Convergence diagnostics for Markov chain Monte Carlo

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Abstract

Markov chain Monte Carlo (MCMC) is one of the most useful approaches to scientific computing because of its flexible construction, ease of use and generality. Indeed, MCMC is indispensable for performing Bayesian analysis. In spite of its widespread use, two critical questions that MCMC practitioners need to address are where to start and when to stop the simulation. Although a great amount of research has gone into establishing convergence criteria and stopping rules with sound theoretical foundation, in practice, MCMC users often decide convergence by applying empirical diagnostic tools. This review article discusses the most widely used MCMC convergence diagnostic tools. Some recently proposed stopping rules with firm theoretical footing are also presented. The convergence diagnostics and stopping rules are illustrated using three detailed examples.
1. INTRODUCTION

Markov chain Monte Carlo (MCMC) methods are now routinely used to fit complex models in diverse disciplines. A Google search for Markov chain Monte Carlo returns over 11.5 million hits. The popularity of MCMC is mainly due to its widespread usage in computational physics and Bayesian statistics, although it is also used in frequentist inference (see e.g. Geyer and Thompson 1995, Christensen 2004).

The fundamental idea of MCMC is that if simulating from a target density \( \pi \) is difficult so that the ordinary Monte Carlo method based on iid samples cannot be used for making inference on \( \pi \), it may be possible to construct a Markov chain \( \{X_n\}_{n \geq 0} \) with stationary density \( \pi \) for forming Monte Carlo estimators. An introduction to construction of such Markov chains, including the Gibbs sampler and the Metropolis Hastings (MH) sampler, can be found in Geyer (2011) (see also Robert and Casella 2004). General purpose MH algorithms are available in the R packages mcmc (Geyer and Johnson 2017) and MCMCpack (Martin et al. 2011). There are several R (R Core Team 2018) packages implementing specific MCMC algorithms for a number of statistical models (see e.g. MCMCpack (Martin et al. 2011), MCMCglmm (Hadfield 2010), geoBayes (Evangelou and Roy 2019)). Here, we do not discuss development of MCMC algorithms, but rather focus on analyzing the Markov chain obtained from running such an algorithm for determining its convergence.

Two important issues that must be addressed while implementing MCMC are where to start and when to stop the algorithm. As we discuss now, these two tasks are related to determining convergence of the underlying Markov chain to stationarity and convergence of Monte Carlo estimators to population quantities, respectively. It is known that under some standard conditions on the Markov chain, for any initial value, the distribution of \( X_n \) converges to the stationary distribution as \( n \to \infty \) (see e.g. Meyn and Tweedie 1993, chapter 13), Roberts and Rosenthal (2004). Since \( X_0 \sim \pi \) and MCMC algorithms produce (serially) correlated samples, the further the initial distribution from \( \pi \), the longer it takes for \( X_n \) to approximate \( \pi \). In particular, if the initial value is not in a high density (\( \pi \)) region, the samples at the earlier iterations may not be close to the target distribution. In such cases, a common practice is to discard early realizations in the chain and start collecting samples only after the effect of the initial value has (practically) worn off. The main idea behind this method, known as burn-in, is to use samples only after the Markov chain gets sufficiently close to the stationary distribution, although its usefulness for Monte Carlo estimation has been questioned in the MCMC community (Geyer 2011). Thus, ideally, MCMC algorithms should be initialized at a high density region, but, if finding such areas is difficult, collection of Monte Carlo samples can be started only after certain iteration \( n' \) when approximately \( X_n' \sim \pi \).

Once the starting value is determined, one needs to decide when to stop the simulation. (Note that, the starting value, here, refers to the beginning of collection of samples as opposed to the initial value of \( X_0 \) of the Markov chain, although these two values can be the same.) Often the quantities of interest regrading the target density \( \pi \) can be expressed as means of certain functions, say \( E_{\pi}g \equiv \int_X g(x)\pi(x)dx \) where \( g \) is a real valued function. For example, appropriate choices of \( g \) makes \( E_{\pi}g \) different measures of location, spread, and other summary features of \( \pi \). Here, the support of the target density \( \pi \) is denoted by \( X \), which is generally \( \mathbb{R}^d \) for some \( d \geq 1 \), although it can be non-Euclidean as well. We later consider vector valued functions \( g \) as well. The MCMC estimator of the population mean \( E_{\pi}g \) is the sample average \( \hat{g}_{n',n} \equiv \frac{\sum_{i=n'}^{n} g(X_i)}{(n-n')} \). If no burn-in is used then \( n' = 0 \). It is known that usually \( \hat{g}_{n',n} \to E_{\pi}g \) as \( n \to \infty \) (see Section 2 for details). In practice, however, MCMC users run the Markov chain for a finite \( n^* \) number of iterations, thus MCMC simulation should be stopped only when \( \hat{g}_{n',n^*} \) has sufficiently converged to \( E_{\pi}g \). The accuracy of the time average estimator \( \hat{g}_{n',n} \) obviously depends on the quality of the samples. Thus, when implementing MCMC methods, it is necessary to wisely conclude Markov chain convergence, and subsequently determine when to stop the simulation. In particular, while premature termination of simulation will most likely lead to inaccurate inference, unnecessarily running longer chains is not desirable.
either as it eats up resources.

Performing theoretical analysis on the underlying Markov chain, an analytical upper bound on its distance to stationarity may be obtained (Rosenthal 1995), which in turn can provide a rigorous method for deciding MCMC convergence and thus finding \( n' \) (Jones and Hobert 2001). Similarly, using a sample size calculation based on an asymptotic distribution of the (appropriately scaled) Monte Carlo error \( \bar{g}_{n', n} - E \), an honest stopping value \( n^* \) can be found. In the absence of such theoretical analysis, often empirical diagnostic tools are used to check convergence of MCMC samplers and estimators, although, as shown through examples in Section 3, these tools can not determine convergence with certainty. Since early 1990’s with the increasing use of MCMC, a great deal of research effort has gone into developing convergence diagnostic tools. These diagnostic methods can be classified into several categories. For example, corresponding to the two types of convergence mentioned before, some of these diagnostic tools are designed to assess convergence of the Markov chain to the stationary distribution, whereas others check for convergence of the summary statistics like sample means, sample quantiles to the corresponding population quantities. The available MCMC diagnostic methods can be categorized according to other criteria as well, for example, their level of theoretical foundation, if suitable for checking joint convergence of multiple variables, whether based on multiple (parallel) chains or a single chain or both, if complemented by a visualization tool or not, if based on moments and quantiles or the kernel density of the observed chain etc. Several review papers on MCMC convergence diagnostics are available in the literature (see e.g. Cowles and Carlin 1996, Brooks and Roberts 1998, Mengersen et al. 1999). Cowles and Carlin (1996) provide a description of 13 convergence diagnostics, and summarize these according to the different criteria mentioned before. While some of these methods are widely used in practice, several new approaches have been proposed since then. In this article, we review some of these tools that are either commonly used by MCMC practitioners or we find these promising.

2. MCMC diagnostics

As mentioned in the introduction, MCMC diagnostic tools are needed for deciding convergence of Markov chains to the stationarity. Also, although in general the longer the chain is run the better Monte Carlo estimates it produces, in practice, it is desirable to use some stopping rules for prudent use of resources. In this section, we describe some MCMC diagnostics that may be used for deciding Markov chain convergence or to stop MCMC sampling. In the context of each method, we also report if it is designed particularly for one of these two objectives.

