Lecture 6: Metropolis Algorithms and Stochastic Sampling

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Last Class: Normal Means Model

- Data Model $Y_i \mid \mu_i, \sigma^2 \overset{ind}{\sim} \mathsf{N}(\mu_i, \sigma^2)$
- Means Model $\mu_i \mid \mu, \sigma^2_\mu \overset{iid}{\sim} \mathsf{N}(\mu, \sigma^2_\mu)$\$
- Found marginal likelihood $\mathcal{L}(\mu, \sigma^2, \sigma^2_\mu)$ by integrating out μ_i with respect to g

$$\mathcal{L}(\mu, \sigma^2, \sigma^2_\mu) \propto (\sigma^2 + \sigma^2_\mu)^{-n/2} \exp\left\{-\frac{1}{2}\frac{\sum_{i=1}^n (y_i - \mu)^2}{\sigma^2 + \sigma^2_\mu}\right\}$$

- Posterior for $\theta = \mu, \sigma^2_\mu$ with $\sigma^2 = 1$

$$\pi(\theta \mid y) = \frac{\pi(\theta)\mathcal{L}(\theta)}{\int_\Theta \pi(\theta)\mathcal{L}(\theta)\, d\theta} = \frac{\pi(\theta)\mathcal{L}(\theta)}{m(y)}$$

- while we can integrate out μ, no closed form for posterior of σ^2_μ given σ^2

Important Sampling Estimate

- Estimate of $m(y)$

$$m(y) \approx \frac{1}{T}\sum_{t=1}^{T} \frac{\pi(\theta^{(t)})\mathcal{L}(\theta^{(t)})}{q(\theta^{(t)})} \qquad \theta^{(t)} \sim q(\theta)$$

- Ratio estimator of $\mathsf{E}[h(\theta) \mid y]$

$$\mathsf{E}[h(\theta) \mid y] \approx \frac{\sum_{t=1}^{T} h(\theta^{(t)}) \frac{\pi(\theta^{(t)})\mathcal{L}(\theta^{(t)})}{q(\theta^{(t)})}}{\sum_{t=1}^{T} \frac{\pi(\theta^{(t)})\mathcal{L}(\theta^{(t)})}{q(\theta^{(t)})}} \qquad \theta^{(t)} \sim q(\theta)$$

- Weighted average with importance weights $w(\theta^{(t)}) \propto \frac{\pi(\theta^{(t)})\mathcal{L}(\theta^{(t)})}{q(\theta^{(t)})}$

$$\mathsf{E}[h(\theta) \mid y] \approx \sum_{t=1}^{T} h(\theta^{(t)}) w(\theta^{(t)}) / \sum_{t=1}^{T} w(\theta^{(t)}) \qquad \theta^{(t)} \sim q(\theta)$$

Issues

- if $q()$ puts too little mass in regions with high posterior density, we can have some extreme weights
- optimal case is that $q()$ is as close as possible to the posterior so that all weights are constant
- Estimate may have large variance
- Problems with finding a good $q()$ in high dimensions $(d > 20)$ or with skewed distributions

Markov Chain Monte Carlo (MCMC)

- Typically $\pi(\theta)$ and $\mathcal{L}(\theta)$ are easy to evaluate

> **Question**
>
> How do we draw samples only using evaluations of the prior and likelihood in higher dimensional settings?

