

(1) 4/15/16 (F) : make-up. (tentative) - still look for a room  
2 - 3:45pm

(2) - Examples of the General Linear Model.

- Simple Regression : Example

(3) - One-way ANOVA

- Chapter 2: LSE & Linear Algebra.

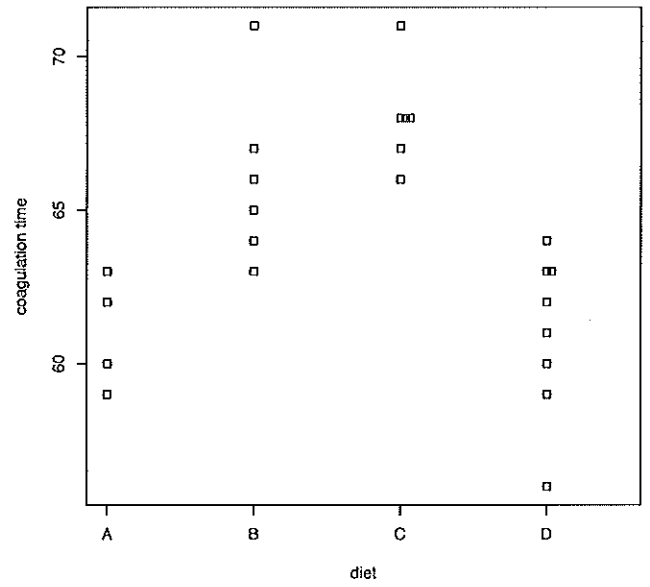
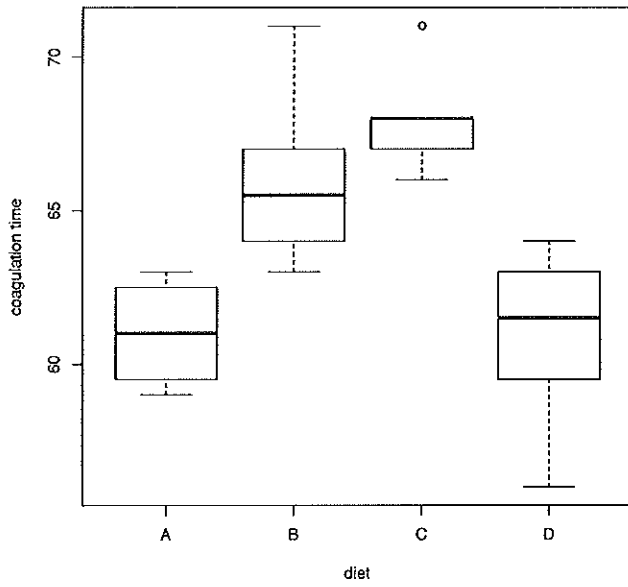
## One-Way ANOVA

in seconds

Dataset comes from a study of blood coagulation times. 24 animals were randomly assigned to four different diets and the samples were taken in a random order (taken from Linear Models with R, page 182)

```
> rm(list=ls(all=TRUE))
> library(faraway)
> data(coagulation)
>
> plot(coag~diet, coagulation, ylab="coagulation time")
> with(coagulation, stripchart(coag ~ diet, vertical=TRUE, metho
```

# One-Way ANOVA



# One-Way ANOVA – parameterization ~~3~~<sup>1</sup>

```

X > options(contrasts=c("contr.sum", "contr.poly"))
  > g2 <- lm(coag ~ diet, coagulation)
  > summary(g2)

```

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij}$$

$i=1, \dots, 4$

Call:

```
lm(formula = coag ~ diet, data = coagulation)
```

$$\sum \alpha_i = 0$$

Residuals:

$$\hat{\mu} = \text{estimated overall mean} = 64$$

Min	1Q	Median	3Q	Max
-5.00	-1.25	0.00	1.25	5.00

Coefficients:

the estimated mean response  
 for A =  $64 - 3 = \underline{61}$

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	64.0000	$\hat{\mu}$ 0.4979	128.537	< 2e-16 ***
diet1	-3.0000	$\hat{\alpha}_1$ 0.9736	-3.081	0.005889 **
diet2	2.0000	$\hat{\alpha}_2$ 0.8453	2.366	0.028195 *
diet3	4.0000	$\hat{\alpha}_3$ 0.8453	4.732	0.000128 ***

---  $\hat{\alpha}_4 = -\hat{\alpha}_1 - \hat{\alpha}_2 - \hat{\alpha}_3 = +3 - 2 - 4 = -3$