2.1. Honest MCMC

In this section, we describe some rigorous methods for finding \( n' \) and \( n^* \) mentioned in the introduction. Let \( f_n \) be the density of \( X_n \). It is known that under some standard conditions (see e.g. Meyn and Tweedie 1993, chap. 13), \( \frac{1}{2} \int_{\mathcal{X}} |f_n(x) - \pi(x)| dx \downarrow 0 \) as \( n \to \infty \), that is, \( X_n \) converges in the total variation (TV) norm to a random variable following \( \pi \). Jones and Hobert (2001) mention that a rigorous way of deciding the convergence of the Markov chain to \( \pi \) is by finding a number \( n' \) such that

\[
\frac{1}{2} \int_{\mathcal{X}} |f_{n'}(x) - \pi(x)| dx < 0.01.
\]

(The cut-off value 0.01 is arbitrary and any predetermined precision level can be used.) Jones and Hobert (2001) propose to use the smallest \( n' \) for which (1) holds as the ‘honest’ value for burn-in.

The above mentioned burn-in hinges on the TV norm in (1), which is generally not available. Constructing a quantitative bound to the TV norm is also often difficult, although significant progress has been made
in this direction [Rosenthal 1995, 2002, Baxendale 2005, Andrieu et al. 2015]. In particular, a key tool for constructing a quantitative bound to the TV norm is using the drift and minorization (d&m) technique [Rosenthal 1995]. The d&m technique has been successfully used to analyze a variety of MCMC algorithms (see e.g. Fort et al. 2003, Jones and Hobert 2004, Roy and Hobert 2010, Vats 2017). The d&m conditions, as we explain next, are also crucial to provide an honest way to check convergence of MCMC estimators of popular summary measures like moments and quantiles of the target distributions.

As in the introduction, let a particular feature of the target density be expressed as $E_{\pi} g$ where $g$ is a real valued function. By the strong law of large numbers for Markov chains, it is known that if $\{X_n\}_{n \geq 0}$ is appropriately irreducible, then $\bar{g}_{n',n} = \sum_{i=n'}^{n+1} g(X_i)/(n-n')$ is a strongly consistent estimator of $E_{\pi} g$, that is, $\bar{g}_{n',n} \to E_{\pi} g$ almost surely as $n \to \infty$ for any fixed $n'$ [Asmussen and Glynn 2011]. Without loss of generality, we let $n' = 0$ when discussing stopping rules, and for the ease of notation, we simply write $\bar{g}_n$ for $\bar{g}_{0,n}$. The law of large numbers justifies estimating $E_{\pi} g$ by the sample (time) average estimator $\bar{g}_n$, as in the ordinary Monte Carlo. If a central limit theorem (CLT) is available for $\bar{g}_n$, that is, for the error $\bar{g}_n - E_{\pi} g$ then a ‘sample size calculation’ based on the width of an interval estimator for $E_{\pi} g$ can be performed for choosing an appropriate value for $n$. Indeed, under some regularity conditions,

$$\sqrt{n} (\bar{g}_n - E_{\pi} g) \overset{d}{\to} N(0, \sigma^2_g) \quad \text{as} \quad n \to \infty,$$

where $\sigma^2_g \equiv \text{Var}_\pi(g(X_0)) + 2 \sum_{i=1}^{\infty} \text{Cov}_\pi(g(X_0), g(X_i)) < \infty$; the subscript $\pi$ indicates that the expectations are calculated assuming $X_0 \sim \pi$. (Note that, due to the autocorrelations present in a Markov chain, $\sigma^2_g \neq \text{Var}_\pi(g(X_0)) = \lambda^2_0$, say.) If $\hat{\sigma}_{g,n}$ is a consistent estimator of $\sigma_g$, then an estimator of the standard error of $\bar{g}_n$, based on the sample size $n$ is $\hat{\sigma}_{g,n}/\sqrt{n}$. Since the standard error $\hat{\sigma}_{g,n}/\sqrt{n}$ allows one to judge the reliability of the MCMC estimate, it should always be reported along with the point estimate $\bar{g}_n$. The standard error also leads to a $100(1-\alpha)/2$ confidence interval for $E_{\pi} g$, namely $\bar{g}_n \pm z_{\alpha/2} \hat{\sigma}_{g,n}/\sqrt{n}$. Here $z_{\alpha/2}$ is the $(1-\alpha/2)$ quantile of the standard normal distribution. The MCMC simulation can be stopped if the half-width of the $100(1-\alpha)/2$ confidence interval falls below a prespecified threshold, say $\epsilon$. [Jones and Hobert 2001] refer to this method as the honest way to stop the chain. Indeed, the fixed width stopping rule (FWSR) [Flegal et al. 2008, Jones et al. 2006] terminates the simulation, the first time after some user-specified $\bar{n}$ iterations that

$$t_* \frac{\hat{\sigma}_{g,n}}{\sqrt{n}} + 1/n \leq \epsilon. \quad \text{(3)}$$

Here, $t_*$ is an appropriate quantile. The role of $\bar{n}$ is to make sure that the simulation is not stopped prematurely due to poor estimate of $\hat{\sigma}_{g,n}$. The value of $\bar{n}$ should depend on the complexity of the problem. [Gong and Flegal 2016] suggest that using $\bar{n} = 10^4$ works well in practice.

For validity of the ‘honest stopping rule’, a CLT [2] for $\bar{g}_n$ needs to exist, and one would need a consistent estimator $\hat{\sigma}_{g,n}$ of $\sigma_g$. For the CLT to hold, the TV norm in [1] needs to converge to zero at certain rate (see [Jones 2004] for different conditions guaranteeing a Markov chain CLT). The most common method of establishing a CLT [2] as well as providing a consistent estimator of $\sigma_g$ has been by showing the Markov chain $\{X_n\}_{n \geq 0}$ is geometrically ergodic, that is, the TV norm [1] converges at an exponential rate [Jones and Hobert 2001, Roberts and Rosenthal 2004]. Generally, geometric ergodicity of a Markov chain is proven by constructing an appropriate d&m condition [Rosenthal 1995, Roy and Hobert 2010]. For estimation of $\sigma^2_g$, while [Mykland et al. 1995], and Hobert et al. [2002] discuss regenerative submission method, [Jones et al. 2006] and [Flegal and Jones 2010] provide consistent batch means and spectral variance methods. Availability of a Markov chain CLT has been demonstrated for myriad MCMC algorithms for common statistical models. Here we provide an incomplete list—linear models [Román and Hobert 2012, 2015], generalized linear models including the probit model [Roy and Hobert 2007, Chakrabarty and Khare 2017], the popular logistic model [Choi and Hobert 2013, Wang and Roy 2018c] and the robit model [Roy 2012].
generalized linear mixed models including the probit mixed model (Wang and Roy 2018b), and the logistic mixed model (Wang and Roy 2018a), quantile regression models (Khare and Hobert 2013), multivariate regression models (Roy and Hobert 2010, Hobert et al. 2018), penalized regression and variable selection models (Khare and Hobert 2013, Roy and Chakraborty 2017, Vats 2017).

So far we have described the honest MCMC in the context of estimating means of univariate functions. The method is applicable to estimation of vector valued functions as well. In particular, if \( g \) is a \( \mathbb{R}^p \) valued function, and if a CLT holds for \( \tilde{g}_n \), that is, if \( \sqrt{n}(\tilde{g}_n - E_{\pi} g) \xrightarrow{d} N(0, \Sigma_g) \) as \( n \to \infty \), for some \( p \times p \) covariance matrix \( \Sigma_g \), then using a consistent estimator \( \hat{\Sigma}_{g,n} \) of \( \Sigma_g \), a \( 100(1 - \alpha)\% \) asymptotic confidence region \( C_\alpha(n) \) for \( E_{\pi} g \) can be formed (see Vats et al. 2019 for details). Vats et al. (2019) propose a fixed volume stopping rule which terminates the simulation the first time after \( \tilde{n} \) iterations that

$$\frac{\text{Vol}(C_\alpha(n))}{n} + \frac{1}{n} \leq \varepsilon,$$

where as in (3), \( \varepsilon \) is the user’s desired level of accuracy. Note that when \( p = 1 \), except the \( 1/n \) terms, the above is same as (3) with \( \varepsilon = 2\varepsilon \). Honest MCMC can also be implemented for estimation of the quantiles (Doss et al. 2014). In order to reduce computational burden, the sequential stopping rules should be checked only at every \( l \) iterations where \( l \) is appropriately chosen. Finally, even if theoretical d&m analysis is not carried out establishing a Markov chain CLT, in practice, FWSR can be implemented using the batch means and spectral variance estimators of \( \sigma_g(\Sigma_g) \) available in the R package mcmcse (Flegal et al. 2012).

