9 Lecture 9: Feb 8

Last time

- Introduction of simple linear regression

Today

- Simple correlation
- The statistical model of the SLR (JF chapter 6)
- Properties of the Least-Squares estimator
- Inference of SLR model

From last lecture: Assume the Gramian matrix has full rank (which actually should be the case, why?)

$$\mathbf{X}^T\mathbf{X} = \begin{bmatrix} n & \sum_i x_i \\ \sum_i x_i & \sum_i x_i^2 \end{bmatrix}$$

Proof:

Some properties:

- (a) $\sum x_i \hat{\epsilon}_i = 0$.
- (b) $\sum \hat{y}_i \hat{\epsilon}_i = 0$ (HW1).

Proof:

Other quantities in Matrix Form

Fitted values

$$\hat{\mathbf{Y}} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} \hat{\beta}_0 + \hat{\beta}_1 x_1 \\ \hat{\beta}_0 + \hat{\beta}_1 x_2 \\ \vdots \\ \hat{\beta}_0 + \hat{\beta}_1 x_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} = \mathbf{X}\hat{\boldsymbol{\beta}}$$

Hat matrix

$$\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}}$$
$$\hat{\mathbf{Y}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$
$$\hat{\mathbf{Y}} = \mathbf{H}\mathbf{Y}$$

where $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ is called "hat matrix" because it turns $\mathbf{Y}$ into $\hat{\mathbf{Y}}$.

Simple correlation

Having calculated the least squares line, it is of interest to determine how closely the line fits the scatter of points. There are many ways of answering it. The standard deviation of the residuals, S_E, often called the *standard error of the regression* or the *residue standard error*, provides one sort of answer. Because of estimation considerations, the variance of the residuals is defined using *degrees of freedom $n-2$*:

$$S_\epsilon^2 = \frac{\sum \hat{\epsilon}_i^2}{n-2}.$$

The residual standard error is,

$$S_\epsilon = \sqrt{\frac{\sum \hat{\epsilon}_i^2}{n-2}}$$

For the Davis's data, the sum of squared residuals is $\sum \hat{\epsilon}_i^2 = 418.87$, and thus the standard error of the regression is

$$S_\epsilon = \sqrt{\frac{418.87}{101-2}} = 2.0569 \text{kg}.$$

On average, using the least-squares regression line to predict measured weight from reported weight results in an error of about 2 kg.

Sum of squares:

- Total sum of squares (TSS) for Y: TSS $= \sum (y_i - \bar{y})^2$
- Residual sum of squares (RSS): RSS $= \sum (y_i - \hat{y}_i)^2$
- regression sum of squares (RegSS): RegSS $=$ TSS $-$ RSS $= \sum (\hat{y}_i - \bar{y})^2$
- RegSS $+$ RSS $=$ TSS

Sample correlation coefficient

Definition: The sample correlation coefficient r_{xy} of the paired data (x_1, y_1), (x_2, y_2), ..., (x_n, y_n) is defined by

$$r_{xy} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})/(n-1)}{\sqrt{\sum (x_i - \bar{x})^2/(n-1) \times \sum (y_i - \bar{y})^2/(n-1)}} = \frac{s_{xy}}{s_x s_y}$$

s_{xy} is called the sample covariance of x and y:

$$s_{xy} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{n-1}$$

$s_x = \sqrt{\sum (x_i - \bar{x})^2/(n-1)}$ and $s_y = \sqrt{\sum (y_i - \bar{y})^2/(n-1)}$ are, respectively, the sample standard deviations of X and Y.

Some properties of r_{xy}:

- r_{xy} is a measure of the linear association between x and y in a dataset.

- correlation coefficients are always between -1 and 1:

$$-1 \leqslant r_{xy} \leqslant 1$$

- The closer r_{xy} is to 1, the stronger the positive linear association between x and y

- The closer r_{xy} is to -1, the stronger the negative linear association between x and y

- The bigger $|r_{xy}|$, the stronger the linear association

- If $|r_{xy}| = 1$, then x and y are said to be perfectly correlated.

- $\hat{\beta}_1 = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sum(x_i - \bar{x})^2} = \frac{s_{xy}}{s_x^2} = r_{xy}\frac{s_y}{s_x}$

R-square

The ratio of RegSS to TSS is called the *coefficient of determination*, or sometimes, simply "r-square". it represents the proportion of variation observed in the response variable y which can be "explained" by its linear association with x.

- In simple linear regression, "r-square" is in fact equal to r_{xy}^2. (But this isn't the case in multiple regression.)

- It is also equal to the squared correlation between y_i and $\hat{y}_i$. (This is the case in multiple regression.)

For Davis's regression of measured on reported weight:

$$\text{TSS} = 4753.8$$
$$\text{RSS} = 418.87$$
$$\text{RegSS} = 4334.9$$

Thus,

$$r^2 = \frac{4334.9}{4753.8} = 1 - \frac{418.87}{4753.8} = 0.9119$$

The statistical model of Simple Linear Regression

Standard statistical inference in simple regression is based on a *statistical model* that describes the population or process that is sampled:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

where the coefficients β_0 and β_1 are the *population regression parameters*. The data are randomly sampled from some population of interest.

- y_i is the value of the response variable

- x_i is the explanatory variable

- ϵ_i represents the aggregated omitted causes of y (i.e., the causes of y beyond the explanatory variable), other explanatory variables that could have been included in the regression model, measurement error in y, and whatever component of y is inherently random.

