Markov Chain Monte Carlo and Stan

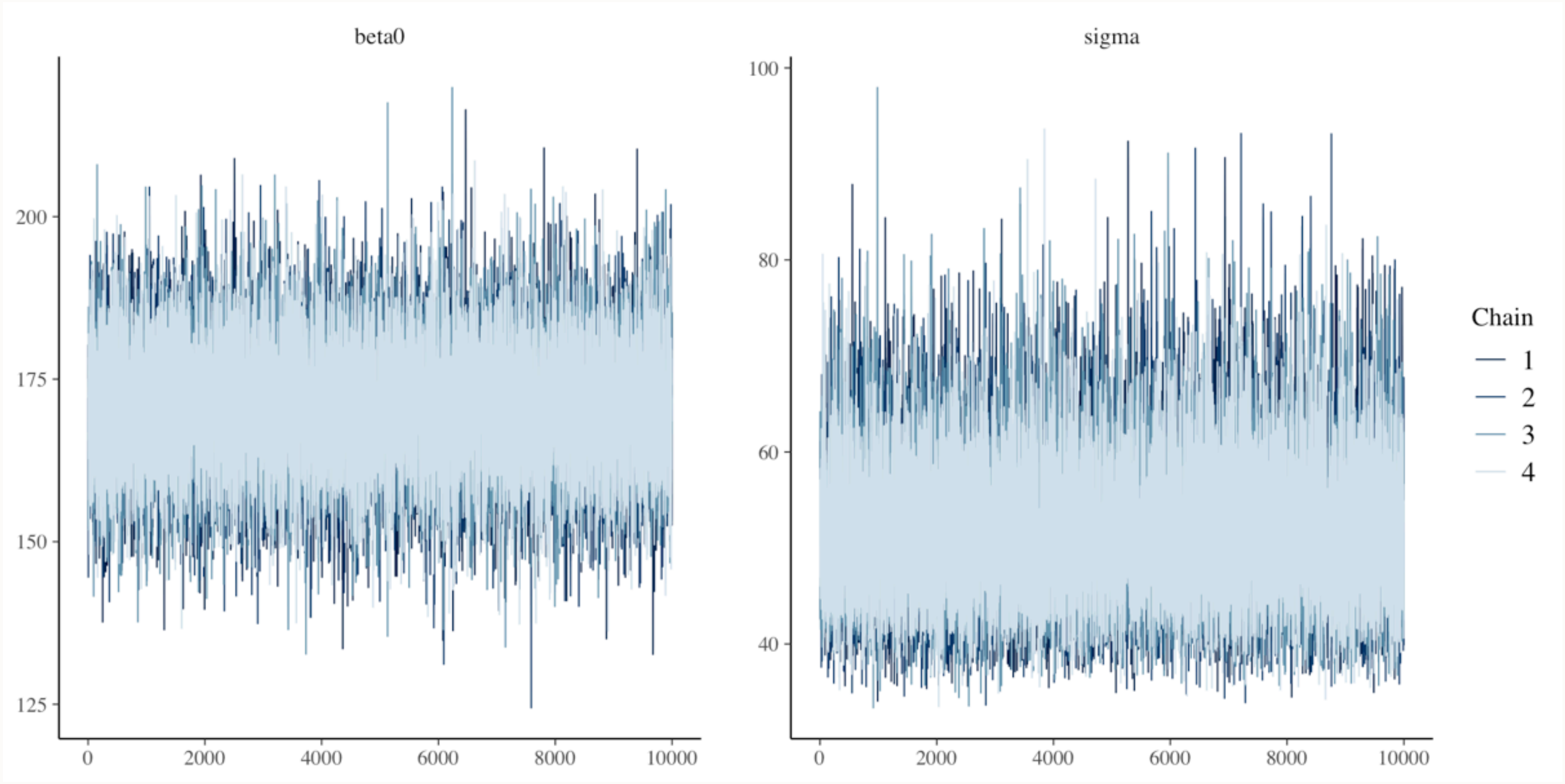
Lecture 3

https://jonathantemplin.com/bayesian-psychometric-modeling-fall-2024/

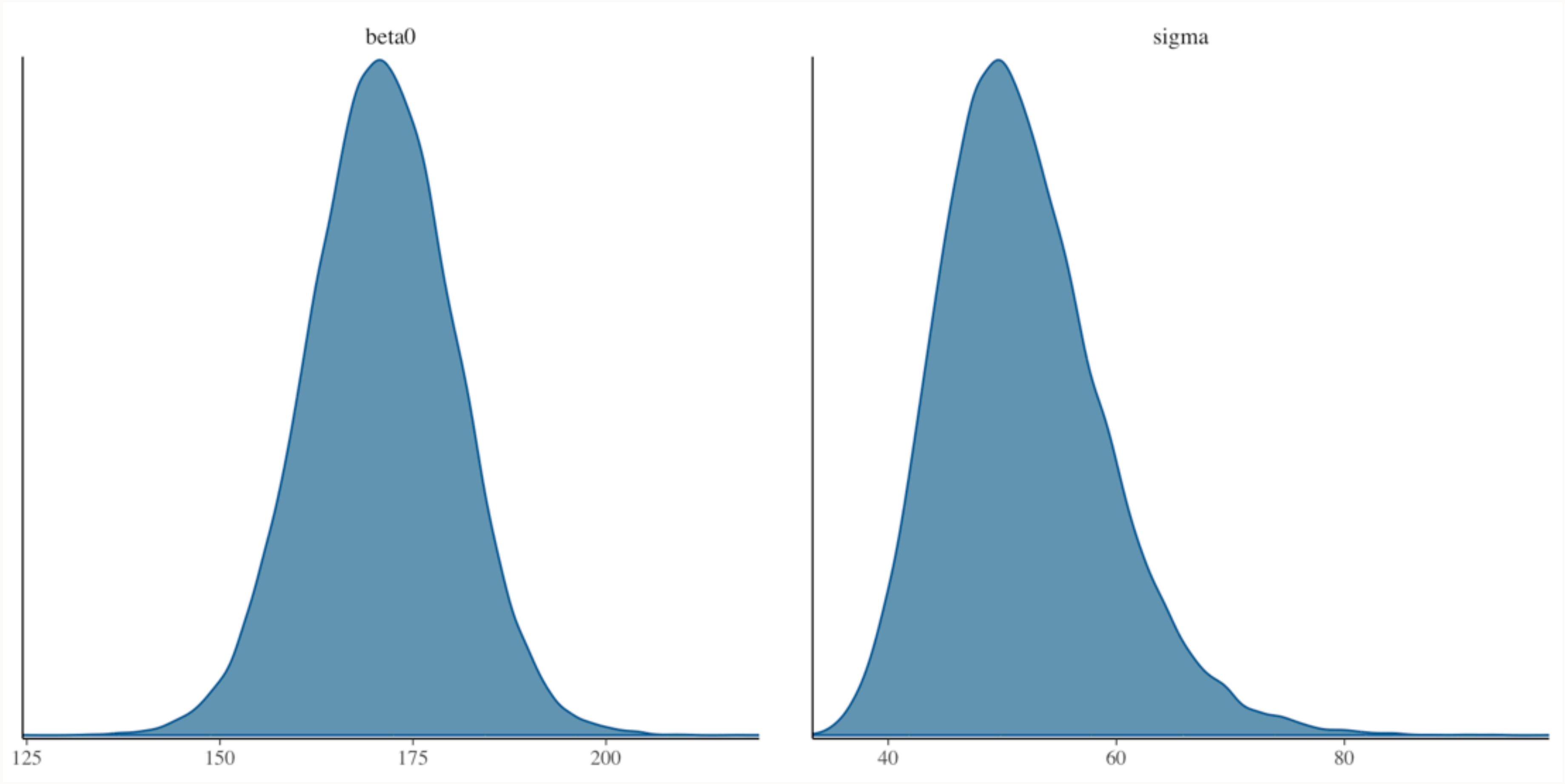
Today's Lecture Objectives

1. An Introduction to MCMC
2. An Introduction to Stan
3. Both with Linear Models

The Markov Chain Timeseries



The Posterior Distribution



Markov Chain Monte Carlo Estimation

Bayesian analysis is all about estimating the posterior distribution

- Up until now, we have worked with posterior distributions that fairly well-known
    - Beta-Binomial had a Beta distribution
    - In general, likelihood distributions from the exponential family have conjugate priors
        - Conjugate prior: the family of the prior is equivalent to the family of the posterior
- Most of the time, however, posterior distributions are not easily obtainable
    - No longer able to use properties of the distribution to estimate parameters

Markov Chain Monte Carlo Estimation

- It is possible to use an optimization algorithm (e.g., Newton-Raphson or Expectation-Maximization) to find maximum value of posterior distribution
  - But, such algorithms may take a very long time for high-dimensional problems
- Variational Bayesian methods also attempt to approximate the center of the posterior distribution (and are faster than optimization algorithms for large models)
- Instead: MCMC "sketches" the posterior by sampling from it – then use that sketch to make inferences
  - Sampling is done via MCMC

Markov Chain Monte Carlo Estimation

- MCMC algorithms iteratively sample from the posterior distribution
  - For fairly simplistic models, each iteration has independent samples
  - Most models have some layers of dependency included
    - Can slow down sampling from the posterior
- There are numerous variations of MCMC algorithms
  - Most of these specific algorithms use one of two types of sampling:
    1. Direct sampling from the posterior distribution (i.e. Gibbs sampling)
       - Often used when conjugate priors are specified
    2. Indirect (rejection-based) sampling from the posterior distribution (e.g., Metropolis-Hastings, Hamiltonian Monte Carlo)

MCMC Algorithms

- Efficiency is the main reason for so many algorithms
    - Efficiency in this context: How quickly the algorithm converges and provides adequate coverage (“sketching”) of the posterior distribution
    - No one algorithm is uniformly most efficient for all models (here model = likelihood prior)
- The good news is that many software packages (stan, JAGS, MPlus, especially) don’t make you choose which specific algorithm to use
- The bad news is that sometimes your model may take a large amount of time to reach convergence (think days or weeks)
- You can also code your own custom algorithm to make things run smoother

