

# Multiple Regression

# 설명변수 2개인 경우 - Data Structure

## ■ 자료구조

	반응변수 response	설명변수 explanatory	
	$y_1$	$x_{11}$	$x_{12}$
$\sim$ 번째 (2)	$y_2$	$x_{21}$	$x_{22}$
	$\vdots$	$\vdots$	$\vdots$
	$y_n$	$x_{n1}$	$x_{n2}$

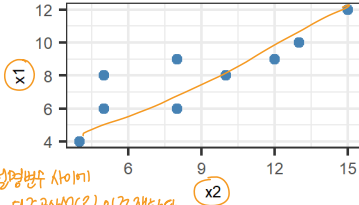
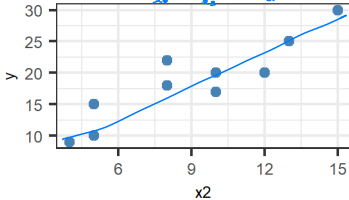
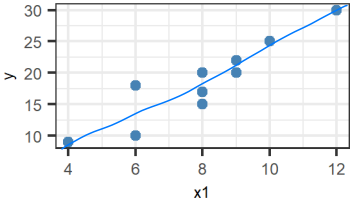
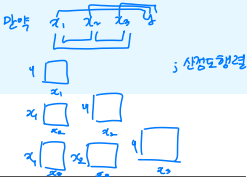
$x_{ij}$   
↓  
 $j = 1, 2$  (설명변수 의미)  
몇 번째 데이터인지 case의 값 의미

# Example

Table: 총판매액의 자료

상점번호	1	2	3	4	5	6	7	8	9	10
광고료 $x_1$ (단위 : 10만 원)	4	8	9	8	8	12	6	10	6	9
상점의 크기 $x_2$ (단위 : 평)	4	10	8	5	10	15	8	13	5	12
총판매액 $y$ (단위 : 100만 원)	9	20	22	15	17	30	18	25	10	20

# Example



설명변수 사이에서  
다중공선성(?)이 존재한다..

# 중회귀모형(Multiple Linear Regression)

## ■ 설명변수가 2개인 다중(선형)회귀모형

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i \quad i = 1, 2, \dots, n$$

- 회귀모수 :  $\beta_0, \beta_1, \beta_2$
- 설명변수(독립변수) :

$$X_1 = (x_{11}, \dots, x_{n1})^\top, X_2 = (x_{12}, \dots, x_{n2})^\top$$

- 반응변수(종속변수) :  $\mathbf{y} = (y_1, \dots, y_n)^\top$
- 오차항 :  $\epsilon = (\epsilon_1, \dots, \epsilon_n)^\top, \epsilon_i \sim_{i.i.d} N(0, \sigma^2)$

# Least Square Estimation

■ 최소제곱추정량 :

$$\hat{y}_{\hat{\beta}} = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2}$$

$$(\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2) = \arg \min_{(\beta_0, \beta_1, \beta_2) \in \mathbb{R}^3} \sum_{i=1}^n \{y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2})\}^2$$

제약조건 3개

$$\frac{\partial S}{\partial \beta_0} = 2 \sum_{i=1}^n (y_i - \underbrace{(\hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2})}_{\hat{y}_{\hat{\beta}}}) (+1) = 0 \quad \Rightarrow \sum e_{\hat{\beta}} = 0$$

$$\textcircled{2} \quad \frac{\partial S}{\partial \beta_1} = 2 \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_{i1} - \beta_2 x_{i2}) (-x_{i1}) = 0 \quad \Rightarrow \sum e_{\hat{\beta}} x_{i1} = 0$$

$$\textcircled{3} \quad \frac{\partial S}{\partial \beta_2} = 2 \sum_{i=1}^n (y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2})) (+x_{i2}) = 0 \quad \Rightarrow \sum e_{\hat{\beta}} x_{i2} = 0$$

# Least Square Estimation

## ■ 정규방정식 (normal equations)

$$\textcircled{1} \sum_{i=1}^n y_i = n\hat{\beta}_0 + \hat{\beta}_1 \sum_{i=1}^n x_{i1} + \hat{\beta}_2 \sum_{i=1}^n x_{i2}$$

$$\sum_{i=1}^n x_{i1}y_i = \hat{\beta}_0 \sum_{i=1}^n x_{i1} + \hat{\beta}_1 \sum_{i=1}^n x_{i1}^2 + \hat{\beta}_2 \sum_{i=1}^n x_{i1}x_{i2}$$

$$\sum_{i=1}^n x_{i2}y_i = \hat{\beta}_0 \sum_{i=1}^n x_{i2} + \hat{\beta}_1 \sum_{i=1}^n x_{i1}x_{i2} + \hat{\beta}_2 \sum_{i=1}^n x_{i2}^2$$

$$\textcircled{1} \sum_{i=1}^n y_i = n\hat{\beta}_0 + \hat{\beta}_1 \sum_{i=1}^n x_{i1} + \hat{\beta}_2 \sum_{i=1}^n x_{i2}$$

