## **Outline**

- Inference on the simple linear regression
- Random Vectors/Matrices
- Simple Linear Regression Model in Matrix Terms
- 4 Estimation of  $\mathbb{E}(Y_h)$
- Estimation vs. Prediction

### Review

Recall the simple linear regression (SLR) model

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \quad \varepsilon_i \sim i.i.d. \ N(0, \sigma^2),$$

for all  $i = 1, \ldots, n$ .

• The least-squares (LS) estimates:

$$\hat{\beta}_{1} = \frac{\sum_{i=1}^{n} (X_{i} - \bar{X})(Y_{i} - \bar{Y})}{\sum_{i=1}^{n} (X_{i} - \bar{X})^{2}},$$

$$\hat{\beta}_{0} = \bar{Y} - \hat{\beta}_{1}\bar{X},$$

$$\hat{\sigma}^{2} = \frac{1}{n-2} \sum_{i=1}^{n} (Y_{i} - \hat{Y}_{i})^{2}.$$

• What are the sampling distributions of  $\hat{\beta}_0$ ,  $\hat{\beta}_1$ , and  $\hat{\sigma}^2$ ?

## Sampling distribution of SLR estimation

Under a simple linear regression model,

$$\begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{pmatrix} \sim \mathcal{MVN} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}, \sigma^2 \begin{bmatrix} \frac{1}{n} + \frac{\bar{X}^2}{\sum_{i=1}^n (X_i - \bar{X})^2} & \frac{-\bar{X}}{\sum_{i=1}^n (X_i - \bar{X})^2} \\ \frac{-\bar{X}}{\sum_{i=1}^n (X_i - \bar{X})^2} & \frac{1}{\sum_{i=1}^n (X_i - \bar{X})^2} \end{bmatrix} \right).$$

Furthermore, let  $\hat{\sigma}^2 = \frac{1}{n-2} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$  be the residual mean square. Then

$$\frac{(n-2)\hat{\sigma}^2}{\sigma^2} \sim \chi_{n-2}^2,$$

and is independent of  $\hat{\beta}_0$  and  $\hat{\beta}_1$ .

This section is to prove the theorem, i.e., the sampling distribution of  $(\hat{\beta}_0, \hat{\beta}_1)^T$  and  $\hat{\sigma}^2$ .

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#### Random Vector and Matrix

- A random vector or a random matrix contains elements that are random variables.
- SLR: The response variables  $Y_1, \ldots, Y_n$  can be written in the form of a random vector

$$\mathbf{Y}_{n\times 1} = \left[ \begin{array}{c} Y_1 \\ \vdots \\ Y_n \end{array} \right]$$

• Alternative notation:  $\mathbf{Y} = (Y_1, \dots, Y_n)'$ .

## Expectation of Random Vector/Matrix

• The expectation of an  $n \times 1$  random vector **Y** is

$$E(\mathbf{Y})_{n\times 1} = [E(Y_i): i = 1, \dots, n] = \begin{bmatrix} E(Y_1) \\ \vdots \\ E(Y_n) \end{bmatrix}$$

• SLR: What is E(Y|X)? Since  $E(Y_i|X) = \beta_0 + \beta_1 X_i$  for i = 1, ..., n,

$$E(\mathbf{Y}|\mathbf{X}) = \begin{bmatrix} \beta_0 + \beta_1 X_1 \\ \vdots \\ \beta_0 + \beta_1 X_n \end{bmatrix}$$

• In general, the expectation of an  $n_1 \times n_2$  random matrix  $\boldsymbol{Y}$  is

$$E(Y)_{n_1 \times n_2} = [E(Y_{ii'}) : i = 1, ..., n_1; i' = 1, ..., n_2].$$

### Variance-Covariance Matrix of Random Vector

 The variance-covariance matrix of an n × 1 random vector Y is

$$Var(\mathbf{Y}) = E[(\mathbf{Y} - E(\mathbf{Y}))(\mathbf{Y} - E(\mathbf{Y}))']$$

$$= \begin{bmatrix} Var(Y_1) & Cov(Y_1, Y_2) & \cdots & Cov(Y_1, Y_n) \\ \cdots & Var(Y_2) & \cdots & Cov(Y_2, Y_n) \\ \vdots & \vdots & & \vdots \\ \cdots & \cdots & Var(Y_n) \end{bmatrix}$$

• Note: Var(Y) is symmetric. Why?  $Cov(Y_i, Y_{i'}) = Cov(Y_{i'}, Y_i)$ .

