Bootstrap & MCMC Tutorial

Contents

Background

Randomization techniques: why do we use them?

Data resampling and randomization methods are most often used for

1. Evaluating uncertainty levels in data
2. Hypothesis testing
3. Improving model fit/performance

Common methods include

- **Bootstrapping**: "pulling yourself up by your bootstraps"; pulling random samples from your data to *evaluate* the distribution of metrics of interest and obtain *confidence intervals* for computed statistics
- **Permutations**: randomizing your data by keeping some parameters constant and varying others, then comparing to a null distribution to ask if your data structure differs significantly from the null expectation; i.e., *hypothesis testing*
- **Markov Chains**: simulate different possible values of model parameters through random sampling, incorporating fixed and random effects; can *improve model performance* when chains are mixed well. This method is based on Bayesian inference, but for the way we will use it in this tutorial, it basically is just a juiced-up generalized linear mixed effects model (GLMM).

Tutorial

Example dataset

The dataset we will use for the tutorial shows feeder visitations by birds in mixed-species flocks in Lincoln, Nebraska. This a summarized version of that dataset which aggregates each individual's number of morning visitations (sumvisits) and compares them to the lowest temperature from the previous night. If you would like to learn more about the original study, you can find it here: https://academic.oup.com/beheco/article/32/3/407/6163219 and the full dataset and code for its analysis can be found here: https://datadryad.org/stash/dataset/doi:10.5061/dryad.x69p8czgr

The original study used a Markov Chain Monte Carlo model to test the effects of overnight temperature on morning feeder visitation by birds in mixed-species flocks. Here, we will be adding a component not used in the original study to demonstrate bootstrapping. The original study also used permutations to test if pairs of birds with a strong social connection had similar foraging activity. The network permutations will not be covered in this tutorial, but the necessary code can be found through the dryad link above.

We will start the tutorial with bootstrapping then move to Markov Chains.

Bootstrapping

Data visualization and exploration

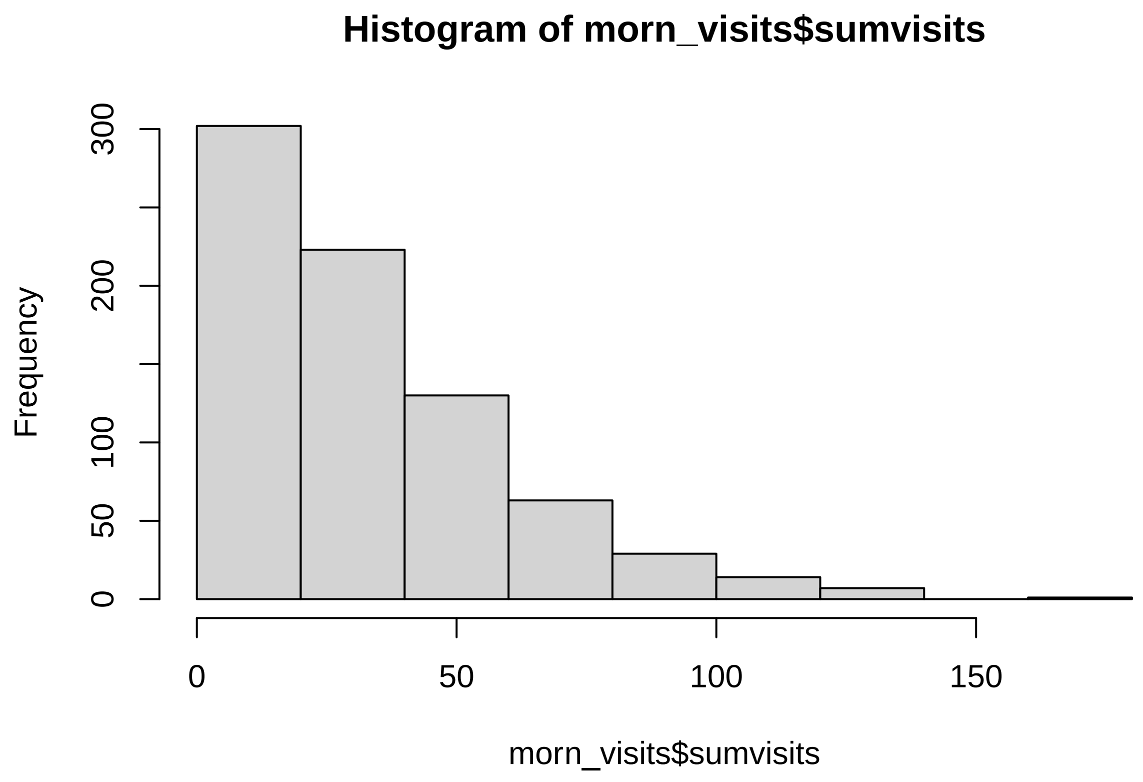
First, we need to load the visitation data and investigate the variables of interest, "sumvisits" (feeder visitation) and "nightlows" (the lowest overnight temperature)

```r
load("morn_visits.dat")

## check out data structure
head(morn_visits)
```

```
##         Date       RFID Species Sex sumvisits  nightlows
## 1 2019-01-27 011016B9B5    WBNU   M        11  -6.722222
## 2 2019-01-29 011016B9B5    WBNU   M         1 -18.888889
## 3 2019-01-30 011016B9B5    WBNU   M        21 -22.222222
## 4 2019-01-31 011016B9B5    WBNU   M        14 -17.777778
## 5 2019-02-01 011016B9B5    WBNU   M        13 -11.722222
## 6 2019-02-02 011016B9B5    WBNU   M         2   1.111111
```

