

$$\frac{y - \bar{y}}{SD_y} = r \frac{x - \bar{x}}{SD_x}$$

$$y = \alpha + \beta x$$

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

$$\sum_i (x_i - \bar{x})(y_i - \bar{y}) = \sum_i x_i (y_i - \bar{y}) = \sum_i (x_i - \bar{x}) y_i$$

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

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}} = r_{xy} \left( \frac{S_{yy}}{S_{xx}} \right)^{1/2}$$

$$S_{xy} = \sum (x_i - \bar{x})(y_i - \bar{y}),$$

$$S_{xx} = \sum (x_i - \bar{x})^2, \quad S_{yy} = \sum (y_i - \bar{y})^2,$$

$$r_{xy} = \frac{S_{xy}}{\sqrt{(S_{xx})(S_{yy})}} \quad (\text{the sample correlation})$$

Fitted value

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i.$$

Residual

$$r_i = y_i - \hat{y}_i \quad \sum_i r_i = 0, \quad \sum_i r_i x_i = 0.$$

$$RSS = \sum_{i=1}^n r_i^2$$

$$\hat{\sigma}^2 = \frac{RSS}{n-p}$$

$$TSS \quad R^2 = r_{xy}^2$$

$$\sum_i (y_i - \bar{y})^2 = \sum_i (y_i - \hat{y}_i + \hat{y}_i - \bar{y})^2 = \sum_i (r_i + \hat{y}_i - \bar{y})^2$$

$$= \sum_i r_i^2 + \sum_i (\hat{y}_i - \bar{y})^2$$

$$= RSS + FSS,$$

$$R^2 = \frac{\sum (\hat{y}_i - \bar{y})^2}{\sum (y_i - \bar{y})^2} = \frac{FSS}{TSS} = \frac{TSS - RSS}{TSS} = 1 - \frac{RSS}{TSS}$$

Regression Through the Origin

$$\sum_i y_i^2 = \sum_i (y_i - \hat{y}_i + \hat{y}_i)^2 = \sum_i (y_i - \hat{y}_i)^2 + \sum_i \hat{y}_i^2$$

$$\hat{\beta}_1 = \frac{\sum_i x_i y_i}{\sum_i x_i^2} \quad \tilde{R}^2 = \frac{\sum_i \hat{y}_i^2}{\sum_i y_i^2} = 1 - \frac{RSS}{\sum_i y_i^2}$$

Properties of LS Estimates

$$\mathbb{E}[y_i | x_i] = \beta_0 + \beta_1 x_i, \quad \text{Cov}[y_i, y_j | x_i, x_j] = \sigma^2 \delta_{ij}$$

$$\delta_{ij} = 1 \text{ if } i = j \text{ and } 0 \text{ if } i \neq j.$$

unbiased

$$\hat{\beta}_1 = \sum_i \frac{(x_i - \bar{x})}{S_{xx}} y_i = \sum_i c_i y_i, \quad \sum_i c_i = 0$$

$$\mathbb{E} \hat{\beta}_1 = \sum_i c_i \mathbb{E} y_i = \sum_i c_i (\beta_0 + \beta_1 x_i) = \beta_1 \left( \sum_i c_i x_i \right) = \beta_1$$

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

$$\mathbb{E} \hat{\beta}_0 = \left( \frac{1}{n} \sum_i \mathbb{E} y_i \right) - \bar{x} \cdot \mathbb{E} \hat{\beta}_1 = \beta_0 + \beta_1 \bar{x} - \beta_1 \bar{x} = \beta_0$$

$$\text{Var}(\hat{\beta}_1) = \text{Var}\left(\sum_i c_i y_i\right) = \sigma^2 \sum_i c_i^2 = \sigma^2 \frac{1}{S_{xx}}$$

$$\text{Var}(\hat{\beta}_0) = \sigma^2 \left( \frac{1}{n} + \frac{\bar{x}^2}{S_{xx}} \right)$$

$$y_i \text{ indep. } \sim N(\beta_0 + \beta_1 x_i, \sigma^2) \quad e_i \text{ iid } \sim N(0, \sigma^2)$$