- construct a Markov chain $\theta^{(t)}$ in such a way the the stationary distribution of the Markov chain is the posterior distribution $\pi(\theta \mid y)$!

$$\theta^{(0)} \xrightarrow{k} \theta^{(1)} \xrightarrow{k} \theta^{(2)} \ldots$$

- $k_t(\theta^{(t-1)}; \theta^{(t)})$ transition kernel
- initial state $\theta^{(0)}$
- choose some nice k_t such that $\theta^{(t)} \to \pi(\theta \mid y)$ as $t \to \infty$
- biased samples initially but get closer to the target
- Metropolis Algorithm (1950's)

Stochastic Sampling Intuition

- From a sampling perspective, we need to have a large sample or group of values, $\theta^{(1)}, \ldots, \theta^{(S)}$ from $\pi(\theta \mid y)$ whose empirical distribution approximates $\pi(\theta \mid y)$.
- for any two sets A and B, we want

$$\frac{\frac{\#\theta^{(s)} \in A}{S}}{\frac{\#\theta^{(s)} \in B}{S}} = \frac{\#\theta^{(s)} \in A}{\#\theta^{(s)} \in B} \approx \frac{\pi(\theta \in A \mid y)}{\pi(\theta \in B \mid y)}$$

- Suppose we have a working group $\theta^{(1)}, \ldots, \theta^{(s)}$ at iteration s, and need to add a new value $\theta^{(s+1)}$.
- Consider a candidate value $\theta^\star$ that is *close* to $\theta^{(s)}$
- Should we set $\theta^{(s+1)} = \theta^\star$ or not?

Posterior Ratio

look at the ratio

$$M = \frac{\pi(\theta^\star \mid y)}{\pi(\theta^{(s)} \mid y)} = \frac{\frac{p(y \mid \theta^\star)\pi(\theta^\star)}{p(y)}}{\frac{p(y \mid \theta^{(s)})\pi(\theta^{(s)})}{p(y)}}$$

$$= \frac{p(y \mid \theta^\star)\pi(\theta^\star)}{p(y \mid \theta^{(s)})\pi(\theta^{(s)})}$$

- does not depend on the marginal likelihood we don't know!

Metropolis Algorithm

- If $M > 1$
  - Intuition: $\theta^{(s)}$ is already a part of the density we desire and the density at $\theta^\star$ is even higher than the density at $\theta^{(s)}$.
  - Action: set $\theta^{(s+1)} = \theta^\star$
- If $M < 1$,
  - Intuition: relative frequency of values in our group $\theta^{(1)}, \ldots, \theta^{(s)}$ "equal" to $\theta^\star$ should be $\approx M = \dfrac{\pi(\theta^\star \mid y)}{\pi(\theta^{(s)} \mid y)}$.
  - For every $\theta^{(s)}$, include only a fraction of an instance of $\theta^\star$.
  - Action: set $\theta^{(s+1)} = \theta^\star$ with probability M and $\theta^{(s+1)} = \theta^{(s)}$ with probability $1 - M$.

Proposal Distribution

- Where should the proposed value $\theta^\star$ come from?
- Sample $\theta^\star$ close to the current value $\theta^{(s)}$ using a **symmetric proposal distribution** $\theta^\star \sim q(\theta^\star \mid \theta^{(s)})$
- $q()$ is actually a "family of proposal distributions", indexed by the specific value of $\theta^{(s)}$.
- Here, symmetric means that $q(\theta^\star \mid \theta^{(s)}) = q(\theta^{(s)} \mid \theta^\star)$.
- Common choice

$$\mathsf{N}(\theta^\star; \theta^{(s)}, \delta^2\Sigma)$$

with Σ based on the approximate $\mathsf{Cov}(\theta \mid y)$ and $\delta = 2.44/\dim(\theta)$ or

$$\mathrm{Unif}(\theta^\star; \theta^{(s)} - \delta, \theta^{(s)} + \delta)$$

Metropolis Algorithm Recap

The algorithm proceeds as follows:

1. Given $\theta^{(1)}, \ldots, \theta^{(s)}$, generate a *candidate* value $\theta^\star \sim q(\theta^\star \mid \theta^{(s)})$.
2. Compute the acceptance ratio

$$M = \frac{\pi(\theta^\star \mid y)}{\pi(\theta^{(s)} \mid y)} = \frac{p(y \mid \theta^\star)\pi(\theta^\star)}{p(y \mid \theta^{(s)})\pi(\theta^{(s)})}.$$