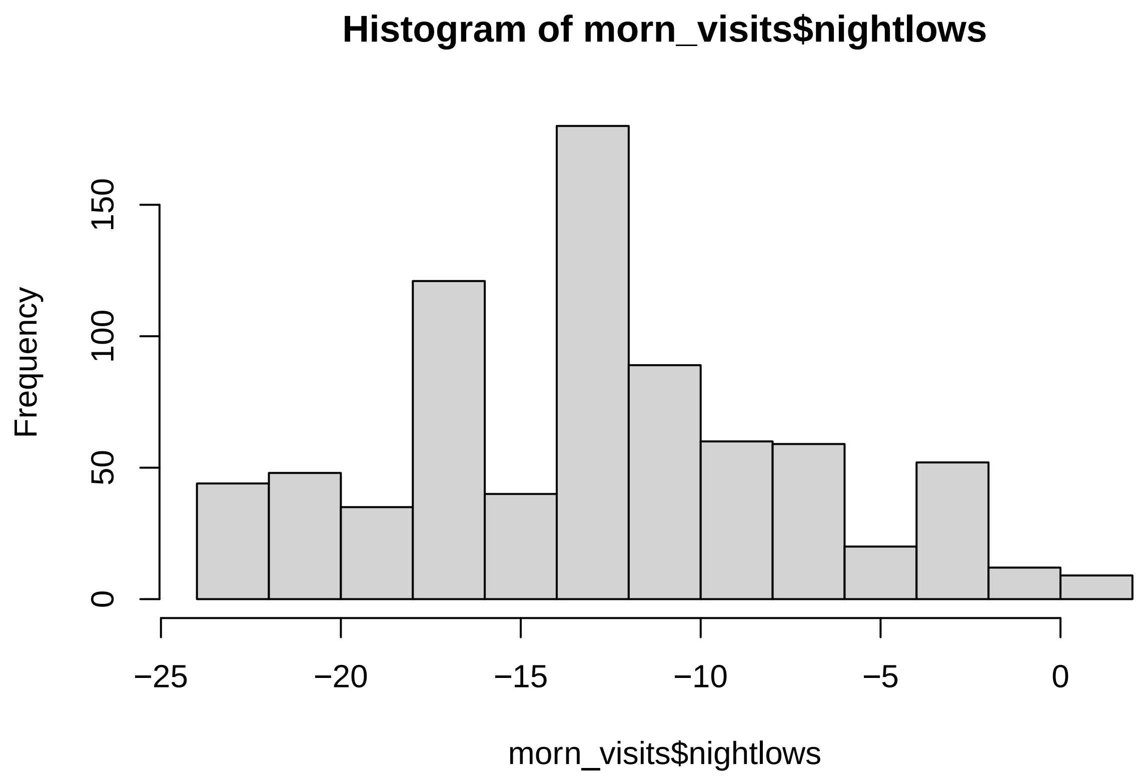
```r
## Let's look at the distributions of our variables of interest
hist(morn_visits$sumvisits)
```



```
## left-biased distribution, aka Poisson
mean(morn_visits$sumvisits)
```

```
## [1] 33.39792
```

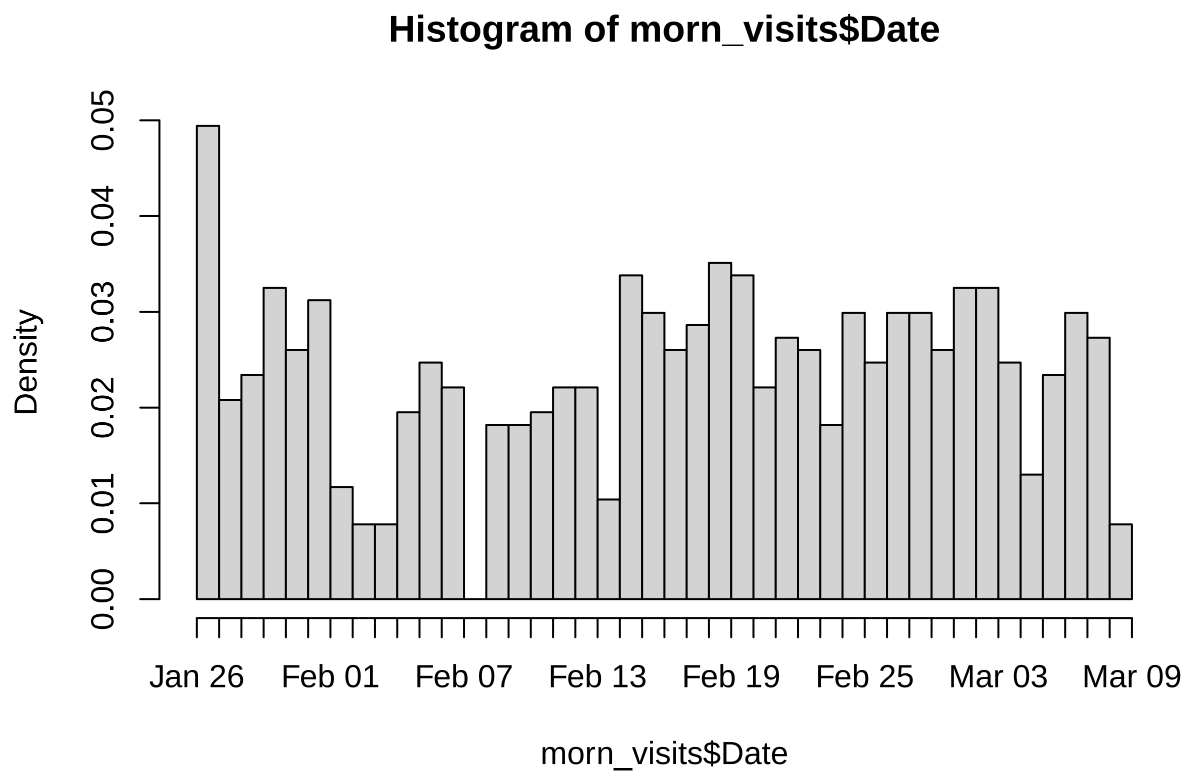
```
hist(morn_visits$nightlows)
```



```
## fairly Gaussian, but not perfect, may need to rescale if model fit is off
mean(morn_visits$nightlows)
```

```
## [1] -12.90478
```

```
hist(morn_visits$Date, breaks = "day")
```



```
## data distribution over the study is fairly even, except for a gap when there were technological issu
```

