

Module 10: Linear Regression

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Agenda

- ▶ Oxygen uptake example
- ▶ Linear regression
- ▶ Multiple Linear Regression
- ▶ Ordinary Least Squares
- ▶ An application to swimmers

Oxygen uptake experiment

Exercise is hypothesized to relate to O_2 uptake

What type of exercise is the most beneficial?

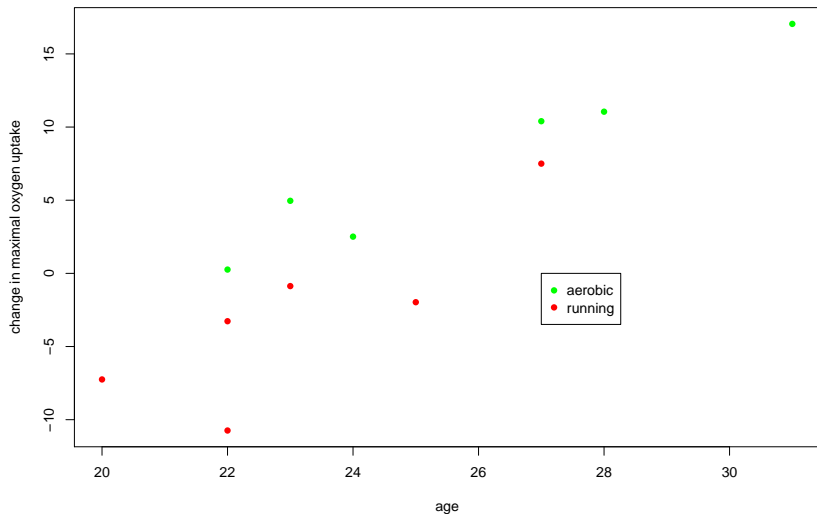
Experimental design: 12 male volunteers.

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 do a running program
4. O_2 uptake measured at end of study

Data

```
# running is 0, 1 is aerobic  
x1<-c(0,0,0,0,0,0,1,1,1,1,1,1)  
# age  
x2<-c(23,22,22,25,27,20,31,23,27,28,22,24)  
# change in maximal oxygen uptake  
y<-c(-0.87,-10.74,-3.27,-1.97,7.50,  
      -7.25,17.05,4.96,10.40,11.05,0.26,2.51)
```

Exploratory Data Analysis



Data analysis

y = change in oxygen uptake

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,

$$\mathbf{y} = \beta_0 + \beta_1 x_2 + \epsilon$$

Linearity means linear in the parameters (β 's).

We could also try the model

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

which is also a linear regression model.

Notation

- ▶ $X_{n \times p}$: regression features or covariates (design matrix)
- ▶ \mathbf{x}_i : i th row vector of the regression covariates
- ▶ $\mathbf{y}_{n \times 1}$: response variable (vector)
- ▶ $\beta_{p \times 1}$: vector of regression coefficients

Goal: Estimation of $p(\mathbf{y} \mid X)$.

Dimensions: $\mathbf{y}_i - \beta^T \mathbf{x}_i = (1 \times 1) - (1 \times p)(p \times 1) = (1 \times 1)$.

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 \mathbf{x} represents a particular covariate we might be interested in, such as age of a person.
- ▶ Denote x_i as the i th **row vector** of the $\mathbf{X}_{n \times p}$ matrix.

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

Notation (continued)

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

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

$$\mathbf{y}_{n \times 1} = \mathbf{X}_{n \times p} \boldsymbol{\beta}_{p \times 1} + \boldsymbol{\epsilon}_{n \times 1}$$

Regression models

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

- ▶ Can we predict \mathbf{Y} as a function of each row in the matrix $X_{n \times p}$ denoted by \mathbf{x}_i .
- ▶ Which \mathbf{x}_i 's have an effect?

