Convergence diagnostics

May 1, 2018

Before using the simulated chain to obtain Monte Carlo estimates, we should first ask ourselves: Has our simulated Markov chain converged to its stationary distribution yet? Unfortunately, this is a difficult question to answer, but we can do several things to investigate.

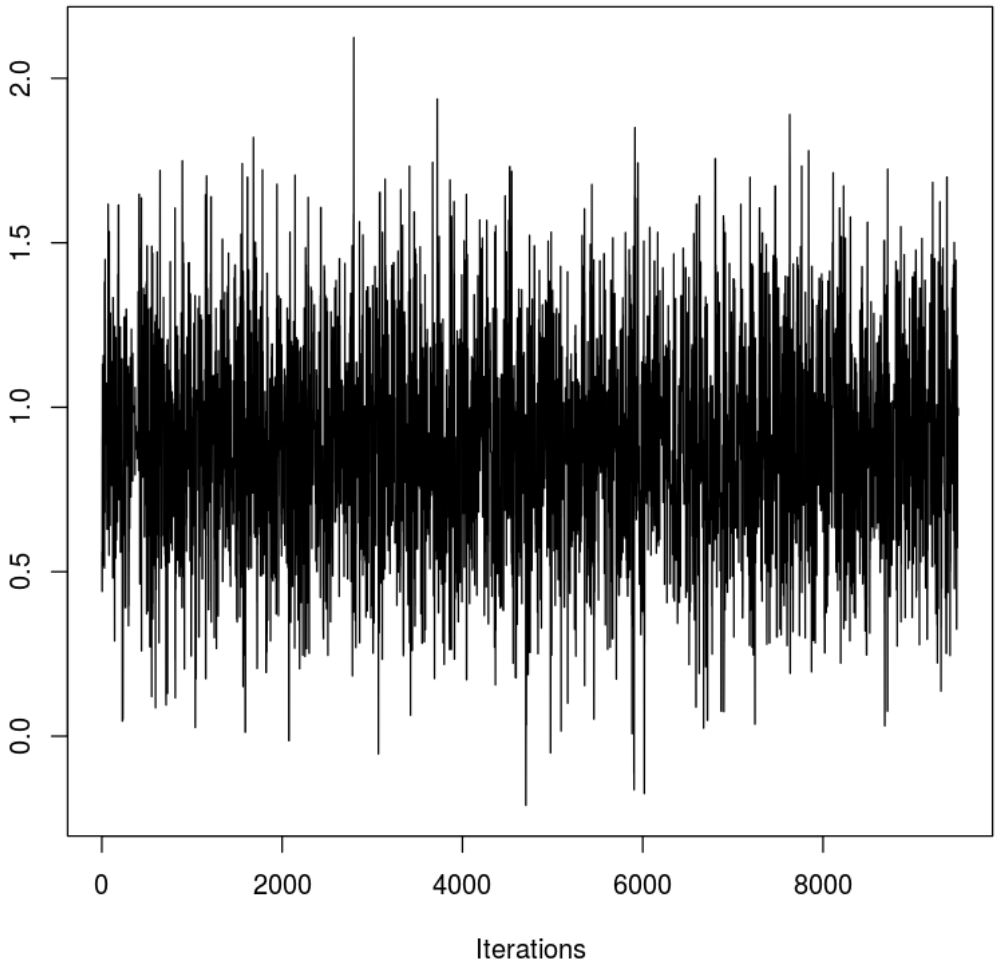
1 Trace plots

Our first visual tool for assessing chains is the trace plot. A trace plot shows the history of a parameter value across iterations of the chain. It shows you precisely where the chain has been exploring.

First, let's talk about what a chain should look like. Here is an example of a chain that has most likely converged.

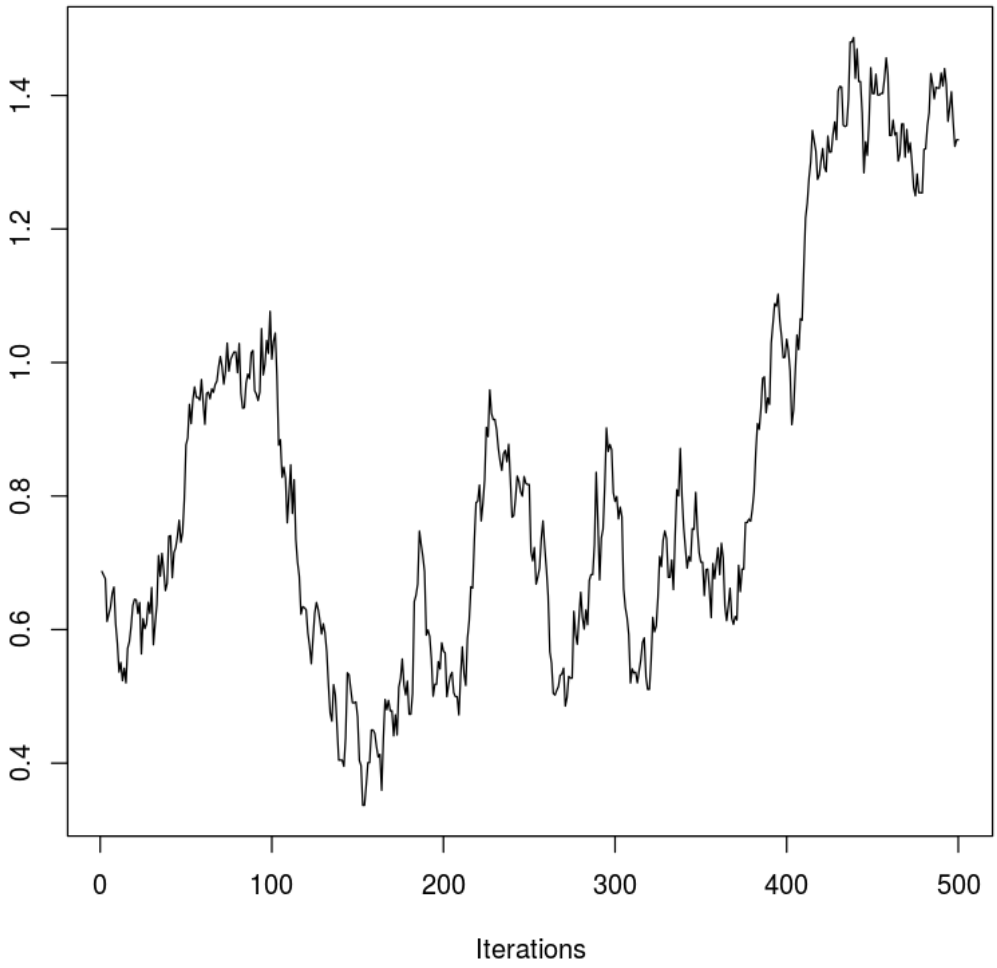
```
In [20]: library(coda)
         setwd("/home/vasilis/Dropbox/Development/Statistics/Bayesian Statistics - Techniques an
         source("Metropolis-Hastings.R")
         set.seed(61)
         post0 = mh(n=n, ybar=ybar, n_iter=10e3, mu_init=0.0, cand_sd=0.9)
         traceplot(as.mcmc(post0$mu[-c(1:500)]))
```

```
List of 2
 $ mu   : num [1:1000] -0.113 1.507 1.507 1.507 1.507 ...
 $ accpt: num 0.122
```



