More MCMC diagnostics

Stat 340: Bayesian Statistics

Tuning MCMC

Three main decisions:

- Selecting the initial values for the parameters
- Determining if/when the chain(s) has converged
- Selecting the number of samples needed to approximate the posterior

Initial values

- The algorithm will eventually converge no matter what initial values you select
- Choosing good starting values will speed up convergence
- It is important to try a few initial values to verify they all give the same result
- Usually 3-5 separate chains is sufficient

Common strategies:

1. Select good initial values using method of moments or MLE
2. Purposely pick bad but different initial values for each chain to check convergence

Convergence diagnostics

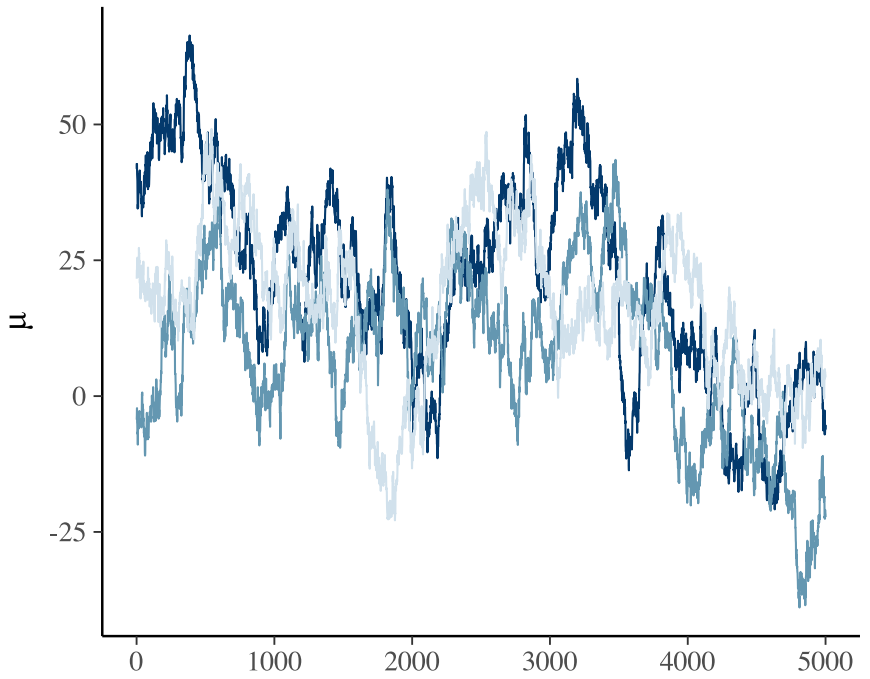
> Don't assume that your Markov chain converged to the desired stationary distribution just because "it worked."

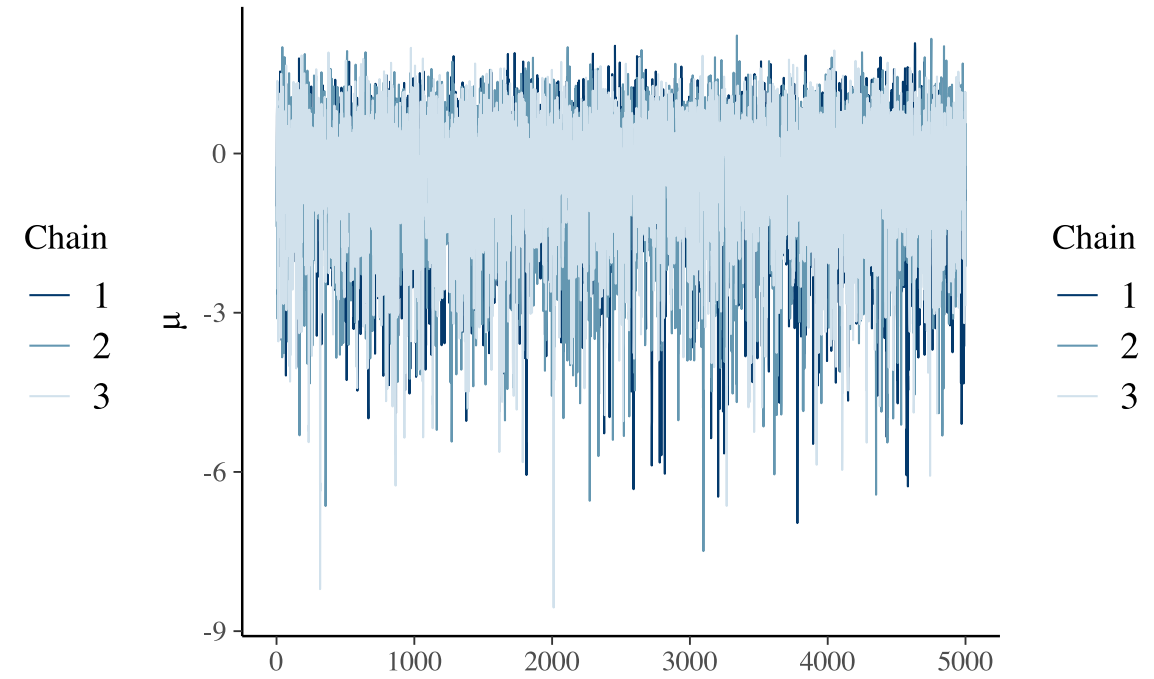
A **"good" Markov chain** should be:

- **Stationary**: draws should within the posterior (stable path around the center of gravity)
- **Well mixed**:
  - successive draws should not be highly correlated
  - each chain should target the same stationary distribution

Your turn

With a neighbor, decide whether each chain is well mixed





Tools already in our toolkit

Did my chains converge?

- Trace plots

Are my chains well mixed?

- ACF plots

Convergence diagnostics

The **coda** R package has dozens of diagnostics

```
library(coda)
```

Did my chains converge?

- Geweke
- Gelman-Rubin

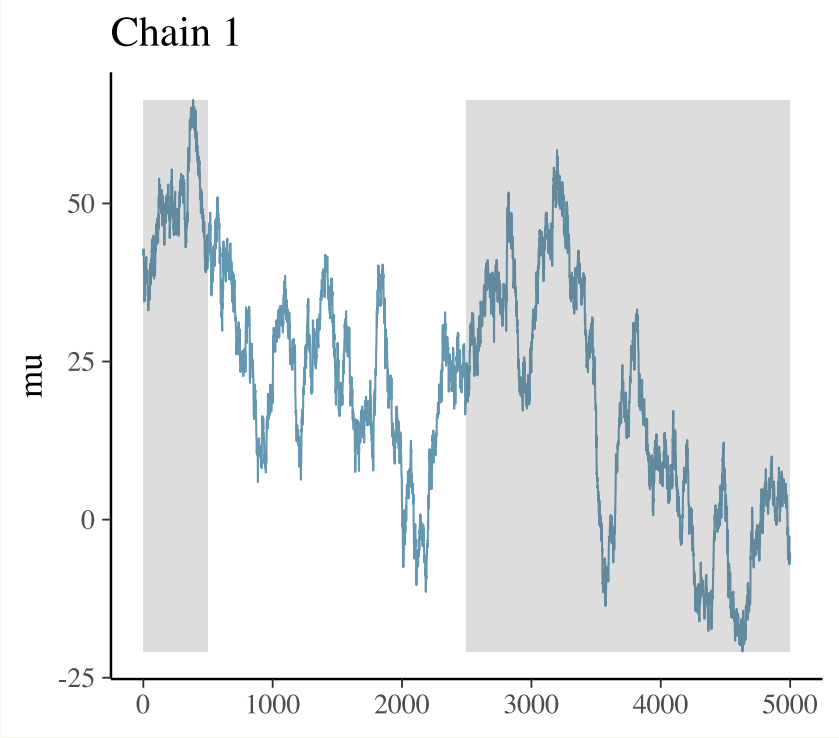
Did I run the sampler long enough after convergence?

- Effective sample size
- Standard errors for the posterior mean estimate

Geweke diagnostic

- **Idea:** a two-sample test comparing the mean of a chain between batches at the beginning versus the end
- By default, JAGS compares the first 10% with the last 50%
- Test statistic is a Z-score with the standard errors adjusted for autocorrelation (so we won't write down the formula)

