Convergence assessment techniques for Markov chain Monte Carlo

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MCMC methods have effectively revolutionised the field of Bayesian statistics over the past few years. Such methods provide invaluable tools to overcome problems with analytic intractability inherent in adopting the Bayesian approach to statistical modelling.

However, any inference based upon MCMC output relies critically upon the assumption that the Markov chain being simulated has achieved a steady state or "converged". Many techniques have been developed for trying to determine whether or not a particular Markov chain has converged, and this paper aims to review these methods with an emphasis on the mathematics underpinning these techniques, in an attempt to summarise the current "state-of-play" for convergence assessment techniques and to motivate directions for future research in this area.

Keywords: MCMC, Gibbs Sampler, Metropolis Hastings, Convergence Rate

1 Introduction

One of the most important implementational problems associated with Markov chain Monte Carlo simulation is caused by the transient phase of the Markov chain, that is the time before the chain settles down to stationary behaviour. In order to reduce the possibility of bias caused by the effect of starting values, iterates within this initial transient phase or *burn in* period are usually discarded. One of the most difficult implementational problems is that of determining the length of the required burn in, since rates of convergence of algorithms on different target distributions vary considerably.

Ideally, we would like to analytically compute or estimate the Markov chain convergence rate and then take sufficient iterations to satisfy any prescribed accuracy criteria. However, this is not possible in general (Tierney,

1994). In fact for Markov chains it is extremely difficult to prove even the existence of a geometric rate of convergence to stationarity (Roberts and Tweedie, 1996b, 1996a) and there are many commonly used algorithms which frequently fail to converge geometrically quickly at all.

Roberts and Polson (1994), Chan (1993) and Schervish and Carlin (1992) provide qualitative geometric convergence results for quite general classes of target densities. However, although these results have theoretical import in ensuring the existence of central limit theorems for instance, they do not offer explicit bounds on the rate of convergence which could be used to determine MCMC sample lengths.

Certain specialised techniques exist to *bound* convergence rates (and hence required burn in lengths) for Markov chains. See for example Lawler and Sokal (1988), Sinclair and Jerrum (1988), Diaconis and Strook (1991), Meyn and Tweedie (1993), and Roberts and Tweedie (1998). However, in general it is difficult to apply these results effectively in the context of MCMC. Notable exceptions include Applegate *et al.* (1990), Amit and Grenander (1991), Amit (1991), Rosenthal (1995a) and Polson (1996).

We argue that because of the fact that theoretical convergence times vary widely (especially in high dimensional problems), and in the absence of any general techniques for

a priori prediction of run lengths, it is necessary to carry out some form of statistical analysis in order to assess convergence. We call such procedures convergence diagnostics. There exist various informal methods for the diagnosis of convergence for example Gelfand's *thick pen technique* (Gelfand *et al.*, 1990), and the use of quantile plots and autocorrelation plots as suggested in Gelfand and Smith (1990). These methods are extremely easy to implement, and can provide a feel for the behaviour of the Markov chain.

However, many more elaborate methods have been proposed in the literature, all of which methods can in some way claim to be more reliable assessors of convergence. This paper aims to review the theory behind these methods, thereby allowing us to make general qualitative statements on the effectiveness of the various techniques. We establish a common notation and show how many of the methods are essentially variations on the same general approach to the problem. We categorise the methods according to the underlying mathematical approach being adopted and suggest improvements and extensions to many of the most common techniques. Thus, we focus on the mathematics of these approaches and not upon their practical implementation. The reader is referred to Cowles and Carlin (1996) for such a review.

As with all statistical procedures, any convergence diagnostic technique cannot be guaranteed to successfully diagnose convergence. In particular, for slowly mixing Markov chains, convergence diagnostics are likely to be unreliable since their conclusions will be based upon output from only a small region of the state space. These ideas are formalised by Asmussen *et al.* (1992). Therefore it is important to emphasise that any convergence diagnostic procedure should not be unilaterally relied upon. Moreover, the use of additional methods for increasing understanding of the target distribution are strongly recommended. There are a number of useful techniques for *a priori* exploration of the target distribution in order to suggest an appropriate Markov chain for simulation and an appropriate collection of starting values. These methods include simulated tempering (see Geyer and Thompson, 1995), simulated annealing (see for example Jennison, 1993 and Applegate *et al.* 1990 in this context) and other mode hunting methods such as that proposed by Gelman and Rubin (1992).

There are also a number of methods which, whilst not actually diagnosing convergence, attempt to "measure" the performance of any particular sampler. These can be used either instead of or in addition to the diagnostic methods to be discussed in this paper. Such methods include that described by Brooks (1998b) which can be applied to problems where the stationary distribution of the sampler is log-concave. In this case, an upper bound can be put on the proportion of the parameter space covered by a particular output sequence. This provides a measure as to how well the chain has explored the parameter space, and an indication as to how well inference based upon the sampler output may reflect characteristics of the stationary distribution.

Before we introduce and discuss the various diagnostic methods, we shall briefly describe the two most common MCMC algorithms, namely the Gibbs sampler and the Metropolis Hastings algorithm. We shall also describe the notation that we will adopt throughout the paper.

We let $X^t \in E \subseteq \mathbb{R}^p$ denote the (p-dimensional) state of an arbitrary chain at time t (simply using X, when $p = 1$). Often, we will refer to several chains run simultaneously, in which case we let X_i^t denote the state of chain i at time t, with $X_{i(j)}^t$ denoting the jth element of the vector X_i^t. It will also be necessary, on occasion, to refer not to the state of a Markov chain directly, but some function of X. Such functions will generally be denoted by $\theta_i^t = \theta(X_i^t)$.

1.1 The Metropolis Hastings algorithm

The Metropolis Hastings algorithm and its application to Monte Carlo sampling, was first described by Hastings (1970) as an extension of the earlier results of Metropolis *et al.* (1953). To construct a Markov chain $\{X^0, \ldots, X^t, \ldots\}$ with state space E, and equilibrium distribution π, the Metropolis Hastings algorithm obtains state X^{t+1} from state X^t as follows. Define q to be an arbitrary Markov transition kernel density (normally either with respect to Lebesgue measure, counting measure or a combination of the two), and let $\alpha(x, y)$ be a function taking values in $[0, 1]$. Then, given that the chain is in state $X^t = x$ at time t, the Metropolis Hastings algorithm generates a candidate value y for the next state X^{t+1}, from the distribution $q(x, \cdot)$. With probability $\alpha(x, y)$ this candidate is accepted as the new state so that $X^{t+1} = y$, otherwise it is rejected and the chain remains at $X^{t+1} = x$.

In this way we obtain a Markov chain with transition kernel with density part

$$\mathcal{K}_H(x^t, x^{t+1}) = q(x^t, x^{t+1})\alpha(x^t, x^{t+1}), \quad x^{t+1} \neq x^t$$

and with

$$\mathbb{P}[X^{t+1} = x^t | X^t = x^t] = 1 - \int_E q(x^t, y)\alpha(x^t, y)\,\mathrm{d}y.$$

There are many acceptance functions α which may be chosen so as to ensure the correct stationary distribution for the chain. However, Peskun (1973) shows that the optimal form for the acceptance function, in the sense that it rejects suitable candidates less often than other forms and therefore mixes quicker, is given by

$$\alpha(x^t, x^{t+1}) = \min\left(\frac{\pi(x^{t+1})q(x^{t+1}, x^t)}{\pi(x^t)q(x^t, x^{t+1})}, \quad 1\right). \quad (1)$$

Note that though the choice of transition kernel q, is arbitrary, it must satisfy certain conditions in order to

guarantee convergence, see for example Roberts and Smith (1994).

1.2 The Gibbs sampler

The Gibbs sampler splits the p-dimensional parameter space into $k \leq p$ blocks. Let $\pi(\boldsymbol{x}) = \pi(\boldsymbol{x}_{(1)}, \ldots, \boldsymbol{x}_{(k)})$, $\boldsymbol{x} \in \mathbb{R}^p$ denote the joint density of $\boldsymbol{x}$ and $\pi_i(\boldsymbol{x}_{(i)}|\boldsymbol{x}_{(-i)})$ denote the full conditional density for the ith element, $\boldsymbol{x}_{(i)}$, of $\boldsymbol{x}$, given each of the other $k - 1$ components, where $\boldsymbol{x}_{(-i)} = \{\boldsymbol{x}_{(j)} : j \neq i\}$ for $i = 1, \ldots, k$. Then the Gibbs sampler, as proposed by Geman and Geman (1984), proceeds as follows.