Signif. codes: 0 \*\*\* 0.001 \*\* 0.01 \* 0.05 . 0.1 1

Residual standard error: 2.366 on 20 degrees of freedom

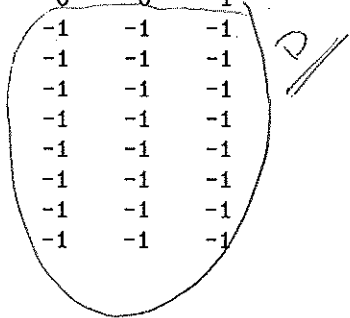
Multiple R-squared: 0.6706, Adjusted R-squared: 0.6212

F-statistic: 13.57 on 3 and 20 DF, p-value: 4.658e-05

# One-Way ANOVA – parameterization §1

```
       $\mu$     $\alpha_1$   $\alpha_2$   $\alpha_3$ 
> model.matrix(g2)
  (Intercept) diet1 diet2 diet3
 1           1     1     0     0
 2           1     1     0     0
 3           1     1     0     0
 4           1     1     0     0
 5           1     0     1     0
 6           1     0     1     0
 7           1     0     1     0
 8           1     0     1     0
 9           1     0     1     0
10          1     0     1     0
11          1     0     0     1
12          1     0     0     1
13          1     0     0     1
14          1     0     0     1
15          1     0     0     1
16          1     0     0     1
17          1    -1    -1    -1
18          1    -1    -1    -1
19          1    -1    -1    -1
20          1    -1    -1    -1
21          1    -1    -1    -1
22          1    -1    -1    -1
23          1    -1    -1    -1
24          1    -1    -1    -1
attr(,"assign")
[1] 0 1 1 1
attr(,"contrasts")
attr(,"contrasts")$diet
[1] "contr.sum"
```

$$\alpha_4 = -\alpha_1 - \alpha_2 - \alpha_3$$



# One-Way ANOVA – parameterization $\chi^2$

```
> g <- lm(coag ~ diet, coagulation)
> summary(g)
Call:
lm(formula = coag ~ diet, data = coagulation)
```

$$y_{ij} = \mu + \alpha_i + e_{ij}$$

$$\alpha_1 = 0$$

$$E(y_{ij}) = E(\mu + \alpha_i + e_{ij})$$

Residuals:

$$= \mu + 0 + 0$$

Min	1Q	Median	3Q	Max
-5.00	-1.25	0.00	1.25	5.00

$$= \mu$$

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	6.100e+01	1.183e+00	51.554	< 2e-16 ***
dietB	5.000e+00	1.528e+00	3.273	0.003803 **
dietC	7.000e+00	1.528e+00	4.583	0.000181 ***
dietD	2.991e-15	1.449e+00	0.000	1.000000

Signif. codes: 0 \*\*\* 0.001 \*\* 0.01 \* 0.05 . 0.1 1

Residual standard error: 2.366 on 20 degrees of freedom

Multiple R-squared: 0.6706, Adjusted R-squared: 0.6212

F-statistic: 13.57 on 3 and 20 DF, p-value: 4.658e-05

# One-Way ANOVA – parameterization 1/2

```
       $\mu$        $\alpha_2$   $\alpha_3$   $\alpha_4$ 
> model.matrix(g)
  (Intercept) dietB dietC dietD
 1           1     0     0     0
 2           1     0     0     0
 3           1     0     0     0
 4           1     0     0     0
 5           1     1     0     0
 6           1     1     0     0
 7           1     1     0     0
 8           1     1     0     0
 9           1     1     0     0
10           1     1     0     0
11           1     0     1     0
12           1     0     1     0
13           1     0     1     0
14           1     0     1     0
15           1     0     1     0
16           1     0     1     0
17           1     0     0     1
18           1     0     0     1
19           1     0     0     1
20           1     0     0     1
21           1     0     0     1
22           1     0     0     1
23           1     0     0     1
24           1     0     0     1
attr(,"assign")
[1] 0 1 1 1
attr(,"contrasts")
attr(,"contrasts")$diet
[1] "contr.treatment"
```

$$y = x\beta + e$$

## One-Way ANOVA – parameterization 2<sup>3</sup>

```
> g1 <- lm(coag ~ diet - 1, coagulation)
```

$$y_{ij} = \theta_i + e_{ij}$$

```
> summary(g1)
```

Call:

```
lm(formula = coag ~ diet - 1, data = coagulation)
```

Residuals:

Min	1Q	Median	3Q	Max
-5.00	-1.25	0.00	1.25	5.00

Coefficients:

	Estimate	Std. Error	t value	Pr(> t )
dietA	61.0000	1.1832	51.55	<2e-16 ***
dietB	66.0000	0.9661	68.32	<2e-16 ***
dietC	68.0000	0.9661	70.39	<2e-16 ***
dietD	61.0000	0.8367	72.91	<2e-16 ***