SLR: What is Var(Y|X)?

$$Var(\mathbf{Y}|\mathbf{X}) = \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix} = \sigma^2 \mathbf{I}_{n \times n}.$$

### Variance-Covariance Matrix of Random Vector

• The random errors  $\varepsilon_1, \dots, \varepsilon_n$  can be written in the form of a random vector

$$\varepsilon_{n\times 1} = \left[ \begin{array}{c} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{array} \right]$$

• SLR: What is  $E(\varepsilon)$ ?

$$E(\varepsilon) = \mathbf{0}_{n \times 1}$$
.

• SLR: What is the variance-covariance matrix of  $\varepsilon$ ?

$$\operatorname{Var}(\varepsilon) = \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix} = \sigma^2 \mathbf{I}_{n \times n}.$$

### **Multivariate Normal Distribution**

• Let  $Y_{n\times 1} = (Y_1, \dots, Y_n)'$  follow a multivariate normal distribution with mean

$$\boldsymbol{\mu}_{n\times 1}=(\mu_1,\ldots,\mu_n)'$$

and variance

$$\Sigma_{n \times n} = [\sigma_{ii'}^2 : i = 1, ..., n; i' = 1, ..., n].$$

We denote this by

$$\mathbf{Y} \sim \mathcal{MVN}(\boldsymbol{\mu}, \boldsymbol{\Sigma}).$$

The probability density function is

$$f(\mathbf{Y}) = \frac{1}{(2\pi)^{n/2} |\Sigma|^{1/2}} \exp\left\{-\frac{1}{2} (\mathbf{Y} - \mu)' \Sigma^{-1} (\mathbf{Y} - \mu)\right\},$$

where  $|\Sigma|$  is the determinant of  $\Sigma$ .

# Preliminaries (Rencher and Schaalj, Chapter 4.4)

### Properties of random vectors

For Y ( $n \times 1$  random vector), A ( $n \times n$  non-random matrix), and b ( $n \times 1$  non-random vector), we have

$$E(AY + b) = AE(Y) + b$$
  
 $Var(AY + b) = AVar(Y)A'$ 

### Properties of Derivative

For  $\theta$  ( $p \times 1$  vector of parameters),  $\mathbf{c}$  ( $p \times 1$  vector of variables), and  $\mathbf{c}$  ( $p \times p$  symmetric matrix of variables), we have

$$\frac{\partial(\theta'\mathbf{c})}{\partial\theta} = \mathbf{c}$$

$$\frac{\partial(\theta'\mathbf{c}\theta)}{\partial\theta} = 2\mathbf{c}\theta$$

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### **Notation**

- Let  $\mathbf{Y}_{n \times 1} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix}$  denote the  $n \times 1$  vector of response variables.
- variables.

   Let  $X_{n \times p} = \begin{bmatrix} 1 & X_{11} & \cdots & X_{p-1,1} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & X_{1n} & \cdots & X_{p-1,n} \end{bmatrix}$  denote the  $n \times p$  design matrix of predictor variables.
- Let  $\varepsilon_{n\times 1}=\begin{bmatrix} \varepsilon_1\\ \vdots\\ \varepsilon_n\end{bmatrix}$  denote the  $n\times 1$  vector of random errors.
- Let  $\beta_{p \times 1} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{p-1} \end{bmatrix}$  denote the  $p \times 1$  vector of regression

coefficients.