### 2.2. Relative fixed width stopping rules

FWSR described in Section 2.1 explicitly address how well the estimator \( \tilde{g}_n \) approximates \( E_{\pi} g \). Recently Flegal and Gong (2015) and Gong and Flegal (2016) discussed relative FWSR in MCMC setting. Flegal and Gong (2015) consider a relative magnitude rule that terminates the simulation when after \( \tilde{n} \) iterations \( t_\varepsilon \hat{\sigma}_{g,n} n^{-1/2} + n^{-1} \leq \varepsilon \hat{g}_n \). Flegal and Gong (2015) also consider a relative standard deviation (SD) FWSR that terminates the simulation when after \( \tilde{n} \) iterations \( t_\varepsilon \hat{\sigma}_{g,n} n^{-1/2} + n^{-1} \leq \hat{\lambda}_{g,n} \), where \( \hat{\lambda}_{g,n} \) is a strongly consistent estimator of the population SD \( \lambda_g \). Asymptotic validity of the relative magnitude and relative SD stopping rules is established by Glynn and Whitt (1992) and Flegal and Gong (2015) respectively. This ensures that the simulation will terminate in a finite time with probability 1.

In Bayesian statistics applications, Flegal and Gong (2015) advocate the use of relative SDFWSR. In the high dimensional settings, that is, where \( g \) is a \( \mathbb{R}^p \) valued function and \( p \) is large, without apriori knowledge of the magnitude of \( E_{\pi} g \), Gong and Flegal (2016) prefer relative SDFWSR over FWSR based on the marginal chains. In the multivariate settings, Vats et al. (2019) argue that stopping rules based on \( p \) marginal chains may not be appropriate as these ignore cross correlations between components and may be dictated by the slowest mixing marginal chain. Vats et al. (2019) propose a relative standard deviation stopping rule involving volume of the \( 100(1 - \alpha)\% \) asymptotic confidence region, that is, \( \text{Vol}(C_\alpha(n)) \). Let \( \hat{\Lambda}_{g,n} \) be the sample covariance matrix. Vats et al. (2019) propose to stop the simulation, the first time after \( \tilde{n} \) iterations that

$$\frac{\text{Vol}(C_\alpha(n))}{n} + \frac{1}{n} \leq \varepsilon(|\hat{\Lambda}_{g,n}|)^{1/2},$$

where \(| \cdot |\) denotes the determinant.

### 2.3. Effective sample size

For an MCMC based estimator, effective sample size (ESS) is the number of independent samples equivalent to (that is, having the same standard error as) a set of correlated Markov chain samples. Although ESS
(based on \(n\) correlated samples) is not uniquely defined, the most common definition \cite{Robert2004} is

\[
\text{ESS} = \frac{n}{1 + 2 \sum_{i=1}^{\infty} \text{Corr}(g(X_0), g(X_i))}.
\]

\cite{Gong2016} rewrite the above definition as \(\text{ESS} = n \lambda_2^2/\sigma_g^2\). In the multivariate setting, that is, when \(g\) is \(\mathbb{R}^p\) valued for some \(p \geq 1\), \cite{Vats2019} define multivariate \(\text{ESS}\) as

\[
\text{mESS} = n \left( \frac{|\Lambda_g|}{|\Sigma_g|} \right)^{1/p}, \quad (5)
\]

where \(\Lambda_g\) is the population covariance matrix. An approach to terminate MCMC simulation is when \(\hat{\text{ESS}} (\hat{\text{mESS}})\) takes a value larger than a prespecified number, where \(\hat{\text{ESS}} (\hat{\text{mESS}})\) is a consistent estimator of \(\text{ESS}\) (\(\text{mESS}\)). Indeed, \cite{Vats2019} mention that simulation can be terminated the first time that \(\hat{\text{mESS}} = n \left( \frac{|\hat{\Lambda}_{g,n}|}{|\hat{\Sigma}_{g,n}|} \right)^{1/p} \geq 2^{2/p} \pi^{2/\epsilon^2} \chi^2_{1-\alpha,p} \epsilon^2\), \(\hat{\text{mESS}}\) is the desired level of precision for the volume of the \((1-\alpha)\%\) asymptotic confidence region, and \(\chi^2_{1-\alpha,p}\) is the \((1-\alpha)\) quantile of \(\chi^2_p\). This \(\text{ESS}\) stopping rule is (approximately) equivalent to the multivariate relative standard deviation stopping rule given in \(\footnote{Gong and Flegal (2016)}\) for details). Note that, \(\text{ESS}\) (\(\text{mESS}\)) per unit time can be used to compare different MCMC algorithms (with the same stationary distribution) in terms of both computational and statistical efficiency. \(\text{ESS}\) is implemented in several R packages including \texttt{coda} \cite{Plummer2006} and \texttt{mcmcse} \cite{Flegal2012}. In the \texttt{mcmcse} package, estimates of \(\text{ESS}\) both in univariate and multivariate settings are available. While \cite{Gong2016} and \cite{Vats2019} provide connection between \(\text{ESS}\) and relative SDFWSR stopping rules, \cite{Vats2018} draw correspondence between \(\text{ESS}\) and a version of the widely used Gelman-Rubin diagnostic presented in the next Section.

### 2.4. Gelman-Rubin diagnostic

Gelman-Rubin (GR) diagnostic appears to be the most popular method for assessing samples obtained from running MCMC algorithms. The GR diagnostic relies on multiple chains \(\{X_{i0}, X_{i1}, \ldots, X_{in-1}\}, i = 1, \ldots, m\) starting at initial points that are drawn from a density that is over-dispersed with respect to the target density \(\pi\). \cite{Gelman1992} describe methods of creating an initial distribution, although in practice, these initial points are usually chosen in some ad hoc way. Using parallel chains, \cite{Gelman1992} construct two estimators of the variance of \(X\) where \(X \sim \pi\), namely, the within chain variance estimate, \(W = \sum_{i=1}^{m} \sum_{j=0}^{n-1} (X_{ij} - \bar{X}_i)^2/(m(n-1))\), and the pooled variance estimate \(\hat{V} = ((n-1)/n)W + B/n\) where \(B/n = \sum_{i=1}^{m} (\bar{X}_i - \bar{X})^2/(m-1)\) is the between chain variance estimate, and \(\bar{X}_i\) and \(\bar{X}\) are the \(i^{th}\) chain mean and the overall mean respectively, \(i = 1, 2, \ldots, m\). Finally, \cite{Gelman1992} compare the ratio of these two estimators to one. In particular, they calculate the potential scale reduction factor (PSRF) defined by

\[
\hat{R} = \frac{\hat{V}}{W}, \quad (7)
\]

and compare it to one. \cite{Gelman1992} argue that since the chains are started from an over-dispersed initial distribution, in finite samples, the numerator in \(\footnote{Gelman and Rubin (1992)}\) overestimates the target variance whereas the denominator
underestimates it, making $\hat{R}$ larger than 1. Simulation is stopped when $\hat{R}$ is sufficiently close to one. The cut-off value 1.1 is generally used by MCMC practitioners as recommended in Gelman et al. (2014). Recently, Vats and Knudson (2018) propose a modified GR statistic where the between chain variance ($B/n$) is replaced with a particular batch means estimator of the asymptotic variance for the Monte Carlo averages $X_n$. This modified definition allows for a connection with ESS and, more importantly, computation of the GR diagnostic based on a single chain. We would like to point out that the expression of $\hat{R}$ given in (7), although widely used in practice, it differs slightly from the original definition given in Gelman and Rubin (1992).