$$\textcircled{1}: \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}_1 - \hat{\beta}_2 \bar{x}_2$$

$$\textcircled{2} \sum e_i x_{i1} = 0$$

$$\begin{aligned} \sum e_i x_{i1} &= \sum e_i (x_{i1} - \bar{x}_1 + \bar{x}_1) \\ &= \sum e_i (x_{i1} - \bar{x}_1) + \bar{x}_1 \underbrace{\sum e_i}_{=0} \end{aligned}$$

$$\begin{aligned} e_i &= y_i - \hat{y}_i = y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \hat{\beta}_2 x_{i2}) \\ &= y_i - \bar{y} + \hat{\beta}_1 \bar{x}_1 + \hat{\beta}_2 \bar{x}_2 - \dots \\ &= (y_i - \bar{y}) - \hat{\beta}_1 (x_{i1} - \bar{x}_1) - \hat{\beta}_2 (x_{i2} - \bar{x}_2) \\ &= \sum (y_i - \bar{y})(x_{i1} - \bar{x}_1) - \hat{\beta}_1 \sum (x_{i1} - \bar{x}_1)^2 - \hat{\beta}_2 \sum (x_{i2} - \bar{x}_2)(x_{i1} - \bar{x}_1) \\ &= S_{(1y)} - \hat{\beta}_1 S_{(11)} - \hat{\beta}_2 S_{(12)} = 0 \end{aligned}$$

?

$$\textcircled{3} \begin{cases} \hat{\beta}_1 S_{(11)} + \hat{\beta}_2 S_{(12)} = S_{(1y)} \\ \hat{\beta}_1 S_{(12)} + \hat{\beta}_2 S_{(22)} = S_{(2y)} \end{cases}$$

$S_{(12)}$   
1번자와 2번자에  
공분산 느낌

$S_{(12)}$ 가 0에 가까워지면...

$$\hat{\beta}_1 = \frac{S_{(1y)}}{S_{(11)}} \div \frac{S_{(2y)}}{S_{(22)}}$$



$$\begin{cases} \hat{\beta}_1 S_{(11)} + \hat{\beta}_2 S_{(12)} = S_{(1y)} \\ \hat{\beta}_1 S_{(12)} + \hat{\beta}_2 S_{(22)} = S_{(2y)} \end{cases}$$

$$\begin{pmatrix} S_{(11)} & S_{(12)} \\ S_{(12)} & S_{(22)} \end{pmatrix} \begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} = \begin{pmatrix} S_{(1y)} \\ S_{(2y)} \end{pmatrix}$$

$$\begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} = \begin{pmatrix} S_{(11)} & S_{(12)} \\ S_{(12)} & S_{(22)} \end{pmatrix}^{-1} \begin{pmatrix} S_{(1y)} \\ S_{(2y)} \end{pmatrix}$$

# 단순 선형 회귀모형

## ■ 행렬의 사용

- $j$  번째 관측치

$$y_j = \beta_0 + \beta_1 x_j + \epsilon_j = \begin{pmatrix} 1 & x_j \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} + \epsilon_j$$

- $n$  개의 관측치

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}$$

# 단순 선형 회귀모형

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

$$\underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}}_{n \times 1} = \underbrace{\begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}}_{n \times 2} \underbrace{\begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}}_{2 \times 1} + \underbrace{\begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}}_{n \times 1}$$

# 단순 선형 회귀모형

## ■ Example

$$y = \begin{pmatrix} 9 \\ 20 \\ 22 \\ 15 \\ 17 \\ 30 \\ 18 \\ 25 \\ 10 \\ 20 \end{pmatrix}, \quad X = \begin{pmatrix} 1 & 4 \\ 1 & 8 \\ 1 & 9 \\ 1 & 8 \\ 1 & 8 \\ 1 & 12 \\ 1 & 6 \\ 1 & 10 \\ 1 & 6 \\ 1 & 9 \end{pmatrix}, \quad \epsilon = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \\ \epsilon_7 \\ \epsilon_8 \\ \epsilon_9 \\ \epsilon_{10} \end{pmatrix}, \quad \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}$$

# 단순 선형 회귀모형

$$\sum (y_i - \beta_0 - \beta_1 x_i)^2$$

최소값을 찾기 위해서..

$$\underline{y} = \underline{X}\underline{\beta} + \underline{\epsilon}$$

## 오차제곱합

$$\sum_{j=1}^n \epsilon_j^2 = \underbrace{\underline{\epsilon}^T}_{1 \times n} \underbrace{\underline{\epsilon}}_{n \times 1} = (\underline{y} - \underline{X}\underline{\beta})^T (\underline{y} - \underline{X}\underline{\beta})$$

$$= \underbrace{(\underline{y}^T - \underline{\beta}^T \underline{X}^T)}_{1 \times 1} (\underline{y} - \underline{X}\underline{\beta}) = \underbrace{\underline{y}^T \underline{y}}_{1 \times 1} - \underbrace{\underline{y}^T \underline{X} \underline{\beta}}_{1 \times 1} - \underbrace{\underline{\beta}^T \underline{X}^T \underline{\beta}}_{1 \times 1} + \underbrace{\underline{\beta}^T \underline{X}^T \underline{X} \underline{\beta}}_{1 \times 1}$$

$$= \underline{y}^T \underline{y} - 2\underline{\beta}^T \underline{X}^T \underline{y} + \underline{\beta}^T \underline{X}^T \underline{X} \underline{\beta}$$

