Convergence Diagnostics

Patrick Lam

Outline

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```
> NormalMHExample <- function(n.sim, n.burnin) {
+     library(mvtnorm)
+     mu.vector <- c(3, 1)
+     variance.matrix <- cbind(c(1, -0.5), c(-0.5, 2))
+     theta.mh <- matrix(NA, nrow = n.sim, ncol = 2)
+     theta.current <- rnorm(n = 2, mean = 0, sd = 4)
+     theta.update <- function(index, theta.current, ...) {
+         theta.star <- rnorm(n = 1, mean = theta.current[index], sd = 2)
+         if (index == 1)
+             theta.temp <- c(theta.star, theta.current[2])
+         else theta.temp <- c(theta.current[1], theta.star)
+         r <- dmvnorm(theta.temp, mu.vector, variance.matrix)/dmvnorm(theta.current,
+             mu.vector, variance.matrix)
+         r <- min(r, 1, na.rm = T)
+         if (runif(1) < r)
+             theta.star
+         else theta.current[index]
+     }
+     for (i in 1:n.sim) {
+         theta.current[1] <- theta.mh[i, 1] <- theta.update(1, theta.current,
+             mu.vector, variance.matrix)
+         theta.current[2] <- theta.mh[i, 2] <- theta.update(2, theta.current,
+             mu.vector, variance.matrix)
+     }
+     theta.mh <- theta.mh[(n.burnin + 1):n.sim, ]
+ }
> mh.draws <- NormalMHExample(n.sim = 5000, n.burnin = 0)
```

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However, there is no guarantee that our chain has converged after M draws.

How do we know whether our chain has actually converged?

We can never be sure, but there are several tests we can do, both visual and statistical, to see if the chain appears to be converged.

Convergence Diagnostics in R

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> mh.draws <- mcmc(mh.draws)
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We can tell the `mcmc()` function to burn-in or drop draws with the `start` and `end` arguments.

`mcmc()` also has a `thin` argument, which only tells it the thinning interval that was used (it does not actually thin for us).

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> summary(mh.draws)

Iterations = 1:5000
Thinning interval = 1
Number of chains = 1
Sample size per chain = 5000

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

       Mean    SD Naive SE Time-series SE
[1,] 3.0282 1.027  0.01453        0.03859
[2,] 0.9997 1.424  0.02014        0.04109

2. Quantiles for each variable:

       2.5%     25%    50%   75% 97.5%
var1  0.864 2.37214 3.0489 3.733 5.016
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The results give the posterior means, posterior standard deviations, and posterior quantiles for each variable.

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The time-series standard error adjusts the “naïve” standard error for autocorrelation.

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We need to do the inspections for every parameter.

Traceplots

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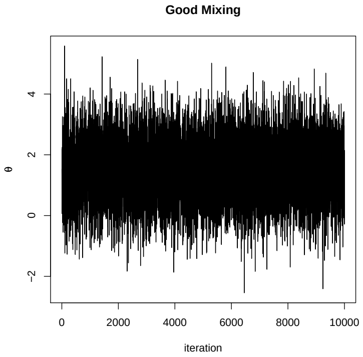

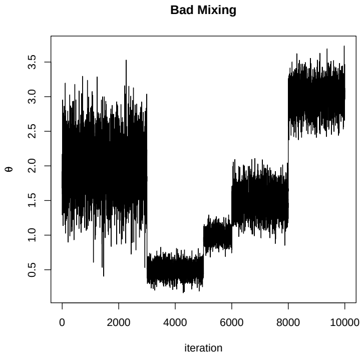

Traceplots and Density Plots

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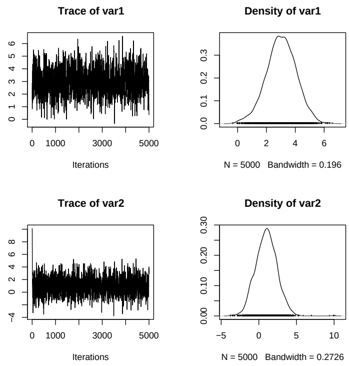
> plot(mh.draws)
```