Brooks and Gelman (1998) propose the multivariate PSRF (MPSRF) to diagnose convergence in the multivariate case. It is denoted by $\hat{R}_p$ and is given by,

$$\hat{R}_p = \max_a a^T \hat{V} a = \frac{n-1}{n} + \left(1 + \frac{1}{m}\right) \lambda_1,$$

where $\hat{V}$ is the pooled covariance matrix, $W^*$ is the within chain covariance matrix, $B^*$ is the between chain covariance matrix and $\lambda_1$ is the largest eigenvalue of the matrix $(W^{*-1}B^*)/n$. As in the univariate case, simulation is stopped when $\hat{R}_p \approx 1$. Recently, Peltonen et al. (2009) have proposed a visualization tool based on linear discriminant analysis and discriminant component analysis which can be used to complement the diagnostic tools proposed by Gelman and Rubin (1992) and Brooks and Gelman (1998). The GR diagnostic can be easily calculated, and is available in different statistical packages including the CODA package (Plummer et al. 2006) in R. To conclude our discussion on the GR diagnostic, note that originally Gelman and Rubin (1992) suggest running $m$ parallel chains, each of length $2n$. Then discarding the first $n$ simulations, $R$ is computed based on the last $n$ iterations. This leads to the waste of too many samples, and we do not recommend it.

2.5. Two spectral density based methods

In this section, we discuss two diagnostic tools based on asymptotic variance estimates of certain statistics to check for convergence to stationarity. Geweke (1992) proposes a diagnostic tool based on the assumption of existence of the spectral density of a related time series. Indeed, for the estimation of $E_g$, the asymptotic variance of $\bar{g}_n$ is $S_g(0)$, the spectral density of $(g(X_t), n \geq 0)$ (treated as a time series) evaluated at zero. After $n$ iterations of the Markov chain, let $\bar{g}_A$ and $\bar{g}_B$ be the time averages based on the first $n_A$ and the last $n_B$ observations. Geweke (1992)’s statistic is the difference $\bar{g}_A - \bar{g}_B$, normalized by its standard error calculated using a nonparametric estimate of $S_g(0)$ for the two parts of the Markov chain. Thus, Geweke (1992)’s statistic is $Z_n = \left(\bar{g}_A - \bar{g}_B\right)/\sqrt{S_g(0)\cdot n_A + S_g(0)\cdot n_B}$. Geweke (1992) suggests using $n_A = 0.1n$ and $n_B = 0.5n$. The $Z$ statistic is calculated under the assumption of independence of the two parts of the chain. Thus, Geweke (1992)’s convergence diagnostic is a $Z$ test of equality of means where autocorrelation in the samples is taken into account while calculating the standard error.

Heidelberger and Welch (1983) propose another method based on spectral density estimates. Heidelberger and Welch (1983)’s diagnostic is based on $B_n(t) = \left(\sum_{i=0}^{\lfloor nt\rfloor} g(X_i) - \lfloor nt\rfloor \bar{g}_n\right)/\sqrt{\frac{nS_g(0)}}$. Assuming that $\{B_n(t), 0 \leq t \leq 1\}$ is distributed asymptotically as a Brownian bridge, the Cramer von Mises statistic $\int_0^1 B_n(t)^2 dt$ may be used to test the stationarity of the Markov chain. The stationarity test is successively applied, first on the whole chain, and then rejecting the first 10%, 20%, ... and so forth of the samples until the test is passed or 50% of the samples have been rejected. Both of these two spectral density-based tools presented here are implemented in the CODA package (Plummer et al. 2006). These are univariate diagnostics although Cowles and Carlin (1996) mention that for Geweke (1992)’s statistic, $g$ may be taken to be $-2$ times the log of the target density when $X = R^d$ for some $d > 1$. Finally, we would like to mention
that the two spectral density based methods mentioned here, just like the ESS and the GR diagnostic, assume the existence of a Markov chain CLT ([2]), emphasizing the importance of the theoretical analysis discussed in Section 2.1.

2.6. Raftery-Lewis diagnostic

Suppose the goal is to estimate a quantile of \( g(X) \), that is, to estimate \( u \) such that \( P_u(g(X) \leq u) = q \) for some prespecified \( q \). Raftery and Lewis ([1992]) propose a method for calculating an appropriate burn-in. They also discuss choosing a run length so that the resulting probability estimate lies in \([q - \epsilon, q + \epsilon]\) with probability \((1 - \alpha)\). Thus the required accuracy \( \epsilon \) is achieved with probability \((1 - \alpha)\). Raftery and Lewis ([1992]) consider the binary process \( W_n \equiv I(g(X_n) \leq u), \) \( n \geq 0 \). Although, in general, \( \{W_n\}_{n \geq 0} \) itself is not a Markov chain, Raftery and Lewis ([1992]) assume that for sufficiently large \( k \), the subsequence \( \{W_{nk}\}_{n \geq 0} \) is approximately a Markov chain. They discuss a method for choosing \( k \) using model selection techniques. The transition probability \( P(W_{nk} = j|W_{(n-1)k} = i) \) is estimated by the usual estimator

\[
\frac{\sum_{l=1}^n I(W_{lk} = j, W_{(l-1)k} = i)}{\sum_{l=1}^n I(W_{lk} = i)},
\]

for \( i, j = 0, 1 \). Here, \( I(\cdot) \) is the indicator function. Using a straightforward eigenvalue analysis of the two-state empirical transition matrix of \( \{W_{nk}\}_{n \geq 0} \), Raftery and Lewis ([1992]) provide an estimate of the burn-in. Using a CLT for \( \sum_{j=0}^{n-1} W_{jk}/n \), they also give a stopping rule to achieve the desired level of accuracy.

To implement this univariate method an initial number \( n_{\text{min}} \) of iterations is used, then it is determined if any additional runs is required using the above techniques. The value \( n_{\text{min}} = \{\Phi^{-1}(1-\alpha/2)\}^2 q(1-q)/\epsilon^2 \) is based on the standard asymptotic sample size calculation for Bernoulli \((q)\) population. Since the diagnostic depends on the \( q \) values, the method should be repeated for different quantiles and the largest among these burn-in estimates can be used. Raftery and Lewis ([1992])’s diagnostic is available in the CODA package (Plummer et al. [2006]).

2.7. Kernel density based methods

There are MCMC diagnostics which compute distance between the kernel density estimates of two chains or two parts of a single chain and conclude convergence when the distance is close to zero. Unlike the widely used GR diagnostic (Gelman and Rubin [1992]) which is based on comparison of some summary moments of MCMC chains, these tools are intended to assess the convergence of the whole distributions. Yu ([1994]) and Boone et al. ([2014]) estimate the \( L^1 \) distance and Hellinger distance between the kernel density estimates respectively. More recently, Dixit and Roy ([2017]) use the symmetric Kullback Leibler (KL) divergence to produce two diagnostic tools based on kernel density estimates of the chains. Below, we briefly describe Dixit and Roy ([2017])’s method.