Multiple Linear Regression (MLR)

Least Squares Estimation

$$\mathbf{y}_{n \times 1} = \mathbf{X}_{n \times p} \boldsymbol{\beta}_{p \times 1} + \mathbf{e}_{n \times 1}, \quad \mathbf{e} \sim N_n(\mathbf{0}, \sigma^2 \mathbf{I}_n)$$

$$RSS = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^t (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

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

$$= \frac{1}{n \sum x_i^2 - (n\bar{x})^2} \begin{pmatrix} \sum x_i^2 & -n\bar{x} \\ -n\bar{x} & n \end{pmatrix} \begin{pmatrix} n\bar{y} \\ \sum x_i y_i \end{pmatrix}$$

$$\hat{\beta}_1 = \frac{-n^2 \bar{x} \bar{y} + n \sum x_i y_i}{n \sum x_i^2 - (n\bar{x})^2} = \frac{\sum x_i y_i - n\bar{x} \bar{y}}{\sum x_i^2 - n\bar{x}^2} = \frac{S_{xy}}{S_{xx}}$$

Fitted value

$$\hat{\mathbf{y}}_{n \times 1} = \mathbf{X} \hat{\boldsymbol{\beta}} = \mathbf{X} (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbf{y} = \mathbf{H}_{n \times n} \mathbf{y}_{n \times 1}$$

$$\text{Residuals } \mathbf{r}_{n \times 1} = \mathbf{y} - \hat{\mathbf{y}} = (\mathbf{I} - \mathbf{H}) \mathbf{y}.$$

$$\text{normal equation } \mathbf{X}^t (\mathbf{y} - \mathbf{X} \hat{\boldsymbol{\beta}}) = \mathbf{0}.$$

$$\mathbf{r} = \mathbf{y} - \mathbf{X} \hat{\boldsymbol{\beta}} \text{ satisfies } \mathbf{X}^t \mathbf{r} = \mathbf{0} \quad \hat{\mathbf{y}}^t \mathbf{r} = \hat{\boldsymbol{\beta}}^t \mathbf{X}^t \mathbf{r} = \mathbf{0}$$

$\mathbf{r}$  is orthogonal to each column of  $\mathbf{X}$  and  $\hat{\mathbf{y}}$ .

The Hat Matrix

$$\mathbf{H}_{n \times n} = \mathbf{X} (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \quad \mathbf{H} \mathbf{X} = \mathbf{X} (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbf{X} = \mathbf{X}$$

$$\text{Symmetric: } \mathbf{H}^t = [\mathbf{X} (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t]^t = \mathbf{X} (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t = \mathbf{H}$$

$$\text{Idempotent}^a: \mathbf{H} \mathbf{H} = \mathbf{H} \mathbf{H}^t = \mathbf{H} \quad \mathbf{H} (\mathbf{I} - \mathbf{H}) = \mathbf{0}_{n \times n}.$$

$$\mathbb{E}(\hat{\boldsymbol{\beta}}) = \mathbb{E}(\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbf{y}$$

$$= (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbb{E} \mathbf{y}$$

$$= (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbf{X} \boldsymbol{\beta} = \boldsymbol{\beta}$$

$$\text{Cov}(\hat{\boldsymbol{\beta}}) = (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \text{Cov}(\mathbf{y}) [(\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t]^t$$

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

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

$$\mathbb{E}(\hat{\mathbf{y}}) = \mathbf{X} \boldsymbol{\beta}, \quad \text{Cov}(\hat{\mathbf{y}}) = \sigma^2 \mathbf{H};$$

$$\mathbb{E}(\mathbf{r}) = \mathbf{0}, \quad \text{Cov}(\mathbf{r}) = \sigma^2 (\mathbf{I}_n - \mathbf{H})$$

$$\mathbb{E}(\hat{\sigma}^2) = \frac{1}{n-p} \mathbb{E} \mathbf{r}^t \mathbf{r} = \frac{1}{n-p} \text{tr}[\mathbb{E} \mathbf{r}^t \mathbf{r}] = \frac{1}{n-p} \text{tr}[\mathbb{E} \mathbf{r} \mathbf{r}^t] = \sigma^2$$

