## Module 9: Linear Regression

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Hoff, Chapter 9

#### Remainder of Semester

#### This week

- Thursday, November 5: Linear Regression
- ► Friday, November 6: Lab 10 (Homework 8)

#### Next week

- Tuesday, November 10: Linear and Logistic Regression
- ► Thursday, November 12: Logistic Regression + Final Exam
- Friday November 13, 5 PM EDT: Homework 8 (last homework + extra credit)

#### Reading period

▶ All OH will be held. Mine will be during class to avoid any conflicts and be more friendly to international students.

#### Final Exam

The final exam is **November 22, 2 PM - 5 PM EDT** (open note/open book)

- $\triangleright$  The material will be on modules 1-9.
- ▶ I will go over more details regarding the exam next week

## Agenda

- ► Motivation: oxygen uptake example
- Linear regression
- Multiple and Multivariate Linear Regression
- Bayesian Linear Regression
- Background on the Euclidean norm and argmin
- Ordinary Least Squares + Exercises
- Setting Prior Parameters
- ► The g-prior
- How does this all fit together

## Oxygen uptake case study

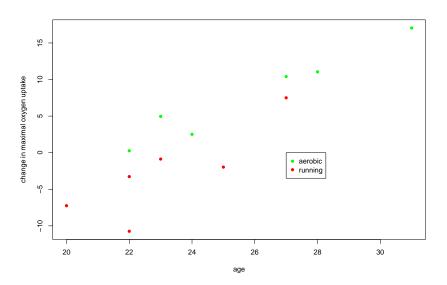
Experimental design: 12 male volunteers.

- 1.  $O_2$  uptake measured at the beginning of the study
- 2. 6 men take part in a randomized aerobics program
- 3. 6 remaining men participate in a running program
- 4.  $O_2$  uptake measured at end of study

What type of exercise is the most beneficial?

#### Data

# Exploratory Data Analysis



## Data analysis

```
y= change in oxygen uptake (scalar) x_1= exercise indicator (0 for running, 1 for aerobic) x_2= age How can we estimate p(y\mid x_1,x_2)?
```

## Linear regression

Assume that smoothness is a function of age.

For each group,

$$y = \beta_o + \beta_1 x_2 + \epsilon$$

Linearity means linear in the parameters ( $\beta$ 's).

### Linear regression

We could also try the model

$$y = \beta_0 + \beta_1 x_2 + \beta_2 x_2^2 + \beta_3 x_2^3 + \epsilon$$

which is also a linear regression model.

#### Notation

- $\triangleright$   $X_{n \times p}$ : regression features or covariates (design matrix)
- $\triangleright$   $x_i$ : *i*th row vector of the regression covariates
- $ightharpoonup y_{n \times 1}$ : response variable (vector)
- $\triangleright$   $\beta_{p\times 1}$ : vector of regression coefficients

## Notation (continued)

$$\mathbf{X}_{n \times p} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ x_{21} & x_{22} & \dots & x_{2p} \\ x_{i1} & x_{i2} & \dots & x_{ip} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix}.$$

- ► A column of x represents a particular covariate we might be interested in, such as age of a person.
- ▶ Denote  $x_i$  as the ith row vector of the  $X_{n \times p}$  matrix.

$$x_i = \begin{pmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{ip} \end{pmatrix}$$

# Notation (continued)

$$\boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{pmatrix}$$

$$\boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

$$\mathbf{y}_{n\times 1} = X_{n\times p}\beta_{p\times 1} + \epsilon_{n\times 1}$$

## Regression models

How does an outcome y vary as a function of the covariates which we represent as  $X_{n \times p}$  matrix?

- ► Can we predict y as a function of each row in the matrix  $X_{n \times p}$  denoted by  $x_i$ .
- $\triangleright$  Which  $x_i$ 's have an effect?

Such questions can be assessed via a linear regression model  $p(\mathbf{y} \mid X)$ .

