Analyzing MCMC output

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Overview

Abstract

Markov chain Monte Carlo (MCMC) is a sampling-based method for estimating features of probability distributions. MCMC methods produce a serially correlated, yet representative, sample from the desired distribution. As such it can be difficult to assess when the MCMC method is producing reliable results. We present some fundamental methods for ensuring a reliable simulation experiment. In particular, we present a workflow for output analysis in MCMC providing estimators, approximate sampling distributions, stopping rules, and visualization tools.

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1 Introduction

Markov chain Monte Carlo (MCMC) algorithms are an essential tool for estimating features of probability distributions encountered in diverse applications (Brooks et al., 2011). The use of MCMC is commonly identified with Bayesian settings, but it is also useful in other situations (see e.g. Caffo et al., 2005; Geyer, 1991; Gjoka et al., 2011).

Suppose, for our application, we have developed a probability distribution \( F \) with support \( \mathcal{X} \subseteq \mathbb{R}^d, \ d \geq 1 \). Our goal is to use fixed, unknown features of \( F \) to make inference about the population. For example, for \( h : \mathcal{X} \to \mathbb{R} \), we may be interested in the expectation\(^1\)

\[
\mu_h = \mathbb{E}_F[h(X)] = \int_{\mathcal{X}} h(x) F(dx).
\]

The apparent simplicity of this hides an array of features, including probabilities, means, moments, and marginal densities associated with \( F \). Accordingly, we will typically want to use several expectations. There are features of \( F \) that are not expectations, such as quantiles, but we will defer discussion of this to Section 3. We collect all the features of \( F \) we want in a \( p \)-dimensional vector, \( \theta \).

We use the notation \( \sim \) to mean “distributed as,” \( \sim \) to mean “approximately distributed as,” \( \not\sim \) to mean “not distributed as,” and \( \approx \) to mean “is approximately equal to.” Often \( F \) is analytically intractable in the sense that directly calculating \( \theta \) is impossible and hence we may turn to estimating \( \theta \) using Monte Carlo sampling methods. We consider only MCMC in which a realization of a (aperiodic, Harris recurrent – for definitions see Meyn and Tweedie (2009)) Markov chain \( \{X_1, X_2, \ldots, X_n\} \) is produce so that for a sufficiently large Monte Carlo sample size \( n \), we have \( X_n \sim F \). We will not discuss how to construct or implement MCMC methods (see Chib and Greenberg, 1995; Robert and Casella, 2013; Robert et al., 2018), but will instead assume that there is already an efficient method for producing the MCMC sample, or output. The output is then used to construct estimators of \( \theta \) so that for a sufficiently large Monte Carlo sample size, \( n \), we have

\[
\hat{\theta}_n = \hat{\theta}(X_1, \ldots, X_n) \approx \theta.
\]

\(^1\)If \( f \) is a probability function, then this notation avoids having separate formulas for the continuous case where \( \mu_h = \int_{\mathcal{X}} h(x)f(x)dx \) and the discrete case where \( \mu_h = \sum_{x \in \mathcal{X}} h(x)f(x) \) but it also applies to more general settings.
In typical implementations of MCMC, the initial state, $X_1$, is drawn from some other distribution than the target, that is, $X_1 \sim F$, which implies $X_n \sim F$ for any finite Monte Carlo sample size $n$. Moreover, there is an inherent serial correlation in the MCMC sample. That is, the Markov chain draws are neither independent nor identically distributed. Thus, there are two common tasks in MCMC output analysis (i) deciding when the simulation has produced a representative sample from $F$, that is, when is $n$ large enough so that $X_n \sim F$, and (ii) when is $n$ sufficiently large to conclude $\hat{\theta}_n \approx \theta$. Notice that the required number of draws may be different for each task. Task (i) is difficult and while there are some rigorous approaches (Rosenthal, 1995), these are typically challenging to implement in practically relevant settings. This has led most practitioners to approach this question by relying on graphical summaries and ad hoc convergence diagnostics; see Section 2. Task (ii) is our main focus and is fundamental to ensuring a reliable simulation experiment. Classical large-sample frequentist methods provide principled, practical solutions for (ii). However, since it is a Markov chain that is being simulated, specialized techniques are required for their implementation; this is covered in some detail in Sections 3–6.