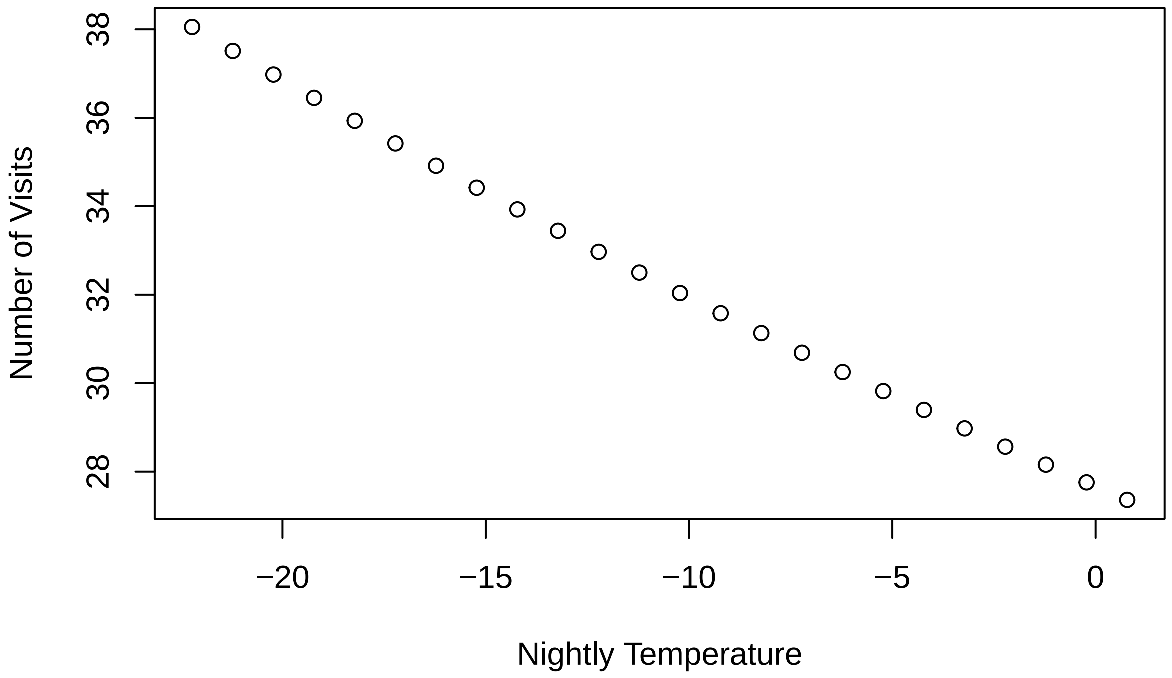
Simple model

Now that we know our data a little better, let's start by running a simple generalized linear model to test the effects of overnight temperature on feeder visitation.

```
glm.1 = glm(formula = sumvisits ~ nightlows, data = morn_visits, family = "poisson")
summary(glm.1)
```

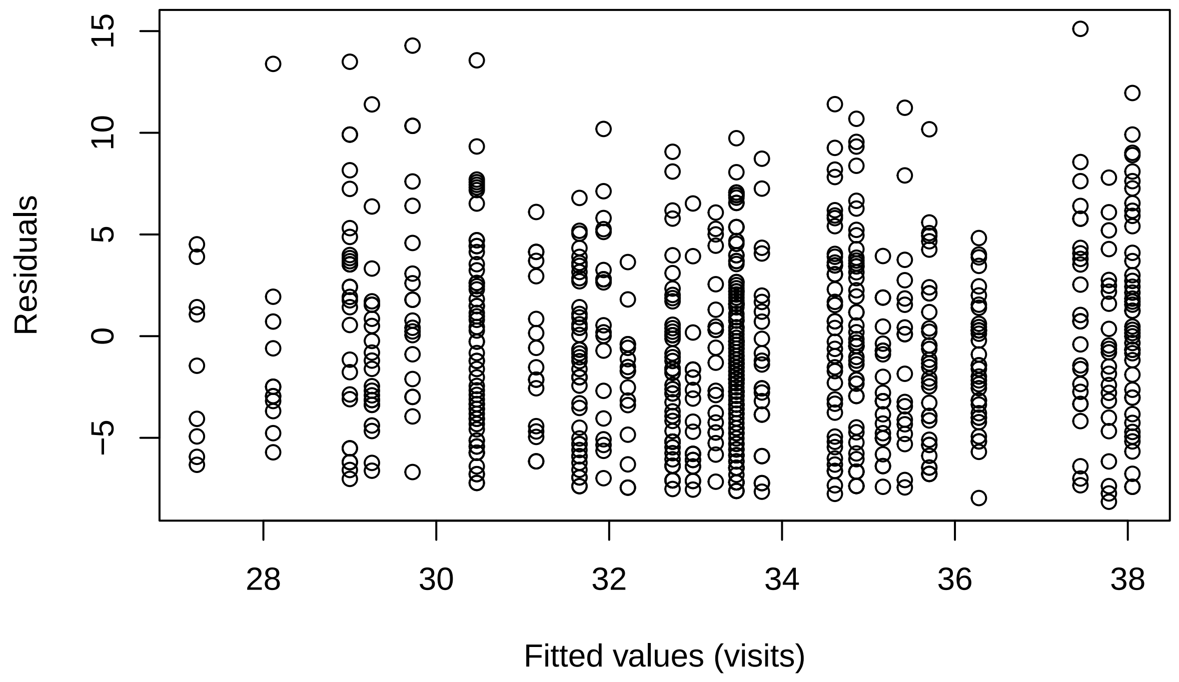
```
##
## Call:
## glm(formula = sumvisits ~ nightlows, family = "poisson", data = morn_visits)
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  3.32029    0.01644  202.01   <2e-16 ***
## nightlows   -0.01434    0.00114  -12.58   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for poisson family taken to be 1)
##
##     Null deviance: 16371  on 768  degrees of freedom
## Residual deviance: 16211  on 767  degrees of freedom
## AIC: 20001
##
## Number of Fisher Scoring iterations: 5
```

```
## Predictive graph for Temperature
temp <- data.frame(nightlows = seq(min(morn_visits$nightlows),max(morn_visits$nightlows)), by = 0.5, Da
temp$Predict <- predict(glm.1, temp, type = "response")
## takes parameters from model and returns values for the response variable
plot(temp$nightlows, temp$Predict, xlab = "Nightly Temperature", ylab = "Number of Visits")
```