Let \( \{X_{ij} : i = 1, 2; j = 1, 2, \ldots, n\} \) be the \( n \) observations obtained from each of the two Markov chains initialized from two points well separated with respect to the target density \( \pi \). The adaptive kernel density estimates of observations obtained from the two chains are denoted by \( p_{1n} \) and \( p_{2n} \) respectively. The KL divergence between \( p_{1n} \) and \( p_{2n} \) is denoted by \( KL(p_{1n} | p_{2n}), i \neq j, i, j = 1, 2 \), that is,

\[
KL(p_{1n} | p_{2n}) = \int_X p_{1n}(x) \log \frac{p_{1n}(x)}{p_{2n}(x)} dx.
\]

Dixit and Roy ([2017]) find the Monte Carlo estimates of \( KL(p_{1n} | p_{2n}) \) using samples simulated from \( p_{1n} \) using the technique proposed by Silverman ([1986], Sec 6.4.1). They use the estimated symmetric KL divergence \( (KL(p_{1n} | p_{2n}) + KL(p_{2n} | p_{1n})/2) \) between \( p_{1n} \) and \( p_{2n} \) to assess convergence where a testing of hypothesis
framework is used to determine the cut-off points. The hypotheses are chosen such that the Type 1 error is concluding that the Markov chains have converged when in fact they have not. The cut-off points for the symmetric KL divergence are selected to ensure that the probability of Type 1 error is below some level, say, 0.05. In case of multiple ($m > 2$) chains, the maximum among ($\binom{m}{2}$) estimated symmetric KL divergence (referred to as Tool 1) is used to diagnose MCMC convergence. Finally, for multivariate examples, that is when $\mathcal{X} = \mathbb{R}^d$ for some $d > 1$, although multivariate Tool 1 can be used, in higher dimensions when kernel density estimation is not reliable, Dixit and Roy (2017) recommend assessing convergence marginally, i.e. one variable at a time, where appropriate cut-off points are found by adjusting the level of significance using Bonferroni’s correction for multiple comparison.

For multimodal target distributions, if all chains are stuck at the same mode, then empirical convergence diagnostics based solely on MCMC samples may falsely treat the target density as unimodal and are prone to failure. In such situations, Dixit and Roy (2017) propose another tool (Tool 2) that makes use of the KL divergence between the kernel density estimate of MCMC samples and the target density (generally known up to the unknown normalizing constant), to detect divergence. In particular, let $\pi(x) = f(x)/c$, where $c = \int_{\mathcal{X}} f(x)dx$ is the unknown normalizing constant. Dixit and Roy (2017)’s Tool 2 is given by

$$T_2^* = \left| \hat{c} - c^* \right| / c^*,$$

where $\hat{c}$ is a Monte Carlo estimate, as described in section 3.3 of Dixit and Roy (2017), of the unknown normalizing constant ($c$), based on the KL divergence between the adaptive kernel density estimate of the chain and $\pi$, and $c^*$ is an estimate of $c$ obtained by numerical integration. Dixit and Roy (2017) discuss that $T_2^*$ can be interpreted as the percentage of the target distribution not yet captured by the Markov chain. Using this interpretation, they advocate that if $T_2^* > 0.05$, then the Markov chain has not yet captured the target distribution adequately. Since (9) involves numerical integration, it can’t be used in high-dimensional examples.

2.7.1. A visualization tool. Dixit and Roy (2017) propose a simple visualization tool to complement their KL divergence diagnostic tool. This tool can be used for any diagnostic method (including the GR diagnostic) based on multiple chains started at distinct initial values, to investigate reasons behind their divergence. Suppose $m (\geq 3)$ chains are run, and a diagnostic tool has revealed that the $m$ chains have not mixed adequately and thus the chains have not yet converged. This indication of divergence could be due to a variety of reasons. A common reason for divergence is formation of clusters among multiple chains. Dixit and Roy (2017)’s visualization tool utilizes the tile plot to display these clusters. As mentioned in Section 2.7 for $m$ chains, the KL divergence tool finds the estimated symmetric KL divergence between each of the ($\binom{m}{2}$) combinations of chains and reports the maximum among them. In the visualization tool, if the estimated symmetric KL divergence for a particular combination is less than or equal to the cut-off value, then the tool utilizes a “grey” tile to represent that the two chains belong to the same cluster else it uses a “black” tile to represent that the two chains belong to different clusters.

Dixit and Roy (2017)’s visualization tool can also be used for multivariate chains. In cases where the diagnostic tool for $d$ variate chains, indicates divergence, for further investigation, the user can choose a chain from each cluster and implement the visualization tool marginally i.e. one variable at a time. This will help the user identify, which among the $d$ variables are responsible for inadequate mixing among the $m$ multivariate chains.
2.8. Graphical methods

In addition to the visualization tool mentioned in Section 2.7.1, we now discuss some of the widely used graphical methods for MCMC convergence diagnosis. The most common graphical convergence diagnostic method is the trace plot. The trace plot is a time series plot which shows the realizations of the Markov chain at each iteration against the iteration numbers. This graphical method is used to visualize how the Markov chain is moving around the state space, that is, how well it is mixing. If the MCMC chain is stuck in some part of the state space, the trace plots show flat bits indicating slow convergence. Such a trace plot is observed for an MH chain if too many proposals are rejected consecutively. On the other hand, for an MH chain if too many proposals are accepted consecutively, then trace plots may move slowly not exploring the rest of the state space. Visible trend or change in spread of the trace plot imply that the stationarity has not been reached yet. It is often said that a good trace plot should look like a hairy caterpillar. For an efficient MCMC algorithm if the initial value is not in the high density region, the beginning of the trace plots show back to back steps in one direction. On the other hand, if the trace plot shows similar pattern throughout, then there is no use in throwing burn-in samples.

Unlike iid sampling, MCMC algorithms result in correlated samples. The lag-\(k\) (sample) autocorrelation is defined to be the correlation between the samples \(k\) steps apart. The autocorrelation plot shows values of the lag-\(k\) autocorrelation function (ACF) against increasing \(k\) values. For fast mixing Markov chains, lag-\(k\) autocorrelation values drop down to (practically) zero quickly as \(k\) increases. On the other hand, high lag-\(k\) autocorrelation values for larger \(k\) indicates presence of high degree of correlation and slow mixing of the Markov chain. Generally, in order to get precise Monte Carlo estimates, Markov chains need to be run a large multiple of the time it takes the ACF to be practically zero.

Another graphical method used in practice is the running mean plot although its use has faced criticism (Geyer 2011). The running mean plot shows the Monte Carlo (time average) estimates against the iterations. This line plot should stabilize to a fixed number as iteration increases. On the other hand, non convergence of the plot indicates that the simulation can not be stopped yet. While the trace plot is used to diagnose Markov chain’s convergence to stationarity, the running mean plot is used to decide stopping times.

In the multivariate case, individual trace, autocorrelation and running mean plots are generally made based on realizations of each marginal chain. Thus the correlations that may be present among different components are not visualized through these plots. In multivariate settings, investigating correlation across (cross correlation) different variables is required to check for the presence of high cross correlation (Cowles and Carlin 1996).

3. Examples

In this section, we use three detailed examples to illustrate the convergence diagnostics presented in Section 2. Using these examples, we also demonstrate that empirical convergence diagnostic tools may give false indication of convergence to stationarity as well as convergence of Monte Carlo estimates.