3. Set

$$\theta^{(s+1)} = \begin{cases} \theta^\star & \text{with probability} \quad \min(M, 1) \\ \theta^{(s)} & \text{with probability} \quad 1 - \min(M, 1) \end{cases}$$

equivalent to sampling $u \sim U(0, 1)$ independently and setting

$$\theta^{(s+1)} = \begin{cases} \theta^\star & \text{if} \quad u < M \\ \theta^{(s)} & \text{if} \quad \text{otherwise} \end{cases}.$$

Notes

- Acceptance probability is

$$M = \min\left\{1, \frac{\pi(\theta^\star)\mathcal{L}(\theta^\star)}{\pi(\theta^{(s)})\mathcal{L}(\theta^{(s)})}\right\}$$

- ratio of posterior densities where normalizing constant cancels!
- The Metropolis chain ALWAYS moves to the proposed $\theta^\star$ at iteration $s+1$ if $\theta^\star$ has higher target density than the current $\theta^{(s)}$.
- Sometimes, it also moves to a $\theta^\star$ value with lower density in proportion to the density value itself.
- This leads to a random, Markov process that naturally explores the space according to the probability defined by $\pi(\theta \mid y)$, and hence generates a sequence that, while dependent, eventually represents draws from $\pi(\theta \mid y)$ (stationary distribution of the Markov Chain).

Summarizing Samples

- Once we obtain the samples, then we are back to using Monte Carlo approximations for quantities of interest!
- we can approximate posterior means, quantiles, and other quantities of interest using the empirical distribution of our sampled values.
- easy to compute the posterior distribution of nonlinear functions of parameters!

$$\psi^{(s)} = g(\theta^{(s)})$$

- some posterior summaries are hard to calculate based on samples $\{\theta^{(s)}\}$
  - mode/MAP (at least for continuous)
  - marginal likelihood $m(y) = \int \pi(\theta) p(y \mid \theta)\, d\theta$

Convergence

We will not cover the convergence theory behind Metropolis chains in detail, but ...

- The Markov process generated under this procedure is **ergodic** (irreducible and aperiodic) and has a unique limiting distribution (stationary distribution)
  - ergodicity means that the chain can move anywhere at each step, which is ensured, if $q(\theta^\star \mid \theta^{(s)}) > 0$ everywhere!
- By construction, Metropolis chains are **reversible**, so that $\pi(\theta \mid y)$ is the stationary distribution
  - Think of reversibility as being equivalent to symmetry of the joint density of two consecutive $\theta^{(s)}$ and $\theta^{(s+1)}$ in the stationary process (which we get by using a symmetric proposal distribution)
  - detailed balance