## Multiple linear regression

Consider the following:

$$y_i = \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + \epsilon_i$$

where

$$x_{i1} = 1$$
 for subject  $i$  (1)  
 $x_{i2} = 0$  for running; 1 for aerobics (2)

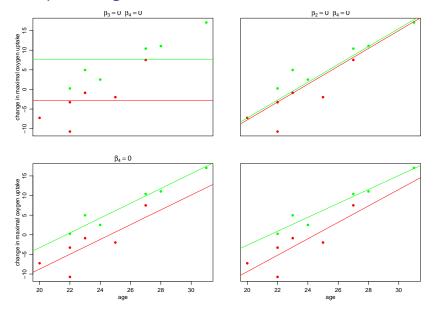
$$x_{i3} = \text{age of subject i}$$
 (3)

$$x_{i4} = x_{i2} \times x_{i3} \tag{4}$$

Under this model,

$$E[\textbf{\textit{y}} \mid \textbf{\textit{x}}] = \beta_1 + \beta_3 \times \textit{age} \text{ if } x_2 = 0$$
 
$$E[\textbf{\textit{y}} \mid \textbf{\textit{x}}] = (\beta_1 + \beta_2) + (\beta_3 + \beta_4) \times \textit{age} \text{ if } x_2 = 1$$

## Least squares regression lines



### Multivariate Setup

Let's assume that we have data points  $(x_i, y_i)$  available for all i = 1, ..., n.

 $\triangleright$  y is the response variable

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}_{n \times 1}$$

 $ightharpoonup x_i$  is the *i*th row of the design matrix  $X_{n \times p}$ .

Consider the regression coefficients

$$\beta = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{pmatrix}_{p \times 1}$$

## Normal Regression Model

The Normal regression model specifies that

- $\triangleright$   $E[Y \mid x_i]$  is linear and
- the sampling variability around the mean is independently and identically (iid) drawn from a normal distribution

$$Y_i = \boldsymbol{\beta}^T \boldsymbol{x}_i + \boldsymbol{\epsilon}_i \tag{5}$$

$$\epsilon_1, \dots, \epsilon_n \stackrel{iid}{\sim} \mathsf{Normal}(0, \sigma^2)$$
 (6)

This implies  $Y_i \mid \beta, \mathbf{x}_i \sim \text{Normal}(\beta^T \mathbf{x}_i, \sigma^2)$ .

## Multivariate Bayesian Normal Regression Model

We can re-write this as a multivariate regression model as:

$$\mathbf{y} \mid X, \beta, \sigma^2 \sim \mathsf{MVN}(X\beta, \sigma^2 I_p).$$

We can specify a multivariate Bayesian model as:

$$\mathbf{y} \mid X, \beta, \sigma^2 \sim \mathsf{MVN}(X\beta, \sigma^2 I_p)$$
  
 $\beta \sim \mathsf{MVN}(0, \tau^2 I_p),$ 

where  $\sigma^2, \tau^2$  are known.

## Bayesian Normal Regression Model

#### The likelihood is

$$p(y_1,\ldots,y_n\mid x_1,\ldots x_n,\beta,\sigma^2) \tag{7}$$

$$=\prod_{i=1}^{n} p(\mathbf{y}_{i} \mid \mathbf{x}_{i}, \boldsymbol{\beta}, \sigma^{2})$$
 (8)

$$(2\pi\sigma^2)^{-n/2} \exp\{\frac{-1}{2\sigma^2} \sum_{i=1}^{n} (\mathbf{y}_i - \boldsymbol{\beta}^T \mathbf{x}_i)^2\}$$
 (9)

$$= (2\pi\sigma^2)^{-n/2} \exp\{-\frac{1}{2}(\mathbf{y} - X\beta)^T (\sigma^2)^{-1} I_p(\mathbf{y} - X\beta)\}$$
 (10)

## Background

The Euclidean norm ( $L^2$  norm or square root of the sum of squares) of  $\mathbf{y} = (y_1, \dots, y_n)$  is defined by

$$\|\mathbf{y}\|_2 = \sqrt{y_1^2 + \ldots + y_n^2}.$$

It follows that

$$\|\mathbf{y}\|_2^2 = y_1^2 + \ldots + y_n^2.$$

Why do we use this notation? It's compact and convenient!

