Nested $\hat{R}$: Assessing Convergence for Markov chain Monte Carlo when using many short chains

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Abstract

When using Markov chain Monte Carlo (MCMC) algorithms, we can increase the number of samples either by running longer chains or by running more chains. Practitioners often prefer the first approach because chains need an initial “warmup” phase to forget their initial states; the number of operations needed for warmup is constant with respect to chain length but increases linearly with the number of chains. However, highly parallel hardware accelerators such as GPUs may allow us to run many chains in parallel almost as quickly as a single chain. This makes it more attractive to run many chains with a short sampling phase. Unfortunately, existing diagnostics are not designed for the “many short chains” regime. This is notably the case for the widely used $\hat{R}$ statistic [e.g. Gelman and Rubin, 1992, Vehtari et al., 2020]. $\hat{R}$ checks for consistency between chains and converges to 1 if the chains produce Monte Carlo estimators in sufficiently good agreement. Convergence to 1 however requires the measured effective sample size (ESS) per chain to be large [Vats and Knudson, 2021], a condition which is incompatible with running many short chains; if diagnosing convergence requires us to run long chains, we cannot reap the benefits of running many short chains in parallel.

We present a generalization of $\hat{R}$, called nested $\hat{R}$, which checks for consistency between groups of chains. $n\hat{R}$ is a useful diagnostic for the many-short-chains regime and works under conditions similar to those that the classic $\hat{R}$ assumes. The main additional requirement is to initialize each chain within a group at the same point. Because properly warmed-up MCMC forgets its starting point, this requirement does not affect the quality of our estimates; it does, however, help us diagnose convergence failures. While $\hat{R}$ converges to 1 only when the number of post-warmup samples is large, $n\hat{R}$ can go to 1 (once the chains are properly warmed up) when either the number of iterations or the number of chains is large. Hence for a sufficiently large number of chains we can where we run many chains in parallel, using a short sampling phase [Lao et al., 2020, Hoffman and Ma, 2020]. New MCMC algorithms, such as ChEES-HMC are particularly well adapted to run many chains, leveraging the parallelization capacities of accelerators [Hoffman et al., 2021]. For many Bayesian inference applications, an effective sample size (ESS) of about 100 may be adequate, in which case we might want to run as many as $\sim$100 chains. Indeed, if the chains are independent and sampling from the stationary distribution, then the number of chains provides a lower bound on the ESS, provided the target distribution has finite variance.

Existing diagnostics are not designed for the regime where we have many chains each made up of only a few iterations. This is notably the case for the widely used $\hat{R}$ statistic [e.g. Gelman and Rubin, 1992, Vehtari et al., 2020]. $\hat{R}$ checks for consistency between chains and converges to 1 if the chains produce Monte Carlo estimators in sufficiently good agreement. Convergence to 1 however requires the measured ESS per chain to be large [Vats and Knudson, 2021], a condition which is incompatible with running many short chains; if diagnosing convergence requires us to run long chains, we cannot reap the benefits of running many short chains in parallel.

We present a generalization of $\hat{R}$, called nested $\hat{R}$, and denoted $n\hat{R}$, which checks for consistency between groups of chains. $n\hat{R}$ is a useful diagnostic for the many-short-chains regime and works under conditions similar to those that the classic $\hat{R}$ assumes. The main additional requirement is to initialize each chain within a group at the same point. Because properly warmed-up MCMC forgets its starting point, this requirement does not affect the quality of our estimates; it does, however, help us diagnose convergence failures. While $\hat{R}$ converges to 1 only when the number of post-warmup samples is large, $n\hat{R}$ can go to 1 (once the chains are properly warmed up) when either the number of iterations or the number of chains is large. Hence for a sufficiently large number of chains we can

1 Work mostly done while an intern at Google Research.
2 Three perspectives on \( \hat{R} \)

Given a random variable, \( \theta \in \Theta \), with a target distribution \( \pi \), and a scalar function of interest, \( f : \Theta \rightarrow \mathbb{R} \), our goal is to estimate the expectation value \( \mathbb{E}_\pi f \), where we assume \( \text{Var}_\pi f \) is finite. We call a Monte Carlo estimator any statistic, \( T \), intended to estimate \( \mathbb{E}_\pi f \). This definition encompasses the traditional Monte Carlo estimator used when doing MCMC sampling but it is deliberately broader. Let \( \Gamma \) be the probability measure which generates \( T \). Any Monte Carlo estimator admits an effective sample size (ESS):

\[
\text{ESS} \triangleq \frac{\text{Var}_\pi f}{\text{Var}_\pi T}. \tag{1}
\]

Consider an MCMC sampler with stationary distribution \( \pi \), which generates \( M \) chains, each with \( N \) iterations. Each chain is initialized at a point \( \theta^{(0m)} \). We denote the \( m \)-th sample from chain \( m \) as \( \theta^{(nm)} \). It is common practice to first “warm up” the sampler for some number of iterations. During the warmup phase, the Markov chains travel to the region where the probability mass concentrates and begin exploring this region [Betancourt, 2018]; early exploration also allows us to tune the parameters of our sampler [e.g. Hoffman and Gelman, 2014; Hoffman et al., 2021]. Once the chain is warmed up, we generate the samples we use for our inference. For ease of notation, we consider estimation of \( \text{Var}_\pi \theta \) and note all our calculations generalize to functions of \( \theta \) with a finite variance.

