Chap 2: Linear Regression

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Outline

1. Least Squares Method

2. Multiple Regression

3. Distribution of $\hat{\beta}$

Simple Linear Regression

- The data consists of $(x_1, y_1), ..., (x_N, y_N)$

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

  - β_0: intercept
  - β_1: slope
  - ε_i: random error

- We obtain β_0 and β_1 via the least squares method.

Least Squares Method

- sum of squares of the residuals,
  we minimize L of the squared distances L between (x_i, y_i) and $(x_i, \beta_0 + \beta_1 x_i)$ over $i = 1, 2, ..., N$.

$$L = \sum_{i=1}^{N} (y_i - \beta_0 - \beta_1 x_i)^2$$

- Then, by partially differentiating L by β_0, β_1 and letting them be zero.

$$\frac{\partial L}{\partial \beta_0} = -2 \sum_{i=1}^{N} (y_i - \beta_0 - \beta_1 x_i) = 0$$

$$\frac{\partial L}{\partial \beta_1} = -2 \sum_{i=1}^{N} (x_i (y_i - \beta_0 - \beta_1 x_i)) = 0$$

- β_0 and β_1 are regarded as constants when differentiating L by β_1 and β_0.

Least Squares Method

- When $\sum_{i=1}^{N}(x_i - \bar{x})^2 \neq 0$,
  $\hat{\beta}_0$, $\hat{\beta}_1$ instead of β_0, β_1 which means that they are not the true values but rather estimates obtained from data.

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{N}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{N}(x_i - \bar{x})^2}$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

- We center the data as follows,

$$\tilde{x}_1 := x_1 - \bar{x}, \cdots, \tilde{x}_N := x_N - \bar{x}, \tilde{y}_1 := y_1 - \bar{y}, \cdots, \tilde{y}_N := y_N - \bar{y}$$

- Center the data results in a zero average.
- The formula for calculating the slope from the centralized data is as follows:

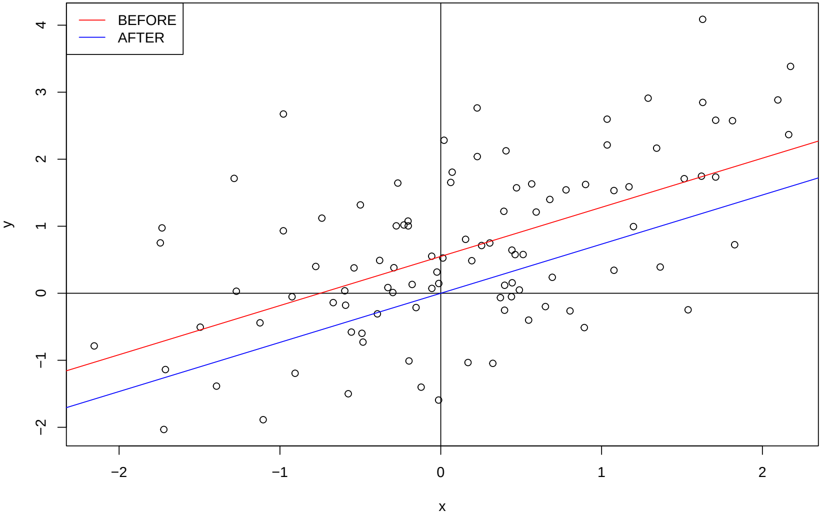
$$\hat{\beta}_1 = \frac{\sum_{i=1}^{N}\tilde{x}_i\tilde{y}_i}{\sum_{i=1}^{N}(\tilde{x}_i)^2}$$

Example

- The two lines l is obtained from the N pairs of data and the least squares method, and l' obtained by shifting l so that it goes through the origin.

```
min.sq=function(x,y){
  x.bar=mean(x);y.bar=mean(y)
  beta.1=sum((x-x.bar)*(y-y.bar))/sum((x-x.bar)^2);beta.0=y.bar-beta.1*x.bar
  return(list(a=beta.0,b=beta.1))
}
a=rnorm(1);b=rnorm(1);
N=100;x=rnorm(N);y=a*x+b+rnorm(N)
plot(x,y);abline(h=0);abline(v=0)
abline(min.sq(x,y)$a,min.sq(x,y)$b,col="red")
x=x-mean(x);y=y-mean(y)
abline(min.sq(x,y)$a,min.sq(x,y)$b,col="blue")
legend("topleft",c("BEFORE","AFTER"),lty=1,col=c("red","blue"))
```

Example



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Multiple Regression with Matrices

We formulate the least squares method for multiple regression with matrices.

- $L := \sum_{i=1}^{N}(y_i - \beta_0 - \beta_1 x_i)^2$,

$$L = \| y - X\beta \|^2 = (y - X\beta)^T (y - X\beta)$$

- If we define,

$$y := \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}, X := \begin{bmatrix} 1 & x_{1,1} & \cdots & x_{1,p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{N,1} & \cdots & x_{N,p} \end{bmatrix}, \beta := \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}$$

- Partial differentiation with L

$$\nabla L := \begin{bmatrix} \frac{\partial L}{\partial \beta_0} \\ \frac{\partial L}{\partial \beta_1} \end{bmatrix} = -2X^T (y - X\beta)$$

Multiple Regression

- Set to zero to find the minimum value

$$-2X^T(y - X\beta) = \begin{bmatrix} -2\sum_{i=1}^{N}(y_i - \sum_{j=0}^{p}\beta_j x_{i,j}) \\ -2\sum_{i=1}^{N}x_{i,1}(y_i - \sum_{j=0}^{p}\beta_j x_{i,j}) \\ \vdots \\ -2\sum_{i=1}^{N}x_{i,p}(y_i - \sum_{j=0}^{p}\beta_j x_{i,j}) \end{bmatrix}$$

- When a matrix X^TX is invertible, we have

$$\hat{\beta} = (X^TX)^{-1}X^Ty$$

When $X^T X$ is irreversible

1. $N < p + 1$

$$rank(X^T X) \leq rank(X) \leq min\{N, p+1\} = N < p + 1$$

   If $N > p$, It is X_particular, So there is no inverse matrix.