따라서 이로 만드는  $\underline{\beta}$ 를 찾자!

$$\begin{aligned} (A+B)^T &= A^T + B^T \\ (AB)^T &= B^T A^T \\ (A^{-1})^T &= (A^T)^{-1} \end{aligned}$$

# 미분법

constant vector

■  $\mathbf{c}, \mathbf{x} : n \times 1$  벡터

$$\overset{1 \times n}{\mathbf{c}^\top} \overset{n \times 1}{\mathbf{x}} = (c_1, \dots, c_n) \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \sum_{i=1}^n c_i x_i$$

- $\mathbf{c}^\top \mathbf{x}$ 의  $\mathbf{x}$ 에 대한 편도함수(partial derivative)  $\frac{\partial(\mathbf{c}^\top \mathbf{x})}{\partial \mathbf{x}} = \mathbf{c}$  와 같은 미분계정

벡터미분  
! 각 element로 미분하여  
행벡터가 됨

$$\frac{\partial(\mathbf{c}^\top \mathbf{x})}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial(\mathbf{c}^\top \mathbf{x})}{\partial x_1} \\ \vdots \\ \frac{\partial(\mathbf{c}^\top \mathbf{x})}{\partial x_n} \end{pmatrix} = \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix} = \mathbf{c}$$

# 미분법

- $\frac{\partial(\mathbf{c}^\top \mathbf{x})}{\partial \mathbf{x}} = \mathbf{c}$ 
 $\frac{\partial(\mathbf{x}^\top \mathbf{c})}{\partial \mathbf{x}} = \mathbf{c}$

- 이차형식  $\mathbf{y}^\top \mathbf{A} \mathbf{y}$   
 $\begin{matrix} \text{1x}n & n \times n & n \times 1 \\ \hline & 1 \times 1 & \end{matrix}$   
 $\mathbf{A} : \text{symmetric} \Rightarrow \frac{\partial(\mathbf{y}^\top \mathbf{A} \mathbf{y})}{\partial \mathbf{y}} = 2\mathbf{A}\mathbf{y}$   
 $\text{대칭행렬}$

$\text{dimension}$  맞춰야 함

$$\mathbf{A} : \text{non-symmetric} \Rightarrow \frac{\partial(\mathbf{y}^\top \mathbf{A} \mathbf{y})}{\partial \mathbf{y}} = (\mathbf{A} + \mathbf{A}^\top) \mathbf{y}$$

# 단순 선형 회귀모형

- 오차제곱합

$$\hat{\beta} = \arg \min \epsilon^T \epsilon$$

$$\sum_{j=1}^n \epsilon_j^2 = \epsilon^T \epsilon = (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) \quad \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}$$

$$\frac{\partial S}{\partial \beta} = \mathbf{y}^T \mathbf{y} - 2\beta^T \overset{2 \times 1}{\mathbf{X}^T} \overset{2 \times n}{\mathbf{X}} \overset{n \times 1}{\mathbf{y}} + \beta^T \mathbf{X}^T \mathbf{X} \beta$$
$$\frac{\partial S}{\partial \beta} = 0 - 2\mathbf{X}^T \mathbf{y} + 2\mathbf{X}^T \mathbf{X} \beta = 0$$

$\beta^T$  배고 계수만 남음

- 정규방정식

$$\underset{(2 \times 1)}{\mathbf{X}^T \mathbf{X}} \hat{\beta} = \mathbf{X}^T \mathbf{y},$$

- 최소제곱합 (LSE)

$$\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1)^T = \hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$



## 단순 선형 회귀모형

$$\mathbf{X}^\top \mathbf{y} = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} \sum y_j \\ \sum x_j y_j \end{pmatrix}$$

$$\mathbf{X}^\top \mathbf{X} = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \end{pmatrix} \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} = \begin{pmatrix} n & \sum x_j \\ \sum x_j & \sum x_j^2 \end{pmatrix}$$

# 단순 선형 회귀모형

$$(\mathbf{X}^\top \mathbf{X})^{-1} = \begin{pmatrix} n & \sum x_j \\ \sum x_j & \sum x_j^2 \end{pmatrix}^{-1} = \begin{pmatrix} \frac{\sum x_j^2}{n \sum x_j^2 - (\sum x_j)^2} & \frac{-\sum x_j}{n \sum x_j^2 - (\sum x_j)^2} \\ \frac{-\sum x_j}{n \sum x_j^2 - (\sum x_j)^2} & \frac{n}{n \sum x_j^2 - (\sum x_j)^2} \end{pmatrix}$$

$$\Rightarrow \hat{\beta} = \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{pmatrix} = \begin{pmatrix} \frac{(\sum x_j^2)(\sum y_j) - (\sum x_j)(\sum x_j y_j)}{n \sum x_j^2 - (\sum x_j)^2} \\ \frac{n \sum x_j y_j - (\sum x_j)(\sum y_j)}{n \sum x_j^2 - (\sum x_j)^2} \end{pmatrix}$$

