not submitted itself. Rather, the text from it was included in a text box in the submission to Bayesian Analysis.

Dear Madam/Sir,

Please find attached our submission to Bayesian Analysis titled “R\*: A robust MCMC convergence diagnostic with uncertainty using gradient-boosted machines”.

MCMC continues to be a mainstay of applied Bayesian inference, and the popularity of software packages implementing flavours of these algorithms is testament to this. The ease with which MCMC can be used for inference masks the ease of its misuse: namely, that unless Markov chains have run until convergence, the resultant samples will be biased. The predominant approach for determining convergence is to run multiple Markov chains in parallel and monitor their summary statistics: typically, by calculating Rhat. Additionally, other summaries like effective sample size (ESS) are gaining traction as useful warning signs for poor convergence.

Both Rhat and ESS are (typically) univariate measures, which examine the sampling distribution along its marginals. This means that Rhat can detect if there is between-chain variation in the marginal distributions of each parameter. It is, however, unable to detect differences in the joint sampling distributions obtained across chains, unless there are differences in the marginals. For instance, for high dimensional target distributions with high correlations between dimensions, this focus on the marginals may falsely detect convergence.

In this paper, we propose a new measure of chain convergence that we call R\*. This measure is based on the observation that, if chains have fully mixed, it should not be possible to discern the individual chain responsible for a particular draw. Building on this idea, we train a machine learning classifier (specifically a gradient-boosted machine) on the chain-labelled MCMC draws and evaluate its performance on a separate test set. If the predictive accuracy is above baseline, this indicates that the draws contain information of the causative chain, and the chains have not mixed.

Here, we evaluate R\* on a number of test problems and show that it provides convergence information complementary to existing measures like Rhat and ESS. We show that, by leveraging all information in the joint distribution, R\* generally provides a more stringent test of convergence than existing measures. It is also a conservative measure and tends not to indicate convergence unless there are sufficient MCMC draws to do so. R\* could straightforwardly be integrated into existing statistical software to provide these additional checks on convergence, and we provide links to an open-source implementation of R\* coded in the R language.

We hope that you will consider this paper for inclusion in Bayesian Analysis and look forward to hearing from you.

Yours faithfully,

Ben Lambert & Aki Vehtari