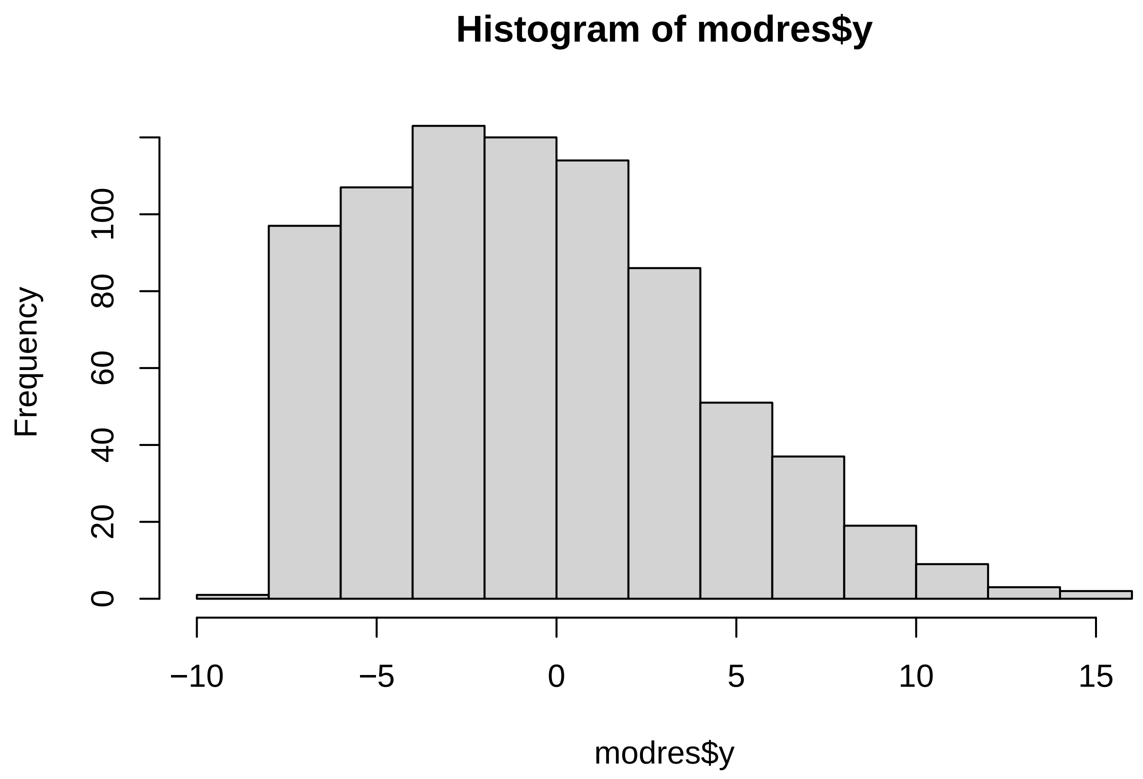


Let’s look at the residuals to assess model fit. The fitted vs. residual plot should have no clear trend and there should be a normal distribution of the residuals.

```
modres = data.frame(x = na.omit(fitted(glm.1)), y = na.omit(resid(glm.1)))
plot(modres$x, modres$y,
     ylab = "Residuals", xlab = "Fitted values (visits)")
```

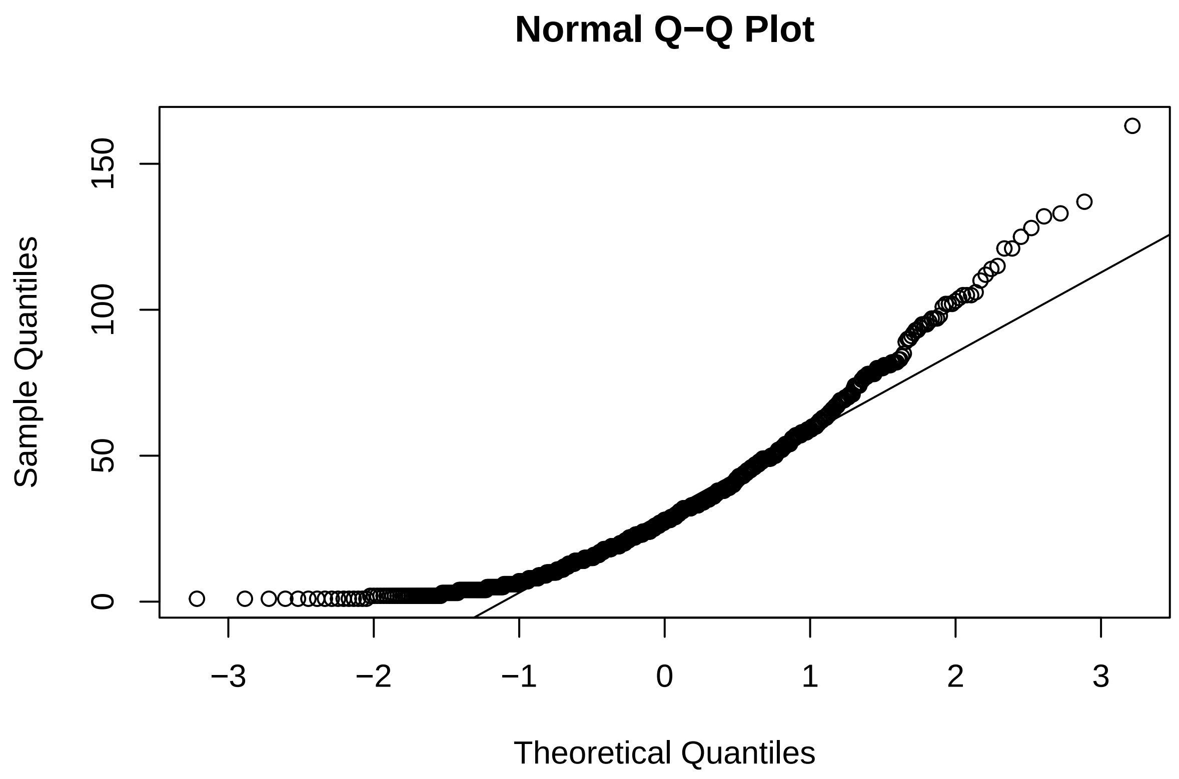


```r
hist(modres$y)
```



Let’s look at the quantiles to assess model fit. The theoretical and sample quantiles should fall along the normal quantiles line.

```r
qqnorm(morn_visits$sumvisits)
qqline(morn_visits$sumvisits)
```



Hm, it's not a perfect model fit. The residuals aren't quite a normal distribution and our Q-Q plot is not quite a straight line. Maybe the model assumptions aren't met or the distribution is thrown off by something. Let's see if we can improve model fit.