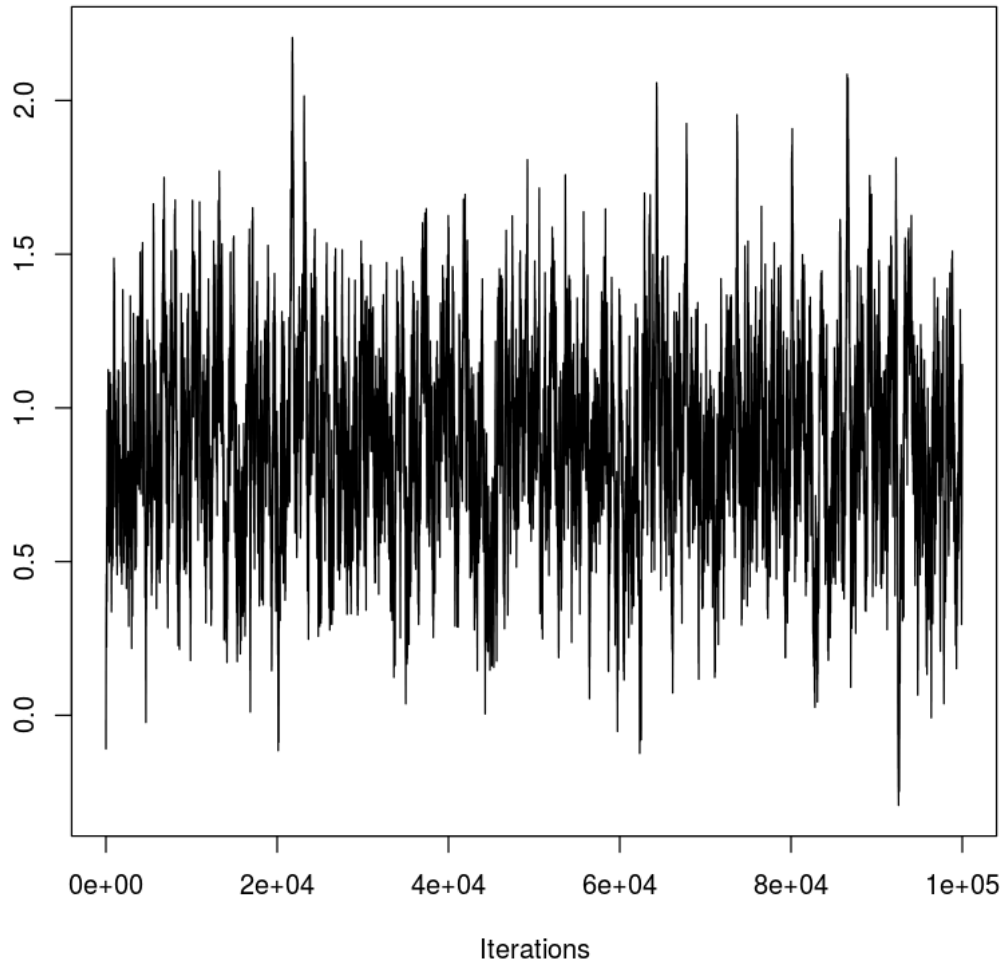
If the chain is stationary, it should not be showing any long-term trends. The average value for the chain should be roughly flat. It should not be wandering as in this example:

```
In [21]: set.seed(61)
         post1 = mh(n=n, ybar=ybar, n_iter=1e3, mu_init=0.0, cand_sd=0.04)
         traceplot(as.mcmc(post1$mu[-c(1:500)]))
```



If this is the case, you need to run the chain many more iterations, as seen here:

```
In [23]: set.seed(61)
         post2 = mh(n=n, ybar=ybar, n_iter=100e3, mu_init=0.0, cand_sd=0.04)
         traceplot(as.mcmc(post2$mu))
```