We begin by picking an arbitrary starting point $\boldsymbol{x}^0$ and then successively sample from the full conditional $\pi_i(\boldsymbol{x}_{(i)}|\boldsymbol{x}_{(-i)})$, by sampling $\boldsymbol{x}^1_{(i)}$ from $\pi_i(\boldsymbol{x}_{(i)}|\boldsymbol{x}^1_{(j)} \ j < i, \ \boldsymbol{x}^0_{(j)} \ j > i)$, $i = 1, \ldots, k$, to generate the next state $\boldsymbol{x}^1$. This process is then repeated to produce a sequence $\boldsymbol{x}^0, \boldsymbol{x}^1, \ldots, \boldsymbol{x}^t, \ldots$ of states from a Markov chain with transition probability

$$\mathscr{K}_G(\boldsymbol{x}, \boldsymbol{y}) = \prod_{l=1}^{k} \pi_l(\boldsymbol{y}_{(l)}|\boldsymbol{y}_{(j)} \text{ for } j < l, \text{ and } \boldsymbol{x}_{(j)} \text{ for } j > l)$$

and which has stationary distribution, π.

Other algorithms commonly used, usually consist of modifications or hybrids of these two methods. See Brooks (1998a) for a comprehensive review of such methods.

1.3 Outline of the Paper

Having introduced the two main MCMC algorithms, we now focus upon techniques for determining whether of not a particular Markov chain has converged to its stationary distribution. Some of the techniques that we shall discuss in this paper, are rather informal statistical methods based on monitoring selected output from the Markov chain itself. Such procedures can often be implemented with little extra computational expense. We broadly term such approaches under the heading *output analysis*, and these are discussed in Section 2.

Other methods try to exploit aspects of the theoretical properties of the sampler, sometimes requiring the monitoring of more complicated functionals of the Markov chain, or even additional simulation. These methods, though still inherently statistical, are typically more complicated to implement than straightforward output analyses and we discuss such approaches in Section 3.

Probabilistic constructions for Markov chains can sometimes suggest alternative ways to implement Markov chains, which are better geared towards convergence assessment. Such approaches switch the emphasis away from empirical diagnostic methods. We discuss exact and approximate techniques based around these ideas in Section 4.

Finally, no convergence diagnostic techniques are foolproof and *a priori* run length determination techniques are rarely available in many practical problems. However notable exceptions do exist, and we discuss analytic estimates for convergence rates and running times of Markov chains in Section 5, together with statistical methods for estimating Markov chain convergence rates.

2 Output analysis

Techniques in this section are amongst the simplest to implement. They require only the output from one or more MCMC simulations, requiring no knowledge of the mechanism generating the output. In particular, all of these methods can be implemented by freely available computer code putting these techniques amongst the most popular of all those proposed in the literature.

2.1 Variance ratio methods

The method of Gelman and Rubin (1992) consists of analysing m independent sequences to form a distributional estimate of the variance of some random variable, given the observations simulated so far. It provides a basis for an estimate of how close the process is to stationarity and, in particular, how much we might expect the estimate to improve with further simulation.

The method is based upon a simple analysis of variance for some scalar functional of interest, $\theta(\boldsymbol{x})$. If θ were known to have variance σ^2 under the target distribution, π then our degree of information about θ could be represented by $1/\sigma^2$. The method of Gelman and Rubin is based upon the idea that if we could estimate σ^2 by $\widehat{V}$, say, from the output of the sample, then the ratio $\widehat{V}/\sigma^2$ provides us with an estimate of what proportion of the total amount of information available about θ has been obtained from the simulations used to construct $\widehat{V}$.

The estimator $\widehat{V}$ is constructed by forming a weighted average of the between and within chain variance estimators. We begin by defining B/n, the variance between the m sequence means as

$$\frac{B}{n} = \frac{1}{m-1} \sum_{i=1}^{m} (\bar{\theta}_i - \bar{\theta}_.)^2,$$

where

$$\bar{\theta}_i = \frac{1}{n} \sum_{t=n+1}^{2n} \theta_i^t, \quad \bar{\theta}_. = \frac{1}{m} \sum_{i=1}^{m} \bar{\theta}_i$$

and $\theta_i^t = \theta(\boldsymbol{x}_i^t)$ is the tth observation of θ from chain i. We then calculate W, the mean of the m within-sequence variances, s_i^2, each of which is based upon $n - 1$ degrees of freedom. Thus, W is given by

$$W = \frac{1}{m} \sum_{i=1}^{m} s_i^2,$$

where

$$s_i^2 = \frac{1}{n-1} \sum_{t=n+1}^{2n} (\theta_i^t - \bar{\theta}_i)^2.$$

Then we define our estimator $\widehat{V}$ by

$$\widehat{V} = \frac{n-1}{n} W + \left(1 + \frac{1}{m}\right) \frac{B}{n}. \tag{2}$$

Having obtained the estimator $\widehat{V}$ we would ideally wish to monitor $\widehat{R} = \widehat{V}/\sigma^2$ as the simulation proceeds, and stop once $\widehat{R}$ is sufficiently close to 1 to indicate that continuing the chain any further would yield little extra information. However, σ^2 is unknown, but can be (under) estimated by W, thus we monitor

$$\widehat{R}_c = \frac{d+3}{d+1} \frac{\widehat{V}}{W},$$

where $(d+1)/(d+3)$ is a correction term compensating for the approximations inherent in the estimator $\widehat{R}_c$, see Gelman and Rubin (1992) and Brooks and Gelman (1998).

Gelman and Rubin (1992) suggest that the value of $\widehat{R}_c$, which is called the *potential scale reduction factor* (PSRF), can be interpreted as a convergence diagnostic as follows. If $\widehat{R}_c$ is large, this suggests that either the estimate of the variance, $\widehat{V}$, can be further decreased by more simulations, or that further simulation will increase W, since the simulated sequences have not yet made a full tour of the target distribution. Alternatively, if the PSRF is close to 1, they argue that we can conclude that each of the m sets of n simulated observations is close to the target distribution.

This original method has subsequently been generalised by Brooks and Gelman (1998). First of all, they suggest alternative implementations of this univariate diagnostic, by proposing the use of moments other than those of second order. Set

$$\widehat{R}_s = \frac{\frac{1}{mn-1} \sum_{i=1}^{m} \sum_{t=n+1}^{2n} |\bar{\theta}_i^t - \bar{\theta}_.|^s}{\frac{1}{m(n-1)} \sum_{i=1}^{m} \sum_{t=n+1}^{2n} |\theta_i^t - \bar{\theta}_i|^s},$$

for $s = 2, 3, 4, \ldots$. Clearly, in the case where $s = 2$, this is directly comparable to the original method. Brooks and Gelman (1998) also suggest an alternative based upon empirical interval lengths.

They construct an interval-based $\widehat{R}$ measure as follows. From each individual chain, take the empirical $100(1-\alpha)\%$ interval, i.e., the $100\frac{\alpha}{2}\%$ and the $100(1-\frac{\alpha}{2})\%$ points of the n simulation draws, thus forming m within-sequence interval lengths. Then, from the entire set of observations, gained from all chains together, calculate the empirical $100(1-\alpha)\%$ interval, gaining a total-sequence interval length. Finally, evaluate $\widehat{R}$ defined as

$$\widehat{R}_{\text{interval}} = \frac{\text{length of total-sequence interval}}{\text{average length of the within-sequence intervals}}. \tag{3}$$

This method is considerably simpler than the original method. It is very easy to implement and does not even require the existence of second moments, let alone normality. $\widehat{R}_{\text{interval}}$ is still a PSRF, but based upon empirical interval lengths as a measure of information, rather than variance estimates.

An alternative method is also provided by Brooks and Gelman (1998), which generalises the original method to consider more than one parameter simultaneously. Let θ denote a vector of parameters, then Brooks and Gelman (1998) estimate the posterior variance-covariance matrix by

$$\widehat{V} = \frac{n-1}{n} W + \left(1 + \frac{1}{m}\right) B/n,$$

where

$$W = \frac{1}{m(n-1)} \sum_{j=1}^{m} \sum_{t=n+1}^{2n} (\theta_j^t - \bar{\theta}_j)(\theta_j^t - \bar{\theta}_j)'$$

and

$$B/n = \frac{1}{m-1} \sum_{j=1}^{m} (\bar{\theta}_j - \bar{\theta}_.)(\bar{\theta}_j - \bar{\theta}_.)',$$

denote the (p-dimensional) within and between-sequence covariance matrix estimates of the p-variate functional θ, respectively.

They then show that if λ_1 is the largest eigenvalue of the symmetric and positive definite matrix $W^{-1}B/n$, then

$$\widehat{R}^p = \frac{n-1}{n} + \left(\frac{m+1}{m}\right) \lambda_1$$

bounds above all of the $\widehat{R}_c$ values associated with any linear function of the univariate elements of θ. They call $\widehat{R}^p$ the Multivariate PSRF (MPSRF). The advantage of the MPSRF is inherent in the fact that it reliably summarises each of the univariate measures in a single value, with only a nominal increase in computational expense. However, the authors suggest combining a number of alternative approaches. For example, for high dimensional problems, the MPSRF may be calculated for all parameters, and the PSRFs for each of the parameters of primary interest.