Distributions of LS Estimates  $\mathbf{y} \sim N_n(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}_n)$

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbf{y} \sim N_p(\boldsymbol{\beta}, \sigma^2 (\mathbf{X}^t \mathbf{X})^{-1})$$

$$\hat{\mathbf{y}} = \mathbf{H} \mathbf{y} \sim N_n(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{H})$$

$$\mathbf{r} = (\mathbf{I}_n - \mathbf{H}) \mathbf{y} \sim N_n(\mathbf{0}, \sigma^2 (\mathbf{I}_n - \mathbf{H}))$$

$$\mathbb{E} \hat{\mathbf{y}} = \mathbf{H} \mathbb{E} \mathbf{y} = \mathbf{H} \mathbf{X} \boldsymbol{\beta} = \mathbf{X} \boldsymbol{\beta} \quad \text{Cov}(\hat{\mathbf{y}}) = \mathbf{H} \sigma^2 \mathbf{H}^t = \sigma^2 \mathbf{H}$$

$$\mathbb{E} \mathbf{r} = (\mathbf{I}_n - \mathbf{H}) \mathbf{X} \boldsymbol{\beta} = \mathbf{0} \quad \text{Cov}(\mathbf{r}) = (\mathbf{I}_n - \mathbf{H}) \sigma^2 (\mathbf{I}_n - \mathbf{H})^t = \sigma^2 (\mathbf{I}_n - \mathbf{H})$$

$$\hat{\sigma}^2 = \frac{\|\mathbf{r}\|^2}{n-p} \sim \sigma^2 \frac{\chi_{n-p}^2}{n-p}$$

Source	df	SS	MS	F
Regression	$p-1$	FSS	$FSS/(p-1)$	$MS(\text{reg})/MS(\text{err})$
Error	$n-p$	RSS	$RSS/(n-p)$	
Total	$n-1$	TSS		
$\frac{MS(\text{reg})}{MS(\text{err})} \sim F_{(p-1), n-p}$				

Nested Models

$$F = \frac{(RSS_0 - RSS_a)/q}{RSS_a/(n-p)} \sim F_{q, n-p}$$

# ANCOVA

$$y = \beta_0 + \beta_1 x + \beta_2 d + \beta_3 (x \cdot d) + e = \begin{cases} \beta_0 + \beta_1 x + e, \\ (\beta_0 + \beta_2) + (\beta_1 + \beta_3)x + e, \end{cases}$$

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & x_1 & 0 \\ 1 & 0 & x_2 & 0 \\ 1 & 1 & x_3 & x_3 \\ 1 & 1 & x_4 & x_4 \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_2 \\ \beta_1 \\ \beta_3 \end{pmatrix}$$

categorical variable  $D$  produces an additive change in  $Y$  and also changes the effect of  $X$  on  $Y$

$$\frac{(\text{RSS}_0 - \text{RSS}_a)/(k-1)}{\text{RSS}_A/(n-p_A)} = \frac{(\text{RSS}_0 - \text{RSS}_a)/(k-1)}{\hat{\sigma}_A^2}$$

which follows  $F_{k-1, n-p_A}$  under the null, where  $\text{RSS}_A$  denotes the

RSS from the biggest model  $Y \sim X + D + X:D$  and  $p_A = 2k$ .

`anova(lm(Y ~ X + D + X:D))`

$H_0$	$H_a$
$Y \sim 1$	$Y \sim X$
$Y \sim X$	$Y \sim X + D$
$Y \sim X + D$	$Y \sim X + D + X:D$

Parallel regression lines

$$y = \beta_0 + \beta_2 d + \beta_1 x + e$$

$\beta_2$ : measures the **change** of the additive effect

Regression lines with equal intercepts but different slopes:

$$y = \beta_0 + \beta_1 x + \beta_3 (x \cdot d) + e$$

$\beta_3$ : measures the **change** of the slope.