https://sta702-F23.github.io/website/

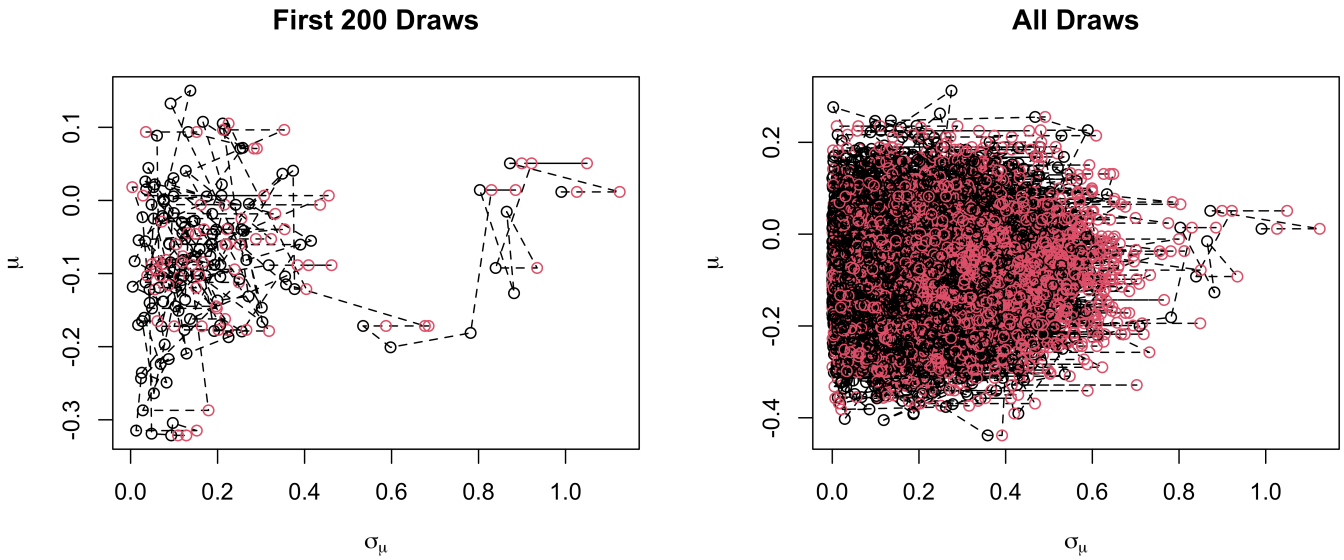
Example

Priors with $\sigma^2 = 1$:

$$p(\mu) \propto 1$$

- Use a Cauchy$(0, 1)$ prior on σ_μ independent of μ and
- Symmetric proposal for μ and σ_τ?
- Try independent normals $\frac{2.44^2}{d}$Cov(θ) where d is the dimension of θ (d = 2)

Samples



- Overall Acceptance probability is 0.6 out of 10^{4} samples
- Goal is around 0.44 in 1 dimension to 0.23 in higher dimensions

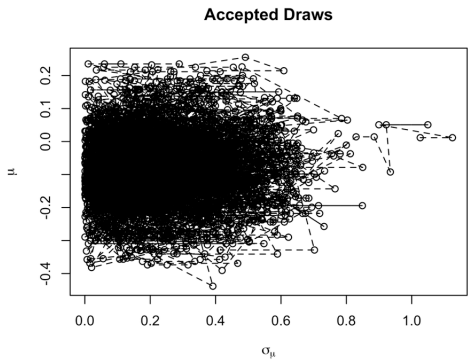
Tuning

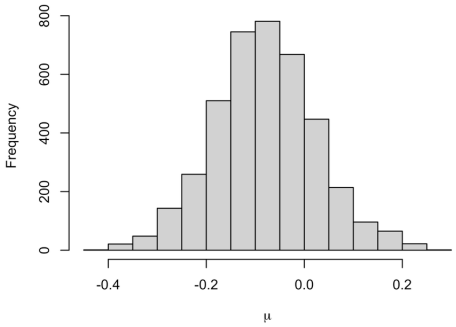
- Sampled values are correlated
- Correlation between samples can be adjusted by selecting an optimal δ (i.e., spread of the distribution) in the proposal distribution
- δ too small leads to $M \approx 1$ for most proposed values, a high acceptance rate, but very small moves, leading to highly correlated chain.
- δ too large can get "stuck" because $\theta^\star$ may be very far away from high density regions, leading to a very low acceptance rate and again high correlation in the Markov chain.
- Burn-in and thinning can help!