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.366 on 20 degrees of freedom

Multiple R-squared: 0.9989, Adjusted R-squared: 0.9986

F-statistic: 4399 on 4 and 20 DF, p-value: < 2.2e-16



# One-Way ANOVA – parameterization ~~2~~<sup>3</sup>

```
       $\theta_1$    $\theta_2$    $\theta_3$    $\theta_4$ 
> model.matrix(g1)
  dietA dietB dietC dietD
1      1      0      0      0
2      1      0      0      0
3      1      0      0      0
4      1      0      0      0
5      0      1      0      0
6      0      1      0      0
7      0      1      0      0
8      0      1      0      0
9      0      1      0      0
10     0      1      0      0
11     0      0      1      0
12     0      0      1      0
13     0      0      1      0
14     0      0      1      0
15     0      0      1      0
16     0      0      1      0
17     0      0      0      1
18     0      0      0      1
19     0      0      0      1
20     0      0      0      1
21     0      0      0      1
22     0      0      0      1
23     0      0      0      1
24     0      0      0      1
attr(,"assign")
[1] 1 1 1 1
attr(,"contrasts")
attr(,"contrasts")$diet
[1] "contr.treatment"
```

AMS 256  
Chapter 2: The Linear Least Squares Problem

Spring 2016

† Notation

1. Vectors: boldface lowercase.

e.g.  $\mathbf{a} = [a_1, \dots, a_n]^T \in \mathbb{R}^n$ ,  $\mathbf{x}$ ,  $\mathbf{y}$ ,  $\mathbf{z}$ ,  $\mathbf{1}$ ,  $\mathbf{0}$

2. Matrices: boldface uppercase.

e.g.  $\underbrace{\mathbf{A}}_{n \times m}$

$\mathbf{A}_j \in \mathbb{R}^n$ : the  $j^{\text{th}}$  column

3. Transpose:  $\mathbf{a}^T$ ,  $\mathbf{A}^T$

† Recall that the form of linear models is

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e},$$

- ▶  $\mathbf{y}$ :  $n \times 1$  vector of observations (random)
- ▶  $\mathbf{X}$ :  $n \times p$  matrix of known constants (*design* matrix)
- ▶  $\boldsymbol{\beta}$ :  $p \times 1$  vector of unobservable parameters
- ▶  $\mathbf{e}$ :  $n \times 1$  vector of unobservable random errors

† Goal: Inference about  $\beta$  and  $\sigma^2$

▶ point estimates

✓ Least squares estimates (**Chapters 2 & 3**):

↪ Find the best approximation of  $\mathbf{y}$  as a linear function of columns of  $\mathbf{X}$

✓ Best linear unbiased estimator (**Chapter 4**):

↪ Assume that  $E(\mathbf{e}) = \mathbf{0}$  and  $\text{Cov}(\mathbf{e}) = \sigma^2 I$  where  $\sigma^2$  is some unknown parameter (will be generalized to  $\text{Cov}(\mathbf{e}) = \sigma^2 \mathbf{V}$  where  $\mathbf{V}$  is a known positive definite matrix)

✓ MLE (**Chapter 5**)

↪ Assume a distribution for the  $\mathbf{e}$

† Goal: Inference about  $\beta$  and  $\sigma^2$  (Contd)

- ▶ tests
- ▶ confidence regions
- ▶ checking the assumptions, model selection

† Applications:

- ▶ Regression Analysis:  $\mathbf{X}^T \mathbf{X}$  is nonsingular (or close to singular)
- ▶ Analysis of Variance:  $\mathbf{X}^T \mathbf{X}$  is singular

\* Example 1: Simple linear regression

Consider the model

$$y_i = \beta_0 + \beta_1 x_i + e_i, \quad i = 1, \dots, n.$$

Write it in the form of linear models.

$$Y = X\beta + e$$

$$\Rightarrow \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix}$$

\* Example 2: Balanced One-Way ANOVA

Consider the model

$$y_{ij} = \mu + \alpha_i + e_{ij}, \quad i = 1, \dots, a \text{ and } j = 1, \dots, n.$$

Write it in the form of linear models.

$$y = X\beta + e$$

$$\Rightarrow \begin{bmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{1n} \\ \vdots \\ y_{an} \end{bmatrix} = \begin{bmatrix} 1_n & 1_n & 0_n & \dots & 0_n \\ 1_n & 0_n & 1_n & \dots & 0_n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1_n & 0_n & 0_n & \dots & 1_n \end{bmatrix} \begin{bmatrix} \mu \\ \alpha_1 \\ \vdots \\ \alpha_a \end{bmatrix} + \begin{bmatrix} e_{11} \\ e_{12} \\ \vdots \\ e_{an} \end{bmatrix}$$