3.1. An exponential target distribution

Let the target distribution be \(\pi(x) = \exp(-x), \; x > 0\). We consider an independence Metropolis sampler with \(\exp(\theta)\) proposal, that is, the proposal density is \(q(x) = \theta \exp(-\theta x), \; x > 0\). We study the independence chain corresponding to two values of \(\theta\), namely, \(\theta = 0.5\) and \(\theta = 5\). Using this example, we illustrate the ‘honest choices’ of burn-in and stopping time described in Section 2.1 as well as several other diagnostic tools. It turns out that, even in this unimodal example, some empirical diagnostics may lead to premature termination of simulation. We first consider some graphical diagnostics for Markov
chain convergence. Since the target density is a strictly decreasing function on (0, ∞), a small value may serve as a reasonable starting value. We run the Markov chain for 1,000 iterations initialized at X_0 = 0.1. Figure 1 shows the trace plots and autocorrelation plots of the Markov chain samples. From the trace plots we see that while the first chain (θ = 0.5) mixes well, the second chain exhibits several flat bits and suffers from slow mixing. Thus from the trace plots, we see that there is no need for burn-in for θ = 0.5, that is, X_0 = 0.1 seems to be a reasonable starting value. On the other hand, for θ = 5, the chain can be run longer to find an appropriate burn-in. This is also corroborated by the autocorrelation plots. When θ = 0.5, autocorrelation is almost negligible after lag 4. On the other hand, for θ = 5, there is significant autocorrelation even after lag 50. Next, using the CODA package (Plummer et al. 2006), we compute Geweke (1992)’s and Heidelberger and Welch (1983)’s convergence diagnostics for the identity function g(x) = x. Using the default n_A = 0.1n and n_B = 0.5n, Geweke (1992)’s Z score for the θ = 0.5 and θ = 5 chains are 0.733 and 0.605 respectively, failing to reject the hypothesis of the equality of means from the beginning and end parts of the chains. Similarly, both the chains pass Heidelberger and Welch (1983)’s test for stationarity. Next, we consider the Raftery and Lewis (1992) diagnostic. When the two samplers are run for 38,415 ([n_{min}] correspond to ε = 0.005, α = 0.05 and q = 0.5) iterations, and Raftery-Lewis diagnostic is applied for different q values (0.1, ..., 0.9), the burn-in estimates for the θ = 5 chain are larger than those for the θ = 0.5 chain, although the overall maximum burn-in (981) is less than 1,000. Finally, we consider the choice of ‘honest burn-in’. Since for θ < 1, π(x)/q(x) = θ^{-1} exp(x(θ − 1)) ≤ θ^{-1} for all x > 0, by Mengersen and Tweedie (1996), we know that
\[
\frac{1}{2} \int_{x} |f_n(x) − \pi(x)| dx ≤ (1 − θ)^n,
\]
that is, an analytical upper bound to the TV norm can be obtained. Thus for θ = 0.5, if n' = [log(0.01)/log(0.5)] = 7, then (1) holds. Thus n' = 7 can be an honest burn-in for the independence Metropolis chain with θ = 0.5. Note that, for θ < 1, the independence chain is geometrically ergodic, for θ = 1, the chain produces iid draws from the target, and for θ > 1, by Mengersen and Tweedie (1996), the independence chain is subgeometric. As mentioned in Jones and Hobert (2001), when θ > 1, the tail of the proposal density is much lighter than that of the target, making it difficult for the chain to move to larger values, and when it does move there, it tends to get stuck.

Next, we consider stopping rules for estimation of the mean of the stationary distribution, that is, E_x X = 1. Based on a single chain, we apply the FWSR (3) to determine the sample size for ε = 0.005 and α = 0.05 (that is, t_α = 1.96). For the independence Metropolis chain with θ = 0.5 starting at X_0 = 0.1545, it takes n' = 323,693 iterations to achieve the cut-off 0.005. The running estimates of the mean along with confidence intervals are given in the left panel of Figure 2. We next run the independence Metropolis chain with θ = 5 for 323,700 iterations starting at X_0 = 0.1. The corresponding running estimates are given in the right panel of Figure 2. Since a Markov chain CLT is not available for the independence chain with θ > 1, we can’t compute asymptotic confidence intervals in this case. From the plot we see that the final estimate (0.778) is far off from the truth (E_x X = 1). Next, we consider ESS. The cut off value for ESS mentioned in (3) with ε = 2 * 0.005 = 0.01 is 153,658. The ESS for the two chains are 163,955 and 1,166 respectively which again shows the presence of large correlation among the MCMC samples for θ = 5. We use the R package mcmcse (Flegal et al. 2012) for computing ESS. Finally, we consider the GR diagnostic. We run four parallel chains for 2,000 iterations starting at 0.1, 1, 2, and 3 respectively each with both θ = 0.5 and θ = 5. We calculate Gelman and Rubin (1992)’s PSRF (7) based on these chains. The plots of iterative R at the increment of every 100 iterations are given in Figure 3. From the plots we see that R for the chain with θ = 0.5 reaches below 1.1 in 100 iterations. On the other hand, the Monte Carlo estimate for E_x X and its standard error based on first 100 iterations for the chain started at 0.1 are 1.109 and 0.111 respectively. Thus, GR diagnostic leads to premature termination of simulation and the inference drawn
from the resulting samples can be unreliable. Lastly, \( \hat{R} \) for the chains with \( \theta = 5 \) takes large (> 16) values even after 2,000 iterations showing that simulation can’t be stopped yet in this case.

3.2. A sixmodal target distribution

This example is proposed by Leman et al. (2009) where the target density is as follows

\[
\pi(x, y) \propto \exp\left(\frac{-x^2}{2}\right) \exp\left(\frac{(\csc y)^5 - x^2}{2}\right), \quad -10 \leq x, y \leq 10.
\]

The contour plot of the target distribution (known up to the normalizing constant) is given in Figure 4 and marginal densities are plotted in Figure 5. The plots of the joint and marginal distributions clearly show that the target distribution is multimodal in nature.

To draw MCMC samples from the target density (10), we use a Metropolis within Gibbs sampler in which X is drawn first and then Y. In this example, we consider only convergence to stationarity, that is, we do not discuss stopping rules here. Through this example, we illustrate that when an MCMC sampler is stuck in a local mode, the empirical convergence diagnostic tools may give false indication of convergence. (Empirical diagnostics may fail even when ‘modes’ are not well defined (Geyer and Thompson 1995).) In order to illustrate the diagnostic tools, as in Dixit and Roy (2017), we consider two cases.
Estimates of the mean
Iterations
Estimate

0 60000 120000 180000 240000 300000
0.8 1.0 1.2 1.4

CI

Estimate

Figure 2
The left plot shows the running estimates of the mean with confidence interval for $\theta = 0.5$. Running mean plot for $\theta = 5$ is given in the right panel. The horizontal line denotes the truth.

Figure 3
Iterative $\hat{R}$ plot (from four parallel chains) for the independence chains (left plot $\theta = 0.5$, right plot $\theta = 5$).

Case 1
In this case, we run four chains wherein two chains (chain 1 and chain 2) are started at a particular mode while the remaining two chains (chain 3 and chain 4) are started at some other mode. Each of the four chains is run for 30,000 iterations. Trace plots of the last one thousand iterations of the four parallel $X$ and $Y$ marginal chains are given in the left panel of Figures 6 and 7 respectively. Trace plots show the divergence of the Markov chains. High ACF values can also be seen from the autocorrelation plots of the marginal chains in Figures 6 and 7.

Next we apply Dixit and Roy (2017)'s bivariate KL divergence Tool 1 on the joint chain. The maximum symmetric KL divergence among the six pairs is 104.89 significantly larger than the cut-off value 0.06. Finally, we use Dixit and Roy (2017)'s visualization tool to identify clusters among the four chains. The result is given in Figure 8 which shows that there are two clusters among the four chains wherein chain 1 and chain 2 form one cluster, while chain 3 and chain 4 form another cluster.

Case 2
In this case also we run four chains but all the chains are started at the same local mode. As in case 1,
all four chains are run for 30,000 iterations. The trace and autocorrelation plots of the marginal chains are given in Figures 9 and 10. From these plots one may conclude mixing of the Markov chains, although the large autocorrelations result in low ESS for the chains. The minimum and maximum mESS (5) computed using the R package mcmcse for the four chains are 412 and 469 respectively.

