

HW1 grading  
Quiz 1 → solution  
PS2 is posted  
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## Lecture 7

Vector representation of MLR continued,  
[ assessing the impact of Gaussian residuals assumption ]

# MLR model expressed in vector notation

We have for each subject  $i, i=1, \dots, n$

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \dots + \beta_p X_{pi} + \varepsilon_i$$

$\mu_i$

error residual

$$\begin{matrix} 1 \\ 2 \\ \vdots \\ n \end{matrix} \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \beta_0 + \beta_1 \begin{pmatrix} X_{11} \\ X_{12} \\ \vdots \\ X_{1n} \end{pmatrix} + \beta_2 \begin{pmatrix} X_{21} \\ X_{22} \\ \vdots \\ X_{2n} \end{pmatrix} + \dots + \beta_p \begin{pmatrix} X_{p1} \\ X_{p2} \\ \vdots \\ X_{pn} \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_p \end{pmatrix}$$

$$\vec{Y}_{n \times 1} = \frac{1}{n} \beta_0 + \beta_1 \vec{X}_{1 \times n} + \beta_2 \vec{X}_{2 \times n} + \dots + \beta_p \vec{X}_{p \times n} + \vec{\varepsilon}_{n \times 1} \rightarrow$$

$$\vec{Y}_{n \times 1} = \begin{pmatrix} 1 & X_1 & X_2 & \dots & X_p \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix} + \vec{\varepsilon}_{n \times 1}$$

$X_{n \times (p+1)}$  design matrix

$\begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}_{p+1 \times 1}$

# MLR model expressed in vector notation

$$\Rightarrow \underset{\sim}{Y}_{n \times 1} = \underset{\sim}{X}_{n \times (p+1)} \underset{\sim}{\beta}_{(p+1) \times 1} + \underset{\sim}{\varepsilon}_{n \times 1}$$

Say  $n=3, p=2 \Rightarrow Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \varepsilon_i$

$$\underset{\sim}{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \end{pmatrix} \quad \underset{\sim}{X} = \begin{bmatrix} \underline{1} & X_{11} & X_{21} \\ 1 & X_{12} & X_{22} \\ 1 & X_{13} & X_{23} \end{bmatrix} \quad \underset{\sim}{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix} \quad \underset{\sim}{\varepsilon} = \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \end{pmatrix}$$

$$\underset{\sim}{X}_{3 \times 3} \underset{\sim}{\beta}_{3 \times 1} = \begin{pmatrix} 1 \cdot \beta_0 + \beta_1 X_{11} + \beta_2 X_{21} \\ 1 \cdot \beta_0 + \beta_1 X_{12} + \beta_2 X_{22} \\ 1 \cdot \beta_0 + \beta_1 X_{13} + \beta_2 X_{23} \end{pmatrix}_{3 \times 1} = \underset{\sim}{\mu}_{3 \times 1}$$

Defines  
the  
mean  
of  $Y_i$   
for  
each  
 $i$

# MLR model expressed in vector notation

What about distribution of  $\underline{\varepsilon}$ ? and  $\underline{y}$ ?

In general, we can define the multivariate normal distribution as:  $\underline{y} \sim \text{MVN}(\underline{\mu}, \underline{V})$

where  $\underline{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$   $\underline{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_n \end{pmatrix}$   $\underline{V} = \begin{bmatrix} v_{11} & v_{12} & \dots & v_{1n} \\ v_{21} & v_{22} & \dots & v_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ v_{n1} & v_{n2} & \dots & v_{nn} \end{bmatrix}$

$v_{ii} = \text{Var}(y_i)$   
 $v_{ij} = v_{ji} = \text{Cov}(y_i, y_j)$

If  $\varepsilon_i \sim N(0, \sigma^2)$ , independent

$$\underline{\varepsilon} \sim \text{MVN}(\underline{0}, \sigma^2 \underline{I})$$

$\underline{I} = \begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix}$  identity matrix

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

$$\underline{V} = \begin{bmatrix} \sigma^2 & & 0 \\ & \ddots & \\ 0 & & \sigma^2 \end{bmatrix}$$

## MLE or LS solution expressed in vector notation

$$\text{MLR model: } \underset{\sim}{Y} = \underset{\sim}{X} \underset{\sim}{\beta} + \underset{\sim}{\varepsilon}, \quad \underset{\sim}{\varepsilon} \sim \text{MVN}(\underset{\sim}{0}, \sigma^2 \underset{\sim}{I})$$

MLE or least squares: Going to drop the " $\sim$ "  
Choose  $\hat{\beta}$  and  $\hat{\sigma}^2$  to minimize  $\sum_{i=1}^n (y_i - x_i \beta)^2$

$$\sum_{i=1}^n (y_i - x_i \beta)^2 = (\underset{1 \times n}{Y} - \underset{n \times 1}{X} \beta) (\underset{n \times 1}{Y} - \underset{n \times 1}{X} \beta)$$

$$U_{\beta}(\beta) = \frac{d}{d\beta} (\underset{1 \times n}{Y} - \underset{n \times 1}{X} \beta)' (\underset{n \times 1}{Y} - \underset{n \times 1}{X} \beta)$$

$$= X' (Y - X\beta)$$

$$\text{Set to 0, solve for } \hat{\beta} = (X'X)^{-1} X'Y$$

$y_i = i^{\text{th row of } Y}$   
 $(y_1 - \mu_1, y_2 - \mu_2) \dots (y_n - \mu_n)$   
 $(y_1 - \mu_1)^2 + (y_2 - \mu_2)^2 + \dots$