Commonalities Across MCMC Algorithms

- Despite having fairly broad differences regarding how algorithms sample from the posterior distribution, there are quite a few things that are similar across algorithms:
  1. A period of the Markov chain where sampling is not directly from the posterior
     - The burnin period (sometimes coupled with other tuning periods and called warmup)
  2. Methods used to assess convergence of the chain to the posterior distribution
     - Often involving the need to use multiple chains with independent and differing starting values
  3. Summaries of the posterior distribution

Commonalities Across MCMC Algorithms

- Further, rejection-based sampling algorithms often need a tuning period to make the sampling more efficient
  - The tuning period comes before the algorithm begins its burnin period

MCMC Demonstration

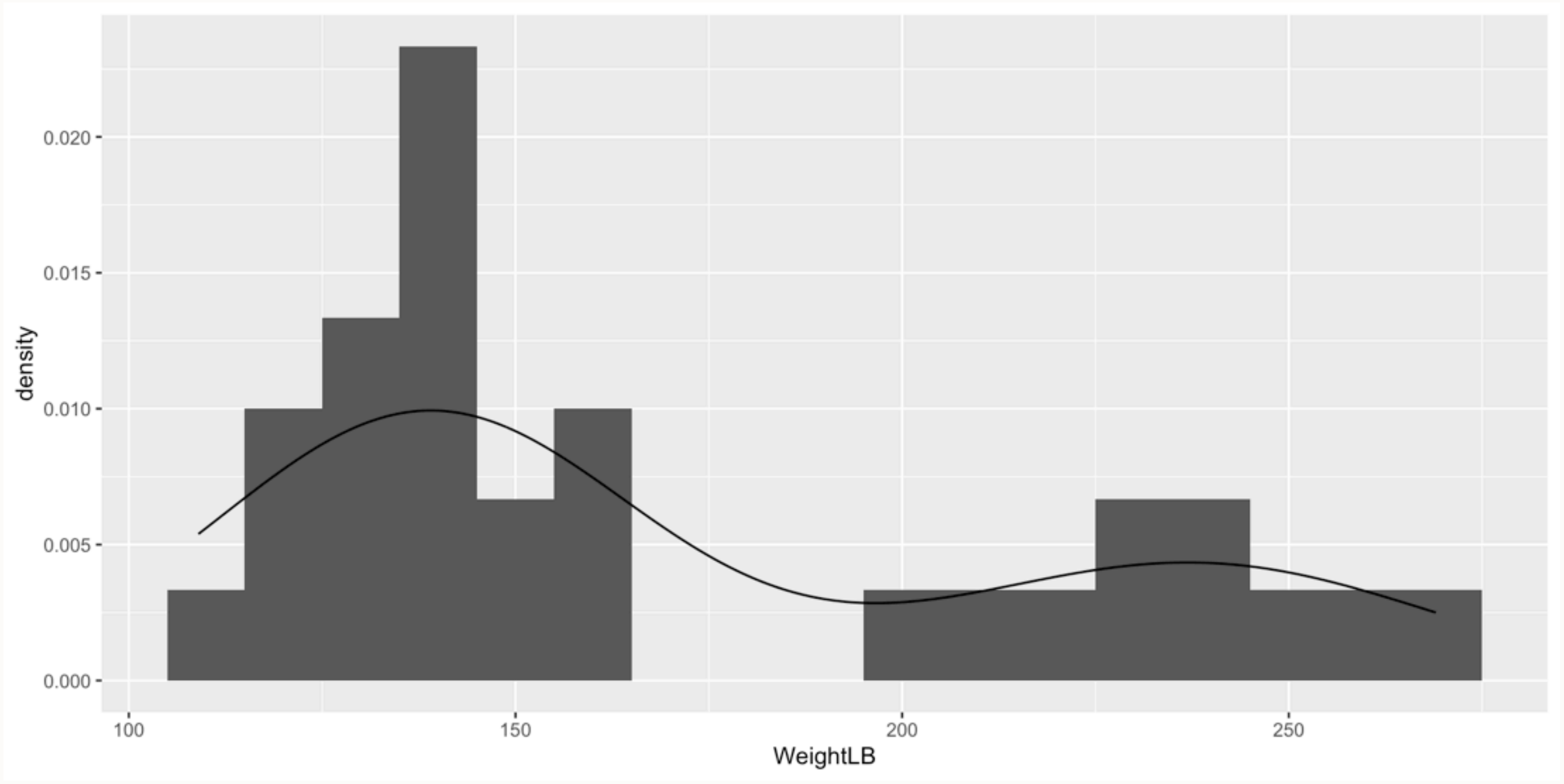
- To demonstrate each type of algorithm, we will use a model for a normal distribution
  - We will investigate each, briefly
  - We will then switch over to stan to show the syntax and let stan work
  - We will conclude by talking about assessing convergence and how to report parameter estimates.