In practice, addressing tasks (i) and (ii) can seem complicated to the uninitiated. Thus, we present a workflow for analyzing output from MCMC addressing these challenges. This is illustrated in the context of a Bayesian example in Section 7.

## 2 Markov chain theory and starting values

The dynamics of a time-homogeneous Markov chain are dictated by its Markov transition kernel

$$P^n(x, A) := \Pr(X_{n+j} \in A \mid X_j = x), \quad n, j \geq 1$$

and $P^1 \equiv P$. If $\nu$ is the initial distribution (i.e. $X_1 \sim \nu$), then $\nu P^n$ is the marginal distribution of $X_n$. Markov chains for MCMC are constructed in such a way that the target distribution $F$, is its stationary distribution. That is, $FP^n = F$, so that if $X_1 \sim F$, then each $X_n \sim F$. Of course, producing $X_1 \sim F$ often is not possible in settings where MCMC is relevant. However, if $\| \cdot \|$ denotes total variation distance, under standard conditions (for
an accessible discussion see Jones and Hobert, 2001; Roberts and Rosenthal, 2004),

\[ \| \nu P^n - F \| \to 0 \text{ as } n \to \infty. \] 

(1)

This implies \( X_n \xrightarrow{d} F \) as \( n \to \infty \). Moreover, the total variation norm in (1) is non-increasing in \( n \) (Meyn and Tweedie, 2009). Hence a representative, although correlated, sample will be produced eventually, that is, for sufficiently large \( n \).

Ideally, we would like to identify \( n^* < \infty \) such that if \( n \geq n^* \), then \( \| \nu P^n - F \| < \epsilon \) for some \( \epsilon > 0 \) so that we could conclude \( X_n \sim F \). Indeed, there are methods for doing so (Jones and Hobert, 2001; Rosenthal, 1995), but they are often so conservative as to be of little practical use or are difficult to apply (Jones and Hobert, 2004). This has forced practitioners to turn to other methods, the most common of which are trace plots of the components of the simulation and so-called convergence diagnostics (Cowles and Carlin, 1996). Perhaps the most commonly used convergence diagnostic was developed by Gelman and Rubin (1992). However, this diagnostic has been shown to have severe limitations (Flegal et al., 2008; Vehtari et al., 2019); see Section 5 for more. In fact, many convergence diagnostics, including the Gelman-Rubin diagnostic, were developed to address task (ii) in Section 1, but are often incorrectly understood to answer task (i). In general, all convergence diagnostics should be used with care since their very use can introduce bias (Cowles et al., 1999). Strictly speaking, convergence does not occur for any finite \( n \) so all they can detect is evidence of non-convergence. Hence diagnostics can never guarantee what we want because absence of evidence of non-convergence is not evidence of convergence. For more discussion on convergence diagnostics see Roy (2019).

While the convergence in (1) holds for any starting value, some will be better than others since the rate of convergence can be affected by the choice of starting value (Rosenthal, 1995). In particular, starting in an area of low probability of \( F \) can lead to slow convergence of the Markov chain (Gilks et al., 1996). If, however, \( X_1 \sim F \), then \( \| FP^n - F \| = 0 \) for all \( n \), and the Markov chain produces exact draws from \( F \) (albeit still correlated). Thus, starting values can have a substantial impact on the quality of the samples. Choosing good starting values can save considerable time in postprocessing and increase confidence in the results.