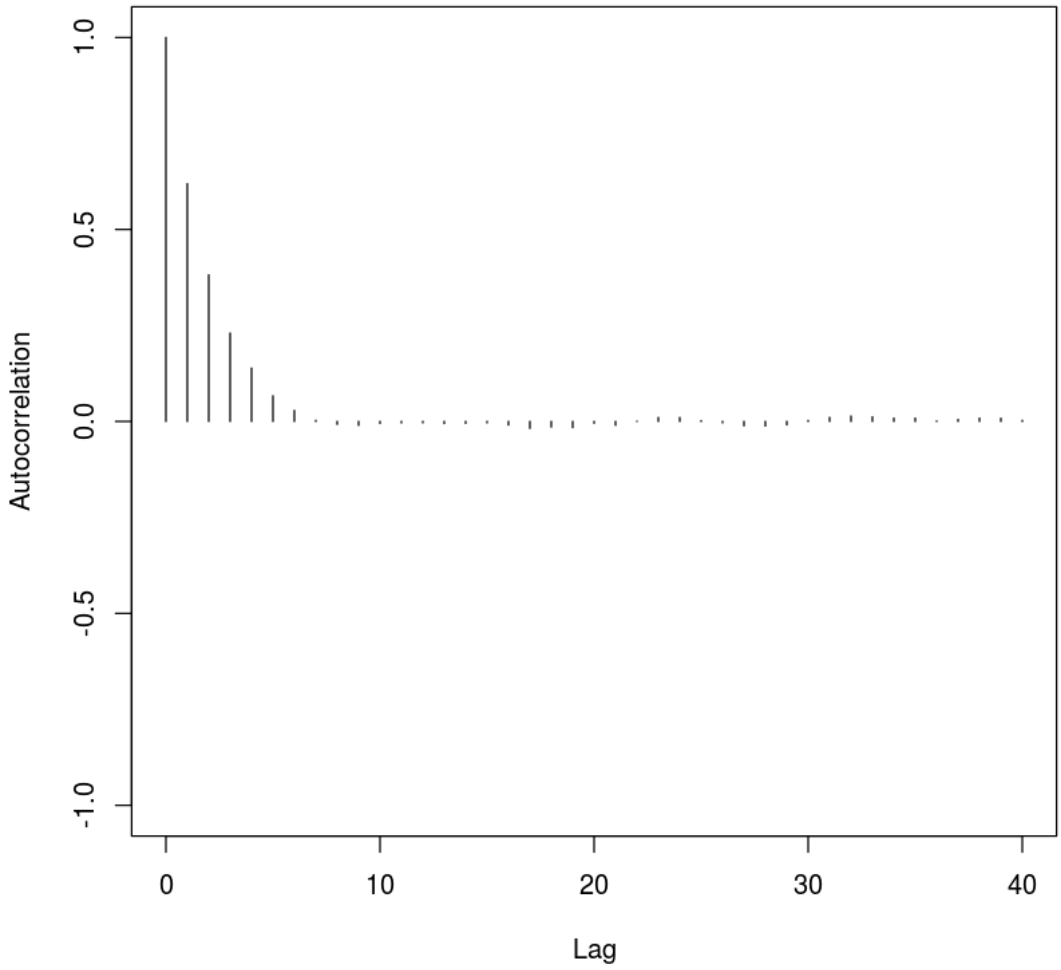


The chain appears to have converged at this much larger time scale.

2 Monte Carlo effective sample size

One major difference between the two chains we've looked at is the level of autocorrelation in each. Autocorrelation is a number between 1 and +1 which measures how linearly dependent the current value of the chain is on past values (called lags). We can see this with an autocorrelation plot:

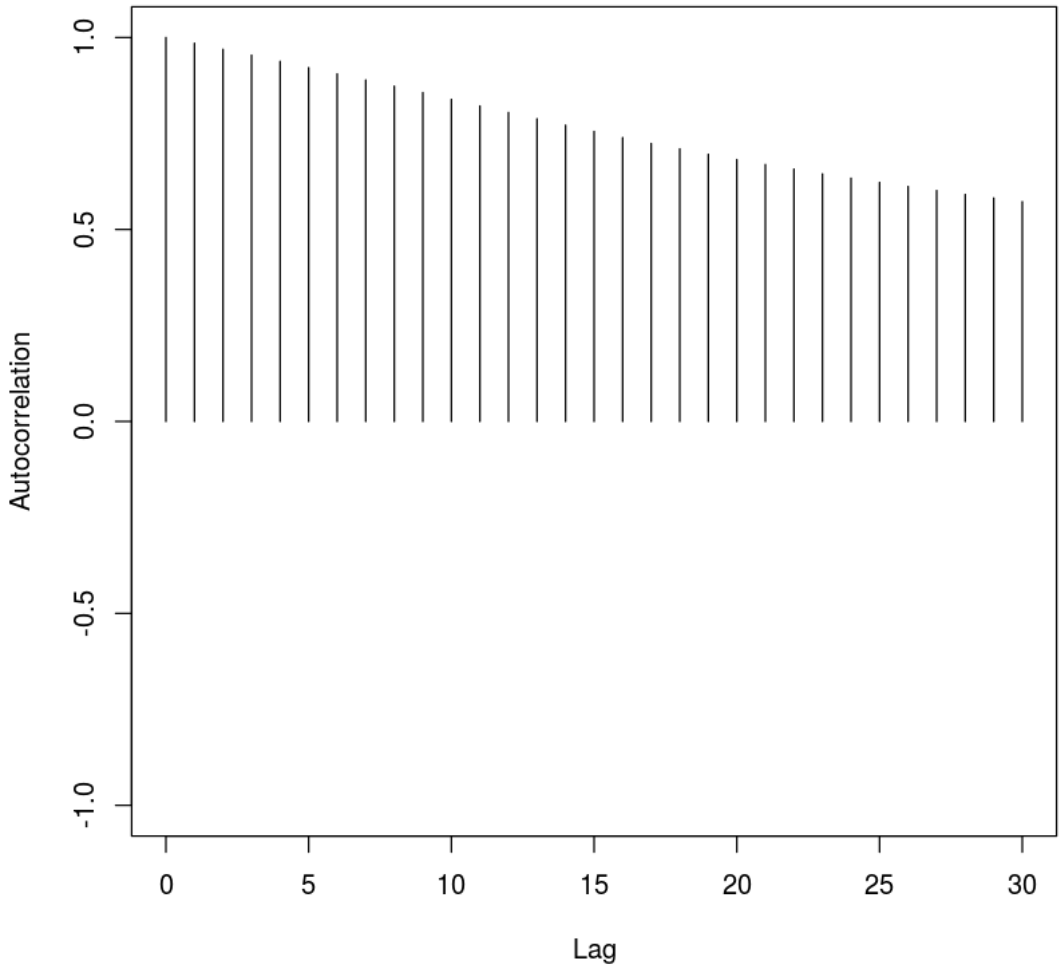
```
In [24]: autocorr.plot(as.mcmc(post0$mu))
```



In [25]: `autocorr.diag(as.mcmc(post0$mu))`

Lag 0	1.000000000
Lag 1	0.619203037
Lag 5	0.066753798
Lag 10	-0.005058642
Lag 50	-0.013328787

In [26]: `coda::autocorr.plot(as.mcmc(post1$mu))`




```
In [27]: autocorr.diag(as.mcmc(post1$mu))
```

Lag 0	1.0000000
Lag 1	0.9850078
Lag 5	0.9213126
Lag 10	0.8387333
Lag 50	0.3834563

Autocorrelation is important because it tells us how much information is available in our Markov chain. Sampling 1000 iterations from a highly correlated Markov chain yields less information about the stationary distribution than we would obtain from 1000 samples independently drawn from the stationary distribution.

Autocorrelation is a major component in calculating the Monte Carlo effective sample size of your chain. The Monte Carlo effective sample size is how many independent samples from the

stationary distribution you would have to draw to have equivalent information in your Markov chain. Essentially it is the mm (sample size) we chose in the lesson on Monte Carlo estimation.