Example Data: Post-Diet Weights

Example Data Link

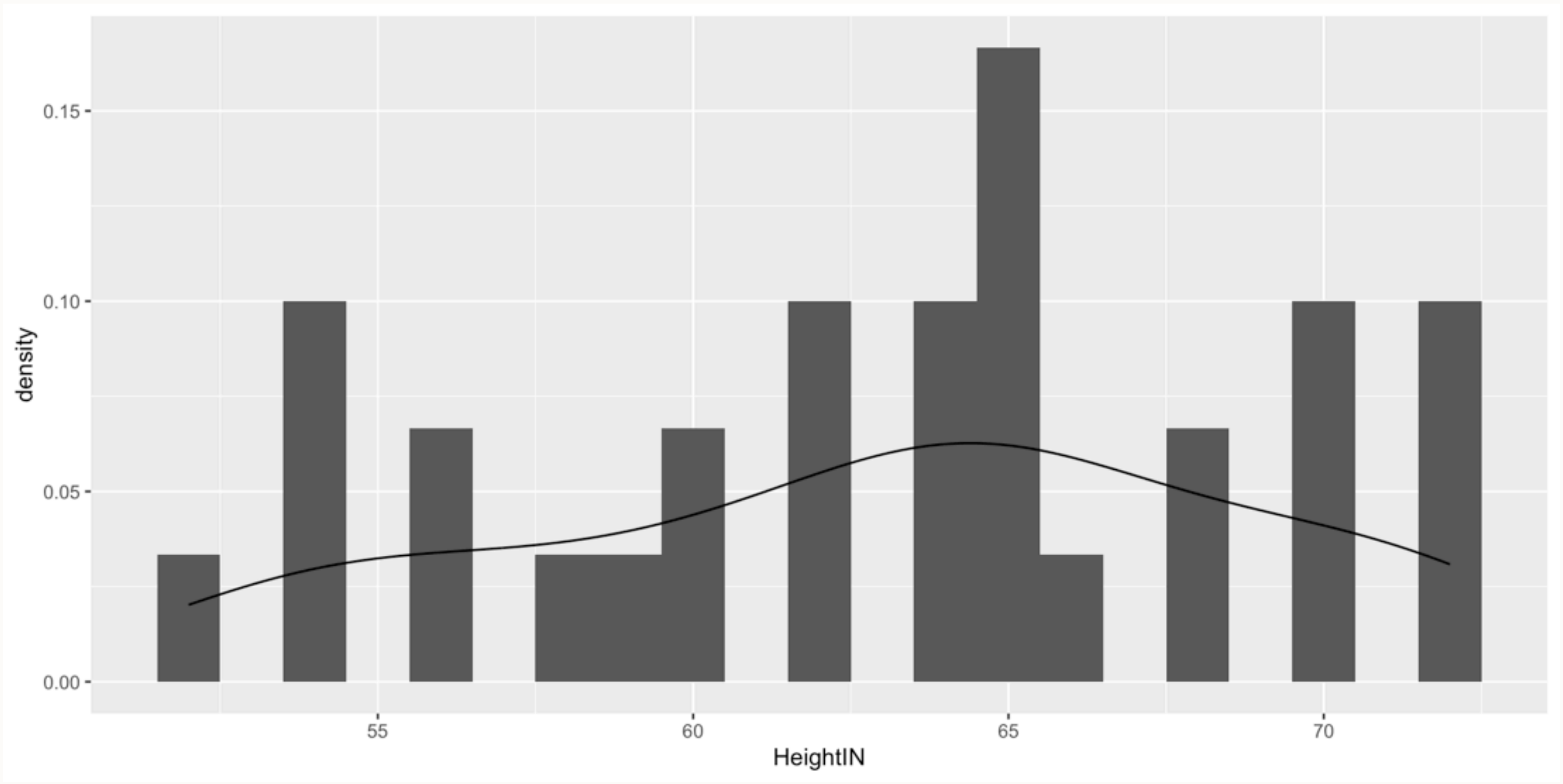
Visualizing Data: WeightLB Variable

```r
DietData = read.csv(file = "DietData.csv")

ggplot(data = DietData, aes(x = WeightLB)) +
  geom_histogram(aes(y = ..density..), position = "identity", binwidth = 10) +
  geom_density(alpha=.2)
```