It is a truism that “Any point you don’t mind having in a sample is a good starting
point.” (Geyer, 2011). While choosing a good starting value may be difficult, it may not be impossible. In fact, it may be possible to start from stationarity via perfect simulation (Huber, 2016), Bernoulli factories (Flegal and Herbei, 2012), or simple accept-reject samplers. When the target distribution is low-dimensional or made low-dimensional by a linchpin variable trick (Archila, 2016), an accept-reject sampler that can produce one sample from the target may be available. Such a sampler is often too computationally burdensome for a full Monte Carlo procedure, but may provide a single draw at reasonable cost.

Starting values are also often obtained by finding a high probability region via optimization. When a closed-form expression is available, using the maximum likelihood estimate can be computationally cheap. Other optimization approaches are certainly possible, but finding a global optimum is in general difficult. Even so, in many situations, any value in a high probability region is a reasonable starting value. In Bayesian settings, practitioners may draw starting values from the (proper) prior distributions of the parameters. This can work particularly well when the prior distributions have been chosen with care. Finally, and particularly when implementing component-wise MCMC methods (Johnson et al., 2013) such as Gibbs samplers, the parameter being updated first may not require a starting value. So it is often a good idea to first update the parameter whose starting value is least trustworthy.

3 Estimation and sampling distributions

Recall that given a realization \( \{X_1, X_2, \ldots, X_n\} \) of the Markov chain we construct an estimator of \( \theta \), \( \hat{\theta}_n = \hat{\theta}(X_1, \ldots, X_n) \) so that \( \hat{\theta}_n \to \theta \) almost surely as \( n \to \infty \). However, no matter how large the (finite) Monte Carlo sample size \( n \), there will be an unknown Monte Carlo error \( \hat{\theta}_n - \theta \). The approximate sampling distribution of the Monte Carlo error is often available through a version of the central limit theorem (CLT), which holds under moment conditions on the functionals and Markov chain mixing conditions (Jones, 2004), both of which require theoretical study to verify in a given application. Jones and Hobert (2001) give an accessible introduction to this theory which has been applied in a number of practically relevant settings (see e.g. Ekvall and Jones, 2019; Hobert et al., 2002; Johnson and Jones, 2015; Khare and Hobert, 2013; Lund and Tweedie, 1996; Roberts and Tweedie, 1996;
Means

In most settings we will want to estimate several expectations. Let $h : \mathcal{X} \to \mathbb{R}^p$ be a function such that $\mathbb{E}_F h(X) = \mu_h$ is of interest. For example, to estimate the mean vector of $F$, $h$ will be the identity function. Estimation is straightforward using a sample mean since the Markov chain strong law ensures

$$\bar{\mu}_n := \frac{1}{n} \sum_{t=1}^{n} h(X_t) \overset{a.s.}{\to} \mu_h \quad \text{as } n \to \infty .$$

If a CLT holds, then there exists a $p \times p$ positive definite matrix, $\Sigma$, such that as $n \to \infty$,

$$\sqrt{n} (\bar{\mu}_n - \mu_h) \overset{d}{\to} N_p(0, \Sigma) .$$

Here, $\Sigma$ encodes the covariance structure for $h$ in the target distribution and the serial lag-covariance due to the Markov chain. More specifically,

$$\Sigma = \sum_{k=-\infty}^{\infty} \text{Cov}_F(h(X_1), h(X_{1+k})) . \quad (2)$$

The subscript $F$ in (2) means that the expectations are calculated under the assumption that $X_1 \sim F$. This does not mean that we need $X_1 \sim F$ for the CLT to hold. Indeed, if the CLT holds for one initial distribution, then it holds for every initial distribution (Meyn and Tweedie, 2009).

Under an independent sampling scheme, $\text{Cov}_F(h(X_1), h(X_{1+k})) = 0$ for all $k \neq 0$, but the Markov chains encountered in MCMC applications exhibit serial dependence. Thus, utilizing the sampling distribution for $\bar{\mu}_n$ to make large-sample inference requires specialized methods for estimating $\Sigma$, which we discuss later.