The classic MCMC estimator is:

\[
\bar{\theta} = \frac{1}{MN} \sum_{m=1}^{M} \sum_{n=1}^{N} \theta^{(nm)}. \tag{2}
\]

A useful perspective is to view this as an average of \( M \) Monte Carlo estimators, \( \bar{\theta}^{(m)} = \sum_{n=1}^{N} \theta^{(nm)} / N \), each based on a single chain.

The \( \hat{R} \) statistic, in its first and simplest iteration as the potential scale reduction factor [Gelman and Rubin, 1992], compares a measure of the total variance across all chains, \( A = \text{Var}_\pi \theta^{(nm)} \), to a measure of within-chain variance, \( W = \mathbb{E}_T \left[ \text{Var}_\pi \left( \bar{\theta}^{(m)} \right) \mid m = m^* \right] \). In words, \( W \) is the expected variance given that the samples are all in the same chain. We estimate these quantities using the sample variance estimators

\[
\hat{W} = \frac{1}{M} \sum_{m=1}^{M} \frac{1}{N-1} \sum_{n=1}^{N} \left( \theta^{(nm)} - \bar{\theta}^{(m)} \right)^2 \tag{3}
\]

and

\[
\hat{A} = \hat{W} + \frac{1}{M-1} \sum_{m=1}^{M} \left( \bar{\theta}^{(m)} - \bar{\theta}^{(-)} \right)^2 \tag{4}
\]

\[\triangleq \hat{W} + \hat{B}.\]

The above expression is motivated by the law of total variance [2] \( \hat{B} \) measures the between-chain variance, \( B = \text{Var}_\pi \bar{\theta}^{(m)} \). We then define \( \hat{R} \triangleq \sqrt{\hat{A} / \hat{W}} \).

If the chains are mixing, we expect the total variance and the within-chain variance to converge to \( \text{Var}_\pi \theta \) as \( N \) grows, meaning \( \hat{R} \) converges to 1. A common practice to assess convergence of the chains is to check that \( \hat{R} \leq 1 + \epsilon \), for some \( \epsilon > 0 \). The choice of \( \epsilon \) varies across the literature, and has evolved over time, starting at \( \epsilon = 0.1 \) and recently using the more conservative value \( \epsilon = 0.01 \) [Vats and Knudson, 2021; Vehtari et al., 2020].

A second perspective on \( \hat{R} \) is due to [Vats and Knudson, 2021] who observe that when the chains are stationary \( \hat{W} / \hat{B} \) is a measure of the effective sample size per chain. Observing that

\[
\hat{R} = \sqrt{\frac{\hat{A}}{\hat{W}}} = \sqrt{1 + \frac{\hat{B}}{\hat{W}}}, \tag{5}
\]

we see that \( \hat{R} \) decays to 1 only once we produce chains with a large effective sample size.

A third perspective is to view \( \hat{R} \) as a measure of agreement between the Monte Carlo estimators produced by each chain. Each chain is distinguished by its initialization point and its seed, but \( \mathbb{E}_T f \) is independent of both of these factors; if either influences our estimator too much then that estimator may not be accurate. Equation 5 shows that \( \hat{R} \) converges to 1 if \( \hat{B} \) is small relative to \( \hat{W} \). For a small \( \epsilon \), such that \( (1 + \epsilon)^2 \approx 1 + 2 \epsilon \), \( \hat{R} \leq 1 + \epsilon \) is approximately equivalent to

\[
\hat{B} \leq 2 \hat{W}. \tag{6}
\]

This inequality establishes a tolerance value for \( \hat{B} \), determined by \( \hat{W} \) and \( \epsilon \).

Once we adopt this perspective two things become clear. First, for small \( N \), the variance of the per-chain

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2The original \( \hat{R} \) uses a slightly different estimator for the within-chain variance when computing \( \hat{A} \). There \( W \) is scaled by \( 1/N \), rather than \( 1/(N - 1) \). This is of little concern when \( N \) is large, but we care about the case where \( N \) is small, and therefore adjust the \( \hat{R} \) statistic slightly.
Monte Carlo estimator stays relatively large, meaning $\hat{B}$ will not be small even if $\text{Var}_\pi \theta^{(-)}$ is. We demonstrate this on the two-dimensional “Banana” distribution,\[\begin{align*}
\theta_1 &\sim \text{Normal}(0, 10); \\
\theta_2 | \theta_1 &\sim \text{Normal}(0.03(\theta_1^2 - 100), 1).
\end{align*}\] (7)

This is a simple transformation of a two-dimensional normal with highly non-convex level sets. After warming up 512 chains for 200 iterations, we only require 1 sampling iteration to achieve a squared error below $\text{Var}_\pi \theta / 100$. Using 4 chains requires a sampling phase with $\sim 200$ iterations (Figure 1). Still $\hat{B}$ is indifferent to the number of chains we run (Figure 2).

Second, $\hat{B}$ focuses on the variance of the per-chain Monte Carlo estimator, not its squared error. $\hat{B}$ therefore cannot detect when all our Monte Carlo estimators suffer from the same bias. A canonical example is a multimodal target $\pi$, with all chains getting stuck with high probability in the same mode after $N$ iterations. Changing the MCMC process, for instance by using overdispersed initializations can help ensure $B$ stays large until we achieve stationarity.