## Background

We would like to find

$$\underset{\boldsymbol{\beta} \in \mathbb{R}^p}{\operatorname{arg min}} \| \boldsymbol{y} - \boldsymbol{X} \boldsymbol{\beta} \|_2^2,$$

where the arg min (the arguments of the minima) are the points or elements of the domains of some function as which the functions values are minimized.

## **Ordinary Least Squares**

We can estimate the coefficients  $\hat{oldsymbol{eta}} \in \mathbb{R}^p$  by least squares:

$$\hat{oldsymbol{eta}} = rg \min_{oldsymbol{eta} \in \mathbb{R}^p} \|oldsymbol{y} - Xoldsymbol{eta}\|_2^2$$

One can show that

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y}$$

The fitted values are

$$\hat{\mathbf{y}} = X\hat{\boldsymbol{\beta}} = X(X^TX)^{-1}X^T\mathbf{y}$$

This is a linear function of  $\mathbf{y}$ ,  $\hat{\mathbf{y}} = H\mathbf{y}$ , where  $H = X(X^TX)^{-1}X^T$  is sometimes called the **hat matrix**.

## Exercise 1 (OLS)

Let SSR denote sum of squared residuals.

$$\min_{\beta} SSR(\beta) = \min_{\beta} \|\boldsymbol{y} - X\beta\|_2^2$$

Show that

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y}.$$

## Ordinary Least squares estimation

Proof: Observe

$$\frac{\partial SSR(\beta)}{\partial \beta} := \frac{\partial \|\mathbf{y} - X\beta\|_2^2}{\partial \beta} \tag{11}$$

$$=\frac{\partial(\mathbf{y}-X\boldsymbol{\beta})^{T}(\mathbf{y}-X\boldsymbol{\beta})}{\partial\boldsymbol{\beta}}$$
(12)

$$= \frac{\partial \mathbf{y}^{\mathsf{T}} \mathbf{y} - 2\beta^{\mathsf{T}} X^{\mathsf{T}} \mathbf{y} + \hat{\beta}^{\mathsf{T}} (X^{\mathsf{T}} X) \beta}{\partial \beta}$$
(13)

$$= -2X^{\mathsf{T}}\mathbf{y} + 2X^{\mathsf{T}}X\boldsymbol{\beta} \tag{14}$$

This implies 
$$-X^T \mathbf{y} + X^T X \beta = 0 \implies \hat{\beta}_{ols} = (X^T X)^{-1} X^T \mathbf{y}$$
.

This is called the **ordinary least squares estimator**. How do we know it is unique?

# Exercise 2 (OLS)

Show that

$$\hat{\boldsymbol{\beta}} \sim MVN(\boldsymbol{\beta}, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}).$$

## Ordinary Least squares estimation

Proof: Recall

$$\hat{\beta} = (X^T X)^{-1} X^T Y.$$

$$E(\hat{\beta}) = E[(X^T X)^{-1} X^T Y] = (X^T X)^{-1} X^T E[Y] = (X^T X)^{-1} X^T X \beta.$$

$$Var(\hat{\beta}) = Var\{(X^{T}X)^{-1}X^{T}Y\}$$

$$= (X^{T}X)^{-1}X^{T}\sigma^{2}I_{n}X(X^{T}X)^{-1}$$

$$= \sigma^{2}(X^{T}X)^{-1}$$
(15)
$$= (15)$$

$$= (15)$$

$$= (15)$$

$$\hat{\boldsymbol{\beta}} \sim MVN(\boldsymbol{\beta}, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}).$$

### Recall data set up

### Recall data set up

```
(x3 < - x2) \#age
##
    [1] 23 22 22 25 27 20 31 23 27 28 22 24
(x2 <- x1) #aerobic versus running
##
    [1] 0 0 0 0 0 0 1 1 1 1 1 1
(x1<- seq(1:length(x2))) #index of person
## [1] 1 2 3 4 5 6 7 8 9 10 11 12
(x4 < - x2*x3)
##
    [1]
        0 0 0 0 0 0 31 23 27 28 22 24
```