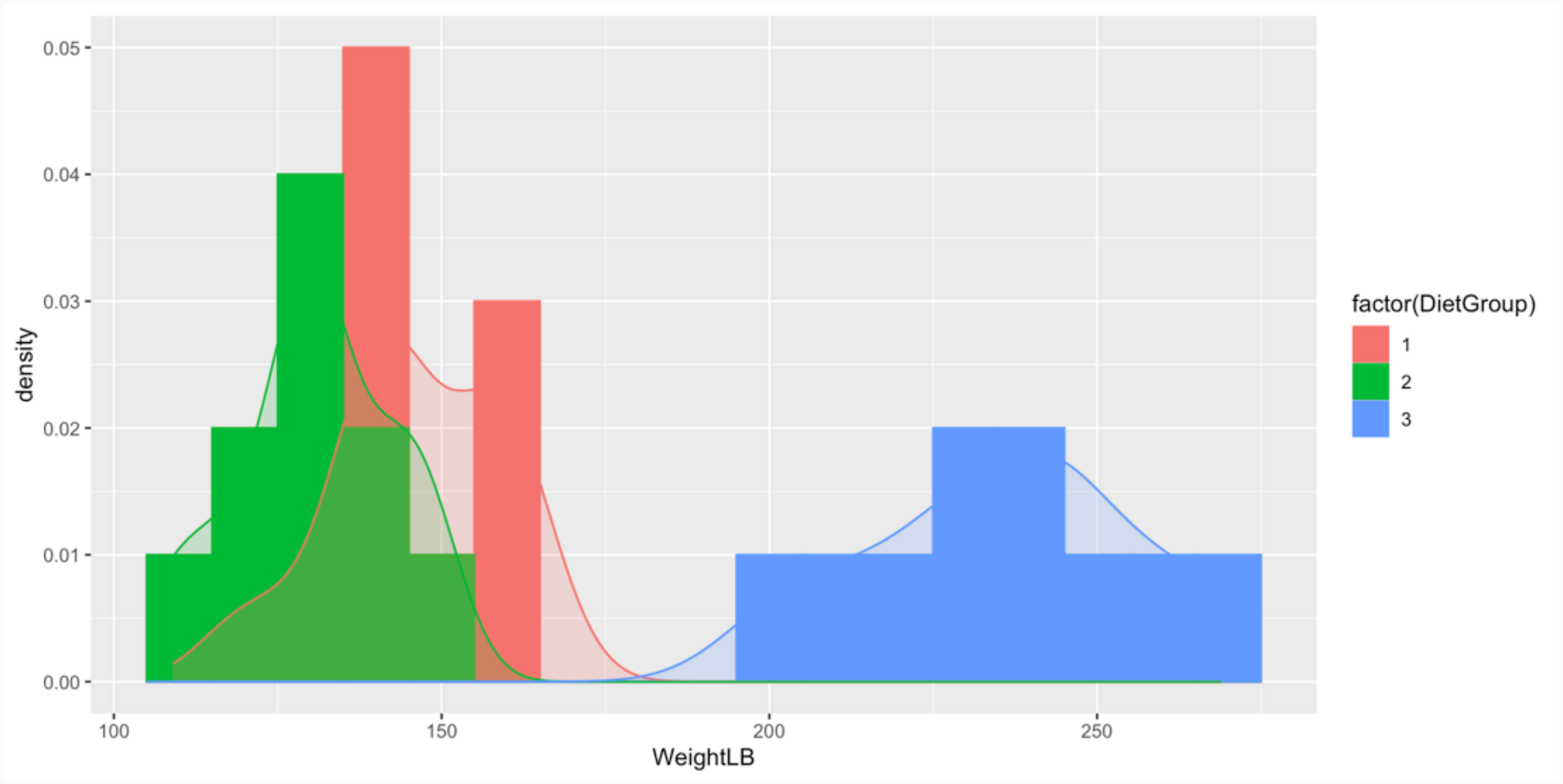
Visualizing Data: HeightIN Variable

```r
ggplot(data = DietData, aes(x = HeightIN)) +
  geom_histogram(aes(y = ..density..), position = "identity", binwidth = 1) +
  geom_density(alpha=.2)
```



Visualizing Data: WeightLB by Group

```r
ggplot(data = DietData, aes(x = WeightLB, color = factor(DietGroup), fill = factor(DietGroup))) +
  geom_histogram(aes(y = ..density..), position = "identity", binwidth = 10) +
  geom_density(alpha=.2)
```



Visualizing Data: Weight by Height by Group

```r
ggplot(data = DietData, aes(x = HeightIN, y = WeightLB, shape = factor(DietGroup), color = factor(Die
  geom_smooth(method = "lm", se = FALSE) + geom_point()
```

Class Discussion: What Do We Do?

Now, your turn to answer questions:

1. What type of analysis seems most appropriate for these data?
2. Is the dependent variable (`WeightLB`) is appropriate as-is for such analysis or does it need transformed?