3 Nested $\hat{B}$

The key idea behind $n\hat{B}$ is to compare Monte Carlo estimators whose variance decreases with both the number of iterations and the number of chains. A natural way to do this is to group chains into super chains. Our MCMC process now has $K$ super chains, each comprising $M$ chains, and we denote $\bar{\theta}^{(n,m,k)}$ the $n$th sample from chain $m$ of super chain $k$. The Monte Carlo estimators compared by $n\hat{B}$ are the sample means of each super chain,

$$\bar{\theta}^{(\cdot),k} = \frac{1}{MN} \sum_{m=1}^{M} \sum_{n=1}^{N} \bar{\theta}^{(n,m,k)}.$$  \hspace{1cm} (8)

Provided we have enough chains per group, $n\hat{B}$ quickly goes to 1, reflecting the high precision of $\bar{\theta}^{(\cdot),k}$ after a few iterations (Figure 2). The new diagnostic follows the same formula as the original $\hat{B}$ except that $\hat{B}$ and $\hat{W}$ are now measures of the between and within-super-chain variances. Overloading our notation, for $n\hat{B}$ we define

$$\hat{B} = \frac{1}{K - 1} \sum_{k=1}^{K} \left( \bar{\theta}^{(\cdot),k} - \bar{\theta}^{(\cdot)} \right)^2$$  \hspace{1cm} (9)

and

$$\hat{W} = \frac{1}{K} \sum_{k=1}^{K} \left[ \frac{1}{M-1} \sum_{m=1}^{M} \left( \bar{\theta}^{(m,k)} - \bar{\theta}^{(\cdot),k} \right)^2 \right] + \frac{1}{M} \sum_{m=1}^{M} \frac{1}{N-1} \sum_{n=1}^{N} \left( \bar{\theta}^{(n,m,k)} - \bar{\theta}^{(\cdot),m,k} \right)^2.$$  \hspace{1cm} (10)

In the special case where $N = 1$ we take the within-chain variance to be 0, meaning the second term in the above equation vanishes. Note this makes $\hat{W}$ smaller and results in a lower tolerance on $\hat{B}$.

It is possible to use rank-normalization on $n\hat{B}$, a technique recently employed to improve $\hat{B}$. One motivation for doing so is to diagnose non-convergence when
π has infinite variance; further benefits are discussed by [Vehtari et al. 2020]. We replace each sample, \( \theta^{(nmk)} \), by its rank across all samples, \( r^{(nmk)} \), and then do an inverse-normal transformation with a fractional offset [Blom 1958] to obtain

\[
z^{(nmk)} = \Phi^{-1} \left( \frac{r^{(nmk)} - 3/8}{NMK + 1/4} \right)
\]  

(11)

\( \pi \hat{R} \) is then computed using \( z^{(nmk)} \) instead of \( \theta^{(nmk)} \). Taking advantage of the normal distribution of \( z \), we work out the distribution of \( \pi \hat{R} \) under the assumption stationarity.

**Lemma 1** Suppose (i) the Markov chains are stationary, (ii) \( N = 1 \), meaning each chain has a single sample, and (iii) \( \hat{B} \) (Equation 9) and \( \hat{W} \) (Equation 10) are computed using rank-normalized samples. Then

\[
\frac{\hat{B}}{\hat{W}} \sim \frac{1}{M} F_{K-1, K(M-1)},
\]  

(12)

The proof is in the Supplement.

### 3.1 Limitations when using independent chains

Unfortunately \( \pi \hat{R} \) as defined above is too optimistic, as illustrated by the following thought experiment. Consider a bimodal target distribution

\[
\pi = 0.3 \text{ Normal}(-10, 1) + 0.7 \text{ Normal}(10, 1),
\]

and suppose each chain is either initialized at -10 or 10 with equal probability. Typical MCMC chains will not be able to mix across the high energy barrier between the modes. As a result, which mode a chain explores depends strongly on initialization, and MCMC incorrectly ascribes (on average) probability mass 0.5 to each mode. The per-chain Monte Carlo estimators are inconsistent, since they estimate the means at different modes. This allows \( \hat{R} \) to diagnose the issue. On the other hand, the per-super-chain Monte Carlo estimators may look consistent and \( \pi \hat{R} \) incorrectly claims convergence.

To see why, let \( \bar{\theta}^{(.,mk)}_N \) be the Monte Carlo estimator we obtain from chain \( m \) of super chain \( k \) after \( N \) iterations. Let \( \sigma_N^2 = \text{Var}(\bar{\theta}^{(.,mk)}_N) \). We use a subscript on the variance because we do not assume stationarity. Because the chains are independent, we have

\[
\text{Var}(\bar{\theta}^{(.,k)}) = \frac{1}{M} \sigma_N^2.
\]

Regardless of whether the chain is stationary or not, this value becomes arbitrarily small for large \( M \). This is not unexpected: we obtain good agreement between MCMC estimators so long as they are based on draws from the same distribution, whether or not it is the stationary distribution. One extreme case would be for \( \pi \hat{R} \) to claim convergence after a single iteration, because all the estimators are accurately computing expectation values with respect to the initialization distribution \( \pi_0 \).

### 3.2 Initialization requirement for the chains

To remedy the above issue, we impose the constraint that all chains within a super chain are initialized at the same point, \( \theta_0^k \). This allows us to track the influence of the initial point. In our thought experiment, the initial point determines which mode each chain explores. Our proposed initialization scheme therefore produces super chains in disagreement with one another, meaning we can now identify with \( \pi \hat{R} \) that our MCMC estimates are unreliable.