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

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}}$$

↑ 노치기

$$\sum x_j^2 - \frac{1}{n}(\sum x_j)^2$$

$$= \sum (x_j - \bar{x})^2 = S_{xx}$$

## 단순 선형 회귀모형

$$\hat{\beta} = \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{pmatrix} = \begin{pmatrix} \frac{(\sum x_j^2)(\sum y_j) - (\sum x_j)(\sum x_j y_j)}{n \sum x_j^2 - (\sum x_j)^2} \\ \frac{n \sum x_j y_j - (\sum x_j)(\sum y_j)}{n \sum x_j^2 - (\sum x_j)^2} \end{pmatrix}$$

# Data Structure and Model

## ■ 자료구조 (설명변수 $p$ 개)

response	explanatory		
$y_1$	$x_{11}$	$\cdots$	$x_{1p}$
$y_2$	$x_{21}$	$\cdots$	$x_{2p}$
$\vdots$	$\vdots$	$\ddots$	$\vdots$
$y_n$	$x_{n1}$	$\cdots$	$x_{np}$

# 중회귀모형(Multiple Linear Regression)

- 설명변수가  $p$ 개인 다중(선형)회귀모형

$$y_i = \beta_0 + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i \quad i = 1, 2, \dots, n$$

- 회귀모수 :  $\beta_0, \beta_1, \dots, \beta_p$  ←  $p+1$ 개
- 설명변수(독립변수) :

$$X_1 = (x_{11}, \dots, x_{n1})^T, \dots, X_p = (x_{1p}, \dots, x_{np})^T$$

- 반응변수(종속변수) :  $Y = (y_1, \dots, y_n)^T$
- 오차항 :  $\epsilon_1, \dots, \epsilon_n, (\sim_{i.i.d} N(0, \sigma^2))$

# 중회귀모형(Multiple Linear Regression)

■ 자료구조 (설명변수  $p$ 개)

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

$$\underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}}_y = \underbrace{\begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix}}_X \underbrace{\begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}}_{\beta} + \underbrace{\begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}}_{\epsilon}$$

# 중회귀모형(Multiple Linear Regression)

## ■ 자료구조

$\text{rank}(X) = p+1$   
설명변수간 상관관계가 없음  
선형적으로 독립

$$\underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}}_{n \times 1} = \underbrace{\begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix}}_{\substack{\underbrace{1 \quad x_1 \quad x_2 \quad \cdots \quad x_p}_{n \times (p+1)}}} \underbrace{\begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}}_{(p+1) \times 1} + \underbrace{\begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}}_{n \times 1}$$

$n \geq p+1$  (∵ 연립방정식 풀이.)

# 중회귀모형(Multiple Linear Regression)

- 설명변수가  $p$ 개인 다중(선형)회귀모형: 행렬형식

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

- 회귀모수 :  $\boldsymbol{\beta} = (\beta_0, \beta_1, \dots, \beta_p)^\top$ ,  $(p+1) \times 1$  vector
- 설명변수(독립변수) :

$$\mathbf{X} = (\mathbf{1}, X_1, \dots, X_p)^\top, \text{ rank}(\mathbf{X}) = p+1, n > p$$

$\mathbf{X} : n \times (p+1)$

- 반응변수(종속변수) :  $\mathbf{y} = (y_1, \dots, y_n)^\top$
- 오차항 :  $\boldsymbol{\epsilon} = (\epsilon_1, \dots, \epsilon_n)^\top \sim N(0, \sigma^2 \mathbf{I}_n)$

$\mathbf{I}_n = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$   
← 항등행렬  
다변량 정규분포



# Least Square Estimation

■ 최소제곱추정량 :

$$\begin{aligned} (\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p) = \\ \arg \min_{(\beta_0, \dots, \beta_p) \in \mathbb{R}^{p+1}} \sum_{i=1}^n \{y_i - (\beta_0 + \beta_1 x_{i1} + \dots + \beta_p x_{ip})\}^2 \end{aligned}$$

또는

$$\hat{\beta} = \arg \min_{\beta \in \mathbb{R}^{p+1}} \underbrace{\|\mathbf{y} - \mathbf{X}\beta\|^2}_{S(\beta)}$$

# Least Square Estimation

$$= \sum \varepsilon_i^2 = \varepsilon^T \varepsilon = (y - X\beta)^T (y - X\beta)$$

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

$$= (y - X\beta)^T (y - X\beta)$$

$$= y^T y - \beta^T X y - y^T X \beta + \beta^T X^T X \beta$$

$$= y^T y - 2y^T X \beta + \beta^T X^T X \beta$$

## ■ 정규방정식

$$\frac{\partial S}{\partial \beta} \Big|_{\hat{\beta}} = -2X^T y + 2X^T X \hat{\beta} = 0 \Rightarrow X^T X \hat{\beta} = X^T y$$

# Least Square Estimation

- 최소제곱추정량 :

$$\hat{\beta} = \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \vdots \\ \hat{\beta}_p \end{pmatrix} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

$\text{rank}(\mathbf{X}) = p+1$   
 $\Leftrightarrow (\mathbf{X}^\top \mathbf{X})^{-1}$  존재함.