Bootstrap a simple statistic

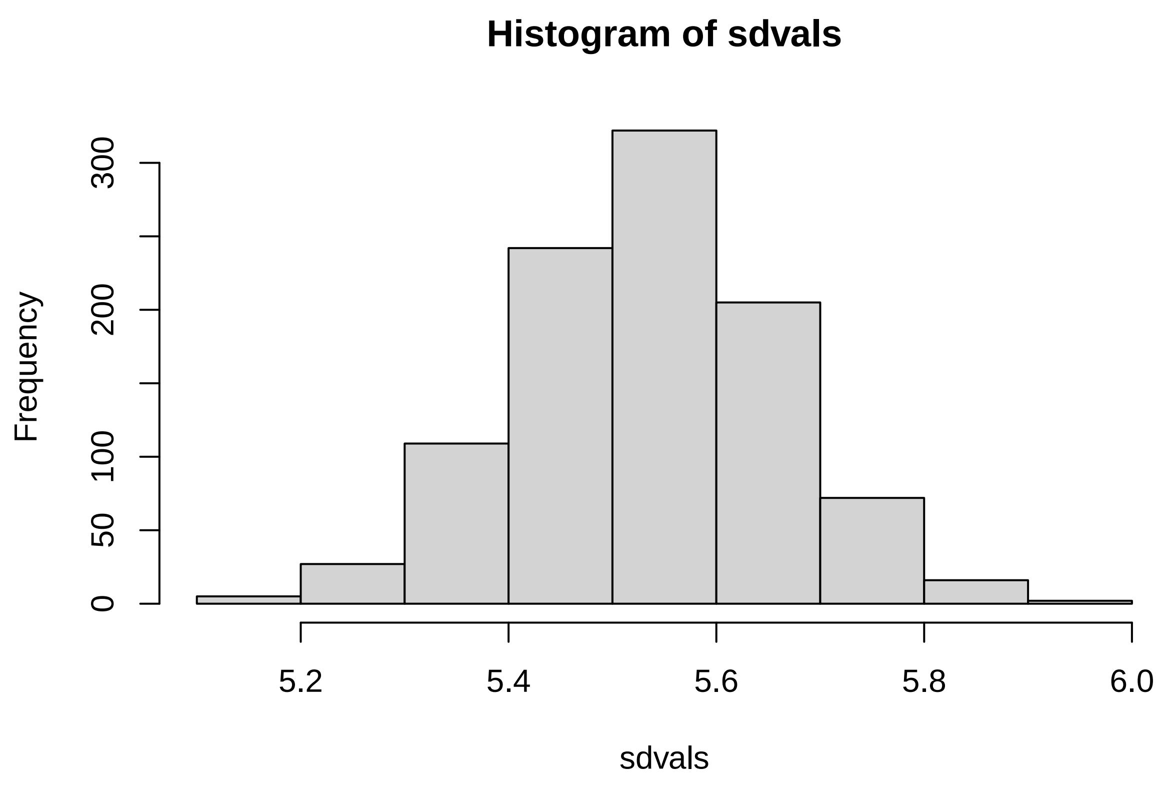
First, to demonstrate the logic behind bootstrapping, let's bootstrap a simple statistic to evaluate our distributions and accuracy. To do this we are going to build a simple function to resample the data and calculate a bootstrap statistic.

```
bootstrap <- function(data, samp_size, calc_statistic, b_iter) {
  boot_statistic <- function() {
    ## randomly sample rows with replacement; enter sample values as samp_size, up to the original samp
    boot_sample = sample(x = data, size = samp_size, replace = T)

    ## apply the statistic of interest
    calc_statistic(boot_sample)
  }
## perform the bootstrap multiple times by changing b_iter
  replicate(n = b_iter, expr = boot_statistic())
}
set.seed(457)
sdvals = bootstrap(data=morn_visits$nightlows, samp_size=nrow(morn_visits), calc_statistic=sd, b_iter=1
```

Now look at the distribution of values.

```r
hist(sdvals)
```



Calculate the 95% confidence intervals.

```r
quantile(sdvals, probs = c(0.025,0.975))
```

```
##     2.5%    97.5% 
## 5.275811 5.780584
```

This example should help you understand some of the logic behind bootstrapping. However, you don't have to write your own function for everything–there are also premade packages in R for bootstrapping, including the *mosaic* package (see here for a specific tutorial on *mosaic* https://rpubs.com/robbsinn/s11) and the *boot* package https://www.mayin.org/ajayshah/KB/R/documents/boot.html. These use wrappers to apply different statistics to your data. They also have a wider variety of options to fine-tune your resampling methods for simple statistics.

```r
library(boot)
??boot
library(mosaic)
```

```
## Warning: package 'mosaic' was built under R version 4.3.3
```

```
??mosaic
```

Bootstrap model outputs

Now let's apply the same logic to the GLM to get a bootstrapped model parameter and calculate confidence intervals. We will do this for our response estimate. Basically, we will run the model a bunch of times, resampling the data each time and grabbing our parameter of interest.