$a n \times (a+1)$



\* Road map:

- Discuss least squares estimates (LSE) and its uniqueness
- Discuss the geometry associated with LSE

† Def

- ▶ (Length of a vector: Euclidean norm) The *length* of a vector  $\mathbf{x}$  is  $\|\mathbf{x}\| \equiv \sqrt{\mathbf{x}^T \mathbf{x}} = (\sum x_i^2)^{1/2}$
- ▶ (Distance between two vectors) The *distance* of two vectors  $\mathbf{x}$  and  $\mathbf{y}$  is a length of their difference, i.e.  $\|\mathbf{x} - \mathbf{y}\|$ .

† Least squares estimate: Find the closest (best) approximation  $\mathbf{X}\beta$  to the observed vector  $\mathbf{y}$  in the Euclidean manner,

$$Q(\beta) = \|\mathbf{y} - \mathbf{X}\beta\|^2 = (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta)$$
$$\Rightarrow \hat{\beta} = \arg \min_{\beta} (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta)$$

## The Least Squares Approach-1/3

★ How to find such  $\beta$ ? (least squares solution:  $\hat{\beta}$ )

$$\begin{aligned}Q(\beta) &= (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) \\&= (\mathbf{y}^T - \beta^T \mathbf{X}^T) (\mathbf{y} - \mathbf{X}\beta) \\&= \mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{X}\beta - \beta^T \mathbf{X}^T \mathbf{y} + \beta^T \mathbf{X}^T \mathbf{X}\beta\end{aligned}$$

- ★ Find the gradient vector
- ★ Set the gradient to zero

## The Least Squares Approach-2/3

\* How to find the gradient vector (Result 2.1)

Let  $\mathbf{a}$  and  $\mathbf{b}$  be  $p \times 1$  vectors and  $\mathbf{A}$  be a  $p \times p$  matrix of constants.  
Then

▶

$$\frac{\partial \mathbf{b}^T \mathbf{a}}{\partial \mathbf{b}} = \frac{\partial \mathbf{a}^T \mathbf{b}}{\partial \mathbf{b}} = \mathbf{a}.$$

▶

$$\frac{\partial \mathbf{b}^T \mathbf{A} \mathbf{b}}{\partial \mathbf{b}} = (\mathbf{A} + \mathbf{A}^T) \mathbf{b}.$$

Recall

$$Q(\beta) = \mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{X} \beta - \beta^T \mathbf{X}^T \mathbf{y} + \beta^T \mathbf{X}^T \mathbf{X} \beta.$$

$$\begin{aligned} \frac{\partial Q(\beta)}{\partial \beta} &= -(\mathbf{y}^T \mathbf{X})^T - \mathbf{X}^T \mathbf{y} + (\mathbf{X}^T \mathbf{X} + (\mathbf{X}^T \mathbf{X})^T) \beta \\ &= -2 \mathbf{X}^T \mathbf{y} + 2 \mathbf{X}^T \mathbf{X} \beta \end{aligned}$$

## The Least Squares Approach-3/3

$$Q(\beta) = \mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{X} \beta - \beta^T \mathbf{X}^T \mathbf{y} + \beta^T \mathbf{X}^T \mathbf{X} \beta.$$

\* Find the gradient vector

\* Set the gradient to zero

$$\cancel{\beta^T} \mathbf{X}^T \mathbf{X} \beta = \cancel{\beta^T} \mathbf{X}^T \mathbf{y}$$

$$\mathbf{X}^T \mathbf{X} \beta = \mathbf{X}^T \mathbf{y}$$

$$\frac{\partial Q}{\partial \beta} = \overbrace{-2\mathbf{X}^T \mathbf{y} + 2\mathbf{X}^T \mathbf{X} \beta} = -2\mathbf{X}^T (\mathbf{y} - \mathbf{X} \beta) = 0$$

$$\Rightarrow \mathbf{X}^T \mathbf{X} \beta = \mathbf{X}^T \mathbf{y} \quad \text{Normal Equations (NEs).}$$

Then solve the NEs for least squares solutions  $\hat{\beta}$ !

\* Example 1 (contd): Simple linear regression

Consider the model

$$y_i = \beta_0 + \beta_1 x_i + e_i, \quad i = 1, \dots, n.$$

Find the NEs.