# Linear Regression in Matrix Terms

The linear regression model in matrix terms is

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

where

$$\boldsymbol{\varepsilon} \sim \mathcal{MVN}(\mathbf{0}, \sigma^2 \boldsymbol{I}).$$

Equivalently, we have

$$\mathbf{Y} \sim \mathcal{MVN}(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}).$$

Why? Since 
$$E(\varepsilon) = \mathbf{0}_{n \times 1}$$
 and  $Var(\varepsilon) = \sigma^2 \mathbf{I}_{n \times n}$ .

$$E(Y) = E(X\beta + \varepsilon) = X\beta + E(\varepsilon) = X\beta$$
  
 $Var(Y) = Var(X\beta + \varepsilon) = Var(\varepsilon) = \sigma^2 I.$ 

## Least Squares Method

Recall that the least squares method for 2-covariates SLR minimizes

$$Q(\beta_0, \beta_1) = \sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 X_i)^2$$

 In general, the least-square for p-covariates can be written as

$$Q(\beta) = (\mathbf{Y} - \mathbf{X}\beta)'(\mathbf{Y} - \mathbf{X}\beta)$$

$$= \mathbf{Y}'\mathbf{Y} - \beta'\mathbf{X}'\mathbf{Y} - \mathbf{Y}'\mathbf{X}\beta + \beta'\mathbf{X}'\mathbf{X}\beta$$

$$= \mathbf{Y}'\mathbf{Y} - 2\beta'\mathbf{X}'\mathbf{Y} + \beta'\mathbf{X}'\mathbf{X}\beta$$

# **Normal Equations**

Let

$$\left(\frac{\partial Q}{\partial \beta}\right)_{p \times 1} = \begin{bmatrix} \frac{\partial Q}{\partial \beta_0} \\ \frac{\partial Q}{\partial \beta_1} \\ \vdots \\ \frac{\partial \beta}{\partial \beta_{p-1}} \end{bmatrix}.$$

• Differentiate Q with respect to  $\beta$  to obtain:

$$\frac{\partial Q}{\partial \beta} = -2\mathbf{X}'\mathbf{Y} + 2\mathbf{X}'\mathbf{X}\beta.$$

• Set the equation above to  $\mathbf{0}_{p\times 1}$  and obtain a set of normal equations:

$$X'X\beta = X'Y.$$

# Estimated Regression Coefficients $\hat{\beta}$

- Let  $\hat{\beta}_{p\times 1}$  denote the least squares estimate of  $\beta$ .
- Thus the least squares estimate of  $\beta$  is

$$\hat{\boldsymbol{\beta}} = \underbrace{(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'}_{\text{non-random}}\boldsymbol{Y}$$

assuming that the matrix X'X is nonsingular and thus invertible.

- What is the distribution of **Y**?
- What is the distribution of  $\hat{\beta} = (\hat{\beta}_0, \dots, \hat{\beta}_{p-1})'$ ?

# Mean and Variance of $\hat{\beta}$

- Recall that  $\hat{\beta} = \underbrace{(X'X)^{-1}X'}_{\text{non-random}} Y$
- What is the expectation of  $\hat{\beta}$ ?

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

• What is the variance-covariance matrix of  $\hat{\beta}$ ?

$$Var(\hat{\beta}) = Var((\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y})$$

$$= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'Var(\mathbf{Y})\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$$

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

• In the special case for simple linear regression with p = 2:

$$\begin{bmatrix} Var(\hat{\beta}_{0}) & Cov(\hat{\beta}_{0}, \hat{\beta}_{1}) \\ Cov(\hat{\beta}_{1}, \hat{\beta}_{0}) & Var(\hat{\beta}_{1}) \end{bmatrix} = \sigma^{2} \begin{bmatrix} \frac{1}{n} + \frac{\bar{X}^{2}}{\sum_{i=1}^{n} (X_{i} - \bar{X})^{2}} & \frac{-\bar{X}}{\sum_{i=1}^{n} (X_{i} - \bar{X})^{2}} \\ \frac{-\bar{X}}{\sum_{i=1}^{n} (X_{i} - \bar{X})^{2}} & \frac{1}{\sum_{i=1}^{n} (X_{i} - \bar{X})^{2}} \end{bmatrix}$$

• What is the distribution of  $\hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1)'$ ?