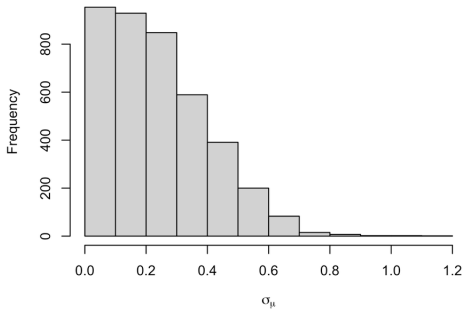
Burn-in

- Convergence occurs regardless of our starting point (in theory), so we can usually pick any reasonable values in the parameter space as a starting point.
- May take a long time to reach high density regions
- Over representation of low density samples given finite iterations
- Generally, we throw out a certain number of the first draws, known as the **burn-in**, as an attempt to make our draws closer to the stationary distribution and less dependent on any single set of starting values.
- However, we don't know exactly when convergence occurs, so it is not always clear how much burn-in we would need.
- If you run long enough you should not need to discard any samples! (ergodicity)

Example







Convergence diagnostics

- Diagnostics available to help decide on number of burn-in & collected samples.
- **Note**: no definitive tests of convergence but you should do as many diagnostics as you can, on all parameters in your model.
- With “experience”, visual inspection of trace plots perhaps most useful approach.
- There are a number of useful automated tests in R.
- **CAUTION**: diagnostics cannot guarantee that a chain has converged, but they can indicate it has not converged.

Diagnostics in R

- The most popular package for MCMC diagnostics in R is `coda`.
- `coda` uses a special MCMC format so you must always convert your posterior matrix into an MCMC object.
- For the example, we have the following in R.

```
#library(coda)
theta.mcmc <- mcmc(theta,start=1) #no burn-in (simple problem!)
```

Diagnostics in R

```
1 summary(theta.mcmc)
```

```
Iterations = 1:10000
Thinning interval = 1
Number of chains = 1
Sample size per chain = 10000

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

             Mean     SD Naive SE Time-series SE
mu       -0.07977 0.1046 0.001046       0.002839
sigma_mu  0.17550 0.1273 0.001273       0.004397

2. Quantiles for each variable:
```

- The naive SE is the **standard error of the mean**, which captures simulation error of the mean rather than the posterior uncertainty.
- The time-series SE adjusts the naive SE for **autocorrelation**.

Effective sample size.

- The **effective sample size** translates the number of MCMC samples S into an equivalent number of independent samples.
- It is defined as

$$\text{ESS} = \frac{S}{1 + 2\sum_k \rho_k},$$

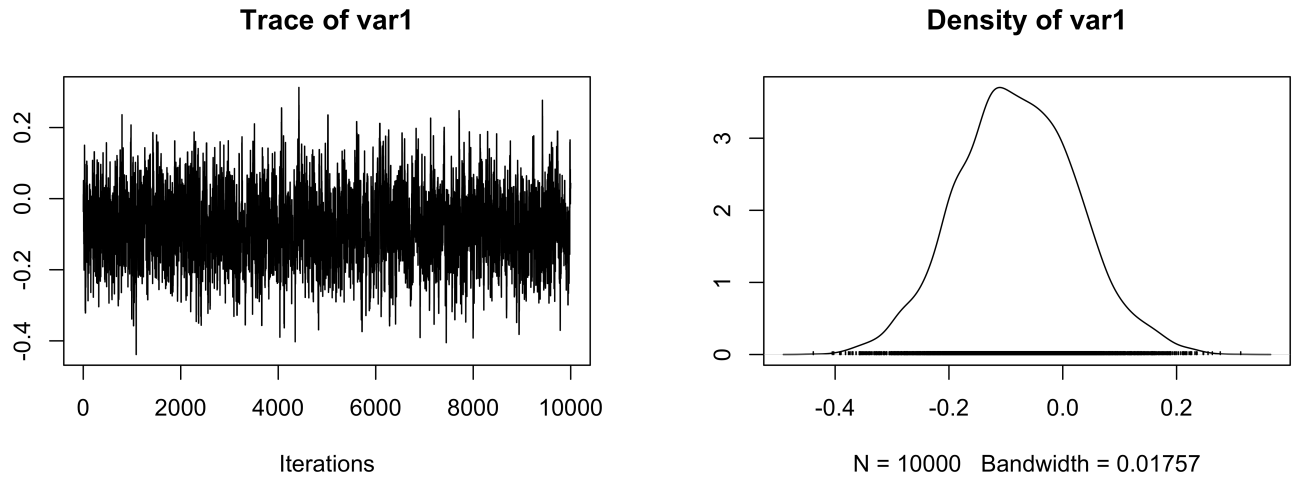
- S is the sample size and ρ_k is the lag k autocorrelation.
- For our data, we have

```
1 effectiveSize(theta.mcmc)
```