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

$$\textcircled{1} X^T X = \begin{bmatrix} 1 & \dots & 1 \\ x_1 & \dots & x_n \end{bmatrix} \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} = \begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix}$$

$$\textcircled{2} X^T y = \begin{bmatrix} 1 & \dots & 1 \\ x_1 & \dots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \end{bmatrix}$$

$$\Rightarrow \underline{\text{NEs}} \quad \begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \end{bmatrix}$$

\* Example 2 (contd): Balanced One-Way ANOVA

Consider the model

$$y_{ij} = \mu + \alpha_i + e_{ij}, \quad i = 1, \dots, a \text{ and } j = 1, \dots, n.$$

Find the NEs.

NEs  $X^T X \beta = X^T y$

$$\textcircled{1} X^T X = \begin{bmatrix} \mathbf{1}_n^T & \mathbf{1}_n^T & \dots & \mathbf{1}_n^T \\ \mathbf{1}_n^T & \mathbf{0}_n^T & \dots & \mathbf{0}_n^T \\ \mathbf{0}_n^T & \mathbf{1}_n^T & \dots & \mathbf{0}_n^T \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_n^T & \mathbf{0}_n^T & \dots & \mathbf{1}_n^T \end{bmatrix} \begin{bmatrix} \mathbf{1}_n & \mathbf{1}_n & \mathbf{0}_n & \dots & \mathbf{0}_n \\ \mathbf{1}_n & \mathbf{0}_n & \mathbf{1}_n & \dots & \mathbf{0}_n \\ \mathbf{1}_n & \mathbf{0}_n & \mathbf{0}_n & \dots & \mathbf{0}_n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{1}_n & \mathbf{0}_n & \mathbf{0}_n & \dots & \mathbf{1}_n \end{bmatrix}$$

$\downarrow \mu$      $\downarrow \alpha_1$      $\downarrow \alpha_2$      $\downarrow \alpha_a$

$$= \begin{bmatrix} na & n & n & \dots & n \\ n & n & 0 & \dots & 0 \\ n & 0 & n & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ n & 0 & 0 & \dots & n \end{bmatrix} \quad (a+1) \times (a+1)$$

$$\textcircled{2} X^T y = \begin{bmatrix} \mathbf{1}_n^T & \mathbf{1}_n^T & \dots & \mathbf{1}_n^T \\ \mathbf{1}_n^T & \mathbf{0}_n^T & \dots & \mathbf{0}_n^T \\ \mathbf{0}_n^T & \mathbf{1}_n^T & \dots & \mathbf{0}_n^T \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0}_n^T & \mathbf{0}_n^T & \dots & \mathbf{1}_n^T \end{bmatrix} \begin{bmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{an} \end{bmatrix} = \begin{bmatrix} \sum y_{ij} \\ \sum y_{1j} \\ \sum y_{2j} \\ \vdots \\ \sum y_{aj} \end{bmatrix} \quad (a+1) \times 1$$

14/64

$$\begin{bmatrix} na & n & \dots & n \\ n & n & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ n & 0 & \dots & n \end{bmatrix} \begin{bmatrix} \mu \\ \alpha_1 \\ \vdots \\ \alpha_a \end{bmatrix} = \begin{bmatrix} \sum y_{ij} \\ \sum y_{1j} \\ \vdots \\ \sum y_{aj} \end{bmatrix}$$

- Normal Equations (NEs)

$$\mathbf{X}^T \mathbf{X} \boldsymbol{\beta} = \mathbf{X}^T \mathbf{y}.$$

↔ **Solving a system of equations,  $\mathbf{Ax} = \mathbf{c}$ .**

- If  $\mathbf{A}$  is nonsingular and square,  $\mathbf{A}^{-1}$  exists and  $\mathbf{A}^{-1}\mathbf{c}$  is the unique solution.
- If  $\mathbf{A}$  is singular or not square, then may not have a solution or infinitely many solutions.

→ **Questions**

- $\exists$  a solution?
- How to find a solution??



† Def **[Vector Space]**: A set  $\mathcal{S} \subset \mathbb{R}^n$  is a vector space if for any  $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbb{R}^n$  and scalar  $\alpha, \beta$ , operations of vector addition and scalar multiplication are defined such that