We have proved the first part of the following theorem.

### Sampling distribution of SLR estimators

Under a simple linear regression model,

$$\left( \begin{array}{c} \hat{\beta}_0 \\ \hat{\beta}_1 \end{array} \right) \sim \mathcal{MVN} \left( \left( \begin{array}{c} \beta_0 \\ \beta_1 \end{array} \right), \sigma^2 \left[ \begin{array}{cc} \frac{1}{n} + \frac{\bar{X}^2}{\sum_{i=1}^n (X_i - \bar{X})^2} & \frac{-\bar{X}}{\sum_{i=1}^n (X_i - \bar{X})^2} \\ \frac{-\bar{X}}{\sum_{i=1}^n (X_i - \bar{X})^2} & \frac{1}{\sum_{i=1}^n (X_i - \bar{X})^2} \end{array} \right] \right).$$

Furthermore, let  $\hat{\sigma}^2 = \frac{1}{n-2} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$  be the residual mean square. Then

$$\frac{(n-2)\hat{\sigma}^2}{\sigma^2} \sim \chi_{n-2}^2,$$

and is independent of  $\hat{\beta}_0$  and  $\hat{\beta}_1$ .

 How to use the above result to perform the hypothesis testing?

$$H_0: \beta_1 = 0$$
, v.s.  $H_A: \beta_1 \neq 0$ 

# Sampling distribution of $\hat{\beta}_1$

We have known that

$$\hat{\beta}_1 \sim N\left(\beta_1, \frac{\sigma^2}{\sum_{i=1}^n (X_i - \bar{X})^2}\right) \Longleftrightarrow \frac{\hat{\beta}_1 - \beta_1}{\sqrt{\frac{\sigma^2}{\sum_{i=1}^n (X_i - \bar{X})^2}}} \sim N(0, 1).$$

• But, we do not know  $\sigma^2$ . A natural (unbiased) estimator of  $\sigma^2$  is

$$\hat{\sigma}^2 = \frac{1}{n-2} \sum_{i=1}^n e_i^2,$$

and  $\frac{(n-2)\hat{\sigma}^2}{\sigma^2} \sim \chi^2_{n-2}$  by previous theorem.

Consider the test statistic

$$\frac{\hat{\beta}_1 - \beta_1}{\sqrt{\frac{\hat{\sigma}^2}{\sum_{i=1}^n (X_i - \bar{X})^2}}} \sim T_{n-2}, \quad \text{where} \quad \hat{\sigma}^2 = \frac{1}{n-2} \sum_{i=1}^n e_i^2$$

• The denominator is also referred to as the estimated standard error of  $\hat{\beta}_1$ .

# Hypothesis Testing for $\beta_1$

A test of interest is:

$$H_0: \beta_1 = 0$$
 vs.  $H_A: \beta_1 \neq 0$ .

• The test statistic is:

$$T = \frac{\hat{\beta}_1 - 0}{\widehat{se}(\hat{\beta}_1)}, \quad \text{where } \widehat{se}(\hat{\beta}_1) = \sqrt{\frac{\hat{\sigma}^2}{\sum_{i=1}^n (X_i - \bar{X})^2}}$$

• Under the  $H_0$  :  $\beta_1 = 0$ ,

$$T = \frac{\hat{eta}_1 - 0}{\widehat{se}(\hat{eta}_1)} \sim T_{n-2}$$

- p-value =  $2 \times P(T_{n-2} > |t^*|)$ , where  $t^*$  is the observed test statistic by plugging the data.
- Similar procedure for CI.