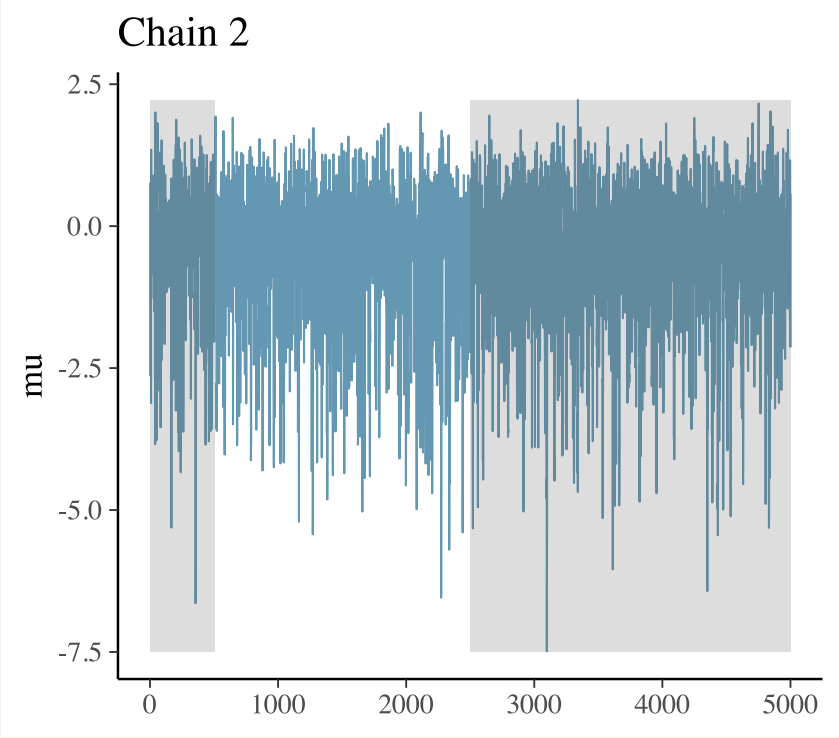
Geweke diagnostic




```
geweke.diag(bad_samples$mcmc[[1]])
```

```
##
## Fraction in 1st window = 0.1
## Fraction in 2nd window = 0.5
##
##    mu
## 2.676
```

Geweke diagnostic



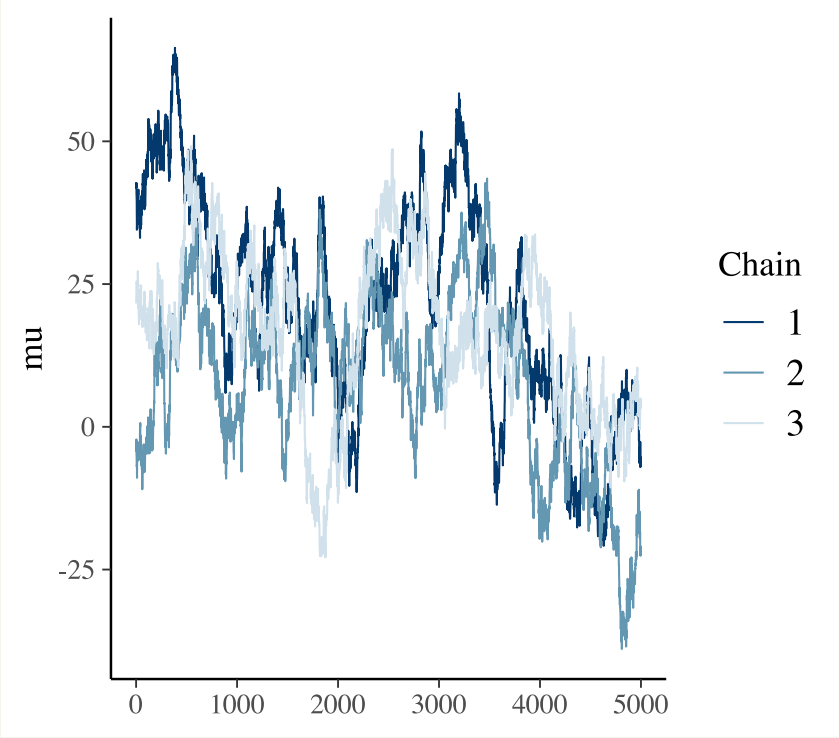

```
geweke.diag(good_samples$mcmc[[2]])
```

```
##
## Fraction in 1st window = 0.1
## Fraction in 2nd window = 0.5
##
##    mu
## 1.704
```

Gelman-Rubin diagnostic

- Effective convergence of Markov chain simulation has been reached when inferences for quantities of interest do not depend on the starting point of the simulations.
- If we run multiple chains, we hope that all chains give same result
- Gelman and Rubin (1992) proposed (essentially) an ANOVA test of whether the chains have the same mean
- R_j is scaled and approaches 1 from above
  - $R_j = 1 \Rightarrow$ perfect convergence
  - $R_j \geq 1.1 \Rightarrow$ red flag