단,  $(\mathbf{X}^\top \mathbf{X})^{-1}$  이 존재하여야 함.

- 추정된 회귀직선 :  $\hat{\mathbf{y}} = \mathbf{X}\hat{\beta} = \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$

# Example

$$\mathbf{y} = \begin{pmatrix} 9 \\ 20 \\ 22 \\ 15 \\ 17 \\ 30 \\ 18 \\ 25 \\ 10 \\ 20 \end{pmatrix}, \quad \mathbf{X} = \begin{matrix} & \begin{matrix} 1 & x_1 & x_2 \end{matrix} \\ \begin{pmatrix} 1 & 4 & 4 \\ 1 & 8 & 10 \\ 1 & 9 & 8 \\ 1 & 8 & 5 \\ 1 & 8 & 10 \\ 1 & 12 & 15 \\ 1 & 6 & 8 \\ 1 & 10 & 13 \\ 1 & 6 & 5 \\ 1 & 9 & 12 \end{pmatrix} \end{matrix}, \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix}, \quad \boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \\ \epsilon_7 \\ \epsilon_8 \\ \epsilon_9 \\ \epsilon_{10} \end{pmatrix}$$

# Example

$$\mathbf{X}^\top \mathbf{X} = \begin{pmatrix} 10 & 80 & 90 \\ 80 & 686 & 784 \\ 90 & 784 & 932 \end{pmatrix}, \quad \mathbf{X}^\top \mathbf{y} = \begin{pmatrix} 186 \\ 1608 \\ 1866 \end{pmatrix}$$

Rocket solver?  
or?  
↓

$$(\mathbf{X}^\top \mathbf{X})^{-1} = \begin{pmatrix} 1.62902 & -0.26385 & 0.06464 \\ -0.26385 & 0.08047 & -0.04222 \\ 0.06464 & -0.04222 & 0.03034 \end{pmatrix}$$

## Example

단순 선형에서

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 \underline{x_2} \quad x_2 \text{ 증가시 } \beta_1 \text{ 만큼 증가..}$$

$$\hat{\beta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} = \begin{pmatrix} -0.651 \\ 1.551 \\ 0.760 \end{pmatrix}$$

- 추정된 회귀직선

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 = -0.651 + 1.551x_1 + 0.760x_2$$

이론 (해석상..)  
↳  $\hat{\beta}_1$ :  $x_2$ 가 변하지 않을 때  $x_1$ 이 1만큼 변하면  $y$ 는  $(1.5)$  만큼 증가  
↳  $\hat{\beta}_2$ :  $x_1$ 가 변하지 않을 때  $x_2$ 가 1단위 증가하면  $y$ 는  $(0.76)$  만큼 증가  
↳ but 실제로는...!!  
    상황과 제약이 있음

# Decomposition of sum of squares

■ 제곱합의 분해 :  $SST = SSE + SSR$

$$\sum_{i=1}^n (y_i - \bar{y})^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2 + \sum_{i=1}^n (\hat{y}_i - \bar{y})^2$$

제곱합의 종류	정의 및 기호	자유도
총제곱합	$SST = \sum_{i=1}^n (y_i - \bar{y})^2$	$n - 1$
잔차제곱합	$SSE = \sum_{i=1}^n (y_i - \hat{y}_i)^2$	$n - \underbrace{(p + 1)}_{\text{제약조건}}$
회귀제곱합	$SSR = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2$	$p$ (설명변수 개수)

# Decomposition of sum of squares

■ 총변동 :  $SST$  (총제곱합)

$$SST = \sum_{i=1}^n (y_i - \bar{y})^2 = \sum_{i=1}^n y_i^2 - n(\bar{y})^2 = \mathbf{y}^\top \mathbf{y} - n(\bar{y})^2$$

또는

$$n(\bar{y})^2 = \frac{1}{n} \left( \sum_{i=1}^n y_i \right)^2 = \mathbf{y}^\top \mathbf{1} \mathbf{1}^\top \mathbf{y} / n$$



# Decomposition of sum of squares

- 회귀모형에 의해 설명되지 않는 변동 :  $SSE$  (잔차제곱합)

$$\begin{aligned} SSE &= \sum_{i=1}^n (y_i - \hat{y}_i)^2 = (\mathbf{y} - \hat{\mathbf{y}})^\top (\mathbf{y} - \hat{\mathbf{y}}) \\ &= (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}})^\top (\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}) \\ &= \mathbf{y}^\top \mathbf{y} - 2\hat{\boldsymbol{\beta}}^\top \mathbf{X}^\top \mathbf{y} + \hat{\boldsymbol{\beta}}^\top \mathbf{X}^\top \mathbf{X} \hat{\boldsymbol{\beta}} \\ &= \mathbf{y}^\top \mathbf{y} - \mathbf{y}^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \\ &= \mathbf{y}^\top \left[ \mathbf{I}_n - \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \right] \mathbf{y} \end{aligned}$$

$$\text{또는 } SSE = \mathbf{y}^\top \mathbf{y} - \hat{\boldsymbol{\beta}}^\top \mathbf{X}^\top \mathbf{y}$$

$$SSE = \sum (y_i - \hat{y}_i)^2 = (\underline{y} - \underline{\hat{y}})^T (\underline{y} - \underline{\hat{y}})$$