 In the wetland species richness example, the summary statistics are:

$$\bar{x} = 0.5210, \ \bar{y} = 7.9483, \ n = 58$$
  
 $\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y}) = -10.7775, \ \sum_{i=1}^{n} (x_i - \bar{x})^2 = 2.3316$   
 $\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = 479.03, \ \sum_{i=1}^{n} (y_i - \bar{y})^2 = 528.84$ 

• The least squares estimated slope is:

$$\hat{\beta}_1 = \frac{-10.7775}{2.3316} = -4.622$$

The least squares estimated intercept is:

$$\hat{\beta}_0 = 7.9483 - (-4.622) \times 0.5210 = 10.357$$

• The estimated error variance is:

$$\hat{\sigma}^2 = \frac{479.03}{56} = 8.554$$

• The estimated standard error of  $\hat{\beta}_1$  is:

$$\widehat{se}(\hat{\beta}_1) \stackrel{\text{def}}{=} \sqrt{\frac{\hat{\sigma}^2}{\sum_{i=1}^n (x_i - \bar{x})^2}} = \sqrt{\frac{8.554}{2.3316}} = 1.915$$

• Note that  $t_{n-2,\alpha/2} = t_{56,0.025} = 2.003$ . Thus, a 95% CI for  $\beta_1$  is

$$\hat{\beta}_1 \pm t_{n-2,\alpha/2} s{\hat{\beta}_1} = -4.622 \pm 2.003 \times 1.915$$
  
=  $-4.622 \pm 3.836$   
=  $[-8.459, -0.785].$ 

• Interpretation: The 95% CI for  $\beta_1$  is [-8.459, -0.785].

 To test whether there is a linear relationship between the # of species and the percent forest cover:

$$H_0: \beta_1 = 0$$
 vs.  $H_A: \beta_1 \neq 0$ .

The observed test statistic is

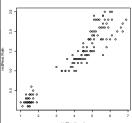
$$t^* = \frac{\hat{\beta}_1}{\widehat{se}(\hat{\beta}_1)} = \frac{-4.622}{1.915} = -2.413.$$

Compared with T<sub>56</sub>, the p-value is

$$2 \times P(T_{56} > 2.413) = 0.0191.$$

• Interpretation: Reject  $H_0$  at  $\alpha = 0.05$  level. There is moderate evidence that there is a linear relationship between # of species and percent forest cover.

# Understanding the R output



## Sampling distribution of SLR estimators

Consider a simple linear regression model. Let  $\hat{\sigma}^2 = \frac{1}{n-2} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2$  be the residual mean square. Then

$$\frac{(n-2)\hat{\sigma}^2}{\sigma^2} \sim \chi^2_{n-2},$$

and is independent of  $\hat{\beta}_0$  and  $\hat{\beta}_1$ . (Proof in next lecture)

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# Estimation of $\mathbb{E}(Y_h)$

- X<sub>h</sub> = the level of X for which we want to estimate the mean response.
- $X_h$  could be observed or not, but should be within the range of  $\{X_i\}$ .
- $\mu_h = \mathbb{E}(Y_h) = \beta_0 + \beta_1 X_h =$ the mean response at  $X_h$ .
- The estimate of  $\mu_h$  is

$$\hat{\mu}_h = \hat{\beta}_0 + \hat{\beta}_1 X_h.$$

•  $\hat{\mu}_h \sim N(\mu_h, \text{Var}(\hat{\mu}_h))$ . Why?

# Estimation of $\mathbb{E}(Y_h)$

• The variance of  $\hat{\mu}_h$  is

$$Var(\hat{\mu}_h) = \sigma^2 \left\{ \frac{1}{n} + \frac{(X_h - \bar{X})^2}{\sum_{i=1}^n (X_i - \bar{X})^2} \right\}.$$
 (proof?)

