Lecture 7: MCMC Diagnostics & Adaptive Metropolis

STA702

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Example from Last Class

- Marginal Likelihood

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

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

- Priors with $\sigma^2 = 1$: $p(\mu) \propto 1$ and $\sigma_\mu \sim \textsf{Cauchy}^+(0,1)$ independent of μ
- Symmetric proposal for μ and σ_τ
- Independent normals centered at current values of μ and σ_μ with covariance $\frac{2.38^2}{d} \textsf{Cov}(\theta)$ where $d = 2$ (the dimension of θ)
- $\delta^2 = 2.38^2/d$ optimal for multivariate normal target Roberts, Gelman, and Gilks (1997) with acceptance rate ranging from 40% to 23.4% (as $d \to \infty$)

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.

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

Diagnostics in R

```r
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

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

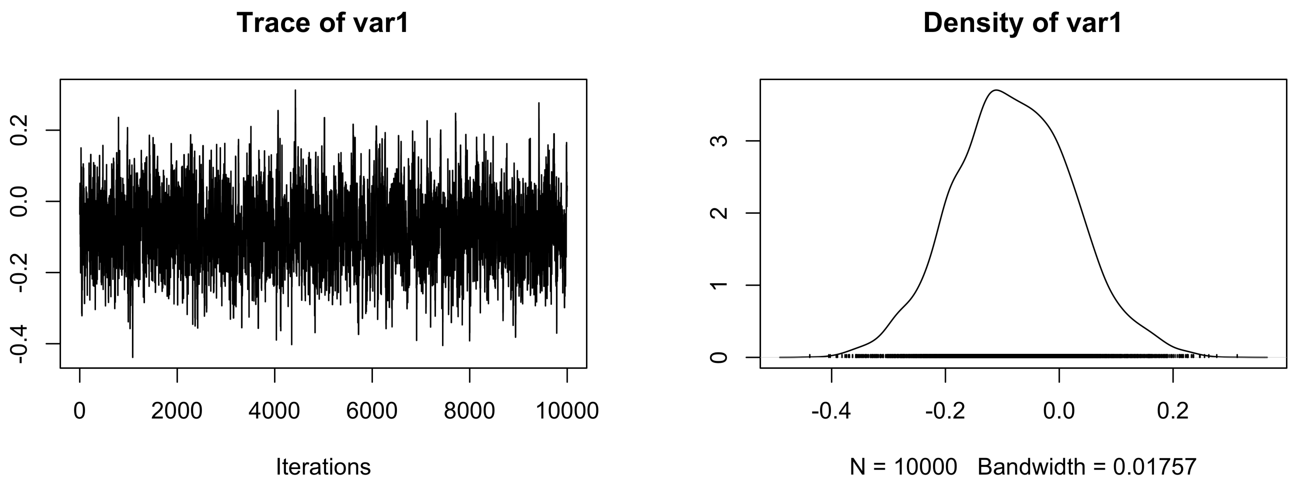
- S is the sample size and ρ_k is the lag k autocorrelation.
- For our data, we have

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

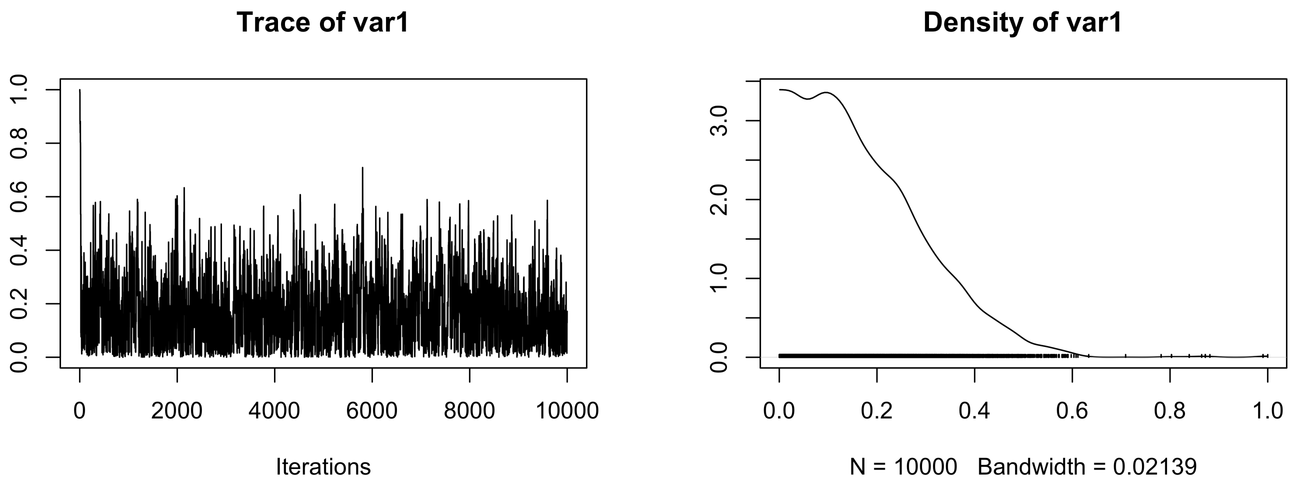
```
       mu  sigma_mu 
1356.6495  838.2613 
```