$$\mathbf{x}_*^t (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{x}_* = \frac{1}{n} + \frac{1}{n-1} (\mathbf{z}^* - \bar{\mathbf{z}})^t \hat{\Sigma}^{-1} (\mathbf{z}^* - \bar{\mathbf{z}}),$$

which is the so-called **Mahalanobis distance** from  $\mathbf{x}_i$  to the center of the

## The QR Decomposition (\*)

How is the LS estimate  $\hat{\beta}$  solved in R? Denote the QR decomposition of  $\mathbf{X}$  as

$$\mathbf{X}_{n \times p} = \mathbf{Q}_{n \times p} \mathbf{R}_{p \times p}$$

where  $\mathbf{Q}$  is an orthogonal matrix (i.e.,  $\mathbf{Q}^t \mathbf{Q} = \mathbf{I}_p$ ) and  $\mathbf{R}$  is an upper triangular matrix, i.e., all the entries in  $\mathbf{R}$  below the diagonal are equal to 0.

$$\begin{aligned} \hat{\beta} &= (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbf{y} \\ (\mathbf{X}^t \mathbf{X})^{-1} &= (\mathbf{R}^t \mathbf{R})^{-1} = \mathbf{R}^{-1} (\mathbf{R}^t)^{-1} \\ \hat{\beta} &= \mathbf{R}^{-1} \mathbf{Q}^t \mathbf{y} \\ \mathbf{R} \hat{\beta} &= \mathbf{Q}^t \mathbf{y} \end{aligned}$$

## Gram-Schmidt (\*)

One method for computing the QR decomposition is the *Gram-Schmidt* algorithm. Let's work with a matrix

$$\mathbf{A}_{n \times p} = [\mathbf{a}_1 \mid \mathbf{a}_2 \mid \cdots \mid \mathbf{a}_p],$$

where  $\mathbf{a}_j$  denotes the  $j$ th column of  $\mathbf{A}$ . Then

$$\begin{aligned} \bullet \mathbf{e}_1 &= \mathbf{a}_1, \quad \mathbf{u}_1 = \frac{\mathbf{e}_1}{\|\mathbf{e}_1\|} \\ \bullet \mathbf{e}_2 &= \mathbf{a}_2 - (\mathbf{a}_2^t \mathbf{u}_1) \mathbf{u}_1, \quad \mathbf{u}_2 = \frac{\mathbf{e}_2}{\|\mathbf{e}_2\|} \\ \bullet \dots \\ \bullet \mathbf{e}_{k+1} &= \mathbf{a}_{k+1} - \sum_{j=1}^k (\mathbf{a}_{k+1}^t \mathbf{u}_j) \mathbf{u}_j, \quad \mathbf{u}_{k+1} = \frac{\mathbf{e}_{k+1}}{\|\mathbf{e}_{k+1}\|} \end{aligned}$$

The resulting QR decomposition is

$$\mathbf{A} = [\mathbf{a}_1 \mid \mathbf{a}_2 \mid \cdots \mid \mathbf{a}_p] = [\mathbf{u}_1 \mid \cdots \mid \mathbf{u}_p] \mathbf{R} = \mathbf{Q} \mathbf{R}.$$

- Affine transformations:**  $\mathbf{W} = \mathbf{a}_{n \times 1} + \mathbf{B}_{n \times m} \mathbf{Z}$ ,

$$\mathbb{E}[\mathbf{W}] = \mathbf{a} + \mathbf{B} \boldsymbol{\mu}, \quad \text{Cov}(\mathbf{W}) = \mathbf{B} \boldsymbol{\Sigma} \mathbf{B}^t.$$

Especially, for  $W = v_1 Z_1 + \cdots + v_m Z_m = \mathbf{v}^t \mathbf{Z}$ ,

$$\mathbb{E}[W] = \mathbf{v}^t \boldsymbol{\mu} = \sum_{i=1}^m v_i \mu_i,$$

$$\text{Var}(W) = \mathbf{v}^t \boldsymbol{\Sigma} \mathbf{v} = \sum_{i=1}^m v_i^2 \text{Var}(Z_i) + 2 \sum_{i < j} v_i v_j \text{Cov}(Z_i, Z_j)$$