2.2 Spectral methods

Functionals of positive-recurrent Markov chains are special cases of stationary time series, so it is natural to use time series methods to try to assess convergence. Here, we discuss two diagnostic methods which use standard techniques from spectral analysis in order to gain variance estimates via the spectral density, $S(\omega)$.

2.2.1 Geweke's spectral density diagnostic

Suppose that we wish to estimate the expected value of some functional, $\theta(X)$. If we let $\theta^t = \theta(X^{(t+n_0)})$, for $t = 1, \ldots, n$ then, given the sequence $\{\theta^t\}$, Geweke (1992) suggests that if the chain has converged by time n_0, then we should accept a test of equal location for two subsequences $\{\theta^t : t = 1, \ldots, n_A\}$ and $\{\theta^t : t = n^*, \ldots, n\}$, where $1 < n_A < n^* < n$. Define $n_B = n - n^* + 1$,

$$\bar{\theta}_A = \frac{1}{n_A} \sum_{t=1}^{n_A} \theta^t \quad \text{and} \quad \bar{\theta}_B = \frac{1}{n_B} \sum_{t=n^*}^{n} \theta^t,$$

and let $\widehat{S}_\theta^A(0)$ and $\widehat{S}_\theta^B(0)$ denote consistent spectral sensitivity estimates for $\{\theta^t : t = 1, \ldots, n_A\}$ and $\{\theta^t : t = n^*, \ldots, n\}$ respectively. Note that elementary spectral analysis illustrates that $\widehat{S}_\theta^A(0)$ is also a consistent estimator for the true variance of θ, allowing for the fact that the set $\{\theta^t : t = 1, \ldots, n_A\}$ is a dependent set of observations, see Ripley (1987) for example.

Then, if the ratios n_A/n and n_B/n are fixed, with

$$\frac{(n_A + n_B)}{n} < 1$$

and if the sequence $\{\theta^t\}$ is stationary, then

$$Z_n = \frac{(\bar{\theta}_A - \bar{\theta}_B)}{\sqrt{\frac{1}{n_A}\widehat{S}_\theta^A(0) + \frac{1}{n_B}\widehat{S}_\theta^B(0)}} \xrightarrow{d} N(0,1) \quad \text{as } n \to \infty. \quad (4)$$

We can use this result to test the null hypothesis of equal location, which, if it is rejected (i.e.; $|Z_n|$ is large), indicates that the chain has not converged by time n_0.

Geweke (1992) suggests taking $n_A = n/10$ and $n_B = n/2$, arguing that these choices meet the assumptions underlying (4) whilst attempting to provide diagnostic power against the possibility that the $\{\theta^t\}$ process was not fully converged early on.

This method could be generalised to make use of multiple replications by using standard Analysis of Variance techniques to test for differences between replications. It might also be generalised to consider the full joint density rather than the marginals by taking the log posterior density as the scalar functional of interest.

In practice, it should be noted that this diagnostic attempts to verify a necessary, but not sufficient, condition for convergence. Thus, it can only inform the user when convergence has not been achieved, and not when it has. Experience with this diagnostic also highlights its sensitivity to the specification of the spectral window. The choice is arbitrary, and there seem to be no general guidelines available. For further discussion of the problems associated with spectral sensitivity estimation, see Ripley (1987).

2.2.2 Heidelberger and Welch's convergence diagnostic

The method of Heidelberger and Welch (1983) confines itself to univariate observations and only single replications. It combines earlier methodology, by Schruben (1982) and Schruben *et al.* (1983), on the application of statistics distributed as Brownian Bridges to the detection of transient phases, with an earlier run length control procedure described by Heidelberger and Welch (1981a, b).

We begin by assuming that, in the steady state, we have a covariance (or weakly) stationary process. This is a reasonable assumption since we are interested in sequences generated from Markov chains, and which therefore have full stationarity.

In order to test the null hypothesis of stationarity, we first suppose that we have a sequence $\{X^t : t = 1, \ldots, n\}$ from a covariance stationary process with unknown spectral density, $S(\omega)$. Then, for $n \geq 1$, we let

$$Y_0 = 0, \quad Y_n = \sum_{t=1}^{n} X^t \quad \text{and} \quad \bar{X} = \frac{1}{n} Y_n,$$

and define

$$\widehat{B}_n(s) = \frac{(Y_{[ns]} - [ns]\bar{X})}{(n\widehat{S}(0))^{\frac{1}{2}}} \qquad 0 \leq s \leq 1,$$

where $[a]$ denotes the greatest integer less than or equal to a, and $\widehat{S}(0)$ is an estimate of the spectral density formed from only the second half of the currently considered data, in order to avoid possible over-estimation in the presence of an initial transient.

Then, for large n, $\widehat{B}_n = \{\widehat{B}_n(s) : 0 \leq s \leq 1\}$ will be distributed approximately as a Brownian Bridge, and we can use various statistics such as the Cramer-von Mises Statistic (von Mises, 1931), the Kolmogorov-Smirnov statistic (Kolmogorov, 1933), or Schruben's statistic (Schruben *et al.*, 1983) to test the null hypothesis of stationarity. Heidelberger and Welch (1983) suggest an iterative procedure, based upon repeated hypothesis tests of these statistics, in order to estimate the length of the burn-in.

This diagnostic uses only single replications and considers only univariate marginals, one at a time. The method may be generalised by making use of the multi-dimensional and multi-sample analogues of the Kolmogorov-Smirnov statistic. See Conover (1965, 1967), Chorneyko and Zing (1982), Fasano and Franceschini (1987) and Ahmad (1976), for example.

Returning to the proposed diagnostic, it should be noted that the stationarity tests will have very little power to detect an initial transient when the run length is shorter than the length of that transient, i.e.; when the whole sample sequence is within the transient phase. It might also

be noted that the sequential use of hypothesis tests should not be performed without some correction factor being combined with the test statistic to allow for the fact that multiple tests are being performed, see Brittain (1987). Finally, we note that, as with Geweke's method, we need to estimate the spectral density at frequency zero. As before, the diagnostic is highly dependent upon this estimate. However, Heidelberger (1981a) suggest a suitable estimator for use with this problem.

2.3 Yu and Mykland's CUSUM method

The CUSUM method is a graphical method which monitors convergence via a CUSUM plot based upon the sampler output. It was proposed by Yu and Mykland (1998) and further discussed in Yu (1995a) and Brooks (1998c). It can be applied to any sampler and can be implemented by generic problem-independent code.

Given the output $\{x^1, ..., x^n\}$, we begin by discarding the initial n_0 iterations, which we believe to correspond to the burn-in period. We then construct CUSUM path plots for some scalar summary statistic θ, as follows:

1. Calculate

$$\widehat{\mu} = (n - n_0)^{-1} \sum_{\tau=n_0+1}^{n} \theta(x^\tau).$$

2. Calculate the CUSUM or partial sum

$$\widehat{S}_t = \sum_{\tau=n_0+1}^{t} [\theta(x^\tau) - \widehat{\mu}] \quad \text{for } t = n_0 + 1, \ldots, n.$$

3. Plot $\{\widehat{S}_t\}$ against t for $t = n_0 + 1, \ldots, n$, connecting successive points by line segments.

Yu and Mykland (1998) argue that the speed with which the chain is mixing is indicated by the smoothness of the resulting CUSUM plot, so that a smooth plot indicates slow mixing, whilst a "hairy" plot indicates a fast mixing rate for θ. They justify their argument by referring to the theoretical work of Lin (1992, p323) which examines the behaviour of partial sums of ϕ-mixing sequences.

In practice, the assessment of smoothness based upon a single plot is, at best, subjective. In order to improve the method, in terms of its subjectivity, Yu and Mykland (1998) suggest adding a "benchmark" CUSUM plot, based upon a sequence of *iid* normal variates with mean and variance matched to estimated moments of the θ sequence. The authors argue that this plot approximates, to the second order, the "ideal" CUSUM path for an *iid* sequence from the target distribution. Thus, a favourable comparison of the two plots, in terms of smoothness and size of excursion, indicates that the chain is mixing well in terms of the statistic, θ. Brooks (1998c) proposes an alternative implementation in an attempt to make this diagnostic more objective.

Let us first obtain a mathematical definition of "hairiness" in the sense discussed by Yu and Mykland (1998). A smooth plot is formed from line segments with the same or similar slope, whilst a perfectly "hairy" plot will consist of line segments which alternately have positive and negative slope, so that each point corresponds to a local optimum. Thus, if we count the number of such points, we get an index of "hairiness" associated with the plot.

If we define

$$d_t = \begin{cases} 1 & \text{if } S_{t-1} > S_t \text{ and } S_t < S_{t+1} \\ & \text{or } S_{t-1} < S_t \text{ and } S_t > S_{t+1}, \\ 0 & \text{else} \end{cases} \quad (5)$$

for all $t = n_0 + 1, \ldots, n - 1$. Then,

$$D_{n_0,n} = \frac{1}{n - n_0} \sum_{t=n_0+1}^{n-1} \mathrm{d}_t$$

takes values between 0 and 1, where a value of 0 indicates a totally smooth plot and a value of 1, indicates maximum "hairiness".