We can understand the behavior of \( \pi \hat{R} \) under this initialization condition via a variance decomposition:

\[
\text{Var}(\bar{\theta}^{(.,k)}) = \mathbb{E} \left[ \text{Var}(\bar{\theta}^{(.,k)} | \theta_0^k) \right] + \text{Var} \left[ \mathbb{E}(\bar{\theta}^{(.,k)} | \theta_0^k) \right].
\]  

(13)

We denote \( B := \text{Var}(\bar{\theta}^{(.,k)}) \), \( B_c := \mathbb{E}[\text{Var}(\bar{\theta}^{(.,k)} | \theta_0^k)] \), and \( B_v := \mathbb{E}[(\text{Var}(\bar{\theta}^{(.,k)} | \theta_0^k)] \). The above equation is in this notation \( B = B_c + B_v \).

Conditional on \( \theta_0^k \), the chains are independent and \( B_c \) behaves as \( \sigma_N^2 \). That is, \( B_c \) goes to 0 either as \( M \) increases or, once we have reached stationarity, as \( N \) increases. \( B_v \), on the other hand, is indifferent to \( M \). For it to decay, the expected value of \( \bar{\theta}^{(.,k)} \) must become independent of \( \theta_0^k \). To use a common phrase, the chains must “forget” where they started.

What we have with this initialization scheme is a useful compromise between \( \hat{R} \) and \( \pi \hat{R} \) applied to independent chains. We term the latter the naive \( \pi \hat{R} \), and save the original term, \( \pi \hat{R} \), devoid of any prefix, for the case where we use one initial point per super chain. \( \pi \hat{R} \) first behaves like \( \hat{R} \) and, as the correlation to the starting point decays, switches to behaving like the naive \( \pi \hat{R} \) if the chains converge. We demonstrate this transient behavior (or lack thereof) on two examples: (i) a Gaussian distribution where the chains mix and the transient behavior occurs; (ii) a mixture of two Gaussian distributions where the chains fail to mix and \( \pi \hat{R} \) does not transition to the naive behavior (Figure 3).

### 3.3 Proper warmup and threshold for \( \pi \hat{R} \)

Our chains are properly warmed up if the first point of each chain is an independent draw from the stationary
distribution. Note that this implies the chains have forgotten their starting point (since some of the chains were initialized at the same point), and that therefore $B_v = 0$. Unfortunately, we cannot directly measure $B_v$. But we can estimate it, and

$$B_v \leq B_v + B_e = B. \quad (14)$$

Hence $B < 2\epsilon \sigma^2_\pi$ implies $B_v < 2\epsilon \sigma^2_\pi$. This latter bound becomes sharper as $B_e$ decays to 0, which we can achieve by either increasing $N$ or $M$. We can therefore set $\epsilon$ to construct a scale-free tolerance on $B_v$, if perhaps a conservative one,

$$\frac{B_e}{\sigma^2_\pi} \leq 2\epsilon - \frac{B_e}{\sigma^2_\pi}. \quad (15)$$

For example, setting $\epsilon = 0.01$ implies we want $B_v$ to be at most 2% of the posterior variance. Suppose we run $M = 128$ chains. Under the assumption of stationarity, $\sigma^2_\pi/B_e = \text{ESS} \geq M$, a lower bound which is attained when $N = 1$. Then

$$0.012 = 0.02 - 1/128 \leq 2\epsilon - B_e/\sigma^2_\pi < 0.02,$$

meaning that even with $N = 1$ the bound is relatively sharp. In our experiments, we find using $N = 5$ works well.

In the special case where $N = 1$, we may take advantage of Lemma 1 to obtain quantiles for the distribution of $n\hat{R}$ under the assumption of stationarity. This assumption acts as a null hypothesis, which we reject if $n\hat{R}$ is too large. The threshold we choose lets us control the Type II error (incorrect claims we have not converged). Unfortunately we cannot control the Type I error (incorrect claims we have converged), because the chains can be almost stationary. In fact finite chains are never stationary and we leave to a future analysis how close to stationarity the chains need to be in order to produce useful Monte Carlo estimators. This can then inform how to calibrate our hypothesis test.

### 3.4 Limitations of $n\hat{R}$

A drawback of $n\hat{R}$, relative to $\hat{R}$, is that our proposed diagnostic is more sensitive to poor initialization. If the initial distribution $\pi_0$ generates samples which share the same bias relative to the target distribution, then the per-super-chain Monte Carlo estimators may appear to be in good agreement even though the chains are still transient. In this scenario $\text{Var}(\hat{\theta}(\cdot))$ does not characterize well the squared error of our Monte Carlo estimator. This can occur if we run a short warmup phase or, somewhat equivalently, if the chains mix slowly. $\hat{R}$’s implicit requirement for long chains enforces long MCMC runs which increases our chances of overcoming the transient behavior. Furthermore, comparing different sections of a chain, as is done with split $\hat{R}$ [Gelman et al., 2013], can help identify transient behaviors. With short chains, this approach is not an option and we need additional analysis, e.g. examining traceplots during the warmup phase. Using overdispersed initialization is generally recommended for any MCMC scheme, a point that deserves further emphasis when using $n\hat{R}$.