## Joint Confidence Region

## Hypothesis Testing

$$t = \frac{\hat{\beta}_j - c}{\text{se}(\hat{\beta}_j)} = \frac{\hat{\beta}_j - c}{\hat{\sigma} \sqrt{[(\mathbf{X}^t \mathbf{X})^{-1}]_{jj}}} \sim T_{n-p} \quad \text{SLR} \quad \frac{\hat{\beta}_1 - c}{\text{se}(\hat{\beta}_1)} = \frac{\hat{\beta}_1 - c}{\hat{\sigma} / \sqrt{S_{xx}}} \sim T_{n-2}$$

$$(\hat{\beta}_j \pm t_{n-p}^{(\alpha/2)} \text{se}(\hat{\beta}_j))$$

$$\text{CI} \quad \hat{\beta}_0 + \hat{\beta}_1 x_* \pm t_{n-2}^{(\alpha/2)} \hat{\sigma} \sqrt{\frac{1}{n} + \frac{(x_* - \bar{x})^2}{S_{xx}}}$$

$$\text{PI} \quad \hat{\beta}_0 + \hat{\beta}_1 x_* \pm t_{n-2}^{(\alpha/2)} \hat{\sigma} \sqrt{1 + \frac{1}{n} + \frac{(x_* - \bar{x})^2}{S_{xx}}}$$

$$\text{se}(\hat{\mu}^*) = \hat{\sigma} \sqrt{(\mathbf{x}^*)^t (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{x}^*}.$$

$$\text{se}(\hat{y}^*) = \hat{\sigma} \sqrt{1 + (\mathbf{x}^*)^t (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{x}^*}.$$

The Gauss-Markov theorem tells us that the BLUE of  $\mu^*$  is

$$\hat{\theta}_{LS} = \mathbf{c}^t \hat{\boldsymbol{\beta}} \quad \hat{\mu}^* = (\mathbf{x}^*)^t \hat{\boldsymbol{\beta}}^t = (\mathbf{x}^*)^t (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{X}^t \mathbf{y}.$$

This is just a linear transformation of  $\mathbf{y}$ , so we can easily derive its variance, and find its standard error.

$$\text{se}(\hat{\mu}^*) = \hat{\sigma} \sqrt{(\mathbf{x}^*)^t (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{x}^*}.$$

A CI for  $\mu^*$  is given by

$$(\hat{\mu}^* - t_{n-p}^{(\alpha/2)} \text{se}(\hat{\mu}^*), \hat{\mu}^* + t_{n-p}^{(\alpha/2)} \text{se}(\hat{\mu}^*)).$$

Just as we can use estimated standard errors and  $t$ -stats to form confidence intervals for a single parameter, we can also obtain a  $(1 - \alpha) \times 100\%$  confidence region for the entire vector  $\boldsymbol{\beta}$ . In particular

$$\boldsymbol{\beta} - \hat{\boldsymbol{\beta}} \sim N(0, \sigma^2 (\mathbf{X}^t \mathbf{X})^{-1}).$$

Thus, the quadratic form

$$\frac{(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})^t \mathbf{X}^t \mathbf{X} (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})}{p \hat{\sigma}^2} \sim F_{p, n-p}.$$

## Simultaneous CIs/PIs

- Consider a simple linear regression  $y_i = \beta_0 + \beta_1 x_i + e_i$ .
- Given a new value  $x^*$ , the  $(1 - \alpha)$  CI for  $\mu^* = \beta_0 + \beta_1 x^*$  is

$$I(x^*) = \left( \hat{\mu}^* \pm t_{n-2}^{(\alpha/2)} \text{se}(\hat{\mu}^*) \right),$$

where

$$\hat{\mu}^* = \hat{\beta}_0 + \hat{\beta}_1 x^*, \quad \text{se}(\hat{\mu}^*) = \hat{\sigma} \sqrt{\frac{1}{n} + \frac{(x^* - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2}}.$$