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

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

바깥싱카이제곱분포!

$$= \underbrace{(I_n - X(X^T X)^{-1} X^T)}_A y$$

$$e = Ay$$

$$SSE = (Ay)^T (Ay) = y^T A^T A y$$

$$A^T A = (I_n - X(X^T X)^{-1} X^T) (I_n - X(X^T X)^{-1} X^T)$$

$$= I_n - 2X(X^T X)^{-1} X^T + X(X^T X)^{-1} X^T \cdot X(X^T X)^{-1} X^T$$

$$= I_n - X(X^T X)^{-1} X^T$$

$$A^T A = A$$

$$\therefore SSE = y^T A y$$

$$y \sim N(\mu, \sigma^2 I_n)$$

$$\underline{\mu} = X\beta$$

$$\boxed{y \sim N(X\beta, I_n \sigma^2)}$$

## Decomposition of sum of squares

$$= \cancel{y^T (I_n - \frac{1}{n} J_n) y} - \cancel{y^T (I_n - X(X^T X)^{-1} X^T) y}$$

- 회귀모형에 의해 설명되는 변동 :  $SSR$  (회귀제곱합)

$$\begin{aligned} SSR &= SST - SSE \\ &= \left[ \mathbf{y}^T \mathbf{y} - n(\bar{y})^2 \right] - \left[ \mathbf{y}^T \mathbf{y} - \hat{\boldsymbol{\beta}}^T \mathbf{X}^T \mathbf{y} \right] \\ &= \hat{\boldsymbol{\beta}}^T \mathbf{X}^T \mathbf{y} - n(\bar{y})^2 \\ &= \mathbf{y}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} - n(\bar{y})^2 \end{aligned}$$

# 분산분석표

## ■ 중회귀모형의 분산분석표

요인	제곱합	자유도(df)	평균제곱(MS)	$F_0$	유의확률
회귀	$SSR$	$p$	$MSR = \frac{SSR}{p}$	$\frac{MSR}{MSE}$	$P(F \geq f)$
잔차	$SSE$	$n - (p + 1)$	$MSE = \frac{SSE}{n - p - 1}$	$\chi^2$ 분모를 대는다.	
계	$SST$	$n - 1$			

# 회귀직선의 유의성 검정

## ■ 회귀직선의 유의성 검정 (F-test)

설명변수가 다의미가 있다.

- 가설 :  $H_0 : \beta_1 = \dots = \beta_p = 0$  vs.  $H_1 : \text{not } H_0$

↳ 제거한 항개는 의미가 있다.

- 검정통계량

$$F = \frac{MSR}{MSE} = \frac{SSR/p}{SSE/(n - (p + 1))} \sim_{H_0} F(p, n - p - 1)$$

- 검정통계량의 관측값 :  $F_0$
- 유의수준  $\alpha$ 에서의 기각역 :  $F_0 > F_\alpha(p, n - p - 1)$
- 유의확률 =  $P(F > F_0)$

## Example

$$SST = \mathbf{y}^\top \mathbf{y} - n(\bar{y})^2$$

$$= 9^2 + 20^2 + \cdots + 20^2 - 10(18.6)^2 = 368.40$$

$$SSR = \hat{\boldsymbol{\beta}}^\top \mathbf{X}^\top \mathbf{y} - n(\bar{y})^2$$

$$= \begin{pmatrix} -0.651 & 1.551 & 0.760 \end{pmatrix} \begin{pmatrix} 186 \\ 1608 \\ 1866 \end{pmatrix} - 10(18.6)^2 = 332.12$$

$$SSE = SST - SSR = 36.28$$

# Example

가설검정 할때 꼭 써주기-

## ■ 회귀직선의 유의성 검정 (F-test)

- 가설 :  $H_0 : \beta_1 = \beta_2 = 0$  vs.  $H_1 : \text{not } H_0$
- 분산분석표

요 인	제곱합	자유도	평균제곱	$F_0$	$F_{0.05}(2, 7)$
회 귀	332.12	2	166.06	32.04**	4.74
잔 차	36.28	7	5.18		
계	368.40	9			

- $F_0 = 32.04 > F_{\alpha}(p, n - p - 1) = F_{0.05}(2, 7) = 4.74$  이므로  
귀무가설 기각

# 회귀모형의 정도

$$\begin{cases} \text{MSE} \downarrow \\ F_0 \uparrow \\ R^2 \uparrow \end{cases}$$

## ■ 회귀모형의 적합도

- $MSE$  평균오차제곱합: 작을수록 좋음
- $F_0 = MSR/MSE$   $F_0 \uparrow \rightarrow SSR \uparrow$ : 모형재해합
- $R^2 = SSR/SST$  1에 가까울수록 좋음
- 회귀계수  $\beta^T = (\beta_0, \beta_1, \beta_2, \dots, \beta_p)$ 의 정확한 추정

↳ 오차가 작다.