The adaptive kernel density estimates of the four chains are visualized in Figure 11. Next, we compute Geweke (1992)'s and Heidelberger and Welch (1983)'s convergence diagnostics for the identity function $g(x) = x$ for all four individual chains. At level 0.05, Geweke (1992)'s diagnostic fails to reject the hypothesis of the equality of means from the beginning and end parts of each chain. Similarly, all chains pass Heidelberger and Welch (1983)'s test for stationarity. Thus both Geweke (1992)'s and Heidelberger and Welch (1983)'s diagnostics fail to detect the non-convergence of the chains to the target distribution. Also, Raftery-Lewis diagnostic fails to distinguish between the chains in Case 1 and Case 2 as it results in similar burn-in estimates in both cases.

We also calculate the PSRF for the marginal chains as well as the MPSRF for the joint chain based on the four parallel chains as the GR diagnostic is often used by practitioners for determining burn-in (Flegal et al. 2008, p. 256). The plots of iterative $\hat{R}$ at the increment of every 1,000 iterations are given in the left
Figure 6
Trace (left panel) and ACF (right panel) plots of the X marginal of the four chains for the sixmodal example in case 1.

Figure 7
Trace (left panel) and ACF (right panel) plots of the Y marginal of the four chains for the sixmodal example in case 1.

Figure 8
Dixit and Roy [2017]'s tile plot in the case 1 of the sixmodal example.
Figure 9
Trace (left panel) and ACF (right panel) plots of the X marginal of the four chains for the sixmodal example in case 2.

Figure 10
Trace (left panel) and ACF (right panel) plots of the Y marginal of the four chains for the sixmodal example in case 2.

PSRFs for the marginal chains reach below 1.1 before 3,000 iterations. The MPSRF (not shown in the plot) also reaches below 1.1 before 6,000 iterations. Since both the PSRF and MPSRF values are close to one, it is often used as sign of convergence to the stationarity.

Since all four chains are stuck at the same local mode, that is, these are not run long enough to move between the modes, the convergence diagnostics including PSRF, MPSRF get fooled into thinking that the target distribution is unimodal, and hence, falsely detect convergence. Laha et al. (2016) demonstrate failures of trace plots, autocorrelation plots and PSRF in diagnosing non-convergence of MCMC samplers in the context of a statistical model used for analyzing rank data (See Hobert et al. (2011) for examples of multimodal targets arising from the popular Bayesian finite mixture models where empirical convergence diagnostic tools face similar issues.). Since these diagnostic tools make use of (only) the samples obtained from the MCMC algorithm and all observations lie around the same mode, they fail to diagnose non-convergence. On the other hand, Dixit and Roy (2017)’s Tool 2 (9) use both MCMC samples and the target density. Since Dixit and Roy (2017)’s Tool 2 requires only one chain and since the PSRF suggest...
that the four chains are similar, we simply choose one of the four chains. Now, $T_2^* = 0.88$ is significantly greater than zero and thus indicates that the chains are stuck at the same mode, further it also indicates that 88% of the target distribution is not yet captured by the Markov chain. Thus Dixit and Roy (2017)'s Tool 2 is successful in detecting the divergence of the chains.

### 3.3. A Bayesian logistic model

In this section, we illustrate MCMC convergence diagnostics in the context of a real data analysis using a popular statistical model. In particular, we fit a Bayesian logistic model on the “Anguilla australis distribution” dataset provided in the R package dismo (Hijmans et al. 2016). Data are available on a number of sites with presence or absence of the short-finned eel (Anguilla australis) in New Zealand, and some environmental variables at these sites. In particular, we fit the “Anguilla_train” data available in the dismo package. Here, the response variable is presence or absence of short finned eel, and six other variables are included as covariates. The six covariates are: summer air temperature (SeqSumT), distance to coast (DSDist), area with indigenous forest (USNative), average slope in the upstream catchment...
(USSlope), maximum downstream slope (DSMaxSlope) and fishing method (categorical variable with five classes namely electric, mixture, net, spot and trap). Thus the data set consists of \((y_i, x_i), i = 1, \ldots, 1000\), where \(y_i\) is the \(i\)th observation of the response variable taking value 1 (presence) or zero (absence), and \(x_i = (1, \tilde{x}_i)\) is the ten dimensional covariate vector, 1 for the intercept and \(\tilde{x}_i\) for the other nine covariates (with four components for the categorical variable fishing method). This example was also used by Dixit and Roy (2017) and Boone et al. (2014) to illustrate their MCMC convergence diagnostic tools.

Denote \(\beta = (\beta_0, \beta_1, \ldots, \beta_9)\) where \(\beta_0\) is the intercept and \((\beta_1, \ldots, \beta_9)\) is the \(9 \times 1\) vector of unknown regression coefficients. We consider the logistic regression model

\[
Y_i | \beta \overset{ind}{\sim} \text{Bernoulli}(F(x_i^T \beta)), \ i = 1, \ldots, 1000,
\]

where \(F(\cdot)\) is the cdf of the logistic distribution, that is,

\[
F(x_i^T \beta) = \frac{\exp(x_i^T \beta)}{1 + \exp(x_i^T \beta)}, \ i = 1, \ldots, 1000.
\]

We consider a Bayesian analysis with a diffuse normal prior on \(\beta\). Thus, the posterior density is

\[
\pi(\beta | y) \propto n \prod_{i=1}^{n} F(x_i^T \beta)^{y_i} \{1 - F(x_i^T \beta)\}^{1-y_i} \phi_{10}(\beta),
\]

where \(\phi_{10}(\beta)\) is the density of \(N(0, 100 I_{10})\). The posterior density \((11)\) is intractable in the sense that means with respect to this density, which are required for Bayesian inference, are not available in closed form.

As in Dixit and Roy (2017) and Boone et al. (2014), we use the MCMClogit function in the R package MCMCpack (Martin et al. 2011) to draw MCMC samples from the target density \(\pi(\beta | y)\). Exact MLE is not available for the logistic likelihood function, neither is the mode of the posterior density \((11)\). But, numerical optimization methods can be used to find approximate MLE or posterior mode, which may then be used as starting values. In order to assess convergence to stationarity, we run three parallel chains with the default tuning values for 5,000 iterations, one initialized at the MLE and the other two initialized at points away from the MLE. Trace plots of the three chains for last 1,000 iterations for the regression coefficients of summer air temperature and distance to coast are given in Figure 13. Trace plots of the other variables look similar. From these plots we see that, there is not much overlap between the three parallel chains. From the frequent flat bits, it follows that the Markov chains move tardily and suffer from slow mixing. Indeed, the default tuning parameters in the MCMClogit function result in low (0.11) acceptance rate. We next set the tuning parameters to achieve around 40% acceptance rate and all analysis in the remaining section is based on these new tuning values. We run the three chains longer (30,000 iterations) to obtain reliable ACF plots. Trace plots of the last 1,000 iterations for each of the three chains for the nine regression coefficients variables are given in Figure 14. From the trace plots we see that convergence of the chains can be further improved. Autocorrelations for all ten variables for one of the chains based on all 30,000 draws are given in Figure 15. Autocorrelations for the other two chains look similar (not included here). Like the trace plots, the autocorrelation plots also reveal that the Markov chains suffer from high autocorrelations. It is further corroborated by the multivariate ESS values which are less than 1,000 for all the three chains. To sample from \((11)\) one may use an alternative MCMC sampler, e.g., the Pólya-Gamma Gibbs sampler (Polson et al. 2013), which is known to be geometrically ergodic (Wang and Roy 2018c, Choi and Hobert 2013). Here we do not use the Pólya-Gamma Gibbs sampler as our goal is to illustrate the convergence diagnostic methods. The MPSRF reaches close to one before 30,000 iterations. Since the Markov chains are 10 dimensional, to maintain an overall Type 1 error rate of \(\alpha = 0.05\), using Bonferroni’s correction, Dixit and Roy
and Roy (2017) advocates the cut-off point 0.01 for the KL Tool 1 for marginal chains. For each of the ten variables, the maximum symmetric KL divergence among the three pairs of chains is computed. It turns out that the marginal chains do not pass the KL Tool 1 test as the maximum symmetric KL divergence takes the value 7.26 for the variable US\text{Slope}. After 30,000 iterations, all marginal chains pass Heidelberger and Welch (1983)'s stationarity test. On the other hand, for each of the three parallel chains, for some of the variables, Geweke (1992)'s Z test turns out to be significant at 0.05 level. Next, we run the chains for another 40,000 iterations. For the last 40,000 iterations, all marginal chains pass Geweke (1992)'s Z test, as well as the the KL Tool 1 test. Also, based on these 40,000 iterations, the maximum burn-in estimate from Raftery-Lewis diagnostic (with $\epsilon = 0.005$, $\alpha = 0.05$) over different quantiles ($q = 0.1, ..., 0.9$) is less than 100 for all 10 variables. We thus use $n' = 70,000$ as the burn-in value.