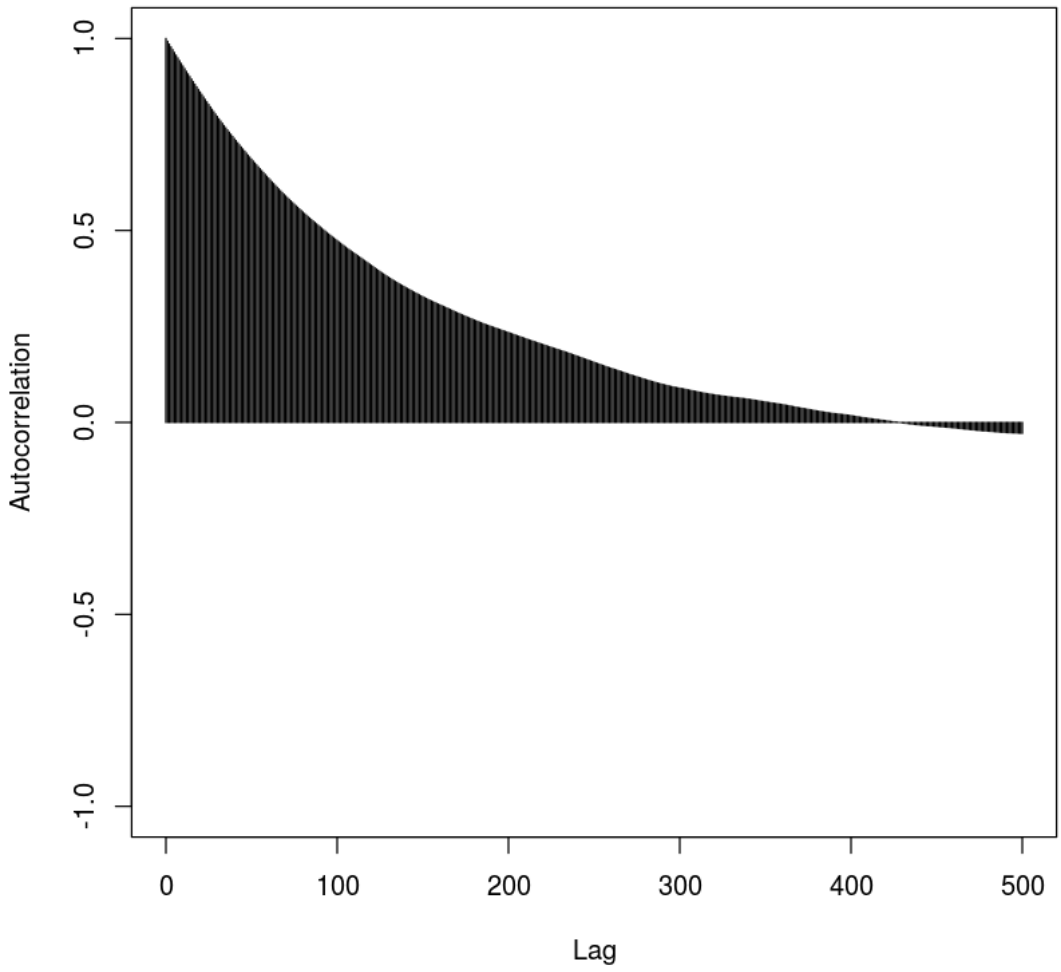
```
In [28]: str(post2) # contains 100,000 iterations
```

```
List of 2
 $ mu   : num [1:100000] -0.0152 -0.1007 -0.0867 -0.1092 -0.0811 ...
 $ accpt: num 0.958
```

```
In [29]: effectiveSize(as.mcmc(post2$mu)) # effective sample size of ~350
```

var1: 373.857993121994

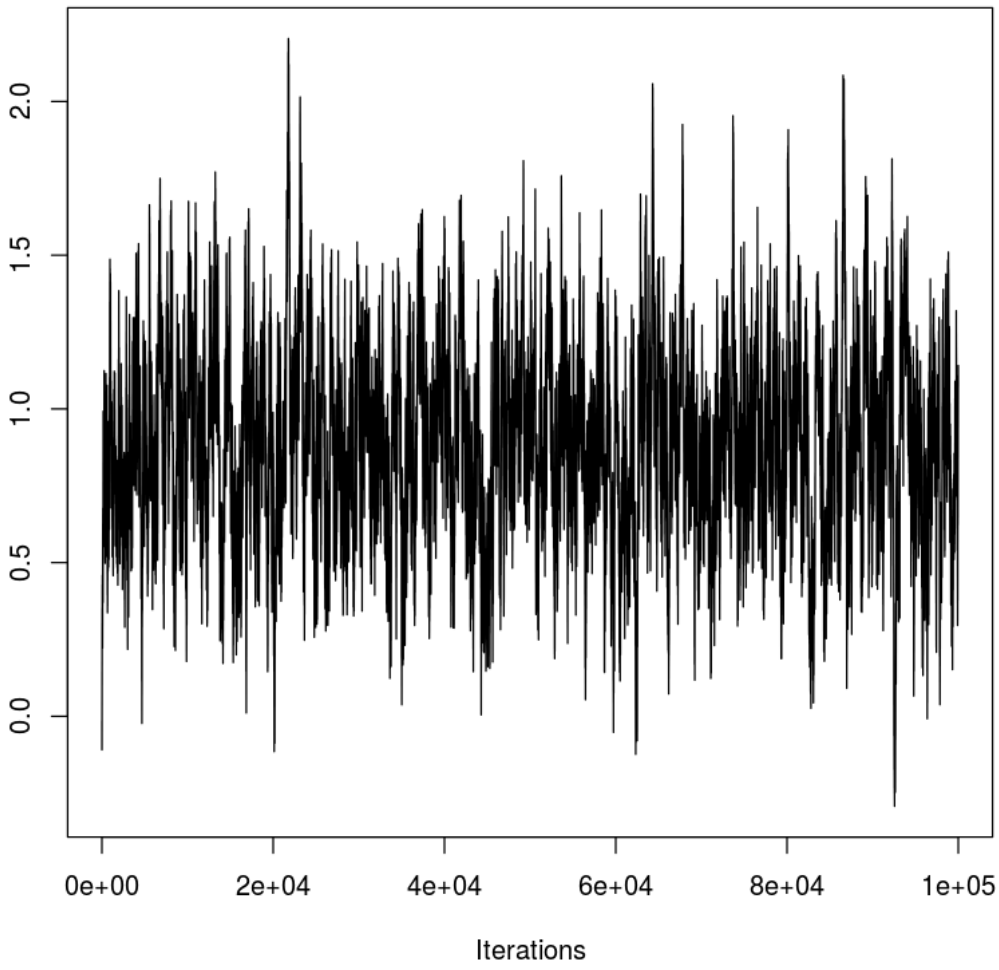
```
In [30]: ## thin out the samples until autocorrelation is essentially 0.
         #This will leave you with approximately independent samples.
         #The number of samples remaining is similar to the effective sample size.
         coda::autocorr.plot(as.mcmc(post2$mu), lag.max=500)
```