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_1$$
$$s.e.(\hat{\beta}_1) = \frac{\sigma^2}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2}}$$



# Estimation of error variance

$$MSE = \hat{\sigma}^2 : \text{불편추정량}$$

## ■ 오차분산 ( $\sigma^2$ )의 추정:

- 잔차 (residual) :  $e_i = y_i - \hat{y}_i$
- 잔차(오차) 제곱합 (residual (or error) sum of squares) :

$$SSE = \sum_{i=1}^n (y_i - \hat{y}_i)^2 = \sum_{i=1}^n e_i^2$$

- 평균제곱오차 (mean squared error) :  $MSE = \frac{SSE}{n - (p + 1)}$
- 오차분산의 추정값 :  $\hat{\sigma}^2 = MSE$

$$E(MSE) = \sigma^2$$

HW

$$SSE = Y^T A Y$$

정리 5.1 통해서

불편추정량으로

보이기

# Coefficient of determination

$$SSE = \sum (y_i - \hat{y}_i)^2$$

$(\beta_0, \beta_1, \dots, \beta_p) =$

$$MSE = \frac{SSE}{n - (p+1)}$$

## ■ 결정계수 (Coefficient of determination)

$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$$

## ■ 수정된 결정계수 (Adjusted multiple correlation coefficient)

$$R^2_{adj} = 1 - \frac{SSE/(n - p - 1)}{SST/(n - 1)}$$

자유도로 나눠줌  $\rightarrow$  평균상승률

ex)

$$\frac{(\beta_1)}{M_1}$$

$$\frac{(\beta_1, \beta_2)}{M_2}$$

$$(\hat{\beta}_0, \hat{\beta}_1) = \underset{\beta_0, \beta_1}{\text{minimize}} (y_i - \hat{y}_i)^2$$

$$\Rightarrow \underset{\beta_0, \beta_1}{\text{minimize}} (y_i - \beta_0 - \beta_1 x_i)^2 = S_1 \quad SSE_1$$

설명 변수가 추가되면  
SSE는 작아지는  
성질이 있다.

$$(\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2) \Rightarrow \underset{\beta_0, \beta_1, \beta_2}{\text{minimize}} (y_i - \beta_0 - \beta_1 x_i - \beta_2 x_i^2)^2 = S_2 \quad SSE_2$$

설명 변수 하나 더 추가..  
SSE... S2에서  $\beta_2=0$ 이라고 생각하는 case

$$\Rightarrow \boxed{S_1 > S_2} \quad \text{무조건..}$$

$$SSE_1 > SSE_2$$

$$\Rightarrow -SSE_1 < -SSE_2$$

$$\Rightarrow 1 - \frac{SSE_1}{SST} < 1 - \frac{SSE_2}{SST}$$

$$\Rightarrow \boxed{R_1^2 < R_2^2}$$

$$\text{Var}(A\mathbf{y}) = A \text{Var}(\mathbf{y}) A^T$$

■  $\hat{\beta}$

$$\begin{aligned} E(\hat{\beta}) &= E \left[ (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \right] \\ &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T E(\mathbf{y}) = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{X} \beta = \beta \end{aligned}$$

부연주장

$$\begin{aligned} \text{Var}(\hat{\beta}) &= \text{Var} \left[ (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \right] \\ &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T [\text{Var}(\mathbf{y})] \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \\ &= (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T (I\sigma^2) \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} = (\mathbf{X}^T \mathbf{X})^{-1} \sigma^2 \end{aligned}$$

■  $\hat{\beta}$ 

$$\begin{aligned} \text{Var}(\hat{\beta}) &= \text{Var} \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_p \end{pmatrix} = \begin{pmatrix} \text{Var}(\hat{\beta}_0) & \text{Cov}(\hat{\beta}_0, \hat{\beta}_1) & \text{Cov}(\hat{\beta}_0, \hat{\beta}_2) & \cdots & \text{Cov}(\hat{\beta}_0, \hat{\beta}_p) \\ & \text{Var}(\hat{\beta}_1) & \text{Cov}(\hat{\beta}_1, \hat{\beta}_2) & \cdots & \text{Cov}(\hat{\beta}_1, \hat{\beta}_p) \\ & & \text{Var}(\hat{\beta}_2) & \cdots & \text{Cov}(\hat{\beta}_2, \hat{\beta}_p) \\ & & & \ddots & \vdots \\ & & & & \text{Var}(\hat{\beta}_p) \end{pmatrix} \\ &= (\mathbf{X}^\top \mathbf{X})^{-1} \sigma^2 := (c_{ij}) \sigma^2 \end{aligned}$$