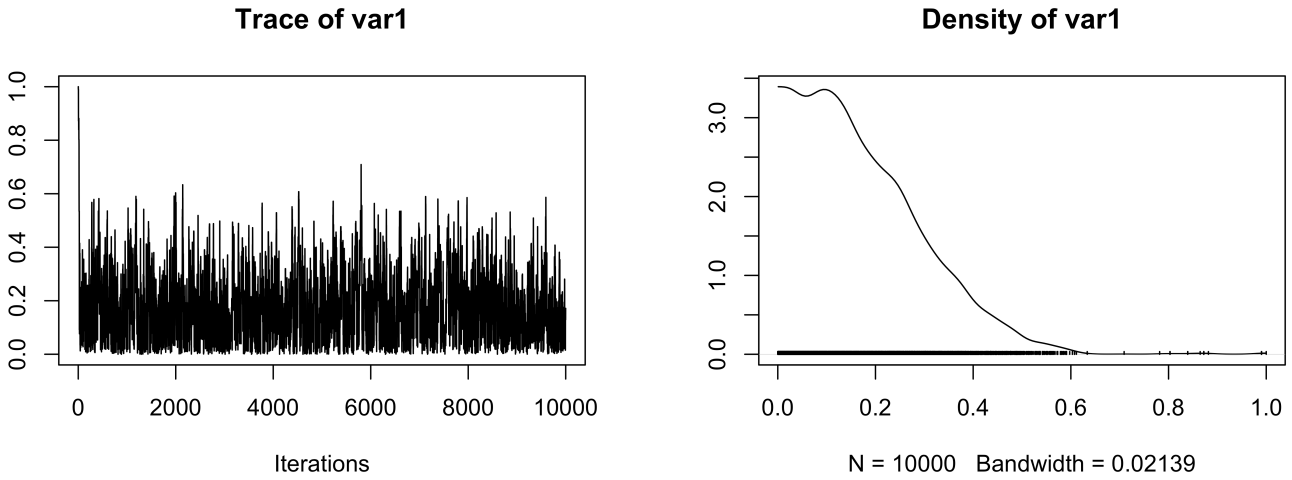
```
       mu  sigma_mu
1356.6495  838.2613
```

- So our 10,000 samples are equivalent to 1356.6 independent samples for μ and 838.3 independent samples for σ_μ.

Trace plot for mean



Trace plot for σ_μ



OK (be careful of scaling in plots!)