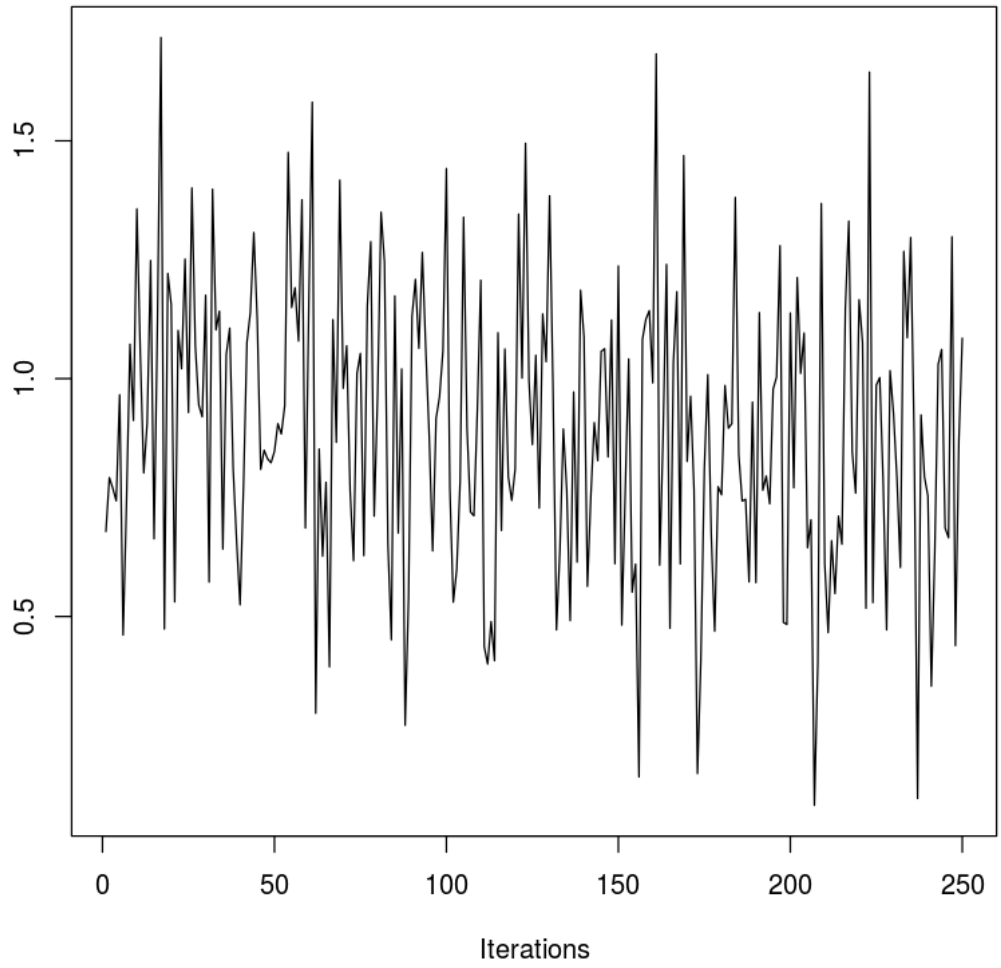
In [31]:
```
thin_interval = 400 # how far apart the iterations are for autocorrelation to be essent
thin_indx = seq(from=thin_interval, to=length(post2$mu), by=thin_interval)
head(thin_indx)
```

1. 400 2. 800 3. 1200 4. 1600 5. 2000 6. 2400

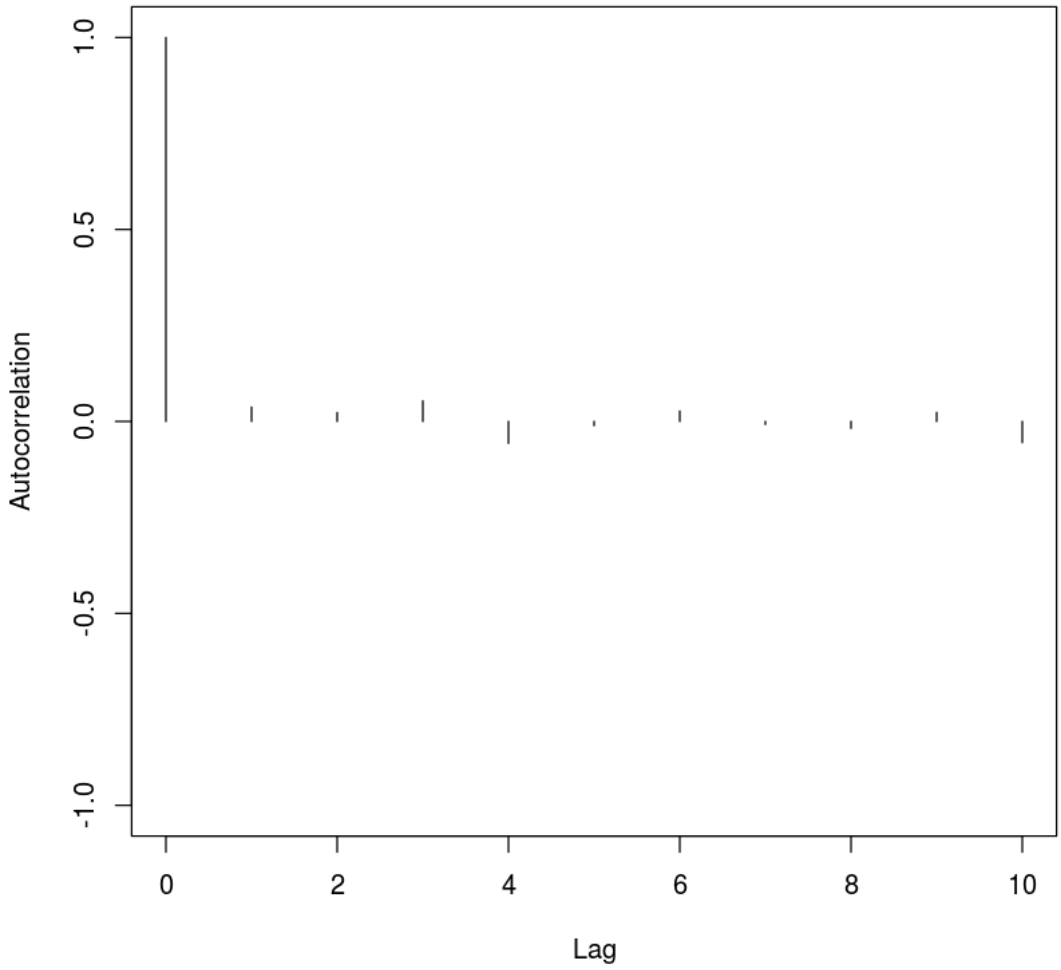
In [32]:
```
post2mu_thin = post2$mu[thin_indx]
traceplot(as.mcmc(post2$mu))
```