Quantiles

In addition to expectations, marginal quantiles are often of interest. Let $h : \mathcal{X} \to \mathbb{R}$, and for $X \sim F$, set $V = h(X)$. Let $F_V$ be the distribution of $V$, and for $0 < q < 1$, the $q$-quantile of $F_V$ is defined as:

$$\phi_q = \inf\{x : F_V(x) \geq q\} .$$
A natural estimator of \( \phi_q \) is the \( \lceil nq \rceil \)th order statistic. If \( \{V_1, V_2, \ldots, V_n\} \) is the transformed process, and \( \{V_{(1)}, V_{(2)}, \ldots, V_{(n)}\} \) are the order statistics, then an estimator of \( \phi_q \) is

\[
\hat{\phi}_q := V_{(j+1)} \text{ where } j < nq \leq j + 1,
\]

and \( \hat{\phi}_q \xrightarrow{a.s.} \phi_q \) as \( n \to \infty \). An approximate sampling distribution for \( \hat{\phi}_q \) is developed by Doss et al. (2014). First, for any \( y \) define,

\[
\sigma^2(y) = \sum_{k=-\infty}^{\infty} \text{Cov}_{F_V}(I(V_1 \leq y), I(V_{1+k} \leq y)),
\]

and let \( f_V \) be the density associated with \( F_V \). Then, as \( n \to \infty \),

\[
\sqrt{n} (\hat{\phi}_q - \phi_q) \xrightarrow{d} N(0, \sigma^2(\phi_q)/f_V(\phi_q)^2).
\]

Here, we present a univariate sampling distribution for the quantiles, but often multiple quantiles may be of interest. The joint sampling distributions of multiple quantiles and of means and quantiles is available in Robertson et al. (2019).

**Functions of expectations**

We are often interested in estimating functions of expectations, in which case a plug-in type estimator is natural, and the approximate sampling distribution may be obtained by an application of the delta method. This includes estimating the covariance matrix of \( F \),

\[
\Lambda = \text{Var}_F(h(X_1)),
\]

with the sample covariance matrix,

\[
\Lambda_n := \frac{1}{n} \sum_{t=1}^{n} (h(X_t) - \bar{\mu}_n)(h(X_t) - \bar{\mu}_n)^T.
\]

A delta method argument similar to the independent and identically distributed setting yields an element-wise sampling distribution for \( \Lambda_n \).

4 **Estimating Monte Carlo error**

The approximate sampling distributions of the previous section provide the keys to assessing the reliability of the simulation effort, that is, addressing task (ii) from Section 1. Construction of confidence regions for \( \mu_h \) to address this problem has attracted substantial interest.
Suppose that $\Sigma_n$ is an estimator of $\Sigma$ in the CLT (2). If $T_{1-\alpha,p,q}^2$ denotes a $1 - \alpha$ quantile from a Hotelling’s $T$-squared distribution with dimensionality $p$ and degrees of freedom $q$, then it is straightforward to construct an asymptotic $100(1 - \alpha)$% confidence region

$$C_\alpha(n) = \{ n(\bar{\mu}_n - \mu_h)^T \Sigma_n^{-1}(\bar{\mu}_n - \mu_h) < T_{1-\alpha,p,q}^2 \}.$$  

The size of $C_\alpha(n)$ will then describe the precision of estimation; we will discuss how to use this information in the sequel. Thus, the main obstacle is estimating the variance in the asymptotic distribution. There are a variety of estimators available that broadly fit into three classes (1) spectral variance estimators (Andrews, 1991; Damerdji, 1991; Flegal and Jones, 2010; Vats et al., 2018), (2) batch means estimators (Chen and Scila, 1987; Liu and Flegal, 2018; Jones et al., 2006; Vats et al., 2019), and (3) initial sequence estimators (Dai and Jones, 2017; Geyer, 1992; Kosorok, 2000). Of these, the most popular are the batch means estimators since they are easy to implement and are computationally efficient.