1.  $(\mathbf{x} + \mathbf{y}) + \mathbf{z} = \mathbf{x} + (\mathbf{y} + \mathbf{z})$
2.  $\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}$
3. There exists a vector  $\mathbf{0} \in \mathcal{S}$  such that  $\mathbf{x} + \mathbf{0} = \mathbf{x} = \mathbf{0} + \mathbf{x}$  for any  $\mathbf{x} \in \mathcal{S}$
4. For any  $\mathbf{x} \in \mathcal{S}$ , there exists  $\mathbf{y} \equiv -\mathbf{x}$  such that  $\mathbf{x} + \mathbf{y} = \mathbf{0} = \mathbf{y} + \mathbf{x}$
5.  $\alpha(\mathbf{x} + \mathbf{y}) = \alpha\mathbf{x} + \alpha\mathbf{y}$
6.  $(\alpha + \beta)\mathbf{x} = \alpha\mathbf{x} + \beta\mathbf{x}$
7.  $(\alpha\beta)\mathbf{x} = \alpha(\beta\mathbf{x})$
8. There exists a scalar  $\xi$  such that  $\xi\mathbf{x} = \mathbf{x}$ . (Typically  $\xi = 1$ )

† Def **[Vector Space]**: in layman's terms,

- ▶ A vector space  $\mathcal{S} \subset \mathbb{R}^n$  is a set of vectors
- ▶ closed under addition and scalar multiplication, that is,  
if  $\mathbf{x}$  and  $\mathbf{y} \in \mathcal{S}$ , then  $\alpha\mathbf{x} + \beta\mathbf{y} \in \mathcal{S}$
- ▶ Contain the vector  $\mathbf{0}$ .

- Ex:  $\mathbb{R}^3 = \{[x, y, z]^T \mid x, y, z \in \mathbb{R}\}$

$$\begin{array}{c}
 \text{y} \\
 \text{n} \times 1
 \end{array}
 =
 \begin{array}{c}
 \text{X} \beta \\
 \text{n} \times \text{p} \quad \text{p} \times 1
 \end{array}
 +
 \begin{array}{c}
 \text{e} \\
 \text{n} \times 1
 \end{array}$$

† Def **[Subspace]**: Let  $\mathcal{S}$  be a vector space, and let  $\mathcal{M}$  be a set with  $\mathcal{M} \subset \mathcal{S}$ .  $\mathcal{M}$  is a subspace of  $\mathcal{S}$  if and only if  $\mathcal{M}$  is a vector space.

M:

- Ex:  $\{[x, y, 0]^T \mid x, y \in \mathbb{R}\}$ : subspace of  $\mathbb{R}^3$  consisting of the  $x - y$  plane

♠ Note: Let  $\mathcal{S}$  be a vector space and let  $\mathbf{x}_1, \dots, \mathbf{x}_r \in \mathcal{S}$ . The set of all linear combinations of  $\mathbf{x}_1, \dots, \mathbf{x}_r$  is a subspace of  $\mathcal{S}$ ;

$$\mathcal{M} = \{ \mathbf{y} \mid \mathbf{y} = \sum c_j \mathbf{x}_j, c_1, \dots, c_r \text{ coefficients} \} \subset \mathcal{S}.$$

The space spanned by the vectors  $x_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$  and  $x_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

consists of vectors  $\begin{bmatrix} a \\ b \end{bmatrix}$ ,  $a, b \in \mathbb{R}$

† Def **[Spanning]**: The set of all linear combinations of  $x_1, \dots, x_r \in \mathcal{S}$  is called the space spanned by  $x_1, \dots, x_r$ . If  $\mathcal{M}$  is a subspace of  $\mathcal{S}$  and  $\mathcal{M}$  equals the space spanned by  $x_1, \dots, x_r$ , then  $\{x_1, \dots, x_r\}$  is called a spanning set for  $\mathcal{M}$ .

† Def **[Column Space]**: The column space of a  $m \times n$  matrix  $\mathbf{A}$ , denoted by  $C(\mathbf{A})$  is the vector space spanned by the columns of the matrix, that is,

$$x_{\beta}$$

$$C(\mathbf{A}) = \{x : \text{there exists a vector } c \text{ such that } \mathbf{Ax} = \mathbf{Ac}\}.$$

In layman's terms, if  $x \in C(\mathbf{A})$ , then  $x$  is a linear combination of columns of  $\mathbf{A}$  (consisting of all vectors (dimension  $m$ ) formed by multiplying  $\mathbf{A}$  by any vector).

$$A = \begin{bmatrix} 1 & -2 \\ 2 & 4 \end{bmatrix}$$

$$\textcircled{1} \quad x = \begin{bmatrix} 3 \\ 6 \end{bmatrix}$$

$$\begin{bmatrix} 3 \\ 6 \end{bmatrix} = c_1 \begin{bmatrix} 1 \\ 2 \end{bmatrix} + c_2 \begin{bmatrix} -2 \\ 4 \end{bmatrix} \Rightarrow \mathbf{Ac} = \begin{matrix} 19/64 \end{matrix}$$

$$c_1 - 2c_2 = 3 \quad \Rightarrow \quad c_1 = 3 + 2c_2$$

$$2c_1 + 4c_2 = 6$$

$$\Rightarrow x \in C(\mathbf{A})$$

$$\textcircled{2} \quad x = \begin{bmatrix} -2 \\ 2 \end{bmatrix} \quad x \notin C(\mathbf{A})$$