In [33]:
```
traceplot(as.mcmc(post2mu_thin))
```



In [34]: `autocorr.plot(as.mcmc(post2mu_thin), lag.max=10)`




```
In [35]: effectiveSize(as.mcmc(post2mu_thin))
```

var1: 250

```
In [36]: str(post0) # contains 10,000 iterations
```

```
List of 2
 $ mu   : num [1:10000] 0 0 0.315 0.315 0.949 ...
 $ accpt: num 0.382
```

```
In [37]: effectiveSize(as.mcmc(post0$mu)) # effective sample size of ~2,500
```

var1: 2537.92418107901

We've now discussed two different interpretations of the effective sample size. The effective sample size can be thought of as **how many independent samples you would need to get the same information** or you could think of it as the **length of chain you would have left over if you removed iterations or thinned the chain until you got rid of the auto correlation**.

The chain from post0 has 10,000 iterations, but an effective sample size of about 2,500. That is, this chain essentially provides the equivalent of 2,500 independent Monte Carlo samples.

Notice that the chain from post0 has 10 times fewer iterations than for post2, but its Monte Carlo effective sample size is about seven times greater than the longer (more correlated) chain. We would have to run the correlated chain for 700,000+ iterations to get the same amount of information from both chains.

It is usually a good idea to check the Monte Carlo effective sample size of your chain. If all you seek is a posterior mean estimate, then an effective sample size of a few hundred to a few thousand should be enough. However, if you want to create something like a 95% posterior interval, you may need many thousands of effective samples to produce a reliable estimate of the outer edges of the distribution. The number you need can be quickly calculated using the Raftery and Lewis diagnostic.

```
In [38]: raftery.diag(as.mcmc(post0$mu))
```

```
Quantile (q) = 0.025
Accuracy (r) = +/- 0.005
Probability (s) = 0.95

 Burn-in  Total Lower bound  Dependence
 (M)      (N)   (Nmin)       factor (I)
 12       13218 3746         3.53
```

```
In [39]: raftery.diag(as.mcmc(post0$mu), q=0.005, r=0.001, s=0.95)
```

```
Quantile (q) = 0.005
Accuracy (r) = +/- 0.001
Probability (s) = 0.95

You need a sample size of at least 19112 with these values of q, r and s
```

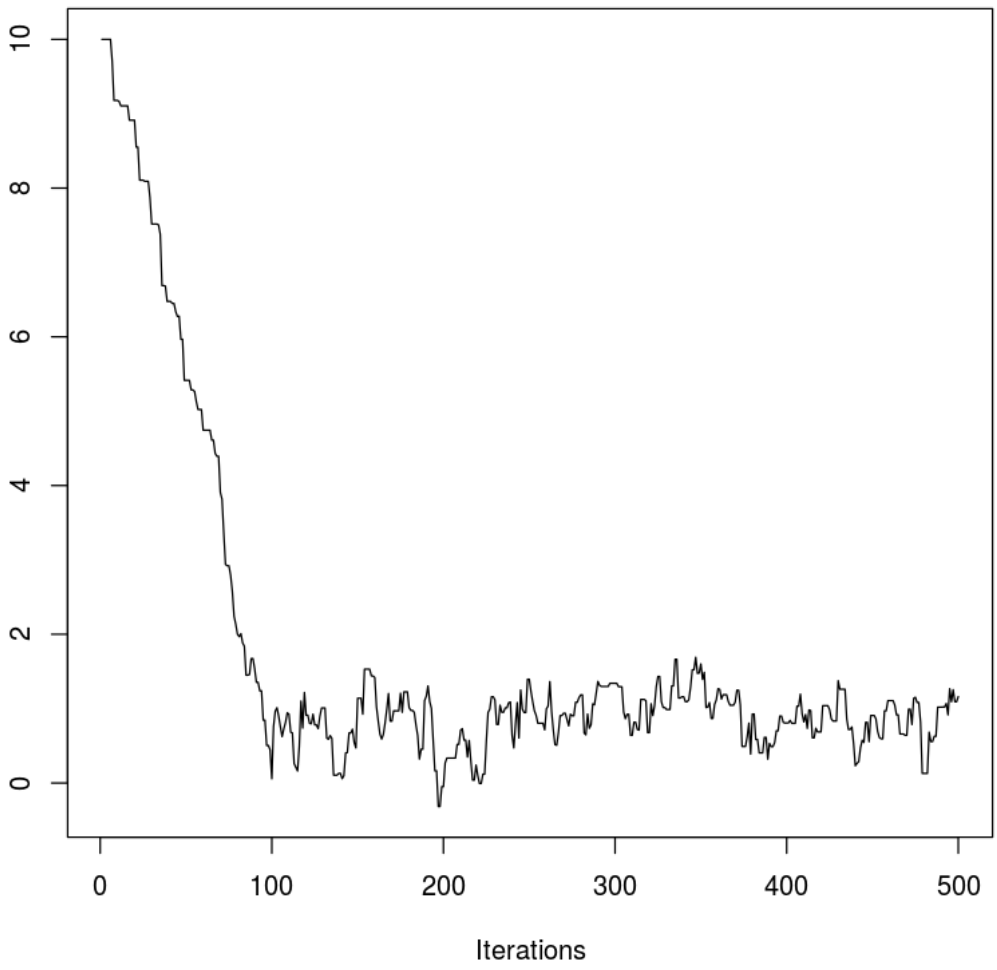
In the case of the first chain from post0, it looks like we would need about 3,700 effective samples to calculate reliable 95% intervals. With the autocorrelation in the chain, that requires about 13,200 total samples. If we wanted to create reliable 99% intervals, we would need at least 19,100 total samples.

3 Burn-in

We have also seen how the initial value of the chain can affect how quickly the chain converges. If our initial value is far from the bulk of the posterior distribution, then it may take a while for the

chain to travel there. We saw this in an earlier example.

```
In [40]: set.seed(62)
         post3 = mh(n=n, ybar=ybar, n_iter=500, mu_init=10.0, cand_sd=0.3)
         traceplot(as.mcmc(post3$mu))
```



Clearly, the first 100 or so iterations do not reflect draws from the stationary distribution, so they should be discarded before we use this chain for Monte Carlo estimates. This is called the "burn-in" period. You should always discard early iterations that do not appear to be coming from the stationary distribution. Even if the chain appears to have converged early on, it is safer practice to discard an initial burn-in.