## Recall data set up

```
(X \leftarrow cbind(x1, x2, x3, x4))
##
        x1 x2 x3 x4
##
    [1,] 1 0 23 0
    [2,] 2 0 22 0
##
    [3,] 3 0 22 0
##
    [4,] 4
           0 25 0
##
    [5,] 5 0 27 0
##
##
    [6,] 6 0 20 0
##
    [7,] 7 1 31 31
##
    [8,] 8 1 23 23
##
    [9,] 9 1 27 27
  [10,] 10 1 28 28
##
##
  [11,] 11 1 22 22
## [12,] 12 1 24 24
```

### OLS estimation in R

```
## using the lm function
fit.ols<-lm(y~ X[,2] + X[,3] +X[,4])
summary(fit.ols)$coef

## Estimate Std. Error t value Pr(>|t|)
## (Intercept) -51.2939459 12.2522126 -4.1865047 0.003052321
## X[, 2] 13.1070904 15.7619762 0.8315639 0.429775106
## X[, 3] 2.0947027 0.5263585 3.9796120 0.004063901
```

## X[, 4] -0.3182438 0.6498086 -0.4897500 0.637457484

# Exercise 3 (Multivariate inference for regression models)

Let

$$\mathbf{y} \mid \boldsymbol{\beta} \sim \mathsf{MVN}(\boldsymbol{X}\boldsymbol{\beta}, \sigma^2 \boldsymbol{I}) \tag{18}$$
$$\boldsymbol{\beta} \sim \mathsf{MVN}(\boldsymbol{\beta}_0, \boldsymbol{\Sigma}_0) \tag{19}$$

Show that the posterior is

$$\beta \mid \mathbf{y}, X \sim \mathsf{MVN}(\beta_n, \Sigma_n)$$
, where

$$\beta_n = E[\beta \mid \mathbf{y}, \mathbf{X}, \sigma^2] = (\Sigma_o^{-1} + (nX^TX)/\sigma^2)^{-1}(\Sigma_o^{-1}\beta_0 + \mathbf{X}^T\mathbf{y}/\sigma^2)$$
  
$$\Sigma_n = \text{Var}[\beta \mid \mathbf{y}, X, \sigma^2] = (\Sigma_o^{-1} + (nX^TX)/\sigma^2)^{-1}$$

Remark: If 
$$\Sigma_o^{-1} << (X^TX)^{-1}$$
 then  $\beta_n \approx \hat{\beta}_{ols}$  If  $\Sigma_o^{-1} >> (X^TX)^{-1}$  then  $\beta_n \approx \beta_0$ 

## Multivariate inference for regression models

The posterior from Exercise 3 can be shown to be

$$\beta \mid \mathbf{y}, X \sim \mathsf{MVN}(\beta_n, \Sigma_n)$$

where

$$\beta_n = E[\beta \mid \mathbf{y}, \mathbf{X}, \sigma^2] = (\Sigma_o^{-1} + (X^T X)/\sigma^2)^{-1}(\Sigma_o^{-1}\beta_0 + X^T \mathbf{y}/\sigma^2)$$

$$\Sigma_n = \text{Var}[\beta \mid \boldsymbol{y}, \boldsymbol{X}, \sigma^2] = (\Sigma_o^{-1} + (X^T X)/\sigma^2)^{-1}$$

## Setting prior parameters

How would you set the prior parameters for

- $ightharpoonup \sigma^2$
- $\triangleright \Sigma_o$
- ▶ β<sub>0</sub>

## Setting prior parameters

- Estimate  $\sigma^2$  by  $\frac{y^Ty \hat{\beta}_{ols}^TX^Ty}{n (p+1)}$  because this is an unbiased estimator of  $\sigma^2$ .
- Set

$$\Sigma_o^{-1} = \frac{(X^T X)}{n\sigma^2},$$

which is known as the unit information prior (Kass and Wasserman, 1995).