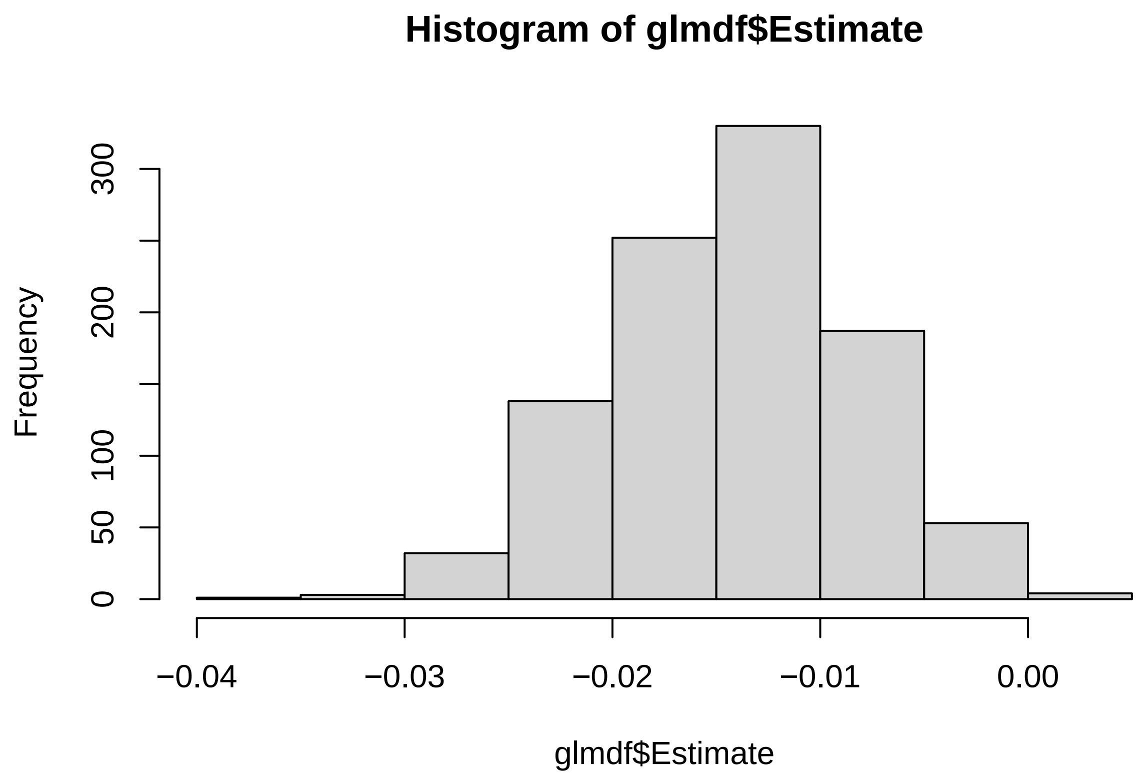
```
library(tidyverse)
##initialize dataframe for our output parameters
glmdf = data.frame(Estimate = numeric())
for(i in 1:1000){
  ## randomly sample rows with replacement up to the original sample size
  sampdata = sample_n(morn_visits, size = nrow(morn_visits), replace = TRUE)
  ## model the effects of interest
  glm_temp = glm(formula = sumvisits ~ nightlows, data = sampdata, family = "poisson")
  ## save the output to our dataframe
  glmdf = rbind(glmdf, data.frame(Estimate = summary(glm_temp)$coefficients[, 1][2]))
}

quantile(glmdf$Estimate,probs = c(0.025,0.975))
```

```
##         2.5%        97.5%
## -0.025744856 -0.003013217
```

```
## get confidence intervals; cool, they do not overlap with zero! If they did, that would mean we canno

hist(glmdf$Estimate)
```



```
## look at the distribution of the parameter
```

Markov Chain Monte Carlo (MCMC) GLMM

Now let's try a different randomization method that also incorporates more complexity from our data. We initially built a simple model with only a response and a single predictor. But in this dataset, we also know there are individuals that may differ in their behavior and we might expect that behavior differs by day, depending on flockmates and other factors. We can incorporate that complexity into the model and into the randomization process itself with MCMC.

Let's run through the logic for MCMC before we continue. These models are complex, and the function we will use "black-boxes" the methods.

```
library(MCMCglmm)
```

```
## Warning: package 'MCMCglmm' was built under R version 4.3.2
```

```
## Warning: package 'coda' was built under R version 4.3.2
```

```
??MCMCglmm
```

The way that MCMC randomizes data is actually by simulating a new data "chain" using a probability of moving from one point to another. As the data is simulated, we might find that data points simulated one after the other are dependent on the previous point. This is important to know because one of the assumptions of a linear model is that data points are independent of each other. To account for this, we can discard every nth data point to maintain independence. We can adjust this with the "thin" argument.

It's also possible that when the chain starts, its first set of simulated data points are less random than as the simulation continues. We may then want to discard osbervations from the beginning of the chain. We can adjust this using the "burnin" argument.

One great thing about the MCMCMglmm package is that it has nifty built-in functions to run diagnostic tests to find the best parameters for the model. We can find the optimum burn-in period, sample size (total), and dependence factor (nth step without losing important info).

```
raftery.diag(morn_visits$sumvisits, q = 0.05)
```

```
##
## Quantile (q) = 0.05
## Accuracy (r) = +/- 0.005
## Probability (s) = 0.95
##
## You need a sample size of at least 7299 with these values of q, r and s
```

```
glmm.1 <- MCMCglmm(fixed = sumvisits~nightlows,
                   random = ~RFID+Date,
                   family = "poisson",
                   data = morn_visits,
                   nitt = 7400,
                   burnin = 100,
                   thin = 1)
```

