Comment: Extracting More Diagnostic Information from a Single Run Using Cusum Path Plot

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The article by Besag, Green, Higdon and Mengersen adds to a series of recent papers (Besag and Green, 1993; Geyer and Thompson, 1992; and Gelman and Rubin, 1992b) in making Markov chain Monte Carlo (MCMC) methods accessible to more statisticians, especially applied statisticians. I am glad to see that different algorithms are reviewed in a unified way and many examples are given. Although the article gives general recommendations as to which algorithms and sampling scans to choose, there is not much discussion on the empirical monitoring of convergence of the Markov chains. Since the convergence issue is very critical to the success of MCMC methods, and something close to my heart, I will make this issue my topic here. In particular, using the prostate cancer example in the article by Besag, Green, Higdon and Mengersen and the Ising model example in Gelman and Rubin (1992a), I illustrate that the cusum path plot in Yu and Mykland (1994) can effectively bring out the local mixing property of the Markov chain.

It had been believed by many MCMC researchers (including this author) that information solely from a single run of a Markov chain can be misleading since, for example, it can get trapped at a local mode of the target density. Consequently, additional information beyond that from a single run has been introduced to the convergence diagnostics. Gelman and Rubin (1992b) proposed a multiple chain approach in the MCMC context, followed by Liu, Liu and Rubin (1992) and Roberts (1992). Yu (1994) introduced additional information to a single run by taking advantage of the unnormalized target density. In the context of Gibbs samplers, Ritter and Tanner (1992) and Cui, Tanner, Sinhua and Hall (1992) suggested diagnostic statistics based on importance weights, using either multiple chains or a single chain. A priori bounds on the convergence rate can be found in Rosenthal (1993) and Mengersen and Tweedie (1993), but unfortunately these theoretical bounds are currently known only in some very special cases. For other references on existing diagnostic tools, see the recent and thorough review by Cowles (1994).

On the other hand, Yu and Mykland (1994) suggest that more information can be extracted from a single run than previously believed. The device is the cusum path plot, which brings out the local mixing behavior of the Markov chain in the direction of a chosen one-dimensional summary statistic, more effectively than the sequential plot. The cases where the cusum path plot works well are those where the mixing behavior is homogeneous across the sample space. For example, in some multimodal examples, the reason that the chain gets trapped at a local mode is because the chain moves around very slowly, even within one mode, and the cusum path plot brings out this local mixing speed even when the sampler is trapped at one mode. As shown below, the Ising model example of Gelman and Rubin (1992a) has a slow local mixing property. One situation in which the cusum path plot fails is a variant on the witch's hat (cf. Cui, Tanner, Sinhua and Hall, 1992; Yu and Mykland, 1994), where the chain has a split mixing behavior: fast in one region and slow in another.

Now we introduce the cusum path plot formally. Let $X_0, X_1, \ldots, X_n$ be a single run of a Markov chain, and let $T(X)$ the chosen one-dimensional summary statistic. Let n_0 be the "burn-in" time, and we construct our cusum statistics based on $T(X_{n_0+1}), \ldots, T(X_n)$ to avoid the initial bias of the chain. What we get out of the cusum plot is the more detailed information we cannot see in the sequential plot of $T(X)$ which MCMC users have been plotting all along.

Denote the observed cusum or partial sum as

$$\hat{S}_t := \sum_{j=n_0+1}^{t} \left[T(X_j) - \hat{\mu}\right] \quad \text{for } t = n_0 + 1, \ldots, n,$$

where

$$\hat{\mu} := \frac{1}{n - n_0} \sum_{j=n_0+1}^{n} T(X_j).$$

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