The multivariate batch means estimator considers non-overlapping batches of the Markov chain and constructs a sample covariance matrix from the sample means of each batch. More formally, let $n = ab$ where $a$ is the number of batches and $b$ is the batch size. For $k = 0, \ldots, a - 1$, define $\bar{Y}_k := b^{-1} \sum_{t=1}^b h(X_{kbi+t})$. The batch means estimator of $\Sigma$ is,

$$\hat{\Sigma}_{n,b} := \frac{b}{a-1} \sum_{k=0}^{a-1} (\bar{Y}_k - \bar{\mu}_n)(\bar{Y}_k - \bar{\mu}_n)^T.$$  

The asymptotic behavior of batch means estimators has been well studied, however small sample performance of batch means estimators can be suspect in the presence of high correlation. Recently, carefully constructed linear combinations of batch means estimators have been proposed for improving finite sample performance of estimators of $\Sigma$ (Liu and Flegal, 2018). Particularly, for an even $b$, they obtain the following flat-top batch means estimator

$$\hat{\Sigma}_n = 2\hat{\Sigma}_{n,b} - \hat{\Sigma}_{n,b/2},$$  

where $\hat{\Sigma}_{n,b/2}$ is the batch means estimator from a batch size of $b/2$.

Ensuring the batch means estimator (or its variants) is strongly and mean-square consistent requires that the batch size $b$ and the number of batches $a$ must be chosen so that both
increase to infinity as $n \to \infty$. The choice of batch size $b$ is critical to the performance of the batch means estimator (Chakraborty et al., 2019; Flegal and Jones, 2010). In particular, Flegal and Jones (2010) show that the mean-squared-optimal batch size is $b \propto n^{1/3}$, where the proportionality constant needs to be estimated separately, and its size depends on the amount of serial correlation in the chain. Flegal et al. (2017) present a parametric method of estimating this proportionality constant, yielding an easily implementable optimal batch size.

5 Stopping the simulation

The justification for using MCMC experiments to estimate features of $F$ is asymptotic, but, in practice, the Monte Carlo sample size $n$ is finite. Thus, the choice of $n$ is crucial to ensuring the reliability of the MCMC experiment. There are several approaches that can be used to terminate the simulation. The simplest is a fixed-time procedure where the practitioner specifies the Monte Carlo sample size before the experiment begins. In this case, we can estimate the Monte Carlo error and, if it is too large, then run the simulation longer. This leads to a sequential fixed-volume or fixed relative-volume approach (Glynn and Whitt, 1992) which terminates simulation at a random time. Discussion of these issues in the context of MCMC and many more details about them can be found in Flegal and Gong (2015), Flegal et al. (2008), Jones et al. (2006), and Vats et al. (2019).

We again focus on estimating a vector of expectations for the sake of specificity. A fruitful approach is to compare the volume of the confidence region, $\text{Vol}(C_n(n))$, to the generalized variance of the target $F$, that is, $|\Lambda|$ where we recall $\Lambda = \text{Var}_F(h(X_1))$ and $|\cdot|$ denotes the determinant. In doing this, Vats et al. (2019) show that simulating until the effective sample size (ESS), defined as

$$\text{ESS} := n \left( \frac{|\Lambda|}{|\Sigma|} \right)^{1/p},$$

is sufficiently large implies that the Monte Carlo error is sufficiently small compared to the variability in the target distribution. ESS provides the number of independent and identically distributed samples that will yield the same generalized Monte Carlo error as the correlated sample. As discussed above, estimators of both $\Lambda$ and $\Sigma$ are available, so that we can easily
estimate it with
\[ \hat{\text{ESS}} := n \left( \frac{|\Lambda_n|}{|\Sigma_n|} \right)^{1/p}. \]
Here \( \Sigma_n \) is any of the estimators of \( \Sigma \) discussed in Section 4. Notice that ESS depends on the function \( h \). It is thus important to first establish the quantities of interest before estimating ESS. When \( p = 1 \), the ESS defined above is the same as the univariate ESS of Kass et al. (1998).