2. Two columns in X coincide.

$$X^T X z = 0 \Rightarrow z^T X^T X_Z = 0 \Rightarrow \| X_z \|^2 = 0 \Rightarrow X_z = 0$$

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Distribution of $\hat{\beta}$ 제목 생각해보기

- y have been obtained from the covariates X multiplied by the (true) coefficients β plus some noise ϵ.

$$y = X\beta + \epsilon$$

- The true β is unknown and different from the estimate $\hat{\beta}$.
- We have estimated $\hat{\beta}$ via the least squares method from the N pairs of data (x_1, y_1),···,$(x_N, y_N) \in R^p$ X R
- $x_i \in R^p$ is the row vector consisting of p values excluding the leftmost one in the ith row of X.

Density function

- We assume that each element $\epsilon_1, \cdots, \epsilon_N$ in the random variable ϵ is independent of the others and Gaussian distribution with mean zero and variance σ^2. $N(0, \sigma^2)$

$$f_i(\epsilon_i) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\epsilon_i^2}{2\sigma^2}}$$

- We may express the distributions of $\epsilon_1, \cdots, \epsilon_N$ by

$$f(\epsilon) = \prod_{i=1}^{N} f_i(\epsilon_i) = \frac{1}{(2\pi\sigma^2)^{N/2}} e^{-\frac{\epsilon^T \epsilon}{2\sigma^2}}$$

This is $N(0, \sigma^2 I)$, I is a unit matrix of size N.

Independent if and only if their covariance is zero

- For the proof,

$$\hat{\beta} = (X^T X)^{-1} X^T (X\beta + \epsilon) = \beta + (X^T X)^{-1} X^T \epsilon$$

- Since the average of $\epsilon \in R^N$ is zero, the average of ϵ multiplied from left by the constant matrix $(X^T X)^{-1} X^T$ is zero.

$$E[\hat{\beta}] = \beta$$

- In general, we say that an estimate is unbiased if its average coincides with the true value.

Covariance matrix of $\hat{\beta}$

- $\hat{\beta}$ and its average β consist of $p+1$ values.
- $V(\hat{\beta}_i) = E(\hat{\beta}_i - \beta_i)^2, i = 0, 1, \cdots, p$, the covariance $\sigma_{i,j} := E(\hat{\beta}_i - \beta_i)(\hat{\beta}_j - \beta_j)^T$ can be defined for each pair $i \neq j$.
- matrix consisting of $\sigma_{i,j}$ in the ith row and jth column as to the covariance matrix of $\hat{\beta}$.

$$E \begin{bmatrix} (\hat{\beta}_0 - \beta_0)^2 & (\hat{\beta}_0 - \beta_0)(\hat{\beta}_1 - \beta_1) & \cdots & (\hat{\beta}_0 - \beta_0)(\hat{\beta}_p - \beta_p) \\ (\hat{\beta}_1 - \beta_1)(\hat{\beta}_0 - \beta_0) & (\hat{\beta}_1 - \beta_1)^2 & \cdots & (\hat{\beta}_1 - \beta_1)(\hat{\beta}_p - \beta_p) \\ \vdots & \vdots & \ddots & \vdots \\ (\hat{\beta}_p - \beta_p)(\hat{\beta}_0 - \beta_0) & (\hat{\beta}_p - \beta_p)(\hat{\beta}_1 - \beta_1) & \cdots & (\hat{\beta}_p - \beta_p)^2 \end{bmatrix}$$

Covariance matrix of $\hat{\beta}$

$$
\begin{aligned}
&E\begin{bmatrix}
(\hat{\beta}_0-\beta_0)^2 & (\hat{\beta}_0-\beta_0)(\hat{\beta}_1-\beta_1) & \cdots & (\hat{\beta}_0-\beta_0)(\hat{\beta}_p-\beta_p) \\
(\hat{\beta}_1-\beta_1)(\hat{\beta}_0-\beta_0) & (\hat{\beta}_1-\beta_1)^2 & \cdots & (\hat{\beta}_1-\beta_1)(\hat{\beta}_p-\beta_p) \\
\vdots & \vdots & \ddots & \vdots \\
(\hat{\beta}_p-\beta_p)(\hat{\beta}_0-\beta_0) & (\hat{\beta}_p-\beta_p)(\hat{\beta}_1-\beta_1) & \cdots & (\hat{\beta}_p-\beta_p)^2
\end{bmatrix} \\
&= E\begin{bmatrix} \hat{\beta}_0-\beta_0 \\ \hat{\beta}_1-\beta_1 \\ \vdots \\ \hat{\beta}_p-\beta_p \end{bmatrix}\left[\hat{\beta}_0-\beta_0, \hat{\beta}_1-\beta_1, \cdots, \hat{\beta}_p-\beta_p\right] \\
&= E(\hat{\beta}-\beta)(\hat{\beta}-\beta)^T = E(X^TX)^{-1}X^T\epsilon(X^TX)^{-1}X^T\epsilon^T \\
&= (X^TX)^{-1}X^TE\epsilon\epsilon^TX(X^TX)^{-1} = \sigma^2(X^TX)^{-1}
\end{aligned}
$$

We have determined that the covariance matrix of ϵ is $E\epsilon\epsilon^T = \sigma^2 I$.

$$\hat{\beta} \sim N(\beta, \sigma^2(X^TX)^{-1})$$