A related limitation of $n\hat{R}$ is that it cannot detect when the chains have converged to a perturbed stationary distribution. This may happen if we are adapting the parameters of the MCMC kernel during warmup, and do not freeze the parameters for enough iterations before sampling. $n\hat{R}$ will detect that all of the chains are sampling from the same distribution, but not that it differs subtly from the stationary distribution. This can be avoided by freezing adaptation earlier, but in any case if we are averaging adaptation signals across many chains, then this undetected bias is likely to be small, since the influence of any one chain on the adaptation is diminished.
4 Adaptive warmup length

When using a short sampling phase, the computation is dominated by the warmup. Which warmup length to use depends on the specific distribution we sample from and the MCMC algorithm we use. Current practice amongst modelers is to prespecify the warmup length and then run a long sampling phase. Only then do we run various diagnostics and if needed adjust the warmup length. This practice means the warmup length is rarely optimal. In this section, we discuss how \( n \hat{R} \) can be used to remedy these problems.

4.1 Existing method

Zhang et al. [2020] propose a cross-chain warmup scheme for Stan’s dynamic Hamiltonian Monte Carlo [Betancourt 2018] Hoffman and Gelman [2014]. This warmup strategy shares tuning parameters by pooling information between chains. Note that ChEES-HMC similarly shares information between chains to tune the sampler. Additionally, rather than run a warmup phase with a fixed length, the cross-chain warmup uses multiple warmup windows of length \( w \). Stan’s default warmup length is 1,000 iterations; the proposed window size \( w = 100 \) or 200. At the end of each window, we compute \( \hat{R} \) as well as the bulk and tail ESS [Vehtari et al. 2020] for the unnormalized log target density using samples from the most recent warmup window. If \( \hat{R} < \hat{R}^* \) and ESS > ESS*, for a prespecified \( \hat{R}^* \) and ESS*, we end the warmup phase. We would like to build on this promising approach.

Our main concern is that the values we should use for \( \hat{R}^* \) and ESS* depend on both \( w \) and the specifics of our target distribution. How to pick the “right” threshold remains an open question, even if we can make a sensible guess. \( n \hat{R} \) lets us address this challenge.

4.2 Revision using \( n \hat{R} \)

We propose the following modification to the adaptive warmup scheme. At the end of each warmup window, we generate 5 sampling iterations and compute \( n \hat{R} \) based on those samples. If \( w \approx 100 \), computing these additional iterations is relatively cheap. We use the threshold proposed in Section 3.3. This use of \( n \hat{R} \) aligns with its natural intent and the window length, \( w \), does not impact our diagnostic.

Additionally, rather than examine the unnormalized log target density, we compute \( n \hat{R} \) for all quantities of interest. While it is convenient to describe how well the chains are mixing using a single scalar, convergence in one quantity may not indicate convergence in all quantities we may care about. We therefore adopt a more conservative approach, but one that is more aligned with the modeler’s goals.

Algorithm 1 summarizes the procedure. We denote the MCMC sampler \( \Gamma \), which admits two arguments: \( \phi \), the tuning parameters of the sampler, and \( \theta \), the current state for all chains. If we draw warmup samples, both \( \phi \) and \( \theta \) are updated at each iteration. When the number of chains we run matches the wanted ESS, we can use the proposed sample, \( \theta_{\text{prop}} \), to construct our Monte Carlo estimators. If the number of chains is smaller than the target ESS, we can run the chains for more iterations until we attain the desired ESS.

Algorithm 1 Adaptive warmup length

Input: MCMC sampler, \( \Gamma \); initial distribution \( \pi_0 \); initial tuning parameters \( \phi_0 \); number of super chains \( K \); number of chains per super chain \( M \); scalar functions of \( \theta \): \( f_1, ..., f_Q \); warmup window length \( w \); max number of steps \( T_{\text{max}} \); sampling window length \( s \); threshold for \( n \hat{R} \), \( 1 + \epsilon \).

1: for \( k = 1 \) to \( K \) do:
   2: Sample \( \theta_0^k \sim \pi_0 \).
   3: Initialize all chains in \( k^{\text{th}} \) group at \( \theta_0^k \).
   4: Set tuning parameters \( \phi = \phi_0 \).
   5: Set chain states \( \theta = \theta_0 \).
   6: for \( t = 1 \) to \( T_{\text{max}} \) do:
      7: Run \( w \) warmup iterations from \( \Gamma(\phi, \theta) \).
      8: Update \( \phi \) and \( \theta \).
      9: Draw \( \theta_{\text{prop}} \) from \( s \) sampling iter from \( \Gamma(\phi, \theta) \).
     10: for \( q = 1 \) to \( Q \) do:
       11: Compute \( n \hat{R} \) for \( f_q(\theta_{\text{prop}}) \).
         12: Check \( n \hat{R} \leq 1 + \epsilon \).
     13: if \( n \hat{R} \) condition met for all \( q \)’s, break.
   14: Return: \( \theta_{\text{prop}} \); \( f_1(\theta_{\text{prop}}), ..., f_Q(\theta_{\text{prop}}); \phi \).

5 Experiments

We study the behavior of \( n \hat{R} \) on four target distributions, which we describe below.

Banana (\( D = 2 \)). See Section 2, Equation 7.