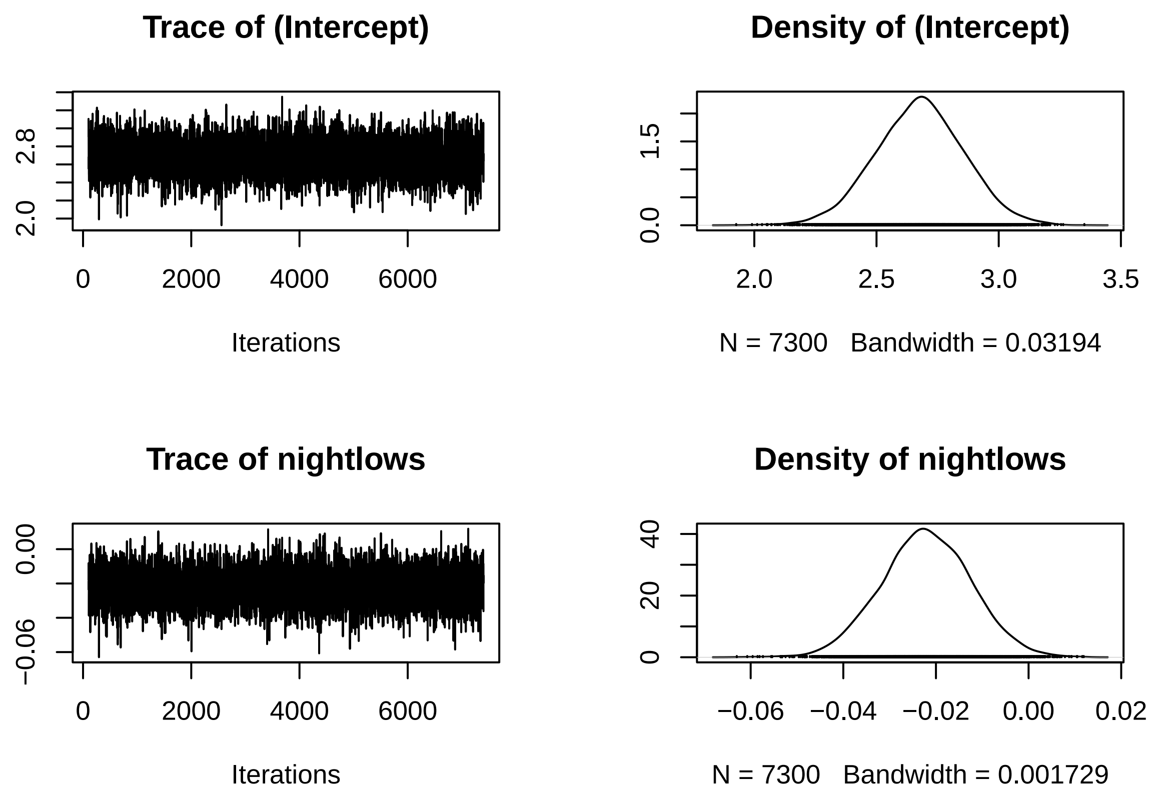
```
## Warning: Unknown or uninitialised column: `family`.
```

```
##
##                        MCMC iteration = 0
##
##  Acceptance ratio for liability set 1 = 0.000315
##
##                        MCMC iteration = 1000
##
##  Acceptance ratio for liability set 1 = 0.397322
##
##                        MCMC iteration = 2000
##
##  Acceptance ratio for liability set 1 = 0.400381
##
##                        MCMC iteration = 3000
##
##  Acceptance ratio for liability set 1 = 0.401224
##
##                        MCMC iteration = 4000
##
##  Acceptance ratio for liability set 1 = 0.400049
##
##                        MCMC iteration = 5000
##
##  Acceptance ratio for liability set 1 = 0.399919
```

```
##
##                          MCMC iteration = 6000
##
##   Acceptance ratio for liability set 1 = 0.399849
##
##                          MCMC iteration = 7000
##
##   Acceptance ratio for liability set 1 = 0.400805
```

Let's look at the residuals. Again, there should be no clear trends–the messier, the better.

```
plot(glmm.1$Sol)
```



These look pretty good.

We can also check overdispersed points to see if there is overlap; this estimates how much between-chain variance could be reduced if the chains were run longer.

```
autocorr(glmm.1$Sol)
```

```
## , , (Intercept)
##
##          (Intercept)     nightlows
## Lag 0    1.000000000  0.6843990990
## Lag 1    0.008967196  0.0114472219
## Lag 5    0.006243232 -0.0002864469
## Lag 10 -0.019514316 -0.0056234806
## Lag 50 -0.016862066 -0.0234951404
##
## , , nightlows
##
##          (Intercept)    nightlows
## Lag 0   0.6843990990  1.000000000
## Lag 1   0.0110591045  0.015821868
## Lag 5   0.0156491389  0.011861528
## Lag 10 -0.0083865158  0.008530944
## Lag 50  0.0005504137 -0.004213824
```

There is very low autocorrelation between points, so that is good.

We can also check model performance by running multiple chains and making sure they are all well mixed. We will use parallel processing to make this part go faster.

```
library(doParallel)
library(foreach)
## Initialize parallel backend
registerDoParallel(cores = 4)
## Use foreach to parallelize the loop
timestamp()
```

```
## ##------ Mon Jun 24 12:52:31 2024 ------##
```

```
set.seed(1)
glmm.mult <- foreach(i = 1:4, .packages = 'MCMCglmm') %dopar% {
    MCMCglmm(fixed = sumvisits~nightlows,
             random = ~RFID+Date,
             family = "poisson",
             data = morn_visits,
             nitt = 7300,
             burnin = 8)
}
timestamp()
```

```
## ##------ Mon Jun 24 12:52:37 2024 ------##
```

```
## Stop parallel backend-- DON'T FORGET TO DO THIS!
stopImplicitCluster()

glmm.mult.1 <- lapply(glmm.mult, function(m) m$Sol)
glmm.mult.1 <- do.call(mcmc.list, glmm.mult.1)
```

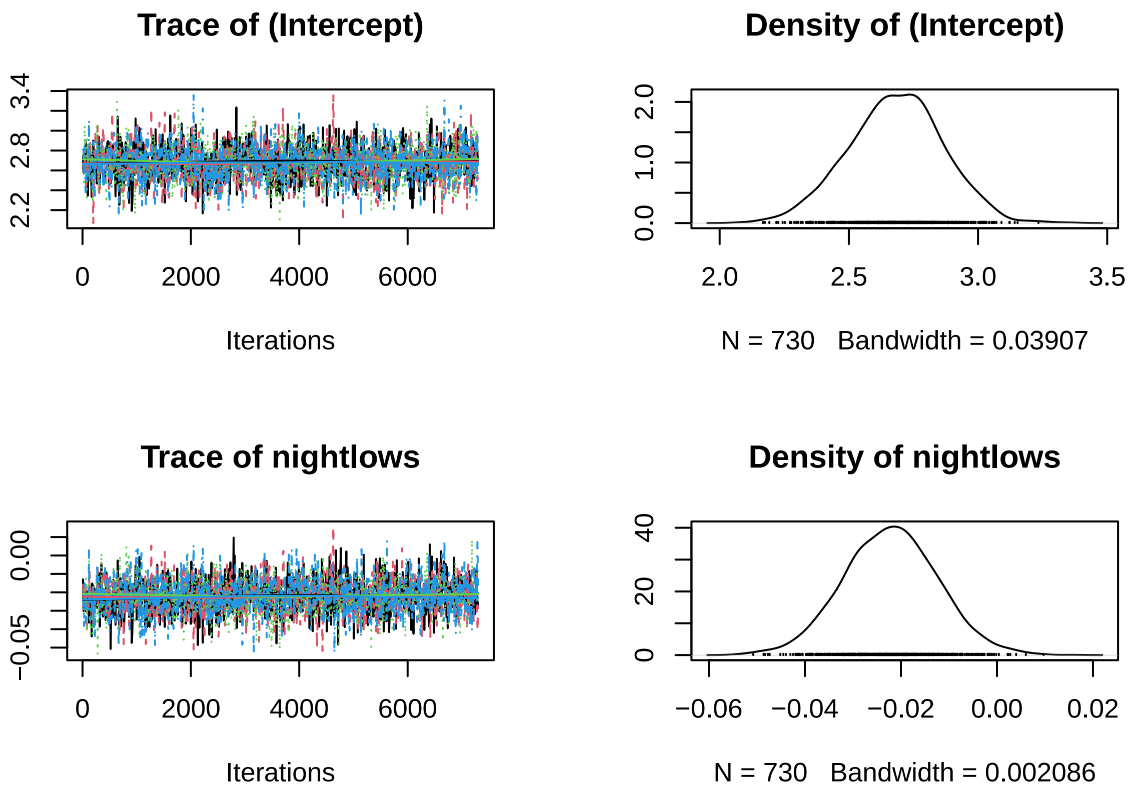
Potential scale reduction factors (PSRF) should be close to one, ideally < 1.2.

```
gelman.diag(glmm.mult.1)
```

```
## Potential scale reduction factors:
##
##             Point est. Upper C.I.
## (Intercept)          1          1
## nightlows            1          1
##
## Multivariate psrf
##
## 1
```