After removing the first 70,000 iterations as initial burn-in, each of the three chains are run for additional 15,000 iterations. Table I presents the PSRF and the maximum symmetric KL divergence (Dixit and Roy (2017)'s KL Tool 1) values based on three parallel chains for all 10 variables. The half-width of 95% confidence interval based on the first chain (started at the MLE) are also tabulated in Table I. All values are given up to three decimal places. MPSRF takes the value 1.004. For the three chains multivariate ESS takes values 515, 520 and 502 respectively. High cross correlation between the Intercept and SeqSumT regression coefficient parameters (-0.984) and between US\text{Native} and US\text{Slope} (-0.558) suggest that mixing of the Markov chain can improve if run on an appropriate lower dimensional space (that is, after dropping some variables) or a reparameterization is used. From Table I we see that all marginal chains pass the KL Tool 1 diagnostic. Also, all PSRF values as well as the MPSRF value reach below the cut-off 1.1. On the other hand, the maximum half-width among the 10 regression parameters is 0.112, much larger than the cut-off 0.01. Doing a simple sample size calculation, based on the pilot sample size 15,000, we find that we need $15,000 \times (0.112/0.01)^2 = 1,881,600$ samples for obtaining confidence intervals with half-width below 0.01.

Finally, we run one of the chains (the chain started at the MLE) for 1,881,600 iterations after a burn-in of $n' = 70,000$ iterations. Thus the chain is stopped after $n^* = 1,951,600$ iterations. In this case, as expected, the maximum half-width of the 95% confidence interval is below 0.01. An estimate of mESS calculated using the mcmcse package is 55,775 which is larger than the cut-off value 55,191 given in (6) for $p = 10$, $\alpha = 0.05$ and $\epsilon = 0.02$. On the other hand, the chain need to be run longer to achieve the cut-off value.
Figure 14
Trace plots of the three chains for the nine regression coefficients variables for the Bayesian logistic model example.

Figure 15
Autocorrelation plots of the ten marginal chains for the Bayesian logistic model example.
Table 1  Application of various MCMC convergence diagnostic tools to the Bayesian logistic model.

| Variable       | R    | half-width | Tool 1 |
|----------------|------|------------|--------|
| Intercept      | 1.000| 0.112      | 0.008  |
| SeqSumT        | 1.000| 0.006      | 0.007  |
| DSResp         | 1.001| 0.000      | 0.005  |
| USNative       | 1.001| 0.025      | 0.004  |
| M - mix        | 1.000| 0.031      | 0.005  |
| M - net        | 1.001| 0.031      | 0.004  |
| M - spot       | 1.000| 0.048      | 0.004  |
| M - trap       | 1.002| 0.051      | 0.004  |
| DSMaxSlope     | 1.000| 0.005      | 0.007  |
| USSlope        | 1.001| 0.002      | 0.004  |

2.20,766 (6) corresponding to \( \varepsilon = 0.01 \). Table 2 gives the estimates of posterior means (Est) of all regression coefficients and their corresponding Monte Carlo standard errors (SE).

Table 2  Estimates of posterior means and standard errors.

| Variable       | \( \beta_0 \) | \( \beta_1 \) | \( \beta_2 \) | \( \beta_3 \) | \( \beta_4 \) | \( \beta_5 \) | \( \beta_6 \) | \( \beta_7 \) | \( \beta_8 \) |
|----------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| Est            | -10.46       | 0.66         | -0.99        | -1.17        | -0.47        | -1.53        | -1.83        | -2.59        | -0.17        | -0.05        |
| \( \text{SE} \times 10^3 \) | 5.73         | 0.32         | 0.00         | 1.52         | 1.46         | 1.65         | 2.76         | 2.35         | 0.24         | 0.08         |

4. Conclusions and discussions

In this article, we discuss several measures for diagnosing convergence of Monte Carlo Markov chains to stationarity as well as convergence of the sample averages based on these chains. Detection of the first is often used to decide a suitable burn-in period, while the second leads to termination of the MCMC simulation. Analytical upper bounds to the TV norm required to obtain an ‘honest burn-in’ maybe difficult to find in practice or may lead to very conservative burn-in values. On the other hand, empirical diagnostics can falsely detect convergence when the chains are not run long enough to move between the modes. For the chains initialized at high density density regions, there is no need for burn-in. If the global mode of the target density can be (approximately) found by optimization then it can be used as the starting value.

Some of the empirical diagnostics for convergence of sample averages may prematurely terminate the simulation and the resulting inference can be far from the truth. Thus, use of fixed width and ESS based stopping rules is recommended. Most of the quantitative convergence diagnostics assumes a Markov chain CLT. While demonstrating the existence of a Markov chain CLT requires some rigorous theoretical analysis of the Markov chain, given the great amount of work done in this direction, validating ‘honest stopping rules’ is not viewed as much an obstacle as in the past.

None of the three examples discussed here used thinning. Thinning, that is, discarding all but every \( k \)th observation, is often used by MCMC practitioners to reduce high autocorrelations present in the Markov chain samples. Since it wastes too many samples, it should be used only if computer storage of the samples is an issue or evaluating the functions of interest \( (q) \) is more expensive than sampling the Markov chain. If thinning is used, convergence diagnostics can be used on the thinned samples.

Some convergence diagnostic tools use parallel chains initialized at different points, or two parts of a single chain. In the presence of multiple modes, if the initial points of the parallel chains are not in distinct high density regions, or the chain is not run long enough to move between the modes, the diagnostics fail to detect the non-convergence. Thus, single long runs should be used to make final inference. Running the chain longer may also result in discovering new parts of the support of the target distribution.
Practitioners should be careful while depending purely on empirical convergence diagnostic tools especially if presence of multiple modes is suspected. Empirical diagnostics can not detect convergence with certainty. Also, if the target is incorrectly assumed to be a proper density, the empirical diagnostic tools may not provide a red flag indicating its impropriety (Athreya and Roy 2014, Hobert and Casella 1996). Over the last two decades, a lot of research has been done to provide honest Monte Carlo sample size calculation for myriad MCMC algorithms for common statistical models. However, theoretical analysis of MCMC algorithms is an ongoing area of research and further important works need to be done. A potential future study involves theoretically verifying the convergence (to zero) of Dixit and Roy (2017)’s statistics based on the KL divergence. Another possible research problem is to construct theoretically valid and computationally efficient MCMC convergence diagnostics in ultrahigh dimensional settings.

ACKNOWLEDGMENTS

The author thanks one anonymous editor for careful and detailed comments on an earlier version of the manuscript. The author also thanks Evangelos Evangelou, Mark Kaiser and Dootika Vats for helpful comments. These valuable suggestions have substantially improved the paper.

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