Logistic regression (\( D = 25 \)). A logistic regression model on the numerical version of the German credit dataset [Dua and Graff, 2017]. There are 24 features and an intercept term. The full model is

\[
\theta \sim \text{Normal}(0, 1); \quad y_n \sim \text{Bernoulli} \left( \frac{1}{1 + e^{-\theta x_n}} \right).
\]

Hierarchical model (\( D = 10 \)). A model describing the effect of an SAT training program, as measured by the performance of students across 8 schools [Rubin, 1981]. We estimate the group mean and the population mean and variance. To avoid a funnel shaped
posterior density, we use a non-centered parameterization:

\[
\mu \sim \text{Normal}(5, 3); \sigma \sim \text{Normal}^+(0, 10) \ ; \eta_n \sim \text{Normal}(0, 1) ; \\
\theta_n, \sigma = \mu + \eta_n \sigma ; \ y_n = \text{Normal}(\theta_n, \sigma) .
\]

**Pharmacokinetics (D = 205).** A hierarchical model describing the diffusion of a drug in the body, using data simulated over 100 patients. We use a one-compartment model with first-order absorption from the gut, described by the differential equation:

\[
m'_{\text{gut}} = -k_1 m_{\text{gut}} ; \ m'_{\text{cent}} = k_1 m_{\text{gut}} - k_2 m_{\text{cent}} .
\]

where \( m \) is the drug mass in the gut and the central compartment (blood and organs into which the drug diffuses profusely). This differential equation admits an analytical solution. Each patient receives a drug dose at a regular interval. The drug plasma concentration is measured over time. Our measurement model is, for each patient indexed by \( n \),

\[
y_n(t) \sim \text{logNormal}(\log m_{\text{cent}}(t), \sigma).
\]

For each patient, we estimate the transmission rates \( k_1^n \) and \( k_2^n \). We use a hierarchical prior on \((k_1^n, k_2^n)\) and estimate the population means and variances for both \( k_1 \) and \( k_2 \). The model is fitted to data sampled from the prior. Further details on the model can be found in the Supplementary Material.

We run Hamiltonian Monte Carlo, using the ChEES adaptive scheme [Hoffman et al., 2021] with 4 super chains, each composed of 32 chains, for a total of 128 chains. We compute the squared error of our Monte Carlo estimators, using long MCMC runs to calculate with high precision the correct posterior mean and variance. Invoking the Central Limit Theorem, we assume \( \bar{\theta} \sim \text{Normal} \) is approximately normally distributed for stationary Markov chains. Then for \( N = 1 \),

\[
\frac{KM}{\text{Var}\theta} (\bar{\theta} - E\theta)^2 \approx \chi^2_1 .
\]

For each model, we compute \( nR \) using 5 samples after warmups of varying lengths \( \ell = (10, 20, 30, \ldots, 100, 200, 300, \ldots, 1000) \). The warmup lengths are not set ahead of time. Rather we use the adaptive warmup scheme in Section 4, starting with a small warmup window, \( w = 10 \), and later expanding this window to \( w = 100 \). The initial short windows have no practical use outside this experimental setting, where they help us monitor the behavior of \( nR \) when the squared error is large. Each adaptive warmup is repeated 10 times. At the end of each window, we record \( nR \) and the squared error of Monte Carlo estimators using a single sample per chain for each dimension. Figure 4 plots the squared error, scaled by \( \frac{KM}{\text{Var}\theta} \), against \( nR \). As desired, there is good correlation between \( nR \) and the squared error, and our diagnostic is consistently large over regions that admit an important squared error. When \( nR < 1.01 \), the squared error mostly falls within the 0.95 coverage area of the \( \chi^2_1 \) distribution. However the fraction of points which fall above the 97.5\textsuperscript{th} quantile somewhat exceeds 0.025 (Table 1), which suggests our diagnostics could be more conservative.

We now use the Eight School model as an illustrative example to highlight further analysis. Using a warmup with length 1,000 is amply sufficient, as can be checked by examining the squared error. Using a warmup with length 1,000 is amply sufficient, as can be checked by examining the squared error. In this scenario, \( nR \) falls consistently below the proposed threshold, bearing a few exceptions, while \( R \) produces values larger than what would be considered acceptable (Figure 5).
\[ n\hat{R} \leq 1.01 \quad n\hat{R} > 1.01 \]

|               | n\hat{R} \leq 1.01 | n\hat{R} > 1.01 |
|---------------|---------------------|------------------|
| Banana        | 0.080               | 0.593            |
| German Credit | 0.042               | 0.636            |
| Eight Schools | 0.053               | 0.466            |
| Pharmacokinetics | 0.036          | 0.812            |

Table 1: Fraction of estimators with a scaled error above the 97.5\textsuperscript{th} quantile of a $\chi^2_1$ distribution with $n\hat{R}$ either below or above 1.01. If the chain is stationary, this number should be close to 0.025.

Figure 5: $n\hat{R}$ and $\hat{R}$ across all 10 parameters of the Eight Schools after a long warmup. $\hat{R}$ is consistently above 1.05, while $n\hat{R}$ is below 1.01.

We run the adaptive warmup algorithm 50 times, using different seeds both for the initialization and the MCMC. Again, we examine the squared error when using one sample per chain and find it to agree reasonably well with what we would expect from independent draws from the stationary distribution. For this relatively simple problem, the warmup length varies between 100 and 1,000 iterations (Figure 6), likely because our initialization strongly influences how quickly the Markov chains reach the stationary distribution. There is no obvious correlation between the observed squared error and the length of the warmup, suggesting the algorithm does a good job of gauging when to stop.