- Ex: Recall  $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$ .

$$\mathbf{X} = \begin{bmatrix} 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

$$\mathbf{X}\boldsymbol{\beta} = \begin{bmatrix} \beta_0 + 2\beta_1 \\ \beta_0 + 3\beta_1 \\ \beta_0 + 4\beta_1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \beta_0 + \begin{bmatrix} 2 \\ 3 \\ 4 \end{bmatrix} \beta_1$$

$\Rightarrow$  Observe  $\mathbf{X}\boldsymbol{\beta} \in C(\mathbf{X})$ .

† Def A system of equations  $\mathbf{Ax} = \mathbf{c}$  is consistent iff there exists a solution  $\mathbf{x}^*$  such that  $\mathbf{Ax}^* = \mathbf{c}$ .

★ Result: A system of equations  $\mathbf{Ax} = \mathbf{c}$  is consistent iff  $\mathbf{c} \in C(\mathbf{A})$ .

♠ Recall NE;

$$\mathbf{X}^T \mathbf{X} \beta = \mathbf{X}^T \mathbf{y}$$

- $\mathbf{X}^T \mathbf{y} \in C(\mathbf{X}^T)$  and  $\mathbf{X}^T \mathbf{X} \beta \in C(\mathbf{X}^T \mathbf{X})$

- Result: for any matrix  $\mathbf{X}$ ,  $C(\mathbf{X}^T \mathbf{X}) = C(\mathbf{X}^T)$  (Result 2.2)

⇒ **The normal equation is consistent (that is,  $\exists$  a solution)**

- **However, still do not know how to find a solution  $\hat{\beta}$ ?**

$$\text{ex. } x_1 = \begin{bmatrix} 1 \\ -1 \\ 3 \end{bmatrix} \quad x_2 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \quad \left. \begin{array}{l} \alpha_1 + \alpha_2 = 0 \\ -\alpha_1 + \alpha_2 = 0 \\ 3\alpha_1 + \alpha_2 = 0 \end{array} \right\} \Leftrightarrow \alpha_1 = \alpha_2 = 0$$

$\Rightarrow x_1$  &  $x_2$  are linearly indep.

$$\text{ex. } x_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad x_2 = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \quad x_3 = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \quad \begin{array}{l} \alpha_1 + \alpha_2 + 2\alpha_3 = 0 \\ -\alpha_1 + 2\alpha_2 + \alpha_3 = 0 \end{array}$$

consider  $\alpha_1 = 1, \alpha_2 = 1$  &  $\alpha_3 = -1 \Rightarrow x_1, x_2$  &  $x_3$  are linearly dep.

† Def [**Linearly dependent**]: Let  $x_1, \dots, x_r$  be vectors in  $\mathcal{S}$ . If there exists scalars  $\alpha_1, \dots, \alpha_r$  not all zero so that  $\sum \alpha_i x_i = 0$ , then  $x_1, \dots, x_r$  are *linearly dependent*.

If such  $\alpha_i$ s do not exist,  $x_1, \dots, x_r$  are *linearly independent*.

† Def [**Basis**]: If  $\mathcal{M}$  is a subspace of  $\mathcal{S}$  and if  $\{x_1, \dots, x_r\}$  is a linearly independent spanning set for  $\mathcal{M}$ , then  $\{x_1, \dots, x_r\}$  is called a *basis* for  $\mathcal{M}$ .

† Recall that for a  $m \times n$  matrix  $\mathbf{A}$ ,  $r(\mathbf{A}) = \#$  of linearly independent rows or columns.

If  $r(\mathbf{A}) = m (\leq n)$ ,  $\mathbf{A}$  has full-row rank.

If  $r(\mathbf{A}) = n (\leq m)$ ,  $\mathbf{A}$  has full-column rank.



† Def [**Singular**]: Let  $\mathbf{A}$  be an  $n \times n$  matrix.

- ▶  $\mathbf{A}$  is *nonsingular* if there exists a <sup>square</sup> matrix  $\mathbf{A}^{-1}$  such that  $\mathbf{A}^{-1}\mathbf{A} = \mathbf{I} = \mathbf{A}\mathbf{A}^{-1}$ .
- ▶ If no such matrix exists, then  $\mathbf{A}$  is *singular*.
- ▶ If  $\mathbf{A}^{-1}$  exists, it is called the inverse of  $\mathbf{A}$ .