- 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!)

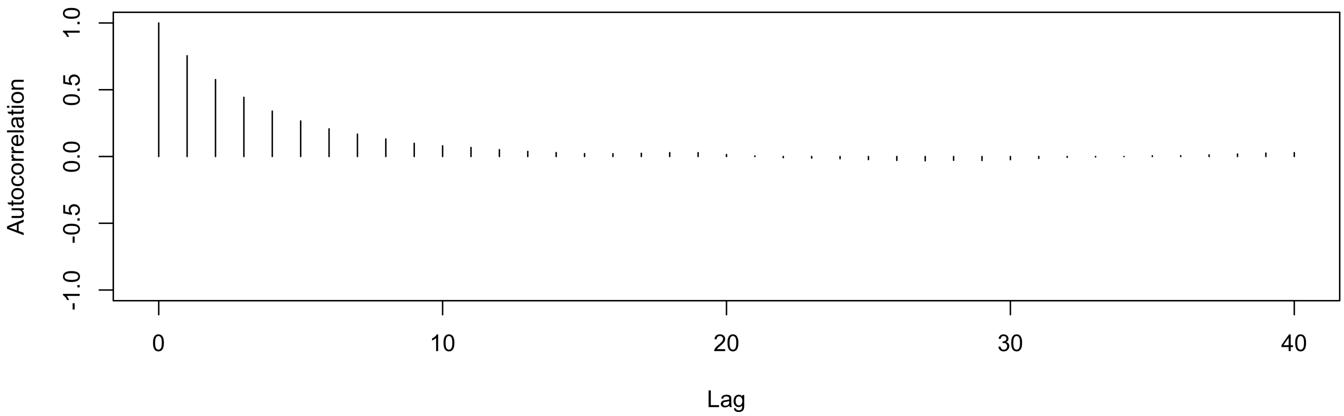
Autocorrelation

- 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

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

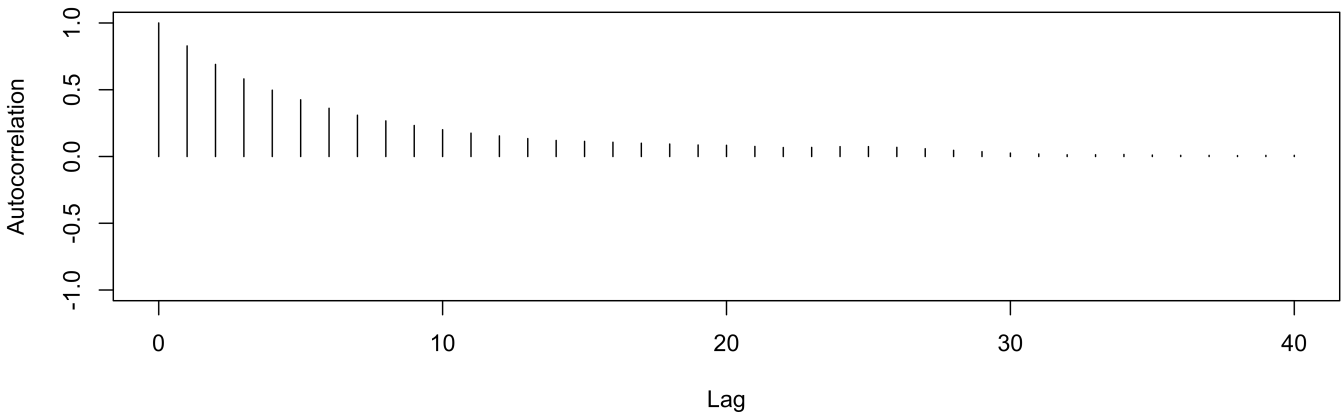
- We expect the autocorrelation to decrease as k increases.
- If autocorrelation remains high as k increases, we have slow mixing due to the inability of the sampler to move around the space well.

Autocorrelation for mean



So-So

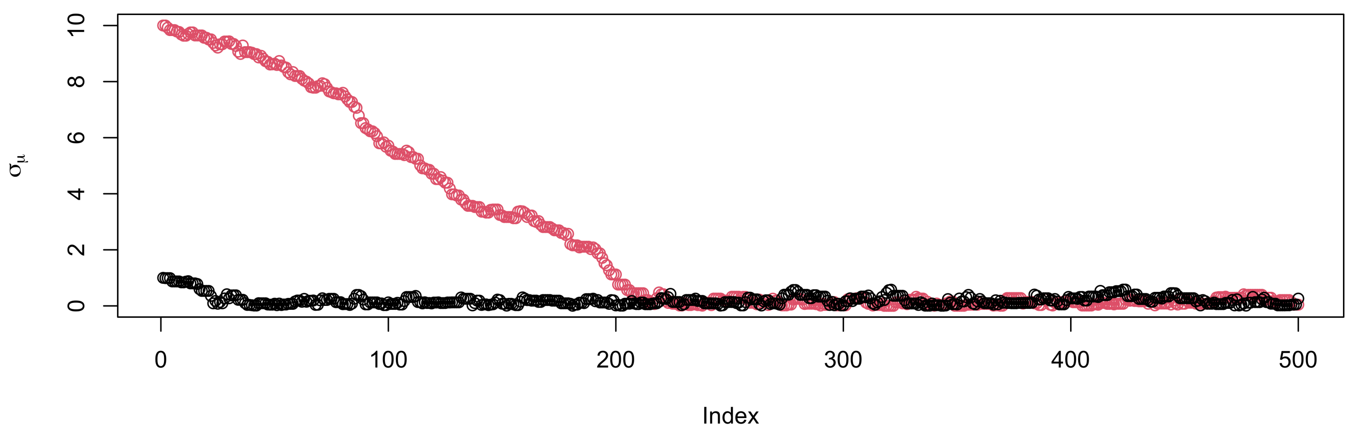
Autocorrelation for variance



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