6 Discussion

$n\hat{R}$ reproduces many of the desirable properties of $\hat{R}$ and can be applied to the regime where we run many chains with a short sampling phase. This makes it a useful tool to monitor MCMC warmup, without the requirement to run long chains. The utility of $n\hat{R}$ lies in its ability to check whether non-independent chains behave as though they were independent, per the notion that a proper warmup should “decouple” chains initialized at the same point. We may be able to relax this condition by starting chains in a super chain within the same region, rather than at the same point. The potential benefits of such an approach would be to cover more ground earlier during the warmup phase, which can improve tuning the sampler. We note that there exist many variations on $\hat{R}$ which can also motivate further improvements to $n\hat{R}$.

In the classic MCMC setting, the warmup phase needs to adapt the tuning parameters of the sampler to ensure the Markov chains move efficiently across the parameter space during the sampling phase. That is we want to reduce the autocorrelation of our Markov chains, in order to generate chains with a large effective sample size. When one sample per chain suffices, autocorrelation is no longer a concern, which raises the possibility that our warmup phase can be less sophisticated and ultimately shorter. On the other hand, tuning the sampler well may be a prerequisite to achieve stationarity and obtain the unavoidable first sample.

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References

M. Betancourt. A conceptual introduction to Hamiltonian Monte Carlo. arXiv:1701.02434v1, 2018.

G. Blom. Statistical Estimates and Transformed Beta-Variables. 1958.

G. Casella and R. L. Berger. Statistical Inference. Wadsworth, 2002.

D. Dua and C. Graff. Ucl machine learning repository. 2017. URL http://archive.ics.ucl.ac.uk/ml

A. Gelman and D. Rubin. Inference from iterative simulation using multiple sequences. Statistical Science, 7(3):457 – 511, 1992.

A. Gelman, J. Carlin, H. Stern, D. Dunson, A. Vehtari, and D. Rubin. Bayesian data analysis, 3rd edition. Chapman & Hall/CRC, 2013.

M. D. Hoffman and A. Gelman. The No-U-Turn Sampler: Adaptively setting path lengths in Hamiltonian Monte Carlo. Journal of Machine Learning Research, 15:1593–1623, April 2014.

M. D. Hoffman and Y. Ma. Black-box variational inference as a parametric approximation to langevin dynamics. International Conference on Machine Learning, 2020.

M. D. Hoffman, A. Radul, and P. Sountsov. An adaptive mcmc scheme for setting trajectory lengths in hamiltonian monte carlo. International Conference on Artificial Intelligence and Statistics, 2021.

J. Lao, C. Suter, I. Langmore, C. Chimisov, A. Saxena, P. Sountsov, D. Moore, R. A. Saurous, M. D. Hoffman, and J. V. Dillon. tfp.mcmc: Modern markov chain monte carlo tools built for modern hardware. arXiv:2002.01184, 2020.

D. B. Rubin. Estimation in parallelized randomized experiments. Journal of Educational Statistics, 6:377 – 400, 1981.

D. Vats and D. Knudson. Rrevisiting the gelman-rubin diagnostic. Statistical Science, 2021.

A. Vehtari, A. Gelman, D. Simpson, B. Carpenter, and P.-C. Bürkner. Rank-normalization, folding, and localization: An improved $\hat{r}$ for assessing convergence of mcmc. Bayesian analysis, 2020. doi: doi:10.1214/20-BA1221.

Y. Zhang, B. Gillespie, B. Bales, and A. Vehtari. Speed up population bayesian inference by combining cross-chain warmup and within-chain parallelization. Journal of Pharmacokinetics and Pharmacodynamics, 47, 2020.
Appendix

This Appendix provides the proof of Lemma 1, which gives us the distribution of the rank-normalized $\hat{\mathbf{nR}}$ when we have one sample per chain, and details for the Pharmacokinetic model used in our numerical experiments (Section 5). The code for running the experiments is available at https://github.com/google-research/google-research/tree/master/nested_rhat. The ReadMe provides instructions on running the code.

A Proof of Lemma 1

Since $N = 1$ we denote our samples $\theta^{(mk)}$, dropping the superscript for the iteration number. By assumption, the chains are stationary and therefore independent and identically distributed. Hence the $\theta^{(mk)}$’s are i.i.d. Thus the $z^{(mk)}$’s are i.i.d as well. Because of rank-normalization, we also have that the $z^{(mk)}$’s are normally distributed and have finite variance.

The proof follows from recovering the ANOVA setting [e.g Casella and Berger 2002]. We write

$$z^{(mk)} = \mu_k + \epsilon_{mk},$$

where $\mu_k = \mathbb{E}z^{(mk)}$ for all $m$.

We now check that the oneway ANOVA assumptions hold:

(i) $\mathbb{E}\epsilon_{mk} = 0$, $\text{Var}\epsilon_{mk} = \sigma^2_m < \infty$, for all $m, k$, and $\text{Cov}(\epsilon_{mk}, \epsilon_{m'k'}) = 0$, $\forall m, m', k, k'$ unless $m = m'$ and $k = k'$.

(ii) The $\epsilon_{ij}$ are independent and normally distributed (normal errors).