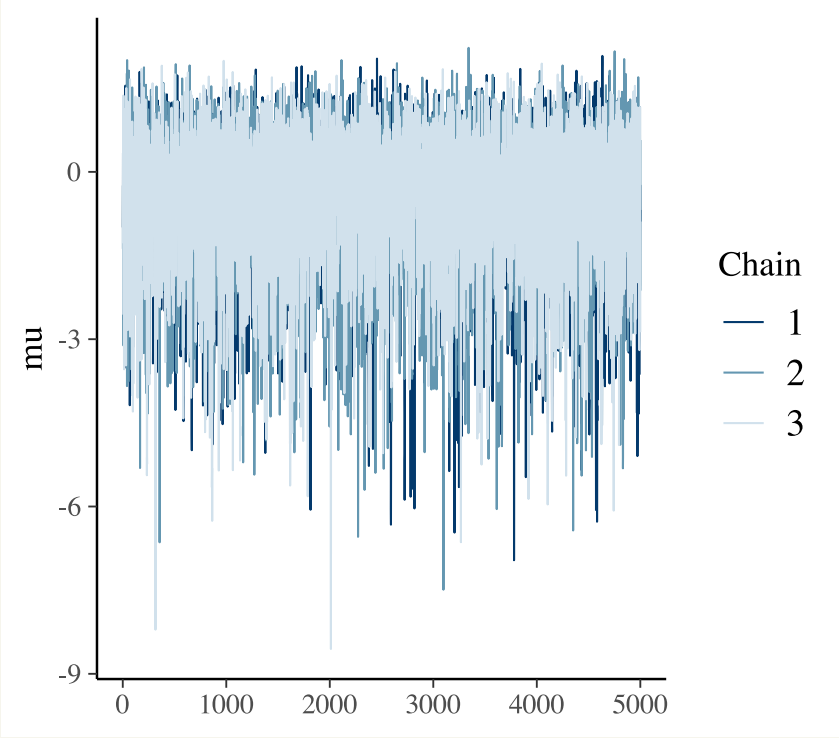
Gelman-Rubin diagnostic




```
gelman.diag(bad_samples$mcmc)
```

```
## Potential scale reduction factors
##
##    Point est. Upper C.I.
## mu       1.06       1.17
```

Gelman-Rubin diagnostic




```
gelman.diag(good_samples$mcmc)
```

```
## Potential scale reduction factors
##
##    Point est. Upper C.I.
## mu          1          1
```

A note on autocorrelation

- Lower values are better, but if the chains are long enough even large values can be OK
- **Thinning** the Markov chain means keeping only every kth draw, where k is chosen so that the autocorrelation is small
- `thin` argument to `run.jags()` implements this
- This is always less efficient than using all samples, but can save memory

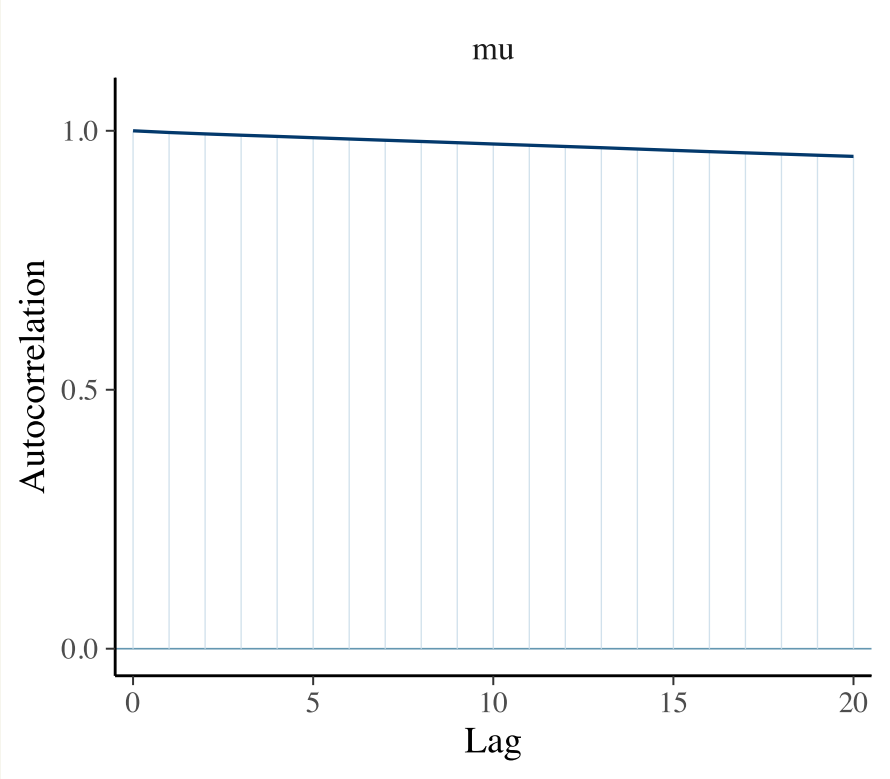
Effective sample size

- Highly correlated samples have less information than independent samples
- $S =$ # MCMC samples after burn in
- **Effective samples size (ESS)**

$$ESS_k = S \Big/ \left(1 + 2\sum_{k=1}^{\infty} \rho(k)\right)$$

- ESS = "equivalent number of independent observations"
- Should be at least a few thousand for all parameters