4 Multiple chains, Gelman-Rubin

If we want to be more confident that we have converged to the true stationary distribution, we can simulate multiple chains, each with a different starting value.

In [41]:
```
set.seed(61)

nsim = 500
post1 = mh(n=n, ybar=ybar, n_iter=nsim, mu_init=15.0, cand_sd=0.4)
post1$accpt
```

0.616

In [42]:
```
post2 = mh(n=n, ybar=ybar, n_iter=nsim, mu_init=-5.0, cand_sd=0.4)
post2$accpt
```

0.612

In [43]:
```
post3 = mh(n=n, ybar=ybar, n_iter=nsim, mu_init=7.0, cand_sd=0.1)
post3$accpt
```

0.844

In [44]:
```
post4 = mh(n=n, ybar=ybar, n_iter=nsim, mu_init=23.0, cand_sd=0.5)
post4$accpt
```

0.53

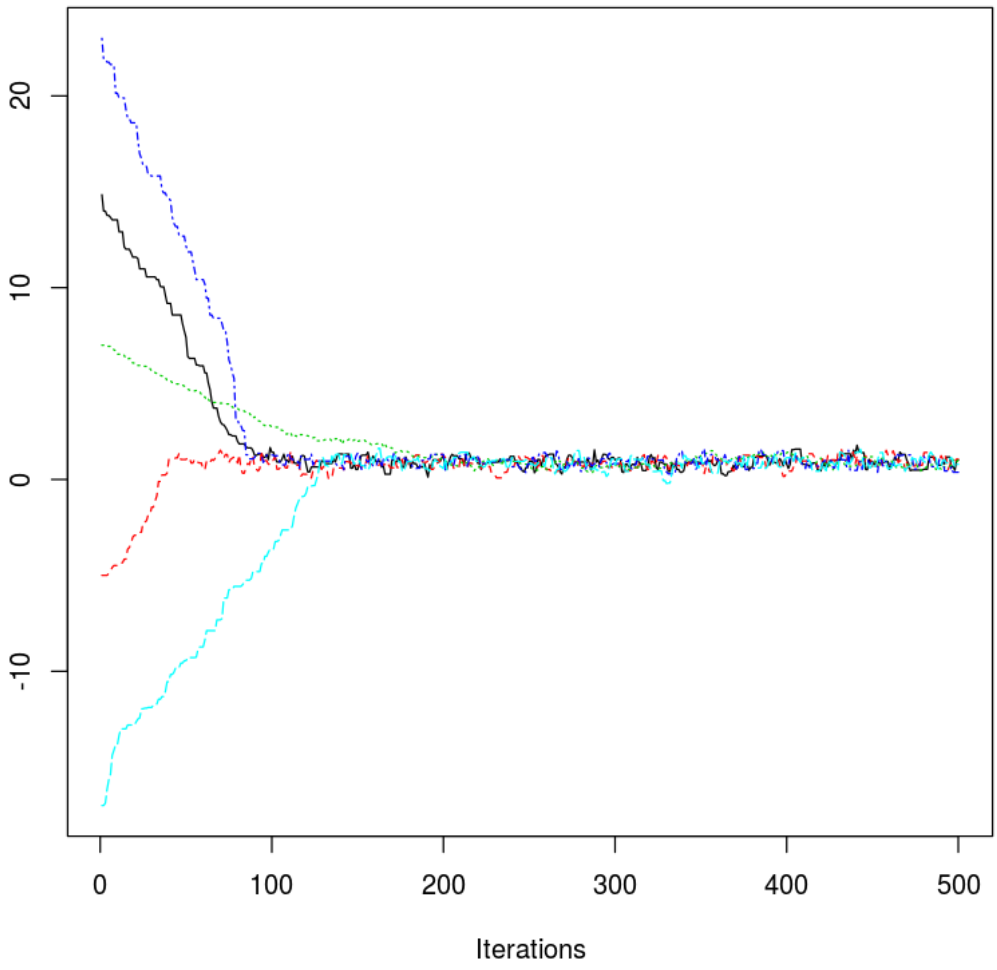
In [45]:
```
post5 = mh(n=n, ybar=ybar, n_iter=nsim, mu_init=-17.0, cand_sd=0.4)
post5$accpt
```

0.618

In [46]:
```
pmc = mcmc.list(as.mcmc(post1$mu), as.mcmc(post2$mu),
                as.mcmc(post3$mu), as.mcmc(post4$mu), as.mcmc(post5$mu))
str(pmc)
```

```
List of 5
 $ :Class 'mcmc'  atomic [1:500] 14.8 14 14 13.8 13.8 ...
  .. ..- attr(*, "mcpar")= num [1:3] 1 500 1
 $ :Class 'mcmc'  atomic [1:500] -5 -5 -5 -5 -4.89 ...
  .. ..- attr(*, "mcpar")= num [1:3] 1 500 1
 $ :Class 'mcmc'  atomic [1:500] 7 7 7 6.94 6.94 ...
  .. ..- attr(*, "mcpar")= num [1:3] 1 500 1
 $ :Class 'mcmc'  atomic [1:500] 23 21.9 21.9 21.8 21.8 ...
  .. ..- attr(*, "mcpar")= num [1:3] 1 500 1
 $ :Class 'mcmc'  atomic [1:500] -17 -17 -16.9 -16.2 -15.7 ...
  .. ..- attr(*, "mcpar")= num [1:3] 1 500 1
 - attr(*, "class")= chr "mcmc.list"
```

```
In [47]: traceplot(pmc)
```