Brooks (1998c) shows that we can treat $D_{n_0,n}$ as a binomial outcome with mean $\frac{1}{2}$ and variance $\frac{1}{4(n-n_0)}$. The Law of Large Numbers ensures that, for large $n - n_0$, the $D_{n_0,n}$ will be approximately normal, so that we can detect a lack of convergence if the $D_{n_0,n}$ statistic lies beyond the bounds

$$\frac{1}{2} \pm Z_{\alpha/2} \sqrt{\frac{1}{4(n - n_0)}}. \quad (6)$$

The original method, whilst quite simple and problem independent, is rather subjective in its graphical interpretation. By introducing the D sequence, it is possible to make the method more quantitative, though this is at the expense of an increase in computation.

Thus, there are various methods which use only the output from one or more replications of the Markov chain in order to diagnose convergence. These are entirely problem-independent methods and are therefore very simple to use. However, a number of problem-specific methods have also been suggested, which use additional information in the form of the transition kernel of the chain, in order to diagnose convergence. We shall discuss these in the next section.

3 Empirical Kernel-Based methods

The methods we discuss in this section use the MCMC simulation output, but also the form of the transition distribution driving the Markov chain, in order to assess convergence. The additional information provided by knowledge of the mechanism generating the output can be utilised to provide a more reliable diagnostic. However,

this is often at the expense of both computational simplicity and expense.

3.1 Weighting methods

Here we discuss two very similar methods for detecting convergence by calculating weighting functions based upon conditional density estimates. The first was proposed by Ritter and Tanner (1992) and attempts to detect convergence of the full joint distribution by monitoring importance weights, calculated from replications of a Gibbs sampler. This method was one of the first to try and assess convergence of the joint distribution and is based upon the method of importance sampling, see Ripley (1987) and Geweke (1989).

If $\mathscr{K}(\cdot, \cdot)$ denotes a Gibbs transition density, then (suppressing dependence on the initial distribution) we can denote the density of X^t by $p^t(x)$, where

$$p^t(x) = \int_E \mathscr{K}(y, x) p^{t-1}(\mathrm{d}y), \quad p^1(x) = \int_E \mathscr{K}(y, x) \pi_0(\mathrm{d}y), \tag{7}$$

and $\pi_0(\cdot)$ denotes the starting distribution for the chain, commonly taken to be a point mass at some point x^0, say.

If we denote the non-normalised stationary distribution by $\tilde{\pi}$ then, at convergence, the importance weights

$$w^t(x) = \frac{\tilde{\pi}(x)}{p^t(x)} \tag{8}$$

should be roughly constant. Of course, $p^t(x)$ is unavailable explicitly, but we can gain an unbiased Monte Carlo approximation in the form of the Rao-Blackwellised estimator

$$\hat{p}^t(x) = \frac{1}{m} \sum_{j=1}^m \mathscr{K}(x_j^{t-1}, x), \tag{9}$$

where $\{x_j^{t-1} : j = 1, \ldots, m\}$ is a sample from p^{t-1}. Ritter and Tanner (1992) suggest sampling from p^{t-1} directly, by drawing m observations at the $(t-1)^{th}$ iteration, i.e. from m parallel replications. This can be very computationally expensive. Alternatively, we may reduce this expense by using the last m states of the chain, $\{x^{t-m}, \ldots, x^{t-1}\}$ since, at convergence, this will simply be a sample from π. This idea can also be extended to the Metropolis Hastings algorithm by a suitable re-definition of p^t (see Gelfand *et al.*, 1992), and to hybrid algorithms such as Metropolis-within-Gibbs, see Müller (1991).

Ritter and Tanner (1992) propose using these importance weights as a convergence diagnostic by running multiple replications of the chain and calculating the weights at equally spaced iterations. Then, for each considered iteration, a histogram of the weights from the different replications is produced until the plots move towards a "spike distribution", indicating convergence.

There are two main problems with this method. Firstly, if the dimension of x is large then we need large m in order for $\hat{p}^t$ to be a good estimate of p^t. Coupled with the need to perform a fairly large number of replications, this means that the method may become computationally very expensive. The need for multiple replications stems from the fact that, since the normalising constant for π is not known, we will not know whether the $\hat{w}^t$'s, (as defined in (8) and substituting $\hat{p}^t$ for p^t), tend to the correct value as $t \to \infty$. It is quite possible that the $\hat{w}^t$'s may remain constant, whilst a mass of π remains unexplored. However, if we use multiple replications and check that they all converge to the same value, then this provides some reassurance that the entire mass of π has been explored. Alternatively, in the special case where we can partition x into $(x_{(1)}, x_{(2)})$ and where the conditionals $p(x_{(1)}|x_{(2)})$ and $p(x_{(2)}|x_{(1)})$ are known standard densities, we may use the weights

$$\hat{w}^t(x_{(1)}, x_{(2)}) = \frac{p(x_{(1)}|x_{(2)})\hat{p}^t(x_{(2)})}{p(x_{(2)}|x_{(1)})\hat{p}^t(x_{(1)})}, \tag{10}$$

where

$$\hat{p}^t(x_{(1)}) = \frac{1}{m} \sum_{j=1}^m p(x_{(1)}|x_{j(2)}^t), \tag{11}$$

and monitor the sequence $\{\hat{w}^t\}$ until it reaches stationarity with mean 1, since both the numerator and denominator are estimates of $p^t(x)$, see Gelfand (1992). This eliminates the need for multiple replications and greatly reduces computational expense.

A similar method to this, called the *Gibbs sampler difference convergence criterion*, was proposed by Zellner and Min (1995) who define their weight function by

$$\hat{w}^t = \hat{p}^t(x_{(1)})p(x_{(2)}|x_{(1)}) - \hat{p}^t(x_{(2)})p(x_{(1)}|x_{(2)}), \tag{12}$$

where each of the densities are normalised, and the $\hat{p}^t$ are as defined in (11). Zellner and Min (1995) argue that if the $\hat{w}^t$ are small, then this indicates that the estimated marginals have converged to the correct values.

Note the clear similarities between this weight function and that proposed by Ritter and Tanner (1992), except here we look at differences rather than a ratio. In fact Zellner and Min (1995) go on to discuss an alternative approach which actually looks at ratios rather than differences, and is directly comparable to the extension of Ritter and Tanner's diagnostic given in (10). However, Zellner and Min (1995) go further than Ritter and Tanner (1992) by attempting to formalise their method within a Bayesian framework, and obtain a posterior density for w, the asymptotic mean of the $\hat{w}^t$, so as to calculate posterior odds relating to the hypotheses

$$H_0 : w = 0 \qquad \text{vs} \qquad H_1 : w \neq 0. \tag{13}$$

Clearly, one of the main drawbacks with this method, as with that of Ritter and Tanner (1992), is the assumption

that we are able to derive explicit conditional posterior densities. This is a strong assumption and restricts the method to only a small class of problems. The method is also restricted to the Gibbs sampler, with no obvious extension to other MCMC algorithms. Also, as with that of Ritter and Tanner, the estimates of the conditionals may be expensive to calculate.

3.2 Normed distance criteria

We shall now discuss four methods which use the transition kernel of the sampler to assess the convergence of the joint density, by using the output from multiple replications.

3.2.1 Liu, Liu and Rubin's L^2 convergence diagnostic

Liu *et al.* (1993) define a scalar global control variable based upon iterates from multiple replications of a Markov chain, reducing the assessment of the convergence of a multi-dimensional Gibbs Sampling procedure to that of a one-dimensional random variable. This control variable incorporates information on the overall convergence of the chain to the target distribution π, and so is more comprehensive than one based solely upon subcomponents. Liu *et al.* (1993) suggest that the method of Gelman and Rubin (1992) can be used to judge the convergence of this control variable and thus convergence of the chain to its stationary distribution.

Liu *et al.* (1993) construct this control variable as follows. At iteration t, we construct a set of $m(m-1)$ values of the variable U, each using two independent parallel chains, i and j, given by

$$U_{ij}^t = \frac{\pi(\mathbf{x}_j^t)}{\pi(\mathbf{x}_i^t)} \frac{\mathscr{K}(\mathbf{x}_j^{t-1}, \mathbf{x}_i^t)}{\mathscr{K}(\mathbf{x}_j^{t-1}, \mathbf{x}_j^t)} \qquad i \neq j, \quad i,j = 1, \ldots, m.$$

Then,

$$U^t = \frac{1}{m(m-1)} \sum_{i \neq j} U_{ij}^t \qquad (14)$$

is an unbiased estimator of the L^2 distance between the t-step transition density $p^t(\cdot)$ and $\pi(\cdot)$.