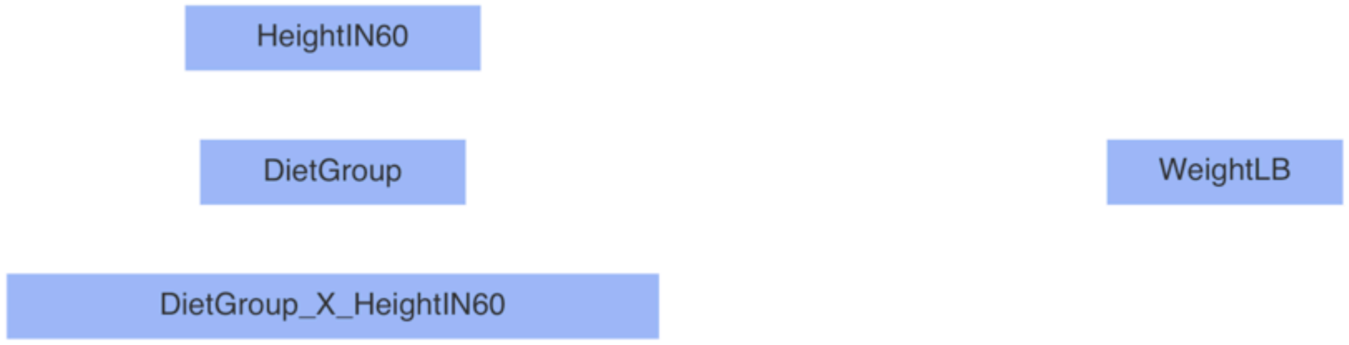
Linear Model with Least Squares

Let's play with models for data…

```r
# center predictors for reasonable numbers
DietData$HeightIN60 = DietData$HeightIN-60

# full analysis model suggested by data:
FullModel = lm(formula = WeightLB ~ 1, data = DietData)

# examining assumptions and leverage of fit
# plot(FullModel)

# looking at ANOVA table
# anova(FullModel)

# looking at parameter summary
 summary(FullModel)
```

```

Call:
lm(formula = WeightLB ~ 1, data = DietData)

Residuals:
   Min     1Q Median     3Q    Max 
-62.00 -36.75 -24.00  49.00  98.00 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  171.000      9.041   18.91   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 49.52 on 29 degrees of freedom
```

Path Diagram of Our Model



Steps in an MCMC Analysis

1. Specify model
2. Specify prior distributions for all model parameters
3. Build model syntax as needed
4. Run Markov chains (specify warmup/burnin and sampling period lengths)
5. Evaluate chain convergence
6. Interpret/report results

Specify Model

- To begin, let's start with an empty model and build up from there
- Let's examine the linear model we seek to estimate:

Where:

Questions:

- What are the *variables* in this analysis?
- What are the parameters in this analysis?

Introduction to Stan

- Stan is an MCMC estimation program
  - Most recent; has many convenient features
  - Actually does several methods of estimation (ML, Variational Bayes)
- You create a model using Stan's syntax
  - Stan translates your model to a custom-built C++ syntax
  - Stan then compiles your model into its own executable program
- You then run the program to estimate your model
  - If you use R, the interface can be seamless

Stan and RStudio

- Stan has its own syntax which can be built in stand-alone text files
  - Rstudio will let you create one of these files in the new file menu
  - Rstudio also has syntax highlighting in Stan files
    - This is very helpful to learn the syntax
- Stan syntax can also be built from R character strings
  - Which is helpful when running more than one model per analysis

Stan Syntax

```stan
data {
  int<lower=0> N;
  vector[N] y;
}

parameters {
  real beta0;
  real<lower=0> sigma;
}

model {
  beta0 ~ normal(0, 1000); // prior for beta0
  sigma ~ uniform(0, 100000); // prior for sigma
  y ~ normal(beta0, sigma); // model for observed data
}
```

- Above is the syntax for our model
  - Each line ends with a semi colon
  - Comments are put in with //

Stan Syntax: R Character Object

```
stanModel = "
data {
  int<lower=0> N;
  vector[N] y;
}

parameters {
  real beta0;
  real<lower=0> sigma;
}

model {
  beta0 ~ normal(0, 1000); // prior for beta0
  sigma ~ uniform(0, 100000); // prior for sigma
  y ~ normal(beta0, sigma); // model for observed data
}
"
```

- Three blocks of syntax needed
  - Data: What Stan expects you will send to it for the analysis (using R lists)
  - Parameters: Where you specify what the parameters of the model are
  - Model: Where you specify the distributions of the priors and data

Stan Data and Parameter Delcaration

Like many compiled languages, Stan expects you to declare what type of data/parameters you are defining:

- `int`: Integer values (no decimals)
- `real`: Floating point numbers
- `vector`: A one-dimensional set of real valued numbers

Sometimes, additional definitions are provided giving the range of the variable (or restricting the set of starting values):

- `real<lower=0> sigma;`

See: https://mc-stan.org/docs/reference-manual/data-types.html for more information

Stan Data and Prior Distributions

- In the model section, you define the distributions needed for the model and the priors
  - The left-hand side is either defined in data or parameters
    - `y ~ normal(beta0, sigma); // model for observed data`
    - `sigma ~ uniform(0, 100000); // prior for sigma`
  - The right-hand side is a distribution included in Stan
    - You can also define your own distributions

See: https://mc-stan.org/docs/functions-reference/index.html for more information

From Stan Syntax to Compilation

```r
# compile model -- this method is for stand-alone stan files (uses cmdstanr)
model00.fromFile = cmdstan_model(stan_file = "model00.stan")

# or this method using the string text in R
model00.fromString = cmdstan_model(stan_file = write_stan_file(stanModel))
```

- Once you have your syntax, next you need to have Stan translate it into C++ and compile an executable
- This is where `cmdstanr` and `rstan` differ
  - `cmdstanr` wants you to compile first, then run the Markov chain
  - `rstan` conducts compilation (if needed) then runs the Markov chain

Building Data for Stan

```r
# build R list containing data for Stan: Must be named what "data" are listed in analysis
stanData = list(
  N = nrow(DietData),
  y = DietData$WeightLB
)

# snippet of Stan syntax:
stanSyntaxSnippet = "
data {
  int<lower=0> N;
  vector[N] y;
}
"
```

- Stan needs the data you declared in your syntax to be able to run
- Within R, we can pass this data to Stan via a list object
- The entries in the list should correspond to the data portion of the Stan syntax
  - In the above syntax, we told Stan to expect a single integer named `N` and a vector named `y`
- The R list object is the same for `cmdstanr` and `rstan`