```
theta.mcmc = mcmc.list(mcmc(theta1, start=5000), mcmc(theta2, star
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

```
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
```

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

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 Results

- more iterations and multiple chains
- thinning to reduce correlations and increase ESS
- change the proposal distribution q
- adaptive Metropolis to tune q

Proposal Distribution

- Common choice

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

- rough estimate of Σ based on the asymptotic Gaussian approximation $\textsf{Cov}(\theta \mid y)$ and $\delta = 2.38/\sqrt{\dim(\theta)}$
- find the MAP estimate (posterior mode) $\hat{\theta}$
- take

$$\Sigma = \left[- \frac{\partial^2 \log(\mathcal{L}(\theta)) + \log(\pi(\theta))}{\partial \theta \partial \theta^T} \right]^{-1}_{\theta = \hat{\theta}}$$

- ignore prior and use inverse of Fisher Information (covariance of MLE)

Learn Covariance in Proposal?

- Can we learn the proposal distribution?
- ad hoc?
  - run an initial MCMC for an initial tuning phase (e.g. 1000 samples) with a fixed δ and estimate $\Sigma(\theta)$ from samples.
  - run more to tweak δ to get acceptance rate between $23\% - 40\%$.
  - fix the kernel for final run
- MCMC doesn't allow you to use the full history of the chain $\theta^{(1)}, \ldots, \theta^{(s)}$ in constructing the proposal distributions as it violates the Markov assumption
- even with no further "learning", no guarantee we will converge to posterior!
- more elegant approach - formal **adaptive Metropolis**
  - keep adapting the entire time!

⚠ ad hoc adaptation may mess up convergence !

Adaptive MCMC

- run RWM with a Gaussian proposal for a fixed number of iterations for $s < s_0$
- estimate of covariance at state s

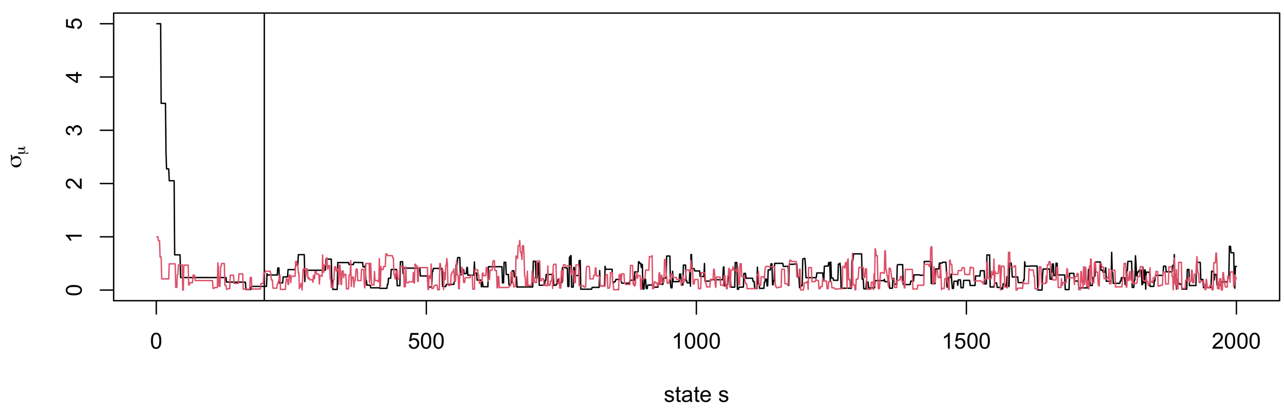
$$\Sigma^{(s)} = \frac{1}{s}\left(\sum_{i=1}^{s} \theta^{(i)}{\theta^{(i)}}^T - s\bar{\theta}^{(s)}{\bar{\theta}^{(s)}}^T\right)$$

- proposal for $s > s_0$ with $\delta = 2.38/\sqrt{d}$

$$\theta^* \sim \mathsf{N}(\theta^{(s)}, \delta^2(\Sigma^{(s)} + \epsilon I_d))$$

- $\epsilon > 0$ insures covariance is positive definite
- if s_0 is too large will take longer for adaptation to be seen
- need conditions for vanishing adaptation e.g. that the proposal depends less and less on recent states in the chain - see Roberts & Rosenthal (2009)for examples and other conditions

Example again



Acceptance rate now around 30-35 % of 10,000 iterations!