Running Mean Plots

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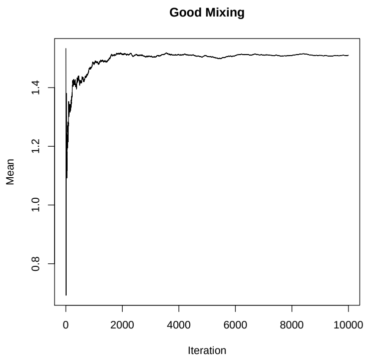

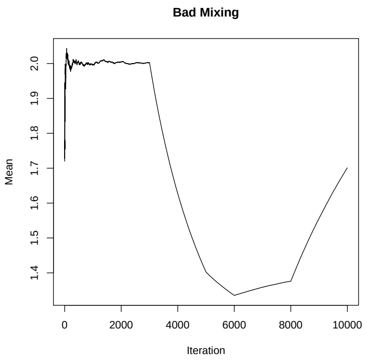

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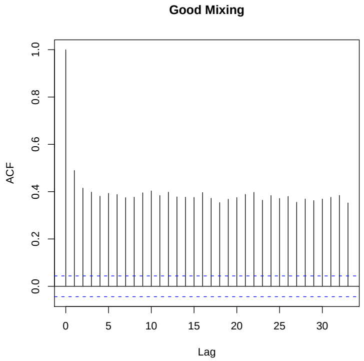
If autocorrelation is still relatively high for higher values of k, this indicates high degree of correlation between our draws and slow mixing.


Good Mixing
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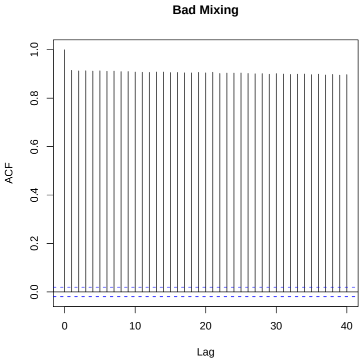
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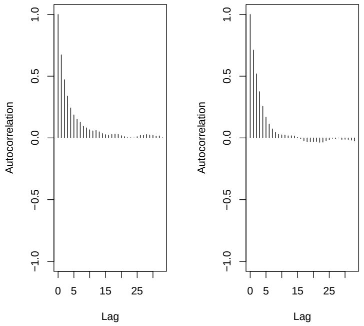
> autocorr.plot(mh.draws)
```



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     var1      var2
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```

To get the acceptance rate, we just want $1-$ rejection rate.

```
> acceptance.rate <- 1 - rejectionRate(mh.draws)
> acceptance.rate

     var1      var2
0.4722945 0.5905181
```

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Gelman and Rubin Multiple Sequence Diagnostic

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4. Calculate the estimated variance of the parameter as a weighted sum of the within-chain and between-chain variance.
5. Calculate the potential scale reduction factor.

Within Chain Variance

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$$W = \frac{1}{m}\sum_{j=1}^{m} s_j^2$$

where

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s_j^2 is just the formula for the variance of the jth chain. W is then just the mean of the variances of each chain.

W likely underestimates the true variance of the stationary distribution since our chains have probably not reached all the points of the stationary distribution.

Between Chain Variance

Between Chain Variance

$$B = \frac{n}{m-1} \sum_{j=1}^{m} (\bar{\theta}_j - \bar{\bar{\theta}})^2$$

where

$$\bar{\bar{\theta}} = \frac{1}{m} \sum_{j=1}^{m} \bar{\theta}_j$$

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This is the variance of the chain means multiplied by n because each chain is based on n draws.

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Because of overdispersion of the starting values, this overestimates the true variance, but is unbiased if the starting distribution equals the stationary distribution (if starting values were not overdispersed).

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When $\hat{R}$ is high (perhaps greater than 1.1 or 1.2), then we should run our chains out longer to improve convergence to the stationary distribution.

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We can then combine the mn total draws from our chains to produce one chain from the stationary distribution.

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```

We then put the *M* chains together into an `mcmc.list`.