A natural question to ask is what ESS is sufficient for reliable estimation? Vats et al. (2019) provide a principled cutoff for the ESS based on the relative quality of estimation. Suppose we are interested in making \( 100(1 - \alpha)\% \) confidence regions of \( \mu_h \) using \( \bar{\mu}_n \) such that the volume of the confidence region is an \( \epsilon \)th fraction of the variability of \( h \) under \( F \). Then simulation can stop the first time
\[
\hat{\text{ESS}} \geq \frac{2^{2/p} \pi}{(p \Gamma(p/2))^{2/p}} \frac{\chi^2_{1-\alpha,p}}{\epsilon^2} := M_{\alpha,\epsilon,p}. \tag{3}
\]
Vats et al. (2019) showed that as \( \epsilon \to 0 \), stopping simulation according to (3) will yield confidence regions with coverage probabilities converging to \( 1 - \alpha \). In practice, we do not check criterion (3) until after some minimum \( n^* \) steps to avoid premature termination due to poor early estimates of \( \Sigma \) and \( \Lambda \). A reasonable choice of \( n^* \) is \( M_{\alpha,\epsilon,p} \), which can be calculated a priori since all quantities are known.

The lower bound in (3) is in the spirit of sample size calculations for a desired half-width of a confidence interval for a simple test of means, where \( \epsilon \) serves the same purpose as a (relative) half-width. The relative tolerance level, \( \epsilon \), can be chosen according to the level of precision in the estimates desired, typically \( \epsilon \leq .05 \). Once \( \hat{\text{ESS}} \) reaches the cutoff, users can stop simulating since they can be \( 100(1 - \alpha)\% \) confident that estimates are within an \( \epsilon \)th level of tolerance relative to the target distribution.

The Gelman-Rubin-Brooks diagnostic of Gelman and Rubin (1992) and Brooks and Gelman (1998) is a popular tool for assessing convergence in task (ii). The original diagnostic estimates \( \Sigma \), by the sample covariance of mean vectors from \( m \) independent chains. Since \( m \) is often small, the original Gelman-Rubin-Brooks statistic has high variability (Flegal et al., 2008; Vats and Knudson, 2018; Vehtari et al., 2019). However, a more robust statistic is achieved if the estimators of \( \Sigma \) described in Section 4 are used in the Gelman-Rubin-Brooks
diagnostic (Vats and Knudson, 2018). In addition, if $\hat{R}_p$ denotes the improved Gelman-Rubin-Brooks statistic, then Vats and Knudson (2018) showed that

$$\hat{R}_p \approx \sqrt{1 + \frac{1}{\text{ESS}}}.$$ 

Thus, there is a direct relationship between ESS and the Gelman-Rubin-Brooks statistic. The above is specifically for a single chain, while a multiple chain statistic is provided in Vats and Knudson (2018).

The Gelman-Rubin-Brooks diagnostic suggests that the simulation be terminated when $\hat{R}_p$ is below a pre-defined cutoff. Vats and Knudson (2018) used the bound in (3) to obtain a cutoff for $\hat{R}_p$: simulation stops the first time

$$\hat{R}_p \leq \sqrt{1 + \frac{1}{M_{\alpha,\epsilon,p}}}.$$ 

However, we recommend using ESS as it is more naturally interpretable and has lower variability in readily available software. Notice that both $\hat{R}_p$ and $\hat{\text{ESS}}$ are aimed at assessing estimation and not ensuring a representative sample; that is, aimed at addressing task (ii) and not task (i) from Section 1.

### 6 Extensions

The practice of thinning (or subsampling) the Markov chain is common. Thinning a Markov chain refers to using every $m$th observation in the simulation. This is often done to reduce autocorrelation, but the resulting process is still a Markov chain with kernel corresponding to $P^m$. Geyer (1992), Link and Eaton (2012), and MacEachern and Berliner (1994) showed that since this comes at the cost of the number of usable samples, the variance of a thinned Monte Carlo estimator is always larger than the variance of the original Monte Carlo estimator.