SLR  
 $\hat{\beta}_1 = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2}$

## Predicted values and residuals in vector notation


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

$$\hat{Y} = X\hat{\beta} = \underbrace{X(X'X)^{-1}X'}_{\substack{n \times (p+1) \quad \text{Hat matrix: } H}} y = HY \quad \begin{matrix} n \times n & n \times 1 \end{matrix}$$

$$\hat{R} = y - \hat{Y} = y - HY = (I - H)y$$

$$\hat{y}_i = \sum_{j=1}^n h_{ij} y_j$$

hat



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## Distribution of $\hat{\beta}$

Note that if  $\underline{Y} \sim \text{MVN}(\underline{\mu}, V)$ , then

$$\underline{AY} \sim \text{MVN}(A\underline{\mu}, \underline{AVA'})$$

$$\hat{\beta} = \underbrace{(X'X)^{-1}X'}_A Y$$

$$\begin{aligned} A' &= [(X'X)^{-1}X']' \\ &= X(X'X)^{-1} \end{aligned}$$

$$E(\hat{\beta}) = E(AY) = E((X'X)^{-1}X'Y) = (X'X)^{-1}X'E(Y) \\ = (X'X)^{-1}X'X\beta = \beta$$

$$\text{Var}(\hat{\beta}) = \text{Var}(AY) =$$

$$(X'X)^{-1}X' \sigma^2 I X(X'X)^{-1}$$

$$\sigma^2 (X'X)^{-1} \underbrace{X'X}_{\text{SLR}} \underbrace{(X'X)^{-1}}_{\hat{\beta}_1 = \sigma^2 / \text{SSX}} = \sigma^2 (X'X)^{-1}$$

## Distribution of $\hat{Y}$

$$\hat{Y} = X\hat{\beta} = X(X'X)^{-1}X'Y = \underline{H}Y$$

$$\hat{Y} \sim \text{MVN}(X\beta, \sigma^2 H)$$

$$E(\hat{Y}) = HE(Y) = HX\beta = X\underbrace{(X'X)^{-1}X'}_I X\beta = X\beta$$

$$\text{Var}(\hat{Y}) = H\text{Var}(Y)H' =$$

$$X(X'X)^{-1}X'\sigma^2 I X(X'X)^{-1}X'$$

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

$$= \sigma^2 X(X'X)^{-1}X' = \sigma^2 H$$





## Properties of the Hat matrix

1) hat matrix is symmetric

$$H' = \left[ X (X'X)^{-1} X' \right]' = X (X'X)^{-1} X'$$

2) hat matrix is idempotent :  $H \cdot H = H$



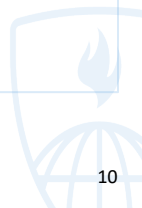
## Distribution of $\hat{R}$

$$\hat{R} = Y - \hat{Y} = Y - HY = \underbrace{(I - H)}_A Y$$

$$\hat{R} \sim \text{MVN}()$$

$$E(\hat{R}) = E(Y - \hat{Y}) = X\beta - X\beta = 0$$

$$\text{Var}(\hat{R}) = \sigma^2 (I - H)$$

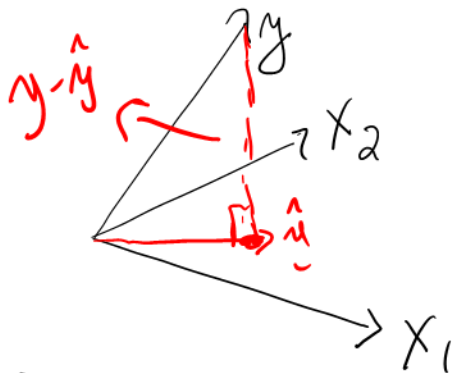


## Relationship between $\hat{Y}$ and $\hat{R}$

$$\begin{aligned}\text{Cov}(\hat{Y}, \hat{R}) &= E \left[ \underbrace{HY}_{HY} \underbrace{\{(I-H)Y\}'}_{(I-H)Y} \right] \\ &= E \left[ HY Y' (I-H) \right] \\ &= H E(Y Y') (I-H) \\ &= H \sigma^2 I (I-H) \\ &= \sigma^2 \underbrace{(H)(I-H)} = 0\end{aligned}$$

# Geometry of least squares

Consider  $y \sim_{n \times 1}$ ,  $X_1 \sim_{n \times 1}$ ,  $X_2 \sim_{n \times 1}$



H projects  $y$  onto the plane spanned by  $X_1, X_2$   
 $\Rightarrow \hat{y} = Hy = X\hat{\beta}$

- 1) minimize the distance between  $y$  and  $\hat{y} = X\hat{\beta}$
- 2) Shortest distance is the one that has a right angle between the predicted value and residual
- 3) residual is orthogonal to the plane spanned by  $X$
- 4) Score equations:  $X'(y - X\hat{\beta}) = 0$

# Simulation study

- ▶ We derived the distribution of the estimated regression coefficients assuming the residuals were Gaussian.
- ▶ Does approximate normality of the estimated regression coefficients hold even when the residuals are non-Gaussian?

$$\hat{\beta} \sim \text{MVA}(\beta, \sigma^2 (X'X)^{-1})$$

## Next time....

- ▶ Deriving the distribution of linear combinations of regression coefficients
- ▶ Deriving the distribution of non-linear combinations of regression coefficients using the Delta method
- ▶ LAB: You will generate the distribution of combinations of regression coefficients using bootstrap!