♣ Th: An  $n \times n$  matrix  $\mathbf{A}$  is nonsingular if and only if  $r(\mathbf{A}) = n$  (full-row & full-column rank), i.e., the columns of  $\mathbf{A}$  form a basis for  $\mathbb{R}^n$ .

★ Note For  $n \times n$   $\mathbf{A}$ ,  $r(\mathbf{A}) = n \Leftrightarrow \mathbf{A}$  is nonsingular.  $|\mathbf{A}| \neq 0$

$p \times p$

★ Result: for any matrix  $\mathbf{X}$  ( $n \times p$ ),  $r(\mathbf{X}^T \mathbf{X}) = r(\mathbf{X})$

★ Result: If  $\mathbf{X}(n \times p)$  has  $r(\mathbf{X}) = p$ , then the  $p \times p$  matrix  $\mathbf{X}^T \mathbf{X}$  is nonsingular.

♠ Recall the NEs;

$$\mathbf{X}^T \mathbf{X} \boldsymbol{\beta} = \mathbf{X}^T \mathbf{y}$$

$\Rightarrow$  If  $r(\mathbf{X}) = p$ ,  $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$ : unique solution

Recall the NLS

$$\begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum x_i y_i \end{bmatrix}$$

If  $r(X^T X) = 2$ ,  $\exists (X^T X)^{-1}$

$$\begin{aligned} \text{nonsingular} \Rightarrow |X^T X| &= n \sum x_i^2 - (\sum x_i)^2 \\ &= n \sum x_i^2 - (n \bar{x})^2 \\ &= n (\sum x_i^2 - n \bar{x}^2) \\ &= n \sum (x_i - \bar{x})^2 > 0 \end{aligned}$$

\* Example 1 (contd): Simple linear regression

Consider the model

$$y_i = \beta_0 + \beta_1 x_i + e_i, \quad i = 1, \dots, n.$$

Find  $\hat{\beta}$ .

$$\begin{aligned} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} &= (X^T X)^{-1} X^T y = \frac{1}{n \sum (x_i - \bar{x})^2} \begin{bmatrix} \sum x_i^2 - \bar{x} \sum x_i \\ -\sum x_i & n \end{bmatrix} \begin{bmatrix} \sum y_i \\ \sum x_i y_i \end{bmatrix} \\ &= \frac{1}{n \sum (x_i - \bar{x})^2} \begin{bmatrix} (\sum x_i^2)(\sum y_i) - (\sum x_i)(\sum x_i y_i) \\ -(\sum x_i)(\sum y_i) + n \sum x_i y_i \end{bmatrix} \end{aligned}$$

①  $\beta_1$

$$\begin{aligned} \beta_1 &= \frac{\sum x_i y_i - \bar{x} \sum y_i}{\sum (x_i - \bar{x})^2} = \frac{\sum (x_i - \bar{x}) y_i}{\sum (x_i - \bar{x})^2} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sum (x_i - \bar{x})^2} \\ &= \frac{S_{xy}}{S_{xx}} \end{aligned}$$

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Observe  
Consider

$$\begin{aligned} \sum (x_i - \bar{x})(y_i - \bar{y}) &= \sum (x_i - \bar{x}) y_i - \sum (x_i - \bar{x}) \bar{y} = \sum (x_i - \bar{x}) y_i \\ &= \sum x_i y_i - n \bar{x} \bar{y} \end{aligned}$$

②  $\beta_0$

$$\beta_0 = \frac{\sum x_i^2 \sum y_i - \sum x_i \sum x_i y_i}{n \sum (x_i - \bar{x})^2} = \frac{\bar{y} (\sum x_i^2 - n \bar{x}^2) + n \bar{y} \bar{x}^2 - \bar{x} \sum x_i y_i}{\sum (x_i - \bar{x})^2}$$

$$= \bar{y} - \bar{x} \frac{(\sum x_i y_i - n \bar{x} \bar{y})}{\sum (x_i - \bar{x})^2} = \bar{y} - \bar{x} \frac{S_{xy}}{S_{xx}} = \bar{y} - \bar{x} \beta_1$$

\* Example 2 (contd): Balanced One-Way ANOVA

Consider the model

$$y_{ij} = \mu + \alpha_i + e_{ij}, \quad i = 1, \dots, a \text{ and } j = 1, \dots, n.$$

Find  $r(\mathbf{X}) = r(\mathbf{X}^T \mathbf{X})$ . =  $a$   
 $(a+1) \times (a+1)$