• The estimated variance of  $\hat{\mu}_h$  is

$$\widehat{\operatorname{Var}(\hat{\mu}_h)} = \hat{\sigma}^2 \left\{ \frac{1}{n} + \frac{(X_h - \bar{X})^2}{\sum_{i=1}^n (X_i - \bar{X})^2} \right\}.$$

It can be shown that

$$rac{\hat{\mu}_h - \mu_h}{\sqrt{\widehat{\mathsf{Var}}(\hat{\mu}_h)}} \sim T_{n-2}.$$

• A  $(1 - \alpha)$  CI for  $\mu_h$  is

$$\hat{\mu}_h \pm t_{n-2,\alpha/2} \sqrt{\widehat{\operatorname{Var}(\hat{\mu}_h)}}.$$

• The estimated mean number of species at  $x_h = 0.10$  is

$$\hat{\mu}_h = \hat{\beta}_0 + \hat{\beta}_1 x_h = 10.357 - 4.622 \times 0.10 = 9.895.$$

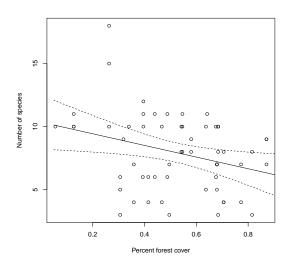
• The estimated variance of  $\hat{\mu}_h$  is

$$\widehat{\text{Var}(\hat{\mu}_h)} = \hat{\sigma}^2 \left\{ \frac{1}{n} + \frac{(\mathbf{x}_h - \bar{\mathbf{x}})^2}{\sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})^2} \right\} 
= 8.554 \left\{ \frac{1}{58} + \frac{(0.10 - 0.521)^2}{2.331} \right\} = 0.80.$$

• The 95% CI for the mean number of species at  $X_h = 0.10$  is

$$\hat{\mu}_h \pm t_{n-2,\alpha/2} \sqrt{\widehat{\text{Var}(\hat{\mu}_h)}} = 9.895 \pm 2.003 \times \sqrt{0.80}$$
  
= 9.895 \pm 1.789 = [8.105, 11.684].

Interpretation:



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- The fitted regression line is  $\hat{y} = 10.357 4.622x$ .
- The estimated error variance is  $\hat{\sigma}^2 = \frac{479.03}{56} = 8.554$ .
- Questions of interest:
  - What is the population mean number of species for a 10% forest cover around the wetland?
  - What is the number of species for a 10% forest cover around a wetland yet to be sampled?
- In both cases, the estimated/predicted value is:

$$\hat{y} = 10.357 - 4.622 \times 0.10 = 9.895.$$

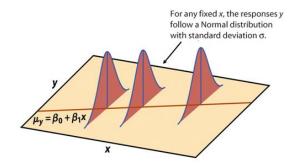
Q: Which quantity has larger uncertainty?

#### Estimation vs. Prediction

#### Simple linear regression model

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \quad \varepsilon_i \sim \text{iid } N(0, \sigma^2), \ i = 1, \dots, n.$$

- mean response at X = 0.1:  $\beta_0 + \beta_1 \times 0.1$
- "new" response at X = 0.1:  $\beta_0 + \beta_1 \times 0.1 + \varepsilon$
- sub-population vs. single observation



### Estimation vs. Prediction

Consider a simple model (with covariate 0)

$$Y_i = \mu + \varepsilon_i, \quad \varepsilon_i \sim \text{iid } N(0, \sigma^2).$$

• Then, estimate  $\mu$  by

$$\hat{\mu} = \bar{Y}$$

What is Var(û)?

$$Var(\bar{Y}) = \frac{\sigma^2}{n}$$
.

2 Also, predict a new observation Y by

$$\hat{Y}_{(\text{new})} = \bar{Y}$$

• What is the variance of the prediction error?

$$Var(Y_{(\text{new})} - \hat{Y}_{(\text{new})}) = Var(Y_{(\text{new})}) + Var(\bar{Y}) = \sigma^2 + \frac{\sigma^2}{n}$$