There are, however, situations where thinning is worthwhile. Geyer (1991) and Owen (2017) argue that when post-processing on the raw MCMC data is expensive, it may be computationally efficient to thin the samples. That is, if the function $h$ is costly to evaluate relative to the time it takes to get more samples, thinning is beneficial. Thinning can also be useful in high-dimensional problems where storing the full MCMC output calls for large
memory requirements. When the original MCMC sample is thinned, all output analysis procedures then apply to the thinned MCMC sample.

Simulating multiple parallel chains is also common practice, and can often be useful in parallel computing environments. However, multiple short runs can be misleading and can retain large estimation bias (however, see Jacob et al., 2020), thus we encourage users to run each chain for as long as they would with a single chain.

Another issue that has received little attention is estimation of higher order moments. These fit naturally into the discussion in Section 3, but bring new practical challenges since, for the same Monte Carlo sample size, estimation quality reduces drastically as moments increase.

Our discussion has focused on the time-homogeneous Markov chains encountered in standard MCMC applications. The theoretical and practical tools required for other simulation techniques can be quite different. For adaptive MCMC, Atchadé (2011) provides estimators for the asymptotic variance of the Monte Carlo estimator. Heck et al. (2019) provide uncertainty quantification for trans-dimensional MCMC methods. However, the literature for these processes is not as rich as traditional MCMC, and would benefit from further work.

7 Example workflow

Using an example, we now illustrate a workflow for MCMC output analysis integrated with useful visualizations. We use a Bayesian reliability model to assess the reliability of liquid crystal display (LCD) projectors. We recognize the target distribution \( F \), establish the function of interest \( h \), choose an appropriate MCMC sampler, choose starting values, visually assess the quality of the MCMC sampler using a preliminary Monte Carlo sample, implement the stopping rules for \( h \), report point estimates, and provide appropriate graphical tools.

Consider the LCD projector data of Hamada et al. (2008). To test the manufacturer’s claim of expected lamp life in an LCD projector being 1500 hours, identical lamps were placed in 31 projectors for various models and their time to failure was recorded. The data is presented in Table 1. For \( i = 1, \ldots, 31 \), let \( t_i \) denote the observed failure time for each
Table 1: LCD time to failure in projection hours for 31 projectors.

|     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|
| 387 | 182 | 244 | 600 | 627 | 332 |
| 300 | 798 | 584 | 660 | 39  | 274 |
| 50  | 34  | 1895| 158 | 974 | 345 |
| 1752| 473 | 81  | 954 | 1407| 230 |
| 380 | 131 | 1205|

lamp. Hamada et al. (2008) assumed that the \( t_i \)'s are a realization from,

\[ T_i \sim \text{Weibull}(\lambda, \beta), \]

where \( \lambda > 0 \) is the scale parameter and \( \beta > 0 \) is the shape parameter. Interest is in estimating the mean time to failure (MTTF) and the reliability function at \( t = 1500 \). Under the Weibull likelihood, the MTTF is

\[ \text{MTTF} = \lambda^{-1/\beta} \Gamma \left( 1 + \frac{1}{\beta} \right), \]

and the reliability function is

\[ R(t) = \exp \left\{ -\lambda t^{\beta} \right\}. \]

Hamada et al. (2008) further assume priors \( \lambda \sim \text{Gamma}(2.5, 2350) \) and \( \beta \sim \text{Gamma}(1, 1) \), where each is parameterized by a shape and rate parameter. The density of the posterior is

\[ f(\lambda, \beta \mid T) \propto \lambda^{32.5} \beta^{31} \left( \prod_{i=1}^{31} t_i \right)^{-1} \exp \left\{ -\lambda \sum_{i=1}^{31} t_i^\beta \right\} \exp\{-\beta\} \exp\{-2350\lambda\}, \]

where the normalizing constant is unknown and we use component-wise MCMC methods (Johnson et al., 2013) to sample from this distribution. The component \( \lambda \) will be updated by a Gibbs step and \( \beta \) will be updated by a Metropolis-Hastings step. The full conditional distribution of \( \lambda \) is

\[ \lambda \mid \beta, T \sim \text{Gamma} \left( 33.5, 2350 + \sum_{i=1}^{31} t_i^\beta \right). \]