# 평균반응 및 개별 $y$ 의 추정량

$$E(\hat{y}) = \mathbf{X}^T E(\hat{\beta}) = \mathbf{X}^T \beta \quad \left( (1 \ x_1 \ \dots \ x_p) \begin{pmatrix} \hat{\beta}_0 \\ \vdots \\ \hat{\beta}_p \end{pmatrix} \right)$$

- $\hat{y} = E(y | \mathbf{X} = \mathbf{x}) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \dots + \hat{\beta}_p x_p = \mathbf{x}^T \hat{\beta}$   
 (하나의 관측값)

$$\text{Var}(\hat{y}) = \text{Var}(\mathbf{x}^T \hat{\beta}) = \mathbf{x}^T \text{Var}(\hat{\beta}) \mathbf{x}$$

- (기댓값: 똑같은)  
 개별관측값  $\hat{y}_s$

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

$\frac{\begin{matrix} (1 \times (p+1)) & (p+1) \times (p+1) & (p+1) \times 1 \\ \hline & 1 \times 1 & \end{matrix}}{1 \times 1}$

$$\text{Var}(\hat{y}_s) = \left[ \underline{1} + \mathbf{x}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x} \right] \sigma^2$$

## Example

- $\text{Var}(\hat{\beta})$

$$\begin{aligned}\text{Var} \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} &= (X^\top X)^{-1} \sigma^2 = \begin{pmatrix} 1.63 & -0.26 & 0.06 \\ -0.26 & 0.08 & -0.04 \\ 0.06 & -0.04 & 0.03 \end{pmatrix} \sigma^2 \\ &= \begin{pmatrix} \text{Var}(\hat{\beta}_0) & \text{Cov}(\hat{\beta}_0, \hat{\beta}_1) & \text{Cov}(\hat{\beta}_0, \hat{\beta}_2) \\ \text{Cov}(\hat{\beta}_0, \hat{\beta}_1) & \text{Var}(\hat{\beta}_1) & \text{Cov}(\hat{\beta}_1, \hat{\beta}_2) \\ \text{Cov}(\hat{\beta}_0, \hat{\beta}_2) & \text{Cov}(\hat{\beta}_1, \hat{\beta}_2) & \text{Var}(\hat{\beta}_2) \end{pmatrix}\end{aligned}$$

## Example

$$\mathbf{x} = \begin{matrix} x_1 & x_2 \\ (1, 10, 10) \end{matrix}$$

- $\text{Var}(\hat{y})$

$$\begin{aligned} \text{Var}(\hat{y}) &= \mathbf{x}^\top (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{x} \sigma^2 \\ &= \begin{pmatrix} 1 & 10 & 10 \end{pmatrix} \begin{pmatrix} 1.63 & -0.26 & 0.06 \\ -0.26 & 0.08 & -0.04 \\ 0.06 & -0.04 & 0.03 \end{pmatrix} \begin{pmatrix} 1 \\ 10 \\ 10 \end{pmatrix} \sigma^2 \\ &= 0.28182 \sigma^2 \end{aligned}$$



# 제곱합의 분포

## ■ 중회귀모형

$$\mathbf{y} = \overbrace{X\boldsymbol{\beta}}^{\text{y의 기대값}} + \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim N(\mathbf{0}, I_n \sigma^2)$$

$$SST = \mathbf{y}^\top \mathbf{y} - n(\bar{y})^2 = \mathbf{y}^\top \left[ I_n - \frac{J_n}{n} \right] \mathbf{y}$$

$$\begin{aligned} SSR &= \mathbf{y}^\top \mathbf{X} (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} - n(\bar{y})^2 \\ &= \mathbf{y}^\top \left[ \mathbf{X} (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top - \frac{J_n}{n} \right] \mathbf{y} \end{aligned}$$

$$SSE = \mathbf{y}^\top \left[ I_n - \mathbf{X} (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \right] \mathbf{y}$$

## 제곱합의 분포

$$\frac{SST}{\sigma^2} \sim \chi^2 \left\{ n - 1, \boldsymbol{\beta}^\top \mathbf{X}^\top \left( I_n - \frac{\mathbf{J}_n}{n} \right) \mathbf{X} \boldsymbol{\beta} / 2\sigma^2 \right\}$$

$$\frac{SSR}{\sigma^2} \sim \chi^2 \left\{ \rho, \boldsymbol{\beta}^\top \mathbf{X}^\top \left( I_n - \frac{\mathbf{J}_n}{n} \right) \mathbf{X} \boldsymbol{\beta} / 2\sigma^2 \right\}$$

$$\frac{SSE}{\sigma^2} \sim \chi^2(n - \rho - 1)$$

## 제곱합의 분포

$$F_0 = \frac{MSR}{MSE} = \frac{(\frac{SSR}{\sigma^2}) / k}{(\frac{SSE}{\sigma^2}) / (n - k - 1)} \sim F'(k, n - k - 1, \lambda)$$

where

$$\lambda = \boldsymbol{\beta}^\top \mathbf{X}^\top \left( I_n - \frac{\mathbf{J}_n}{n} \right) \mathbf{X} \boldsymbol{\beta} / 2\sigma^2$$