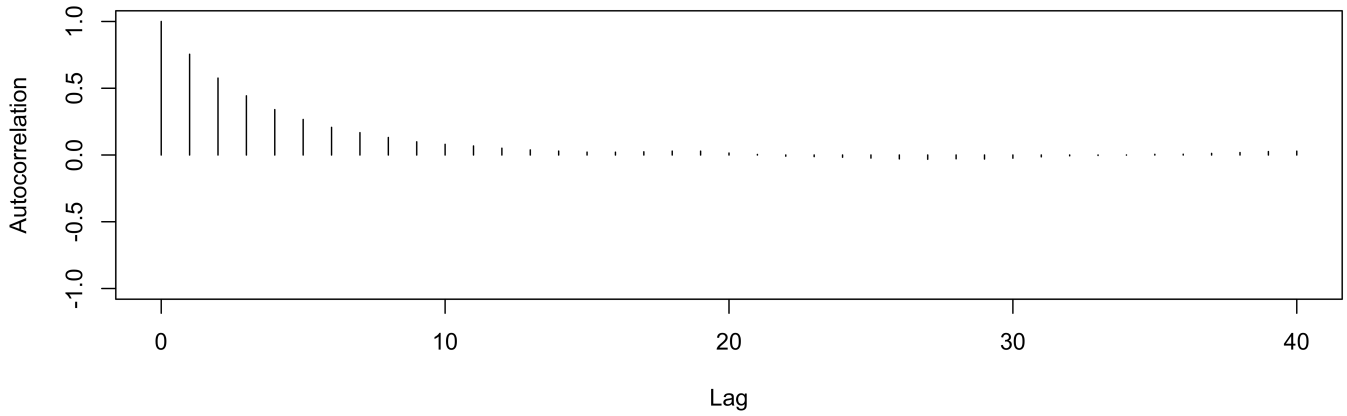
Autocorrelation

- Another way to evaluate convergence is to look at the autocorrelation between draws of our Markov chain.
- The lag k autocorrelation, ρ_k, is the correlation between each draw and its kth lag, defined as

$$\rho_k = \frac{\sum_{s=1}^{S-k}(\theta_s - \bar{\theta})(\theta_{s+k} - \bar{\theta})}{\sum_{s=1}^{S-k}(\theta_s - \bar{\theta})^2}$$

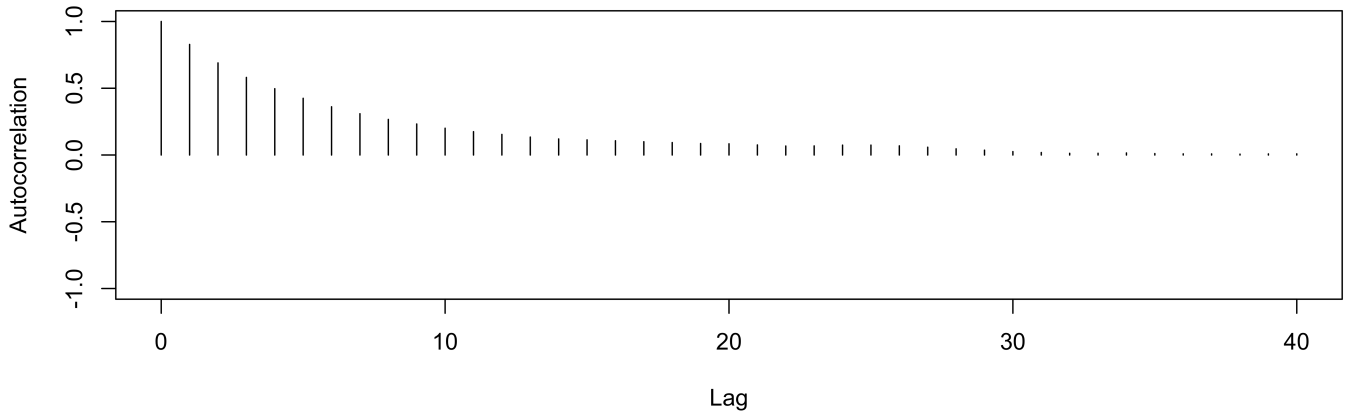
- We expect the autocorrelation to decrease as k increases.
- If autocorrelation remains high as k increases, we have slow mixing due to the inability of the sampler to move around the space well.