The full conditional distribution for \( \beta \) is not available in closed-form, so we implement a Metropolis-Hastings step, yielding a Metropolis-within-Gibbs sampler (see Robert and
Casella, 2013). The proposal distribution is a $N(\cdot, \cdot^2)$, which yields an approximately optimal acceptance probability as suggested by Roberts et al. (1997). We update $\lambda$ first, followed by $\beta$, thus a starting value is only needed for $\beta$. We start from the MLE of $\beta$ which is approximately 1.12.

We are interested in estimating MTTF and $R(1500)$ to contest the manufacturers’ claims. Thus, the function whose posterior mean is of interest $h$ is

$$h(\lambda, \beta) = \left( \frac{1}{\beta} \right) \frac{\lambda^{-1/\beta} \Gamma\left(1 + \frac{1}{\beta}\right)}{\exp\left\{-\lambda t^\beta\right\}}.$$  

Here $p = 2$ and setting the relative tolerance to be $\epsilon = .05$ and $\alpha = .05$ yields a minimum ESS of 7529 using (3). We first run the MCMC sampler for $n^* = 7529$ steps as a check to see whether the sampler is exploring the state space adequately and mixing well. Any issues with the sampler may be addressed in such preliminary steps before a long run for a final analysis is reported. Figure 1 shows the trace plots of $\lambda$ and $\beta$, which indicates that there are no obvious mixing problems. This initial run yields $\hat{\text{ESS}} = 1196$ which is noticeably smaller than its cutoff. Seeing this, we run the sampler for 92471 more steps yielding an overall sample size of 1e5. The final $\text{ESS} = 11834 > 7529$ which indicates we are 95% confident that the simulation has terminated with a relative tolerance smaller than $\epsilon = .05$.

Figure 2 shows the autocorrelation in MTTF and $R(1500)$ along with a cross-correlation plot and the Monte Carlo confidence region for $\bar{\mu}_n$. MTTF has little autocorrelation and

Figure 1: Trace plots of $\lambda$ and $\beta$ for an initial run of the Markov chain.
$R(1500)$ has significant autocorrelation over lag 50. A multivariate analysis of the MCMC output is critically important in this example as seen by the cross-correlation plot. The cross-correlation plot at zero indicates the correlation between MTTF and $R(1500)$ in the posterior distribution. This correlation along with the lag correlations would be completely ignored by a univariate analysis. The resulting confidence region constructed using the batch means estimator and the sampling distribution in (2) captures this cross-correlation structure.

![Autocorrelation and cross-correlation plots](image)

Figure 2: Autocorrelation and cross-correlation plots of MTTF and $R(1500)$. Also, a 95% confidence region for the Monte Carlo average of MTTF and $R(1500)$.

The final estimates of MTTF and $R(1500)$ are 596.8 and 0.073 respectively. The MTTF of 596.8 is significantly far from 1500 with a 95% credible interval of (434, 834). The reliability function at a failure time of 1500 is also low with a 95% credible interval of (0.020, 0.163). The marginal density plots with the respective mean and quantiles are given in Figure 3, along with simultaneous uncertainty plotted for all 6 estimates using the methods of Robertson.
et al. (2019). The error bands around the estimates are nearly indistinguishable from the estimates themselves, indicating a small Monte Carlo error.

Figure 3: Marginal density plots with mean and 95% credible intervals marked. Simultaneous uncertainty bands are drawn, but are nearly indistinguishable from the estimates.

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