Given the global control variable, U^t, Liu *et al.* (1993) propose two ways to utilise it as a convergence diagnostic. The first is to separate the chains into $\frac{m}{2}$ independent pairs and construct the $\{U^t\}$ sequence for each pair. They then suggest using the method of Gelman and Rubin (1992) to diagnose the convergence of these $\frac{m}{2}$ paired sequences individually, and comparing the results. The second method is to produce the sample cumulative density function of U, based upon iterations $t = n+1, \ldots, 2n$ and use Smirnov-statistic based tests to assess convergence in a manner similar to that proposed by Heidelberger and Welch (1983).

One drawback of methods based upon this global control variable is that its variance can be extremely large, making the estimate of the L^2 distance in (14) unreliable. This problem can be overcome by constructing U from the log U_{ij}, but then we lose the direct interpretability which makes this method attractive. Alternatively, we can improve the estimate by taking a large value of m, but this is computationally expensive. A second drawback which is encountered when we use the Gelman and Rubin-style implementation is in the justification of the assumption of normality for the U^t, though some of the extensions proposed by Brooks and Gelman (1998) may overcome this problem.

This method also has problems with interpretability and is problem specific, requiring different code to be written for each problem in order to produce the required output.

3.2.2 Roberts's L^2 convergence diagnostic

This diagnostic uses a density ratio statistic to assess the L^2 convergence of the distribution of the chain as a whole, using samples from several independent replications of a Markov chain with finite Hilbert-Schmidt norm. Thus, the method is essentially restricted to the analysis of the output from a reversible Gibbs sampler, see Roberts (1994).

Here we run m replications of the chain from starting points $\mathbf{x}_i^0$ $i = 1, \ldots, m$, where each starting point produces a sample path $\{\mathbf{x}_i^t : t = 0, 1, 2, \ldots\}$, and define our scalar control variable by

$$\chi_{ij}^t = \frac{\mathscr{K}(\mathbf{x}_i^0, \mathbf{x}_j^{2t-1})}{\pi(\mathbf{x}_j^{2t-1})},$$

where $\mathscr{K}$ is the transition density for the chain with equilibrium distribution π. Roberts suggests the following diagnostic procedure for the case where multiple replications are possible. We define

$$D_t = \frac{1}{m} \sum_{i=1}^m \chi_{ii}^t \quad \text{and} \quad I_t = \frac{1}{m(m-1)} \sum_{i \neq j} \chi_{ij}^t,$$

where the dependence term, D_t, measuring the dependence of the current value of the chain upon the starting point, gives us an indication as to how well the chain has mixed, and I_t denotes an interaction term. Roberts (1994) then suggests that we might monitor D_t and I_t until they both reach stationarity and have similar location.

We have the same drawback with this method as with that of Liu *et al.*, in that the variance of the χ_{ij}^t can be very large. As before, this can be reduced by considering the log χ_{ij}^t which, in this case, retains an appealing interpretation in terms of the Kullback-Leibler distance. Another drawback is associated with the interpretation of the diagnostic. The output from the diagnostic is in the form of

two sequences with different variances, but which have the same asymptotic location. This complicates the decision as to whether or not convergence has been achieved. However, the I_t sequence is less variable than the D_t sequence thus, in practice, it may be easier to interpret convergence if we define

$$I_t(i) = \frac{1}{m-1} \sum_{j \neq i} \chi_{ij}^t,$$

and monitor the $I_t(i)$ sequences for $i = 1, \ldots, m$.

3.2.3 Yu's L^1 diagnostic

The method proposed by Yu (1995b), attempts to diagnose convergence of the full density by monitoring a plot based upon the output of a single replication of the chain.

If $\{x^t : t = 0, 1, 2, \ldots\}$ is the output from a p-dimensional Markov chain with stationary density $\pi(\mathbf{x}) = c\tilde{\pi}(\mathbf{x})$, where $\tilde{\pi}$ is known and c is the unknown normalisation constant for π, then Yu suggests the following procedure.

First, we define a kernel estimator of π, with bandwidth, b_n, by

$$\hat{\pi}_n(\mathbf{x}) = \frac{1}{n} \sum_{t=1}^{n} h_{b_n}(\mathbf{x} - \mathbf{x}^t), \text{ where } h_\sigma(\mathbf{x}) = \frac{1}{\sigma^p} K\left(\frac{|\mathbf{x}|}{\sigma}\right),$$

$K(\cdot)$ is some one-dimensional bounded symmetric kernel, such that $\int_{\mathbb{R}^p} K(|\mathbf{x}|)d\mathbf{x} = 1$, and $|\cdot|$ denotes the Euclidean norm in $\mathbb{R}^p$.

Then, we define an estimate of the normalisation constant by

$$\hat{c}_\sigma = \frac{1}{n(n-1)} \sum_{t=1}^{n} \sum_{\tau \neq t} \frac{h_\sigma(\mathbf{x}^t - \mathbf{x}^\tau)}{\tilde{\pi}(\mathbf{x}^\tau)},$$

and choose some subset, A, of the support of π, and an increment value, t_0. Beginning at time $t = t_0$, we estimate the optimal bandwidth, b_t, for the kernel density estimate, by the method described by Silverman (1986), and based upon the data, $\mathbf{x}^0, \ldots, \mathbf{x}^t$. Given b_t, we estimate the L^1 distance over A between the kernel density estimator $\hat{\pi}_t$ and π, by

$$\hat{D}_t(A) = \int_A |\hat{\pi}_t(\mathbf{x}) - \hat{c}_{b_t}\pi(\mathbf{x})| \, d\mathbf{x}.$$

This process is repeated for times $t = t_0, 2t_0, 3t_0, \ldots$, until a plot of the $\hat{D}_t(A)$ values settles below some critical value, which Yu suggests should be taken as 0.3.

Like the other kernel-based methods, the method of Yu (1995b) is both problem specific (in that the form of $\tilde{\pi}$, is required) and computationally expensive. The output is rather difficult to interpret, though this can be improved by running several independent chains and plotting the resultant $\hat{D}_t(A)$ sequences together. However, the critical

value of 0.3, is rather arbitrary and may be better suited to some problems than others.

It should also be noted that the choice of the set A is of vital importance since, as Yu points out, the diagnostic plot may falsely diagnose convergence if both the sample path and the set A omit the same mode(s) of π. However, Yu's method has an advantage over those of Liu *et al.* and Roberts in that the $\hat{D}_t(A)$ statistic stabilises sample-wise, rather than in expectation, i.e., it is the expectation of the U_{ij}^t and χ_{ij}^t statistics that provide estimates of the respective L^2 distances, whereas $\hat{D}^t$ is a direct estimate of the corresponding L^1 distance.

In the next section, we provide another method for diagnosing convergence, by estimating L^1 distances between transition densities of different chains. Like that of Liu, this method also has the advantage of providing a statistic which stabilises sample-wise.

3.2.4 The total variation diagnostic

Brooks *et al.* (1997) suggest a new approach to diagnosing convergence which attempts to obtain an upper bound to the L^1 distance between full-dimensional kernel estimates from different chains, using ideas similar to those of rejection sampling, (see Smith and Gelfand, 1992).

Brooks *et al.* (1997) suggest that we run m independent chains and split each chain into blocks of n_0 observations, with $\mathbf{x}_i^t$ denoting the state of chain i at time t. Then for the lth block of the ith chain we can define

$$K_{il}(\mathbf{x}) = \sum_{t=(l-1)n_0+1}^{ln_0} \frac{\mathcal{K}(\mathbf{x}_i^t, \mathbf{x})}{n_0} \tag{15}$$

where $\mathcal{K}(\mathbf{x}, \mathbf{y})$ is the one-step transition kernel for the chain moving from state $\mathbf{x}$ to $\mathbf{y}$. Thus, $K_{il}(\mathbf{x})$ is a Rao-Blackwellised estimate of the density of $\mathbf{X}$ in block l of chain i. Finally, we form a mean between chain distance by

$$B_l = \frac{1}{m(m-1)} \sum_{i=1}^{m} \sum_{j \neq i} \hat{r}_{ij}(l) \tag{16}$$

where $\hat{r}_{ij}(l)$ is given by

$$\hat{r}_{ij}(l) = 1 - \min\left(1, \frac{K_{il}(\mathbf{x})}{K_{jl}(\mathbf{x})}\right)$$

for some $\mathbf{x}$ sampled from the density $K_{jl}(\cdot)$, and estimates the L^1 distance between $K_{il}(\cdot)$ and $K_{jl}(\cdot)$, see Brooks *et al.* (1997).

Brooks *et al.* (1997) suggest monitoring the B_l values over blocks $l = 1, 2, \ldots$ to assess convergence. They highlight the interpretability of the diagnostic suggesting that convergence is indicated by a characteristic jump point in the B_l value, which is a physical manifestation of the "cut-off phenomenon" of Diaconis (1988, p91). The diagnostic can also be applied to a wide variety of samplers, though

they discuss only the Metropolis Hastings algorithm and the Gibbs sampler.