▶ Set  $\beta_0 = \hat{\beta}_{ols}$ . (This centers the prior distribution of  $\beta$  around the OLS estimate).

### Why are these reasonable choices?

### Setting prior parameters

- ▶ Do you think that the posterior would be sensitive to the choice of these parameters?
- ▶ How could you improve upon our choices regarding priors on  $\beta_0$  and  $\Sigma_0$ ?

### The g-prior

To improve things by doing the **least amount of calculus**, we can put a *g-prior* on  $\beta$  (not  $\beta_0$ ).

The g-prior on  $\beta$  has the following form:

$$\beta \mid \mathbf{X}, \sigma^2 \sim MVN(0, g \ \sigma^2(\mathbf{X}^T \mathbf{X})^{-1}),$$

where g is a constant, such as g = n.

It can be shown that (Zellner, 1986):

- g shrinks the coefficients and can prevent overfitting to the data
- 2. if g=n, then as n increases, inference approximates that using  $\hat{\beta}_{ols}$

## The g-prior

Under the g-prior, it follows that

$$\beta_n = E[\beta \mid \mathbf{y}, \mathbf{X}, \sigma^2]$$

$$= \left(\frac{X^T X}{g \sigma^2} + \frac{X^T X}{\sigma^2}\right)^{-1} \frac{X^T y}{\sigma^2}$$
(20)

$$= \frac{g}{g+1} (X^T X)^{-1} X^T y = \frac{g}{g+1} \hat{\beta}_{ols}$$
 (22)

$$\Sigma_n = \text{Var}[\beta \mid \mathbf{y}, \mathbf{X}, \sigma^2]$$

$$= \left(\frac{X^T X}{g \sigma^2} + \frac{X^T X}{\sigma^2}\right)^{-1} = \frac{g}{g+1} \sigma^2 (X^T X)^{-1}$$
(24)

$$\left(\begin{array}{ccc} g\sigma^2 & \sigma^2 \end{array}\right) & g+1 \\
= \frac{g}{g+1} \operatorname{Var}[\hat{\beta}_{ols}] \tag{25}$$

## Prior on $\Sigma_0$

What prior would you place on  $\Sigma_0$  and why?

## Next steps

- ► How do all these concepts fit together? How can you build a hierarhical model using linear regression and the tools that you've learned?
- I recommend doing the derivations from this module on your own.
- ▶ I recommend reading through Hoff to solidify you knowledge. This material is around page 153, but chapter 9 is helpful regarding being complementary to this material.
- ➤ You could also code this up to further solidify you knowledge of this, but you'll get practice on this with lab 10 and homework 8.

## Linear Regression Applied to Swimming (Lab 10)

- ► We will consider Exercise 9.1 in Hoff very closely to illustrate linear regression.
- The data set we consider contains times (in seconds) of four high school swimmers swimming 50 yards.
- ▶ There are 6 times for each student, taken every two weeks.
- ► Each row corresponds to a swimmer and a higher column index indicates a later date.
- ► This corresponds with Lab 10 and Homework 8 (the last homework)!

#### Data set

```
read.table("data/swim.dat",header=FALSE)

## Warning in read.table("data/swim.dat", header = FALSE):
## found by readTableHeader on 'data/swim.dat'

## V1 V2 V3 V4 V5 V6

## 1 23.1 23.2 22.9 22.9 22.8 22.7

## 2 23.2 23.1 23.4 23.5 23.5 23.4

## 3 22.7 22.6 22.8 22.8 22.9 22.8

## 4 23.7 23.6 23.7 23.5 23.5 23.4
```

# Full conditionals (Task 1)

We will fit a separate linear regression model for each swimmer, with swimming time as the response and week as the explanatory variable. Let  $y_i \in \mathbb{R}^6$  be the 6 recorded times for swimmer i. Let

$$X_i = \begin{bmatrix} 1 & 1 \\ 1 & 3 \\ \dots & \\ 1 & 9 \\ 1 & 11 \end{bmatrix}$$

be the design matrix for swimmer *i*. Then we use the following linear regression model:

$$\begin{aligned} Y_i &\sim \mathcal{N}_6 \left( X_i \beta_i, \tau_i^{-1} \mathcal{I}_6 \right) \\ \beta_i &\sim \mathcal{N}_2 \left( \beta_0, \Sigma_0 \right) \\ \tau_i &\sim \mathsf{Gamma}(a, b). \end{aligned}$$

Derive full conditionals for  $\beta_i$  and  $\tau_i$ .

