Appraisal of jump distributions in ensemble-based sampling algorithms

Sanda Dejanic, Andreas Scheidegger, Jörg Rieckermann, and Carlo Albert

Eawag, Swiss Federal Institute of Aquatic Science and Technology, Dübendorf, Switzerland (sanda.dejanic@eawag.ch)

Sampling Bayesian posteriors of model parameters is often required for making model-based probabilistic predictions. For complex environmental models, standard Monte Carlo Markov Chain (MCMC) methods are often infeasible because they require too many sequential model runs. Therefore, we focused on ensemble methods that use many Markov chains in parallel, since they can be run on modern cluster architectures. Little is known about how to choose the best performing sampler, for a given application. A poor choice can lead to an inappropriate representation of posterior knowledge. We assessed two different jump moves, the stretch and the differential evolution move, underlying, respectively, the software packages EMCEE and DREAM, which are popular in different scientific communities. For the assessment, we used analytical posteriors with features as they often occur in real posteriors, namely high dimensionality, strong non-linear correlations or multimodality. For posteriors with non-linear features, standard convergence diagnostics based on sample means can be insufficient. Therefore, we resorted to an entropy-based convergence measure. We assessed the samplers by means of their convergence speed, robustness and effective sample sizes. For posteriors with strongly non-linear features, we found that the stretch move outperforms the differential evolution move, w.r.t. all three aspects.