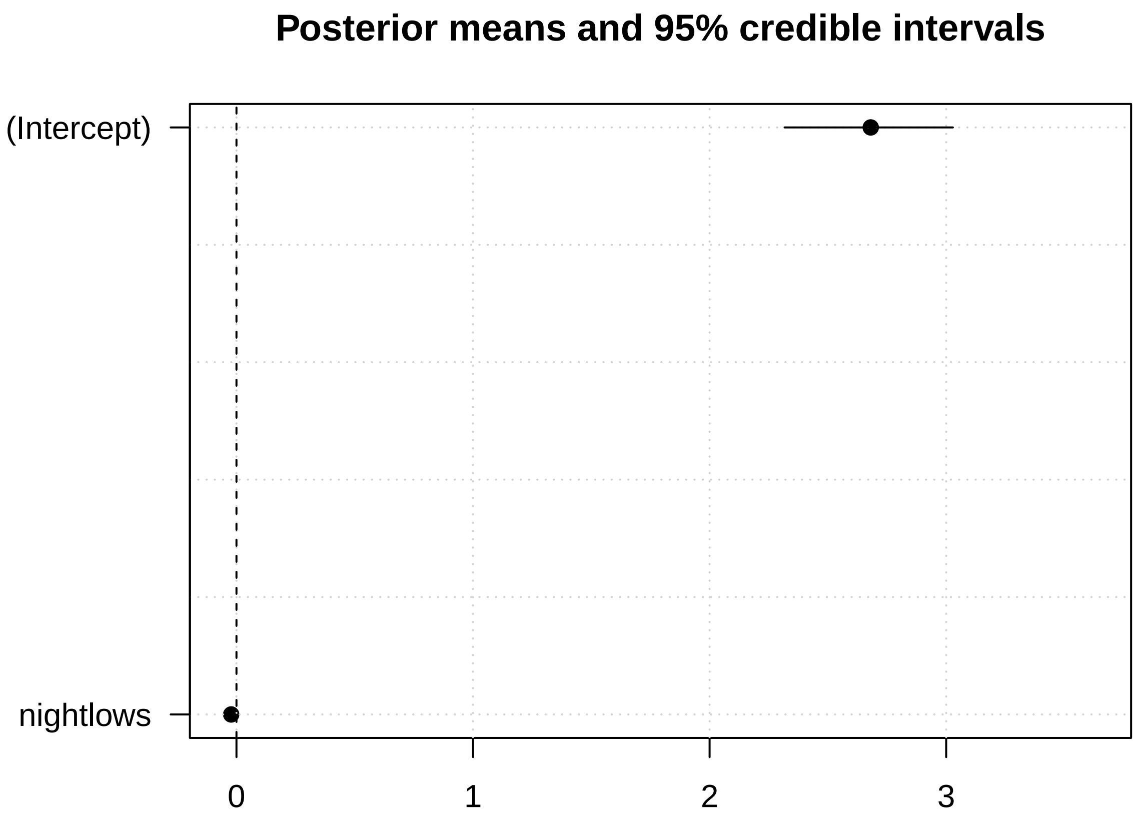
PSRF value is good, now let's look at the chains to make sure they are well mixed. For this plot, no line color should stand out in its own pattern, it should still be super messy, this means the chains all converged on similar answers and that the model fit is good.

```
plot(glmm.mult.1)
```



These look well mixed, so we can be confident that we have a good model fit. MCMC also gives us confidence intervals, so we can also assess the accuracy of our model parameters. We can also use confidence intervals for simple hypothesis testing; i.e., if the parameters overlap with zero, we absolutely cannot reject the null hypothesis, but if not and p-values fall below 0.05, we can reject with relative confidence. FYI the following plot code was adapted from a MCMCglmm tutorial (link at the bottom of the page).

```
  x <- summary(glmm.mult.1)
  n <- dim(x$statistics)[1]
  par(mar=c(2, 7, 4, 1))
  plot(x$statistics[,1], n:1,
       yaxt="n", ylab="",
       xlim=range(x$quantiles)*1.2,
       pch=19,
       main="Posterior means and 95% credible intervals")
  grid()
  axis(2, at=n:1, rownames(x$statistics), las=2)
  arrows(x$quantiles[,1], n:1, x$quantiles[,5], n:1, code=0)
  abline(v=0, lty=2)
```



The basic procedure I described was adopted from ECOLOGICAL MODELS AND DATA IN R: 7.3 - MARKOV CHAIN MONTE CARLO (PAGE 233). There are many more details there. I also used a custom function from an intro to MCMCglmm resource, which follows this same procedure and adds some more details. You should peruse to find more examples and more detailed explanation: https://github.com/tmalsburg/MCMCglmm-intro. And one more resource: http://cran.nexr.com/web/packages/MCMCglmm/vignettes/CourseNotes.pdf

Another great resource for understanding these types of Bayesian models is Richard McElreath's Statistical Rethinking course: https://github.com/rmcelreath/stat_rethinking_2023.