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

Multiple linear regression

Consider the following:

$$\mathbf{Y}_i = \beta_1 \mathbf{x}_{i1} + \beta_2 \mathbf{x}_{i2} + \beta_3 \mathbf{x}_{i3} + \beta_4 \mathbf{x}_{i4} + \epsilon_i$$

where

$$x_{i1} = 1 \text{ for subject } i \quad (1)$$

$$x_{i2} = 0 \text{ for running; } 1 \text{ for aerobics} \quad (2)$$

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

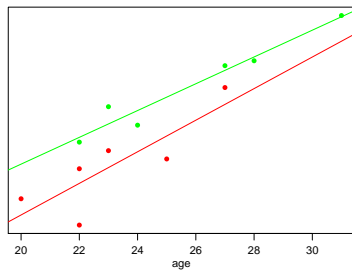
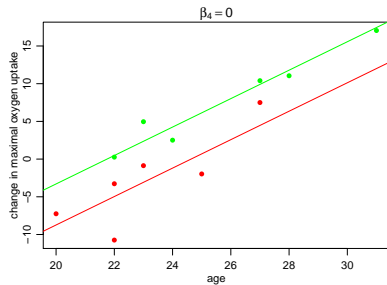
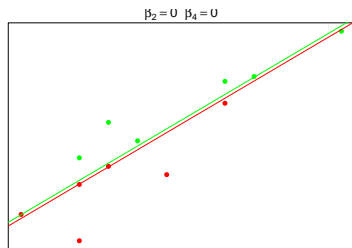
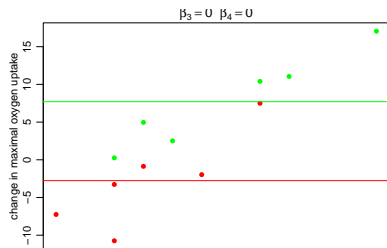
$$x_{i4} = x_{i2} \times x_{i3} \quad (4)$$

Under this model,

$$E[\mathbf{Y} \mid \mathbf{x}] = (\beta_1 + \beta_3) \times \text{age if } x_2 = 0$$

$$E[\mathbf{Y} \mid \mathbf{x}] = (\beta_1 + \beta_2) + (\beta_3 + \beta_4) \times \text{age if } x_2 = 1$$

Least squares regression lines



Multivariate Setup

Let's assume that we have data points $(\mathbf{x}_i, \mathbf{y}_i)$ available for all $i = 1, \dots, n$.

- ▶ y is the response variable

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

- ▶ \mathbf{x}_i is the i th row of the design matrix $\mathbf{X}_{n \times p}$.

Consider the regression coefficients

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

Normal Regression Model

The Normal regression model specifies that

- ▶ $E[Y | x]$ is linear and
- ▶ the sampling variability around the mean is independently and identically (iid) drawn from a normal distribution

$$Y_i = \beta^T x_i + \epsilon_i \quad (5)$$

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

We can specify a simple Bayesian model as the following:

$$\mathbf{y} | X, \beta, \sigma^2 \sim \text{MVN}(X\beta, \sigma^2 I)$$

$$\beta \sim \text{MVN}(0, \tau^2 I)$$

Normal Regression Model (continued)

This specifies the density of the data:

$$p(y_1, \dots, y_n \mid x_1, \dots, x_n, \beta, \sigma^2) \quad (7)$$

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

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

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

Ordinary Least Squares

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

$$\hat{\beta} = \arg \min_{\beta \in \mathbb{R}^p} \|\mathbf{y} - X\hat{\beta}\|_2^2$$

This gives

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

(Check: does this match the expressions for univariate regression, without and with an intercept?)

The fitted values are

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

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

Ordinary Least squares estimation

Let SSR denote sum of squared residuals.

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

Then

$$\frac{\partial SSR(\hat{\beta})}{\partial d\hat{\beta}} = \frac{\partial(\mathbf{y} - \mathbf{X}\hat{\beta})^T(\mathbf{y} - \mathbf{X}\hat{\beta})}{\partial d\hat{\beta}} \quad (11)$$

$$= \frac{\partial \mathbf{y}^T \mathbf{y} - 2\hat{\beta}^T \mathbf{X}^T \mathbf{y} + \hat{\beta}^T (\mathbf{X}^T \mathbf{X}) \hat{\beta}}{\partial d\hat{\beta}} \quad (12)$$

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

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

Called the ordinary least squares estimator. When is it unique?