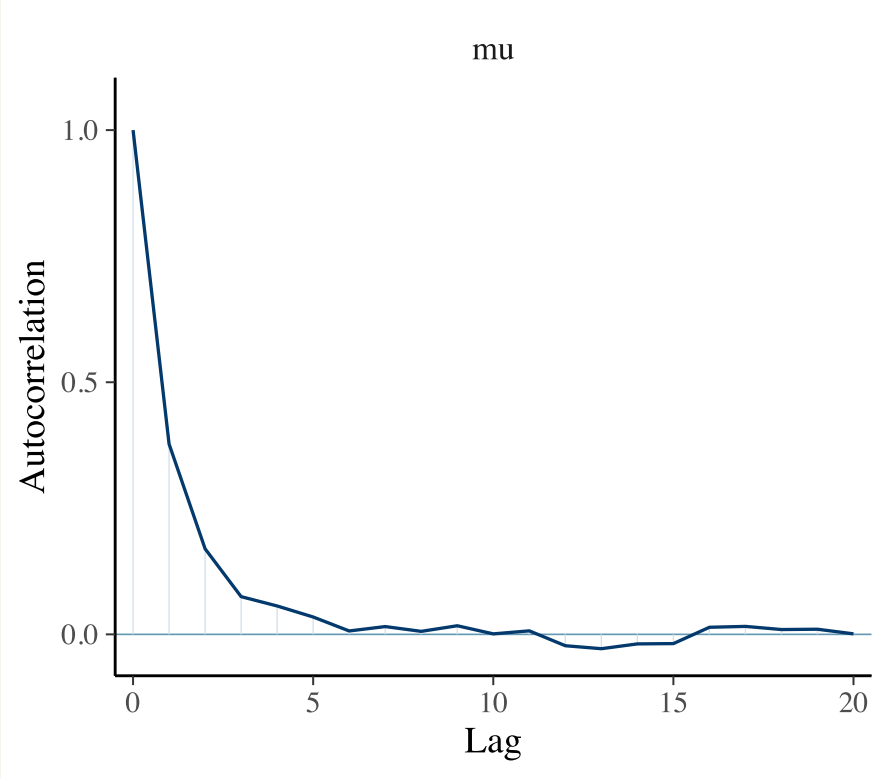
Effective sample size




```
# ESS for single chain of mu1
# n.iter = 5000
effectiveSize(bad_samples$mcmc[[1]])
```

```
##        mu
## 6.062577
```

Effective sample size




```
# ESS for single chain of mu1
# n.iter = 5000
effectiveSize(good_samples$mcmc[[1]])
```

```
##       mu
## 2119.896
```

Standard errors of posterior mean estimates

- Assuming independence the standard error is

$$\text{Naive SE} = \frac{s}{\sqrt{S}}$$

  where s = sample SD

- A more realistic standard error is

$$\text{Time-series SE} = \frac{s}{\sqrt{ESS}}$$

- If the SE is too large, rerun the MCMC algorithm for a larger number of samples

Standard errors of posterior mean estimates

```
summary(bad_samples$mcmc)
##
## Iterations = 2001:7000
## Thinning interval = 1
## Number of chains = 3
## 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
##         15.455         17.026          0.139          3.341
##
## 2. Quantiles for each variable:
##
##    2.5%     25%     50%     75%   97.5%
## -17.812   3.998  15.898  27.229  48.263
```

Standard errors of posterior mean estimates

```
summary(good_samples$mcmc)
##
## Iterations = 2001:7000
## Thinning interval = 1
## Number of chains = 3
## 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
##       -0.56146        1.26084         0.01029        0.01574
##
## 2. Quantiles for each variable:
##
##    2.5%     25%     50%     75%   97.5%
## -3.6330 -1.2123 -0.3600  0.3301  1.2965
```

What to do if the chains haven't converged?

- Increase the number of iterations
- Tune the Metropolis candidate distribution
- Use better initial values
- Use a more advanced algorithm
- Simplify/reparameterize the model
- Use (more) informative priors