(iii) $\sigma^2_m = \sigma^2$ for all $m$ (homoscedasticity).

Condition (i) follows from our definition of $\mu_k$ and the fact the $z^{(mk)}$ have finite variance. The zero covariance condition follows from the independence of the $z^{(mk)}$’s. Condition (ii) is verified because of the rank-normalization. Condition (iii) follows from the assumption of stationarity, as it implies all our samples are identically distributed.

The null ANOVA is that $\mu_1 = \mu_2 = ... = \mu_K$, which holds because of stationarity.

Let

$$S^2_p = \frac{1}{MK - K} \sum_{k=1}^{K} \sum_{m=1}^{M} \left( z^{(mk)} - \bar{z}^{(k)} \right)^2,$$

$$= \frac{1}{K} \sum_{k=1}^{K} \frac{1}{M - 1} \sum_{m=1}^{M} \left( z^{(mk)} - \bar{z}^{(k)} \right)^2, \quad \tag{17}$$

and note that $S^2_p = \hat{W}$, in the special case where $N = 1$. Then following the argument by Casella and Berger [2002, chapter 11] we have that

$$\sum_{k=1}^{K} M \left( \bar{z}^{(k)} - \bar{\bar{z}} \right)^2 W \sim (K - 1)F_{K-1, MK-K}. \quad \tag{18}$$

Rearranging the terms,

$$\frac{1}{K - 1} \sum_{k=1}^{K} \left( \bar{z}^{(k)} - \bar{\bar{z}} \right)^2 W = \frac{\hat{B}}{\hat{W}} \sim \frac{1}{M} F_{K-1, MK-K}, \quad \tag{19}$$

as desired. □
B Pharmacokinetic model

The one-compartment pharmacokinetic model with first-order absorption from the gut describes the diffusion of a drug compound inside a patient’s body. Oral administration of a bolus drug dose induces a discrete change in the drug mass inside the patient’s gut. The drug is then absorbed into the central compartment, which represents the blood and organs into which the drug diffuses profusely. This diffusion process is described by the ordinary differential equation:

\[
\frac{d m_{\text{gut}}}{dt} = -k_1 m_{\text{gut}} \\
\frac{d m_{\text{cent}}}{dt} = k_1 m_{\text{gut}} - k_2 m_{\text{cent}},
\]

(20)

which admits the analytical solution, when \( k_1 \neq k_2 \),

\[
m_{\text{gut}} = m_{\text{gut}}^0 \exp(-k_1 t) \\
m_{\text{cent}} = \frac{\exp(-k_2 t)}{k_1 - k_2} \left( m_{\text{gut}}^0 k_1 (1 - \exp[(k_2 - k_1)t] + (k_1 - k_2)m_{\text{cent}}^0) \right).
\]

(21)

Here \( m_{\text{gut}}^0 \) and \( m_{\text{cent}}^0 \) are the initial conditions at time \( t = 0 \).

A patient typically receives multiple doses. To model this, we solve the differential equations between dosing events, and then update the drug mass in each compartment, essentially resetting the boundary conditions before we resume solving the differential equations. In our example, this means adding \( m_{\text{dose}} \), the drug mass administered by each dose, to \( m_{\text{gut}}(t) \) at the time of the dosing event. We denote \( x \) the dosing schedule.

Our measurement model is given by

\[
y(t) \sim \text{logNormal}(m_{\text{cent}}(t, x), \sigma).
\]

(22)

This is somewhat of a simplification because in practice we measure the drug plasma concentration, e.g. using blood sample, not the drug mass and the volume of the central compartment is unknown.

Each patient receives a total of 14 doses, taken every 12 hours. Measurements are taken at times \( t = (0.083, 0.167, 0.25, 0.5, 0.75, 1, 1.5, 2, 3, 4, 6, 8) \) hours after the 1st, 2nd, and 13th, and before all other dosing events.

We simulate data for 100 patients and for each patient, indexed by \( n \), we estimate the coefficients \( (k_1^n, k_2^n) \). We use a hierarchical prior to pool information between patients and estimate the population parameters \( (k_1^{\text{pop}}, k_2^{\text{pop}}) \), with a non-centered parameterization. The full Bayesian model is given by

_hyperpriors_

\[
k_1^{\text{pop}} \sim \text{logNormal}(\log 1, 0.1) \\
k_2^{\text{pop}} \sim \text{logNormal}(\log 0.3, 0.1) \\
\sigma_1 \sim \text{logNormal}(\log 0.15, 0.1) \\
\sigma_2 \sim \text{logNormal}(\log 0.35, 0.1) \\
\sigma \sim \text{logNormal}(-1, 1)
\]

_hierarchical priors_

\[
\eta_1^n \sim \text{Normal}(0, 1) \\
\eta_2^n \sim \text{Normal}(0, 1) \\
k_1^n = k_1^{\text{pop}} \exp(\eta_1^n \sigma_1) \\
k_2^n = k_2^{\text{pop}} \exp(\eta_2^n \sigma_2)
\]

likelihood

\[
y_n \sim \text{logNormal}(\log m_{\text{cent}}(t, k_1^n, k_2^n, x), \sigma)
\]
Note we fit the model on the unconstrained scale, meaning the Markov chains explore the parameter space of, for example, $\log k_{\text{pop}}^1 \in \mathbb{R}$, rather than $k_{\text{pop}}^1 \in \mathbb{R}^+$. 