Ordinary Least squares estimation

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

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

$$\text{Var}(\hat{\beta}) = \text{Var}\{(X^T X)^{-1} X^T \mathbf{Y}\} \quad (14)$$

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

$$= \sigma^2 (X^T X)^{-1} \quad (16)$$

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

Recall data set up

```
# running is 0, 1 is aerobic  
x1<-c(0,0,0,0,0,0,1,1,1,1,1,1)  
# age  
x2<-c(23,22,22,25,27,20,31,23,27,28,22,24)  
# change in maximal oxygen uptake  
y<-c(-0.87,-10.74,-3.27,-1.97,7.50,  
      -7.25,17.05,4.96,10.40,11.05,0.26,2.51)
```

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 0 31 23 27 28 24
```

Recall data set up

```
(X <- 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 |

Multivariate inference for regression models

$$\mathbf{y} \mid \boldsymbol{\beta} \sim \text{MVN}(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}) \quad (17)$$

$$\boldsymbol{\beta} \sim \text{MVN}(\boldsymbol{\beta}_0, \boldsymbol{\Sigma}_0) \quad (18)$$

The posterior can be shown to be

$$\boldsymbol{\beta} \mid \mathbf{y}, \mathbf{X} \sim \text{MVN}(\boldsymbol{\beta}_n, \boldsymbol{\Sigma}_n)$$

where

$$\boldsymbol{\beta}_n = E[\boldsymbol{\beta} \mid \mathbf{y}, \mathbf{X}, \sigma^2] = (\boldsymbol{\Sigma}_0^{-1} + (\mathbf{X}^T \mathbf{X})^{-1} / \sigma^2)^{-1} (\boldsymbol{\Sigma}_0^{-1} \boldsymbol{\beta}_0 + \mathbf{X}^T \mathbf{y} / \sigma^2)$$

$$\boldsymbol{\Sigma}_n = \text{Var}[\boldsymbol{\beta} \mid \mathbf{y}, \mathbf{X}, \sigma^2] = (\boldsymbol{\Sigma}_0^{-1} + (\mathbf{X}^T \mathbf{X})^{-1} / \sigma^2)^{-1}$$

Multivariate inference for regression models

The posterior can be shown to be

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

where

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

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

Remark: If $\Sigma_o^{-1} \ll (X^T X)^{-1}$ then $\beta_n \approx \hat{\beta}_{ols}$

If $\Sigma_o^{-1} \gg (X^T X)^{-1}$ then $\beta_n \approx \beta_0$

Posterior inference applied to Oxygen uptake

To continue the rest of the oxygen uptake example, please refer to 9.2 in Hoff (commentary and code).

Linear Regression Applied to Swimming

- ▶ 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.

Data set

```
read.table("https://www.stat.washington.edu/~pdhoff/Book/Data")
```

| ## | | 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:

$$Y_i \sim \mathcal{N}_6(X_i \beta_i, \tau_i^{-1} \mathcal{I}_6)$$

$$\beta_i \sim \mathcal{N}_2(\beta_0, \Sigma_0)$$

$$\tau_i \sim \text{Gamma}(a, b).$$

Derive full conditionals for β_i and τ_i .

Solution (Task 1)

The conditional posterior for β_i is multivariate normal with

$$\mathbb{V}[\beta_i \mid Y_i, X_i, \tau_i] = (\Sigma_0^{-1} + \tau X_i^T X_i)^{-1}$$

$$\mathbb{E}[\beta_i \mid Y_i, X_i, \tau_i] = (\Sigma_0^{-1} + \tau_i X_i^T X_i)^{-1}(\Sigma_0^{-1} \beta_0 + \tau_i X_i^T Y_i).$$

while

$$\tau_i \mid Y_i, X_i, \beta \sim \text{Gamma} \left(a + 3, b + \frac{(Y_i - X_i \beta_i)^T (Y_i - X_i \beta_i)}{2} \right).$$

These can be found in in Hoff in section 9.2.1.

Task 2

Complete the prior specification by choosing a , b , β_0 , and Σ_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.

- This is left as an exercise.