```
> mh.list <- mcmc.list(list(mh.draws1, mh.draws2, mh.draws3, mh.draws4,
+     mh.draws5))
```

We then run the diagnostic with the `gelman.diag()` function.

[1] Brooks, Stephen P. and Andrew Gelman. 1997. "General methods for monitoring convergence of iterative simulations." *Journal of Computational and Graphical Statistics* 7: 434-455.

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```
> gelman.diag(mh.list)

Potential scale reduction factors:

     Point est. 97.5% quantile
[1,]       1.00           1.00
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Multivariate psrf

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The results give us the median potential scale reduction factor and its 97.5% quantile (the psrf is estimated with uncertainty because our chain lengths are finite).

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We also get a multivariate potential scale reduction factor that was proposed by Gelman and Brooks.[1]

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We can see how the potential scale reduction factor changes through the iterations using the `gelman.plot()` function.

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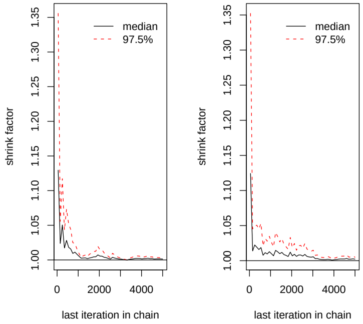

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Geweke Diagnostic

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The **Geweke diagnostic** takes two nonoverlapping parts (usually the first 0.1 and last 0.5 proportions) of the Markov chain and compares the means of both parts, using a difference of means test to see if the two parts of the chain are from the same distribution (null hypothesis).

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The test statistic is a standard Z-score with the standard errors adjusted for autocorrelation.

```
> geweke.diag(mh.draws)

Fraction in 1st window = 0.1
Fraction in 2nd window = 0.5

  var1   var2
0.6149 0.1035
```

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Raftery and Lewis Diagnostic

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If we define some acceptable tolerance r for q and a probability s of being within that tolerance, the **Raftery and Lewis diagnostic** will calculate the number of iterations N and the number of burn-ins M necessary to satisfy the specified conditions.

Raftery and Lewis Diagnostic

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If we define some acceptable tolerance r for q and a probability s of being within that tolerance, the **Raftery and Lewis diagnostic** will calculate the number of iterations N and the number of burn-ins M necessary to satisfy the specified conditions.

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In practice, we can also just test our normal chain to see if it satisfies the results that the diagnostic suggests.

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3. Select a probability s, which is the desired probability of being within (q-r, q+r).
4. Run a "pilot" sampler to generate a Markov chain of minimum length given by rounding up

$$n_{\min} = \left[\Phi^{-1}\left(\frac{s+1}{2}\right)\frac{\sqrt{q(1-q)}}{r}\right]^2$$

where $\Phi^{-1}(\cdot)$ is the inverse of the normal CDF.

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> raftery.diag(mh.draws, q = 0.025, r = 0.005, s = 0.95)

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

 Burn-in  Total Lower bound  Dependence
 (M)      (N)   (Nmin)       factor (I)
 18       20149 3746         5.38
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  High dependence factors (> 5) are worrisome and may be due to influential starting values, high correlations between coefficients, or poor mixing.

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Nevertheless, it often works well with simple models.

Outline

Heidelberg and Welch Diagnostic

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The diagnostic consists of two parts.

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3. If null hypothesis is rejected, discard the first 10% of the chain. Calculate the test statistic and accept or reject null.
4. If null hypothesis is rejected, discard the next 10% and calculate the test statistic.
5. Repeat until null hypothesis is accepted or 50% of the chain is discarded. If test still rejects null hypothesis, then the chain fails the test and needs to be run longer.

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```
> heidel.diag(mh.draws)

     Stationarity start     p-value
     test         iteration
var1 passed       1         0.834
var2 passed       1         0.693

     Halfwidth Mean Halfwidth
     test
var1 passed    3.03 0.0756
var2 passed    1.00 0.0805
```