Running Markov Chains in `cmdstanr`

```r
# run MCMC chain (sample from posterior)
model00.samples = model00.fromFile$sample(
  data = stanData,
  seed = 1,
  chains = 4,
  parallel_chains = 4,
  iter_warmup = 10000,
  iter_sampling = 10000
)
```

Running Markov Chains in `rstan`

```r
rstan_options(auto_write = TRUE)
options(mc.cores = parallel::detectCores())

# example MCMC analysis in rstan
model00.rstan = stan(
  model_code = stanModel,
  model_name = "Empty model",
  data = stanData,
  warmup = 10000,
  iter = 20000,
  chains = 4,
  verbose = TRUE
)
```

- Rstan takes the model syntax directly, then compiles and runs the chains
- The first two lines of syntax enable running one chain per thread (parallel processing)
  - As chains are independent, running them simultaneously (parallel) shortens wait time considerably
- The `verbose` option is helpful for detecting when things break
- The same R list supplies the data to Stan

MCMC Process

- The MCMC algorithm runs as a series of discrete iterations
  - Within each iteration, each parameter of a model has an opportunity to change its value
- For each parameter, a new parameter is sampled at random from the current belief of posterior distribution
  - The specifics of the sampling process differ by algorithm type (we’ll have a lecture on this later)

MCMC Process

- In Stan (Hamiltonian Monte Carlo), for a given iteration, a proposed parameter is generated
  - The posterior likelihood "values" (more than just density; includes likelihood of proposal) are calculated for the current and proposed values of the parameter
  - The proposed values are accepted based on the draw of a uniform number compared to a transition probability
- If all models are specified correctly, then regardless of starting location, each chain will converge to the posterior if run long enough
  - But, the chains must be checked for convergence when the algorithm stops

Example of Bad Convergence

Examining Chain Convergence

- Once Stan stops, the next step is to determine if the chains converged to their posterior distribution
  - Called convergence diagnosis
- Many methods have been developed for diagnosing if Markov chains have converged
  - Two most common: visual inspection and Gelman-Rubin Potential Scale Reduction Factor (PSRF; quick reference)

Examining Chain Convergence

- Visual inspection
  - Want no trends in timeseries – should look like a caterpillar
  - Shape of posterior density should be mostly smooth
- Gelman-Rubin PSRF (denoted with)
  - For analyses with multiple chains
  - Ratio of between-chain variance to within-chain variance
  - Should be near 1 (maximum somewhere under 1.1)

Setting MCMC Options

- As convergence is assessed using multiple chains, more than one should be run
  - Between-chain variance estimates improve with the number of chains, so I typically use four
  - Others have two; more than one should work
- Warmup/burnin period should be long enough to ensure chains move to center of posterior distribution
  - Difficult to determine ahead of time
  - More complex models need more warmup/burnin to converge
- Sampling iterations should be long enough to thoroughly sample posterior distribution
  - Difficulty to determine ahead of time
  - Need smooth densities across bulk of posterior
- Often, multiple analyses (with different settings) is what is needed

The Markov Chain Timeseries

The Posterior Distribution

Assessing Our Chains

```
model00.samples$summary()
```

```
# A tibble: 3 × 10
  variable   mean median    sd   mad     q5    q95  rhat ess_bulk ess_tail
  <chr>     <dbl>  <dbl> <dbl> <dbl>  <dbl>  <dbl> <dbl>    <dbl>    <dbl>
1 lp__     -129.  -128.   1.02 0.735 -131.  -128.   1.00   17577.   22523.
2 beta0     171.   171.   9.44 9.31   155.   186.   1.00   29639.   25175.
3 sigma      51.8   51.0  7.20 6.84    41.5   64.8  1.00   29147.   24620.
```

- The summary function reports the PSRF (rhat)
- Here we look at our two parameters: and
- Both have , so both would be considered converged
- `lp__` is posterior log likelihood—does not necessarily need examined
- `ess_` columns show effect sample size for chain (factoring in autocorrelation between correlations)
  - More is better

Results Interpretation

- At long last, with a set of converged Markov chains, we can now interpret the results
  - Here, we disregard which chain samples came from and pool all sampled values to use for results
- We use summaries of posterior distributions when describing model parameters
  - Typical summary: the posterior mean
    - The mean of the sampled values in the chain
  - Called EAP (Expected a Posteriori) estimates
  - Less common: posterior median

Results Interpretation

- Important point:
  - Posterior means are different than what characterizes the ML estimates
    - Analogous to ML estimates would be the mode of the posterior distribution
  - Especially important if looking at non-symmetric posterior distributions
    - Look at posterior for variances

Results Interpretation

- To summarize the uncertainty in parameters, the posterior standard deviation is used
  - The standard deviation of the sampled values in the chain
  - This is the analogous to the standard error from ML
- Bayesian credible intervals are formed by taking quantiles of the posterior distribution
  - Analogous to confidence intervals
  - Interpretation slightly different – the probability the parameter lies within the interval
  - 95% credible interval notes that parameter is within interval with 95% confidence
- Additionally, highest density posterior intervals can be formed
  - The narrowest range for an interval (for unimodal posterior distributions)