# Solution (Task 1)

The conditional posterior for  $\beta_i$  is multivariate normal with

$$V[\beta_{i} | Y_{i}, X_{i}, \frac{\tau_{i}}{\tau_{i}}] = (\Sigma_{0}^{-1} + \frac{\tau_{i}}{\tau_{i}} X_{i}^{T} X_{i})^{-1}$$

$$\mathbb{E}[\beta_{i} | Y_{i}, X_{i}, \frac{\tau_{i}}{\tau_{i}}] = (\Sigma_{0}^{-1} + \frac{\tau_{i}}{\tau_{i}} X_{i}^{T} X_{i})^{-1} (\Sigma_{0}^{-1} \beta_{0} + \frac{\tau_{i}}{\tau_{i}} X_{i}^{T} Y_{i}).$$

while

$$au_i \mid Y_i, X_i, eta \sim \mathsf{Gamma}\left(a+3\,,\ b+rac{(Y_i-X_ieta_i)^T(Y_i-X_ieta_i)}{2}
ight).$$

These can be found in in Hoff in section 9.2.1.

I highly recommend that you derive these as practice for the final exam.

### Task 2

Complete the prior specification by choosing  $a, b, \beta_0$ , and  $\Sigma_0$ . Let your choices be informed by the fact that times for this age group tend to be between 22 and 24 seconds.

# Solution (Task 2)

Choose a = b = 0.1 so as to be somewhat uninformative.

Choose  $\beta_0 = [23 \ 0]^T$  with

$$\Sigma_0 = \begin{bmatrix} 5 & 0 \\ 0 & 2 \end{bmatrix}$$
.

This centers the intercept at 23 (the middle of the given range) and the slope at 0 (so we are assuming no increase) but we choose the variance to be a bit large to err on the side of being less informative.

## Gibbs sampler (Task 3)

Code a Gibbs sampler to fit each of the models. For each swimmer i, obtain draws from the posterior predictive distribution for  $y_i^*$ , the time of swimmer i if they were to swim two weeks from the last recorded time.

# Posterior Prediction (Task 4)

The coach has to decide which swimmer should compete in a meet two weeks from the last recorded time. Using the posterior predictive distributions, compute  $\Pr\{y_i^* = \max(y_1^*, y_2^*, y_3^*, y_4^*)\}$  for each swimmer i and use these probabilities to make a recommendation to the coach.

### Final Grades

I am proposing to drop your lowest exam grade (out of Exam I, Exam II, and the Final Exam).

► Homework: 30 percent

► Highest Exam: 35

Second Highest Exam: 35

So your two highest exam scores will be weighted evenly and you lowest exam score will be completely dropped.

Yes, you still must take the final exam.

### Course Evaluations

- I would be very appreciative if you would fill out the course evaluations
- ► They are located on DukeHub
- Directions: https://assessment.trinity.duke.edu/studentscourse-evaluations
- ▶ If there is a 100 percent response rate, I will give everyone in the course 1 point on their final exam grade.

### Exam II

- ▶ Students did extremely well on problems 1 and 2.
- You should feel very proud of how you did on these problems. Great job!

### Exam II

There were issues on both problems 3 and 4.

Due to this, I'm releasing Exam II: https://github.com/resteorts/modernbayes/blob/master/exercises/final-exam/exam2-2020-version2.pdf

No solutions will be posted to encourage you to work through these derivations on your own. See a member of the TA Team if you have a question, and make sure to bring your derivation with you so we can help understand how best to help you!