One advantage of this method over the alternative methods for diagnosing convergence of the joint density, is that it is easily adapted to measure convergence of particular multivariate densities. This may be particularly useful in high dimensional problems, where assessing convergence of the full joint density may be prohibitively expensive. In this case, the L^1 diagnostic can be used to assess convergence of the joint density of a subset of the parameters, perhaps those that are of principal interest.

In terms of computational expense, this method compares favourably with the methods of Liu *et al.* (1993) and Roberts (1994). However, for most problems, the evaluation of the diagnostic sequence typically increases the execution time for the sampler by an order of magnitude. One might argue that the added computational expense is acceptable in order to gain a reliable and interpretable diagnostic. It is really a matter of how much we are willing to "pay" in order to obtain such a diagnostic.

4 Regeneration and coupling methods

Here, we consider methods for diagnosing convergence motivated by the two important probabilistic constructions: coupling times and regeneration times.

First consider the following theoretical construction that motivates the use of coupling diagnostics. Let $\mathbf{X}_1$ and $\mathbf{X}_2$ be discrete time processes, marginally having distributions which are realisations from the Markov chain of interest, started at different starting distributions, say $\mathbf{X}_i^0 \sim \mu_i^0$, $i = 1, 2$. We do not prescribe any particular dependence structure between the two chains, except to stipulate that the joint process $(\mathbf{X}_1, \mathbf{X}_2)$ be Markov. Indeed $\mathbf{X}_1$ and $\mathbf{X}_2$ will commonly be constructed in a highly dependent way.

Such a construction is called a *coupling* of $\mathbf{X}_1$ and $\mathbf{X}_2$, and if we let $\tau = \inf\{t : \mathbf{X}_1^t = \mathbf{X}_2^t\}$, τ is known as the coupling time of the construction. If μ_i^0 is taken to be the stationary distribution π, then the celebrated *coupling inequality* (see for example Lindvall, 1992 p.12) ensures that

$$\sup_A \big(\mathbb{P}[\mathbf{X}_2^t \in A] - \pi(A) \big) \le \mathbb{P}[\tau > t].$$

Therefore if the probability that coupling has occurred by time t is high, then the distribution of $\mathbf{X}_2^t$ is a good approximation to π. This construction motivates the following diagnostic introduced by Johnson (1996) and subsequently extended by Reutter and Johnson (1995).

4.1 Johnson's coupling diagnostic

The Johnson diagnostic was first proposed for the Gibbs sampler, though refinements due to Rutter and Johnson

(1995) extend its natural application to more general Hastings-Metropolis situation.

Let $\boldsymbol{U} = \{u_{(j)}^t : j = 1, \ldots, k, \ t = 1, 2, \ldots\}$ be an array of independent standard uniform random variables, and let $\boldsymbol{x}^t = \{x_{(j)}^t : j = 1, \ldots, k\}$ denote the tth sample vector in a sequence of draws from the Gibbs sampler. Finally, let $F(\cdot|\cdot)$ denote the conditional cumulative distribution associated with π, with corresponding quantile function, $F^{-1}(\cdot|\cdot)$. Then the coupled Gibbs sampler algorithm can be defined as follows.

We begin with m starting vectors, $\boldsymbol{x}_i^0 \quad i = 1, \ldots, m$ drawn from a distribution overdispersed with respect to π. Then, at time t, we set element j of each chain i, to be

$$[x_{i(j)}^t = F^{-1}(u_{(j)}^t | x_{i(1)}^t, \ldots, x_{i(j-1)}^t, x_{i(j+1)}^{t-1}, \ldots, x_{i(k)}^{t-1}), \quad (17)$$

where $x_{i(j)}^t$ is the jth component of the vector $\boldsymbol{x}_i^t$, the state of chain i at iteration t. If $|\boldsymbol{x}_i^t - \boldsymbol{x}_l^t| \le \epsilon \quad \forall \, i \ne l$, $i, l \in \{1, \ldots, m\}$ and some $\epsilon > 0$, this suggests that the paths have coalesced and we stop at time t. Otherwise we continue to the next time period and repeat the process.

Variations on this theme involve situations where the inversion step in (17) is not needed because of the existence of fully conjugate prior distributions. In this case, we can simply make the random draws for each chain by feeding the same seed to the random number generator. However, if this is not the case, then the implementation of this diagnostic can become rather complicated and computationally expensive.

The diagnostic produces appealing and easily interpretable graphical output, and in many situations can be surprisingly easy to implement, despite the need to produce problem specific computer code for its implementation. However, since the coupling inequality does *not* state that $\mathbf{X}_2^\tau \sim \pi$ (which is false in general), in order to attempt to justify this diagnostic using the coupling inequality, the procedure described in (1)–(3) needs to be carried out many times, and even then uncertainty remains about how well we can find an over-dispersed starting distribution that approximates π. The overall procedure may therefore be very computationally expensive.

4.2 Methods for regenerative chains

Here, we consider the case where we have a Markov chain $\{X^1, \ldots, X^n\}$, which *regenerates* at times $\{\tau_t : t = 1, \ldots, T\}$, and has stationary density π. A Markov chain X is said to regenerate at time τ if the Markov chain sample path before and after τ are independent conditioned on τ. For finite Markov chains, it is easy to spot regeneration times, for example just set τ_t to be the tth visit of the chain to the state $\boldsymbol{x}^0$. For continuous state spaces, regeneration times are not in general naturally available and need to be constructed artificially.

Suppose that we wish to estimate $\mathbb{E}_\pi(\theta)$, based upon observations from the process, for some function θ. Then, the usual method is to form an ergodic estimate,

$$\frac{1}{N}\sum_{t=1}^{N}\theta(\boldsymbol{x}^t).$$

In this case, the Central Limit Theorem gives us that, if the $\boldsymbol{x}^t$ are *iid* random variables with finite variance, then

$$\frac{1}{\sqrt{N}}\sum_{t=1}^{N}\theta(\boldsymbol{x}^t)-\sqrt{N}\mathbb{E}_\pi[\theta(\boldsymbol{x}^t)]\stackrel{d}{\longrightarrow}N(0,\sigma_\theta^2),\ \text{as}\ N\to\infty.$$

However, since the $\boldsymbol{x}^t$ are realisations from a Markov chain, they will not be independent, nor will they necessarily have identical distributions. Thus, the traditional ergodic estimate of $\mathbb{E}_\pi(\theta)$ is biased and Central Limit Theorems need not apply.

However, since the process is regenerative, if we observe the process for a fixed number of tours T, say, let

$$n_t = \tau_t - \tau_{t-1}$$

and

$$S_t = \sum_{s=\tau_{t-1}+1}^{\tau_t}\theta(\boldsymbol{X}^s)\qquad t=1,\ldots,T,$$

then $\sum_{t=1}^{T}S_t/\sum_{t=1}^{T}n_t$ *is* a consistent estimator for $\mathbb{E}_\pi(\theta)$, by the Law of Large Numbers and the Renewal Theorem, see Lindvall (1992).

In order to assess convergence of a regenerative chain run for T tours, Mykland *et al.* (1995) suggest plotting τ_t/τ_T against t/T, which they refer to as a scaled regeneration quantile, or *SRQ* plot. Since the $\{\tau_t\}$ form a renewal process with constant probability of regeneration, the τ_t will be uniformly distributed so that, for large T, the SRQ plot should resemble a straight line.

Deviations from a straight line occur when relatively long tours are encountered. This is consistent with a highly positively skewed distribution for the length of the regeneration times, which is in turn indicative of a slowly mixing Markov chain. The deviation from a straight line can be quantified by fitting an intercept-slope model to the observed data and assessing the fit of the model.

The main problem with this method is in the introduction of regeneration points into the MCMC sampler. This is straightforward in the case of a discrete state space, since regenerations can occur each time the chain enters a particular pre-determined state (or set of states). In the general state space case, Mykland *et al.* (1995) use Nummelin's Splitting technique (Nummelin, 1984) to introduce regenerations, and show how to introduce regenerations in a limited number of special cases. However Gilks *et al.* (1996) show that the artificial construction of such regeneration times is effectively limited to small dimensional problems, so that these extensions have limited practical appeal.

As an alternative diagnostic, Robert (1996) proposes the following method. Given a renewal set (or *atom*) A, Robert shows that

$$\frac{\tau_T}{T}\xrightarrow{T\to\infty}\mathbb{E}_\pi[\tau_2-\tau_1]=\mu_A,\ \text{say}$$

and, under suitable regularity conditions provided by Robert (1996),

$$\sqrt{T}\sum_{t=1}^{T}(S_t-n_t\mathbb{E}_\pi[\theta(\boldsymbol{x})])\stackrel{d}{\longrightarrow}N(0,\sigma_A^2).$$

Now, σ_A^2 can be estimated by

$$\widehat{\sigma}_A^2=\sum_{t=1}^{T}\left(S_t-n_t\sum_{t=1}^{T}\frac{S_t}{N}\right)^2$$

and μ_A, by N/T. Thus, σ_θ^2 can be estimated by

$$\widehat{\sigma}_\theta^2(A)=\widehat{\sigma}_A^2/\widehat{\mu}_A,$$

for all atoms of the chain. Thus, Robert suggests stopping the simulation once the estimators $\widehat{\sigma}_\theta^2(A)$ stabilise to the same value for a collection of different atoms, $A\in\mathscr{A}$.