Autocorrelation for mean



So-So

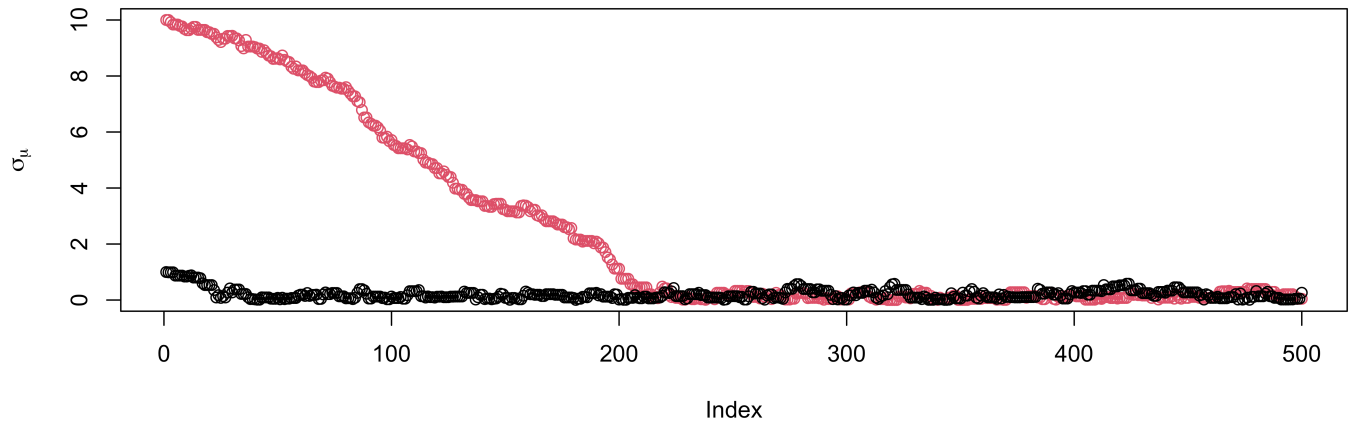
Autocorrelation for variance



worse

Gelman-Rubin

Gelman & Rubin suggested a diagnostic R based on taking separate chains with dispersed initial values to test convergence



Gelman-Rubin Diagnostic

- Run m > 2 chains of length 2S from overdispersed starting values.
- Discard the first S draws in each chain.
- Calculate the pooled within-chain variance W and between-chain variance B.

$$R = \frac{\frac{S-1}{S}W + \frac{1}{S}B}{W}$$

- numerator and denominator are both unbiased estimates of the variance if the two chains have converged
  - otherwise W is an underestimate (hasn't explored enough)
  - numerator will overestimate as B is too large (overdispersed starting points)
- As $S \to \infty$ and $B \to 0, R \to 1$
- version in R is slightly different

Gelman-Rubin Diagnostic

```
1 theta.mcmc = mcmc.list(mcmc(theta1, start=5000), mcmc(theta2, star
2 gelman.diag(theta.mcmc)
```

```
Potential scale reduction factors:

         Point est. Upper C.I.
mu                1          1
sigma_mu          1          1

Multivariate psrf

1
```

- Values of $R > 1.1$ suggest lack of convergence
- Looks OK
- See also `gelman.plot`

Geweke statistic

- Geweke proposed taking two non-overlapping parts of a single Markov chain (usually the first 10% and the last 50%) and comparing the mean of both parts, using a difference of means test
- The null hypothesis would be that the two parts of the chain are from the same distribution.
- The test statistic is a z-score with standard errors adjusted for autocorrelation, and if the p-value is significant for a variable, you need more draws.
- Output in R is the Z score

Geweke Diagnostic

- The output is the z-score itself (not the p-value).

```
1 geweke.diag(theta.mcmc)
```

```
[[1]]

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

      mu sigma_mu
 -0.7779   0.7491


[[2]]

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

Practical advice on diagnostics

- There are more tests we can use: Raftery and Lewis diagnostic, Heidelberger and Welch, etc.
- The Gelman-Rubin approach is quite appealing in using multiple chains
- Geweke (and Heidelberger and Welch) sometimes reject even when the trace plots look good.
- Overly sensitive to minor departures from stationarity that do not impact inferences.
- Most common method of assessing convergence is visual examination of trace plots.

Improving

- more iterations and multiple chains
- thinning to reduce correlations and increase ESS e.g. if autocorrelation drops to near zero at say lag 5, keep every 5th draw
- change the proposal distribution q