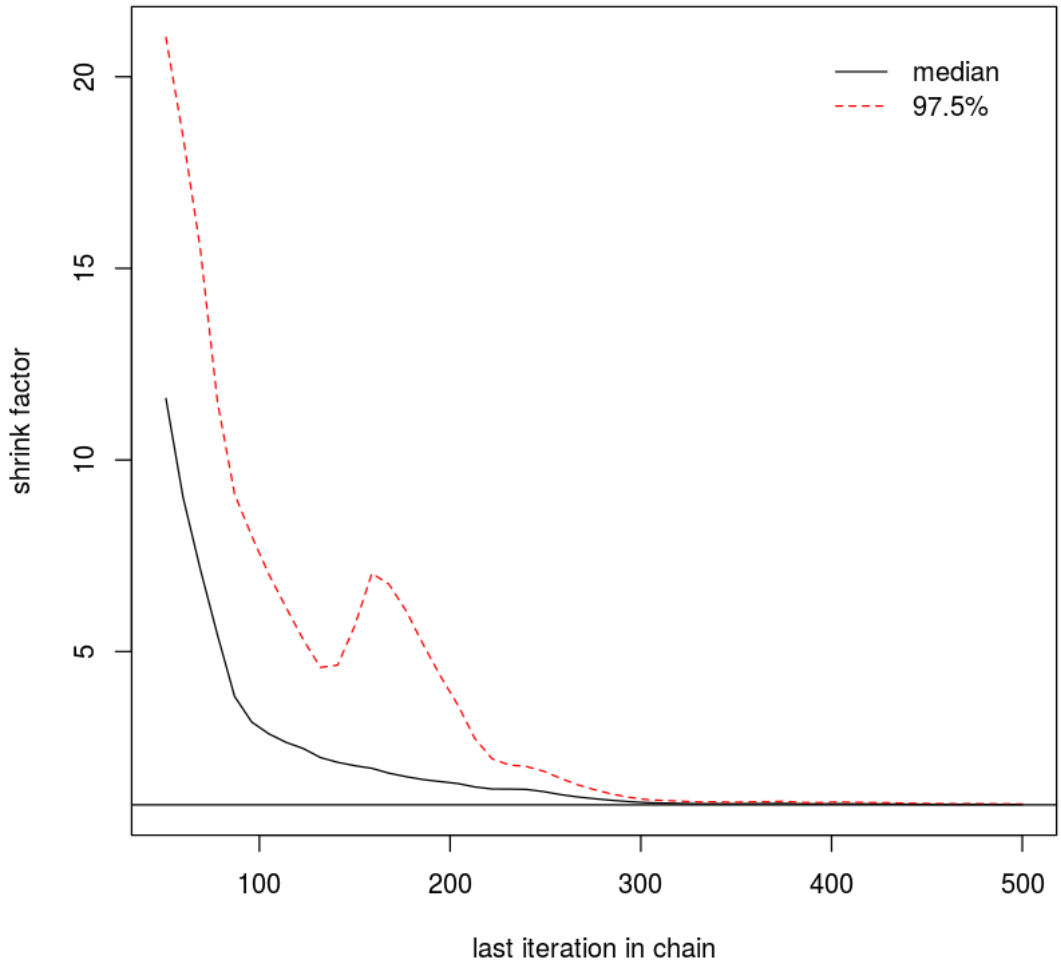
It appears that after about iteration 200, all chains are exploring the stationary (posterior) distribution. We can back up our visual results with the Gelman and Rubin diagnostic. This diagnostic statistic calculates the variability within chains, comparing that to the variability between chains. If all chains have converged to the stationary distribution, the variability between chains should be relatively small, and the potential scale reduction factor, reported by the the diagnostic, should be close to one. If the values are much higher than one, then we would conclude that the chains have not yet converged.

```
In [48]: gelman.diag(pmc)

Potential scale reduction factors:
```

```
     Point est. Upper C.I.
[1,]       1.01       1.02
```

```
In [49]: gelman.plot(pmc)
```



From the plot, we can see that if we only used the first 50 iterations, the potential scale reduction factor or "shrink factor" would be close to 10, indicating that the chains have not converged. But after about iteration 300, the "shrink factor" is essentially one, indicating that by then, we have probably reached convergence. Of course, we shouldn't stop sampling as soon as we reach convergence. Instead, this is where we should begin saving our samples for Monte Carlo estimation.

5 Monte Carlo estimation

If we are reasonably confident that our Markov chain has converged, then we can go ahead and treat it as a Monte Carlo sample from the posterior distribution. Thus, we can use the techniques we learned to calculate posterior quantities like the posterior mean and posterior intervals from the samples directly.

```
In [50]: nburn = 1000 # remember to discard early iterations
         post0$mu_keep = post0$mu[-c(1:1000)]
         summary(as.mcmc(post0$mu_keep))
```

```
Iterations = 1:9000
Thinning interval = 1
Number of chains = 1
Sample size per chain = 9000

1. Empirical mean and standard deviation for each variable,
   plus standard error of the mean:

          Mean             SD       Naive SE Time-series SE
      0.889449       0.304514       0.003210       0.006295

2. Quantiles for each variable:

  2.5%    25%    50%    75%  97.5%
0.2915 0.6825 0.8924 1.0868 1.4890
```

```
In [51]: mean(post$mu_keep > 1.0) # posterior probability that mu  > 1.0
```

0.342222222222222

6 Review

** Question 1**

Why is it important to check your MCMC output for convergence before using the samples for inference?

a. Convergence diagnostics provide a guarantee that your inferences are accurate.

b. Pre-convergence MCMC samples are useless.

c. You can cut your Monte Carlo error by a factor of two if you strategically select which samples to retain.

d. If the chain has not reached its stationary distribution (the target/posterior), your samples will not reflect that distribution.

Answer 1

d.

Monte Carlo samples from the incorrect distribution will likely produce misleading results.

Question 2

Suppose you have multiple MCMC chains from multiple initial values and they appear to traverse the same general area back and forth, but struggle from moderate (or high) autocorrelation. Suppose also that adjusting the proposal distribution q is not an option. Which of the following strategies is likely to help increase confidence in your Monte Carlo estimates?

a. Retain only the 80% of samples closest to the maximum likelihood estimate.

b. Run the chains for many more iterations and check for convergence on the larger time scale.

c. Discard fewer burn-in samples to increase your Monte Carlo effective sample size.

d. Add more chains from more initial values to see if that reduces autocorrelation.

Answer 2

b.

Proper MCMC algorithms come with a theoretical guarantee of eventual convergence to the target distribution. Chains with very high autocorrelation may require an impractical number of iterations, but it is worth checking to see if a longer chain yields acceptable results.

Question 3

Suppose the Gelman and Rubin diagnostic computed from multiple chains reports a scale reduction factor much higher than 1.0, say 8.0. What is the recommended action?

a. Discontinue use of the model, since there is little hope of reaching the stationary distribution.

b. Use the samples for inference as this high scale reduction factor indicates convergence.

c. Continue running the chain for many more iterations.

d. Thin the chain by discarding every eighth sample.

Answer 3

c.

A high scale reduction factor indicates that the chains are not yet exploring the same space, so we need to provide them more iterations to converge.

Question 4

Which of the following Monte Carlo statistics would require the largest MCMC effective sample size to estimate reliably? Assume the target distribution is unimodal (has only one peak).

a. 15 percentile of the target distribution

b. 97.5 percentile of the target distribution

c. Median of the target distribution

d. Mean of the target distribution

Answer 4

b.

The outer edges of the distribution are sampled less frequently and therefore susceptible to changes between simulations. The Raftery and Lewis diagnostic can help you decide how many iterations you need to reliably estimate outer quantiles of the target distribution.