The difficulty with this method, as with that of Mykland *et al.* (1995), is that it is often very difficult to obtain atoms for chains defined on a general state space. Thus, this method is of limited practical value in the general state space case.

However, for a discrete chain, as we explained earlier, atoms are easy to find, since the chain can be allowed to regenerate each time $X^t=X^*$, for some pre-determined state, X^*. Robert (1996) suggests taking the state which has greatest mass under π or, if the state space is large, a collection of states with "significant" mass under π, in order to ensure a reasonable regeneration rate. Thus, in the discrete case, it is easy to construct several atoms $A_1,\ldots,A_k$ and calculate $\widehat{\sigma}_\theta^2(A_i)$ for $i=1,\ldots,k$, stopping when the sample paths of these statistics converge.

5 Eigenvalue bounds and semi-empirical methods

Most (but not all) MCMC algorithms used in practice, converge to stationarity geometrically quickly. That is, there exists a measurable function $V\geq 1$, and a constant $\rho<1$ such that

$$\|P^t(\boldsymbol{x},\cdot)-\pi(\cdot)\|\leq V(\boldsymbol{x})\rho^n\qquad(18)$$

where P^t denotes the t step transition distribution for the Markov chain, and $\|\cdot\|$ denotes total variation distance, see for example Roberts and Tweedie (1996b). Furthermore, suitably well-behaved Markov chains exhibit an eigen-expansion for their transition probabilities, implying that

$$P^t(\boldsymbol{x},A)-\pi(A)=a(\boldsymbol{x},A)\lambda_1^n+O(\lambda_2^n)\qquad(19)$$

where $|\lambda_2| < |\lambda_1| < 1$. See Roberts (1994) for a discussion of sufficient conditions for such an expansion. In this section we concentrate on methods which either estimate $a(\cdot)$ and λ_1 or analytically estimate $V(\cdot)$ and ρ.

It is clearly of interest to be able to estimate λ_1, but how useful knowledge about λ_1 is (and indeed how valid the procedure for estimating it) depends upon the existence of an expansion such as (19). Furthermore, we also need $|\lambda_2|$ to be significantly smaller than $|\lambda_1|$ so that its effect on the estimation procedure for λ_1 is negligible.

There are many situations for which MCMC algorithms reasonably satisfy these assumptions, for example Gibbs samplers on densities which are well approximated by Gaussians. However there are others for which (18) holds but (19) does not, for instance the independence sampler on a continuous space (see Smith and Tierney, 1996).

Two rather different procedures have been proposed for estimation of principle eigenvalues in the MCMC context on the basis of expansions of the form (19). A direct method based on (19) is proposed by Garren and Smith (1995). Whereas Raftery and Lewis (1992) propose a method for estimating a probability of interest $\pi(A)$ say, by assessing the convergence of a binary process derived from the original chain.

5.1 Garren and Smith's convergence rate estimator

Suppose $\{X^t\}$ is a sequence from a Markov chain with state space E, and stationary distribution $\pi(\cdot)$, and take some subset $A \subseteq E$. Garren and Smith (1995) define

$$Z^t = I_{(X^t \in A)}, \qquad \rho_t = \mathbb{E}(Z^t), \quad \text{and} \quad \rho = \lim_{t \longrightarrow \infty} \rho_t. \quad (20)$$

Then, Garren and Smith (1995) attempt to estimate ρ and assume that there exists an expression in terms of the eigenvalues of the transition kernel, of the form

$$\rho_t = \rho + a_2 \lambda_2^t + O(|\lambda_3|^t), \quad (21)$$

where $|\lambda_3| < |\lambda_2| < 1$ and $a_2 \in \mathbb{R}$.

The assumptions underlying (21) are difficult to check in practice. Limited theoretical results exist to justify this assumption, for example (21) holds whenever the transition kernel is self-adjoint (that is the Markov chain is reversible), its Hilbert-Schmidt norm is finite (see for example Roberts, 1992), and its two principal eigenvalues have unit multiplicity.

However, the Hilbert-Schmidt condition is rarely checkable (though see Roberts, 1992), and in fact fails for virtually all Metropolis-Hastings algorithms. Furthermore the multiplicity of the second eigenvalue is very rarely easy to verify. More worrying is that (21) itself frequently fails in examples for MCMC where we can identify the spectrum of the Markov chain.

Given that (21) holds, Garren and Smith (1995) propose the following estimation scheme. Fix integers n_0 and n with $1 \le n_0 < n$, and run m independent replications of the chain $\{X_i^t : 0 \le t \le n\}$ $i = 1, \ldots, m$, each starting with the same initial distribution f_0, taken to be a point mass at some point x^0. Then, define

$$\bar{Z}^t = \frac{1}{m} \sum_{i=1}^{m} I_{(X_i^t \in A)},$$

where X_i^t is the tth observation from chain i, and I denotes the indicator function. Thus, $\bar{Z}^t$ is the sample frequency of the event $\{X_t \in A\}$ over the m replications. Finally, we define estimators $\widehat{\rho}$, $\widehat{a}_2$ and $\widehat{\lambda}_2$ of ρ, a_2 and λ_2 respectively, which minimise

$$S(\rho, a_2, \lambda_2) = \sum_{t=n_0+1}^{n} (\bar{Z}^t - \rho - a_2 \lambda_2^t)^2.$$

Garren and Smith (1995) suggest a heuristic approach to assessing convergence, given these estimates. They note that as n increases the estimates for a_2 and λ_2 become unstable (with the standard errors increasing) and they suggest taking the largest value of n for which plots of both $\widehat{a}_2$ and $\widehat{\lambda}_2$ remain stable. A suitable value for n_0 may then be found by ignoring the $O(|\lambda_3|^t)$ term in (21), and imposing the condition that $|\rho_t - \rho| \le \epsilon$, for some $\epsilon > 0$, then

$$n_0 = \frac{\log\left(\frac{\epsilon}{|\widehat{a}_2(n)|}\right)}{\log |\widehat{\lambda}_2(n)|}.$$

The main drawback to this diagnostic is the computational expense of the method, due to the problem of choosing a value of m which leads to good estimators of ρ, a_2 and λ_2. Garren and Smith (1995) suggest that m should be "large" in comparison to n, and suggest taking values as large as 5000. Such large numbers of replications may cause serious problems for many practical applications and results in a considerable loss of computational efficiency. Note also that each of these replications have the same starting point and so they do little to help explore the different regions of the parameter space. Garren and Smith (1995) discuss the possibility of using multiple replications from different starting points, but show that this would require prohibitively long sample runs in order to gain reasonable estimators.

5.2 Raftery and Lewis' Convergence Rate Estimator

Raftery and Lewis (1992) consider the problem of calculating the number of iterations necessary to estimate a posterior quantile from a single run of a Markov chain. They propose a 2-state Markov chain model fitting procedure based upon a pilot analysis of output from the original chain.

Suppose that we wish to estimate a particular posterior quantile for some function θ of a parameter (or set of pa-

rameters) X, i.e.; we wish to estimate from observational data the value of u such that

$$\mathbb{P}(\theta(X) \le u) = q$$

for some pre-prescribed q and so that, given our estimate $\widehat{u}$, $\mathbb{P}(\theta(X) \le \widehat{u})$ lies within $\pm r$ of the true value, say, with probability p.

Raftery and Lewis (1992) propose a method to calculate first of all the length of the "burn-in" period n_0, and secondly the number of further iterations, n, required to estimate the above probability to within the required accuracy. They suggest that we run the MCMC algorithm for an initial n_0 iterations, which we discard, and then a further n iterations which we thin by storing every s^{th}, and provide a method to determine the values of n_0, n and s. Here, we are interested only with the value of n_0 which estimates the number of iterations required before convergence is "achieved". This can be calculated as follows.

First, we calculate $\theta^t = \theta(X^t)$ where X^t is the state of the chain at time t, and then form $Z^t = I_{(\theta^t \le u)}$, where I is the indicator function. Then, Z^t is a binary process derived from a Markov chain by marginalisation and truncation but is not a Markov chain itself. We then take the subsequence $\{Z_s^t\}$ where $Z_s^t = Z^{1+(t-1)s}$.

The binary process $\{Z^t\}$ is not Markov in general. However for large enough $s \ge 1$, $\{Z_s^t\}$ will well approximate a Markov chain. The Raftery and Lewis procedure is based around this assumption, choosing s after observing a pilot sample of the data. In fact, they sequentially use BIC ratios to select s, though other ways of doing this are clearly possible.