Our Results

```
model00.samples$summary()
```

```
# A tibble: 3 × 10
  variable   mean median    sd   mad     q5    q95  rhat ess_bulk ess_tail
  <chr>     <dbl>  <dbl> <dbl> <dbl>  <dbl>  <dbl> <dbl>    <dbl>    <dbl>
1 lp__     -129.  -128.   1.02 0.735 -131.  -128.   1.00   17577.   22523.
2 beta0     171.   171.   9.44 9.31   155.   186.   1.00   29639.   25175.
3 sigma      51.8   51.0  7.20 6.84    41.5   64.8  1.00   29147.   24620.
```

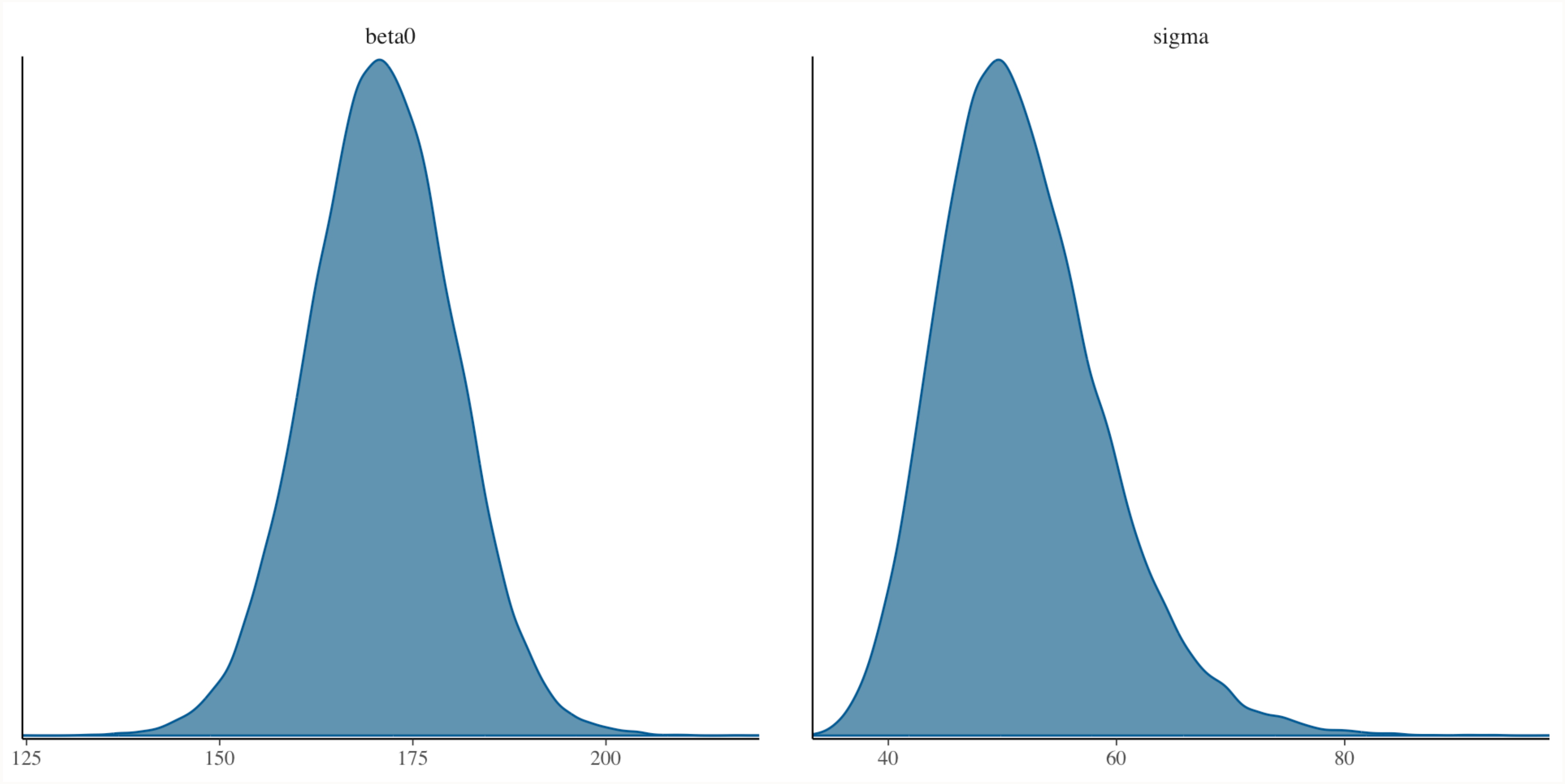
```
hdi(model00.samples$draws("beta0"), credMass = .9)
```

```
  lower   upper
155.015 185.762
attr(,"credMass")
[1] 0.9
```

```
hdi(model00.samples$draws("sigma"), credMass = .9)
```

```
  lower   upper
40.2305 63.0083
attr(,"credMass")
[1] 0.9
```

The Posterior Distribution



Wrapping Up

- This lecture covered the basics of MCMC estimation with Stan
- Next we will use an example to show a full analysis of the data problem we started with today
- The details today are the same for all MCMC analyses, regardless of which algorithm is used