Once s is established, the approximate transition matrix of $\{Z_s^t\}$ is approximated empirically by the obvious estimator $\widehat{R}$, with i,jth element

$$\widehat{R}_{ij} = \frac{\#\{t : Z_s^t = j, \ Z_s^{t-1} = i\}}{\#\{t : \ Z_s^{t-1} = i\}} \qquad i,j = 0, 1.$$

Since eigen-analysis of $\widehat{R}$ is straightforward, convergence diagnostic procedures both for the convergence in distribution of $\{Z_s^t\}$ and for convergence to a pre-specified accuracy of ergodic estimates are easily constructed.

The main strengths of this method lie in its ease of implementation and in its focus upon the accuracy of ergodic averages. However, the method relies upon three levels of approximation: the Markov approximation, the choice of s and the estimation of $\widehat{R_{ij}}$.

A further word of caution regarding this method is provided by Brooks and Roberts (1997) who further stress the fact that this method estimates the convergence rate of the chain only for the quantile of interest and does not provide any information as to the convergence rate of the chain as a whole. In fact they show that in the case of the independence sampler the convergence rate estimate provided by Raftery and Lewis lies below the convergence rate

of the full chain and that the choice of q is of critical importance to the estimate obtained. Thus, some care should be taken in selecting a suitable q value. In particular, the routine use of $q = 0.025$, suggested both in the literature and within the S-Plus and Fortran code that the original authors distribute, should not be adopted as a general rule, since it may lead to a strong underestimate of the true length of the burn-in period. When interested in a number of quantiles, it may be most sensible to run the procedure for a number of different u-values and take the largest of the resulting estimated burn-in lengths, but in the case where quantiles themselves are not of interest, this method should be used with caution.

5.3 Geometric Convergence Bounds

Because of the uncertainties associated with eigenvalue estimation outlined above, it is appealing to search for analytic inequalities of the form (18). However, for Markov chains which provably satisfy (18), it is rare for useful bounds on V and ρ to be attainable in even moderately complicated statistical models. The one technique which has made inroads into this problem is the coupling approach introduced by Rosenthal (1995b) and extended by Roberts and Tweedie (1998), which gives a flexible approach for computing ρ and V which can (in some cases at least) be applied to MCMC problems (see Rosenthal, 1995a, b, c).

This method is based upon the idea of running two chains independently, one of which is started from the stationary distribution π, and the other from some initial distribution π_0 and both with t-step transition kernel $P^t(\cdot, \cdot)$. Let C be a small set, i.e.;

$$\pi(C) > 0 \quad \text{and} \quad P^t(x, \cdot) \ge \epsilon v(\cdot) \quad \forall x \in C , \qquad (22)$$

and for some integer $t \ge 1$, constant $\epsilon > 0$ and probability measure v on E. Such a condition is called a *minorisation condition*. We shall also need to use a Lyapunov *drift* condition: there exists a function $V : E \to [1, \infty)$ and constants $\lambda < 1$ and $b < \infty$ such that for all $x \in E$,

$$\mathbb{E}(V(X^1)|X^0 = X) \le \lambda V(x) + b I_{(x \in C)} \qquad (23)$$

Intuitively, (23) forces the Markov chain to shrink at a geometric rate (as measured by V) towards C, and (22) allows any two copies of the Markov chain in C to couple with probability ϵ. Quantifying this idea in terms of the various constants ϵ, λ, b etc. leads to the result that if (22) and (23) hold with C being a small set given by $C = \{x; \ V(x) \le d\}$ for some constant $d \ge 1$. Then there exist constants $\rho < 1$, α and β (which are functions of ϵ, b, $V(x)$, λ and d) such that

$$\|P^n(x, \cdot) - \pi(\cdot)\| \le (\alpha + \beta n)\rho^n . \qquad (24)$$

See Roberts and Tweedie (1998) for further details and an explicit statement of the constants involved.

This method can require a substantial amount of analytical work in order to calculate the various quantities in the given upper bound. Often also, the bounds obtained are too poor to be of any practical value. However, this method has been applied to a number of statistical problems, see Rosenthal (1995a,b,c), and Roberts and Rosenthal (1998). The approach remains the most promising avenue for analytic estimation of Markov chain running times.

An interesting idea to make these ideas more accessible and generally applicable is to use simulation techniques to calculate the constants α and ϵ, see Cowles and Rosenthal (1998). Although promising, this approach still remains rather computationally expensive, and the bounds obtained can still be very poor.

Similar, computable, bounds have also been derived by Meyn and Tweedie (1994). However, for complex target distributions, the approximations necessary in order for any of these bounds to be analytically tractable, lead to bounds too weak to be of much practical value.

It is possible to construct less general, but rather more accurate results applicable to certain classes of problems. For example, Roberts and Sahu (1997) give exact expressions for the rate of convergence of various types of Gibbs sampler on Gaussian target densities. For distributions close to Gaussian, corresponding approximations can be obtained, see Roberts and Sahu (1996). Some related results are given by Amit (1991). Similarly, Polson (1996) discusses approaches to the estimation of the convergence rate by the case for log-concave target distributions on a lattice, using a particular form of the Metropolis algorithm. Finally, Liu (1994) provides a method for exact calculation of the rate of convergence for the independence sampler. If the importance weight, $w(x)$, has a finite maximum w^* for some $x = x^* \in E$, then the convergence rate of the chain is given by $\rho = 1 - 1/w^*$. Thus, the independence sampler converges geometrically to π, whenever $w^* < \infty$. This result is further discussed by Mengersen and Tweedie (1995) and extended by Smith and Tierney (1996), and is particularly easy to use. However, no similar results exist for more general samplers such as the Gibbs sampler or the Metropolis-Hastings algorithm.

6 Discussion

It is clear that the usefulness of convergence assessment methods is limited by their potential unreliability. They will always be useful in diagnosing transient behaviour, but it is much more dangerous to try and assert stationarity from their use. In this paper, we have tried to broaden the scope of techniques beyond empirically calculated convergence summary statistics. However, many of the theoretical techniques are difficult to apply, so the scope of their application is also limited.

In addition, currently implemented MCMC algorithms commonly involve simulating Markov chains in complicated spaces with no metric space structure, such as the so-called *reversible jump* algorithm (see Green 1995). For these problems, most of the techniques considered in Sections 2 and 3 are unlikely to be effective. Finding techniques that are specifically geared to these algorithms is an important problem which requires further research, see Brooks (1997).

One way of avoiding the problem of deciding when convergence has *occurred* is the recent idea of "exact" or "perfect" simulation algorithms. These constructions allow us to simulate Markov chains which began at some point infinitely far back in the past, so that at time zero, after an infinite number of iterations, the chain will have reached its stationary distribution. The problem is then that since we can't actually start these chains infinitely far back in the past, how do would we know where they would be at time zero? However, a recent paper by Propp and Wilson (1996) shows how the use of combined forward and backward simulation can be used to answer this question.

Suppose that the state space for the Markov chain E say, is finite, and that we are able to carry out the following 'backwards' simulation. For a fixed $N \in \mathcal{N}$, start a Markov chain sample path from each point in E, at time $-N$. Call these chains $\{X_1, \ldots, X_{|E|}\}$ say. The $|E|$ chains can be constructed in a dependent way, though once coupled, we stipulate that they remain together, that is for $N \leq s < t \leq 0$,

$$X_i^s = X_j^s \Rightarrow X_i^t = X_j^t.$$

We examine the set $\{X_i^0, \ i \in E\}$. It is possible that all $|E|$ chains have coupled by time 0, so that $\{X_i^0, \ i \in E\}$ consists of a unique point. In this case, there is no dependence of X_i^0 on its initial value i, and it can be shown that the distribution of X_i^0 is π. If $\{X_i^0; \ i \in E\}$ is not a singleton, we repeat the simulation, this time started at time $-2N$, though using the same sample paths on the time period $\{-N, \ldots, 0\}$ as for the first simulation. Now we continue to double the length of the simulation until we reach a situation where $\{X_i^0; \ i \in E\}$ is a singleton.

This procedure may seem rather complicated, though its subtle differences from the procedure suggested by Johnson (1996) ensure that in this case, as soon as $\{X_i^0; \ i \in E\}$ is a singleton, the distribution of that point is *exactly* the target distribution, π. Thus, we can exactly simulate from π and hence the names often given to these simulation methods: *exact* or *perfect* simulation.

On the other hand, the simulation procedure is very cumbersome and for most practical problems, it is difficult if not impossible to simulate chains simultaneously from all possible starting points. The pure application of this idea is therefore (for the moment at least) restricted to a small class of problems where special structure of the state space needs only two processes to be constructed simultaneously,

a 'top' and a 'bottom' process. Particularly innovative algorithms of this kind have appeared in the stochastic geometry literature, see Kendall (1997) and Møller (1997). Moreover an inevitable cross-fertilisation between the coupling constructions of Section 5.3 and the perfect simulation literature is beginning to develop (see for example Murdoch and Green, 1997).

Despite its current practical limitations, the idea already promises to become an active research area, and undoubtedly practical simulation procedures of this kind (at least for some classes of problems) will eventually become available.

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