Key assumptions of SLR

The key assumptions of the SLR model concern the behavior of the errors, equivalently, the distribution of y conditional on x:

- *Linearity.* The expectation of the error given the value of x is 0: $\mathbf{E}\left(\epsilon\right) \equiv \mathbf{E}\left(\epsilon|x_i\right) = 0$. And equivalently, the expected value of the response variable is a linear function of the explanatory variable: $\mu_i \equiv \mathbf{E}\left(y_i\right) \equiv \mathbf{E}\left(y_i|x_i\right) = \mathbf{E}\left(\beta_0 + \beta_1 x_i + \epsilon_i|x_i\right) = \beta_0 + \beta_1 x_i$.

- *Constant variance.* The variance of the errors is the same regardless of the value of x: $\mathbf{Var}\left(\epsilon|x_i\right) = \sigma_\epsilon^2$. The constant error variance implies constant conditional variance of y on given x: $\mathbf{Var}\left(y|x_i\right) = \mathbf{E}\left((y_i - \mu_i)^2\right) = \mathbf{E}\left((y_i - \beta_0 - \beta_1 x_i)^2\right) = \mathbf{E}\left(\epsilon_i^2\right) = \sigma_\epsilon^2$. (Question: why the last equal sign?)

- *Normality.* The errors are independent identically distributed with Normal distribution with mean 0 and variance σ_ϵ^2. Write as $\epsilon_i \overset{iid}{\sim} N(0, \sigma_\epsilon^2)$. Equivalently, the conditional distribution of the response variable is normal: $y_i \overset{iid}{\sim} N(\beta_0 + \beta_1 x_i, \sigma_\epsilon^2)$.

- *Independence.* The observations are sampled independently.

- *Fixed X, or X measured without error and independent of the error.*

  - For experimental research where X values are under direct control of the researcher (i.e. X's are fixed). If the experiment were replicated, then the values of X would remain the same.

  - For research where X values are sampled, we assume the explanatory variable is measured without error and the explanatory variable and the error are independent in the population from which the sample is drawn.

- *X is not invariant.* X's can not be all the same.

Figure 9.1 shows the assumptions of linearity, constant variance, and normality in SLR model.
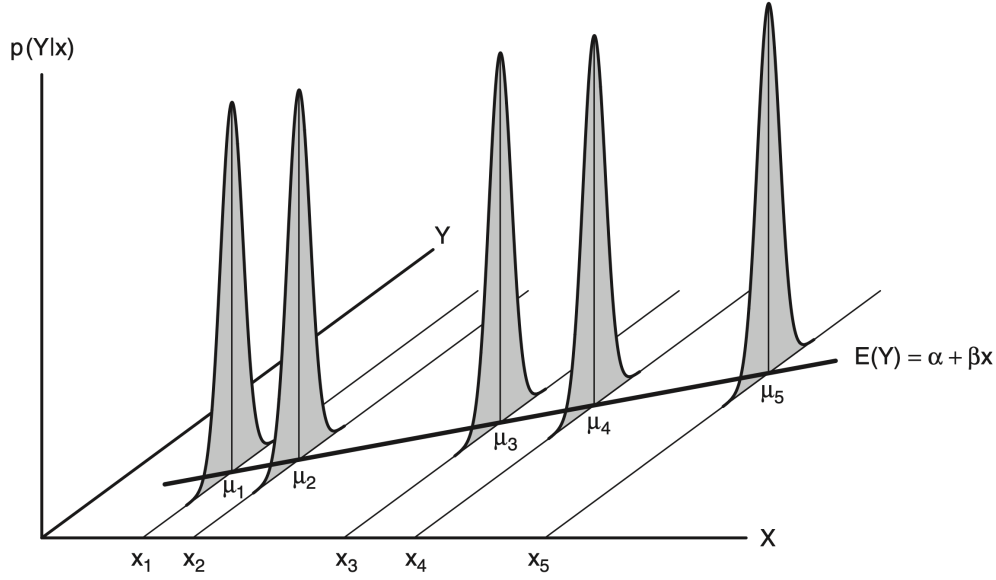
Figure 9.1: The assumptions of linearity, constant variance, and normality in simple regression. The graph shows the conditional population distributions $\Pr(Y|x)$ of Y for several values of the explanatory variable X, labeled as $x_1, x_2, \ldots, x_5$. The conditional means of Y given x are denoted $\mu_1, \ldots, \mu_5$.

Properties of the Least-Squares estimator

Under the strong assumptions of the simple regression model, the sample least squares coefficients $\hat{\beta}_{ls}$ have several desirable properties as estimators of the population regression coefficients β_0 and β_1:

- The least-squares intercept and slope are *linear estimators*, in the sense that they are linear functions of the observations y_i.
  Proof:

- The sample least-squares coefficients are *unbiased estimators* of the population regression coefficients:
$$\mathbf{E}\left(\hat{\beta}_0\right) = \beta_0$$
$$\mathbf{E}\left(\hat{\beta}_1\right) = \beta_1$$

  Proof:

- Both $\hat{\beta}_0$ and $\hat{\beta}_1$ have simple sampling variances:
$$\mathrm{Var}(\hat{\beta}_0) = \frac{\sigma_\epsilon^2 \sum x_i^2}{n \sum (x_i - \bar{x})^2}$$
$$\mathrm{Var}(\hat{\beta}_1) = \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2}$$

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Proof:

- Rewrite the formula for $\text{Var}(\hat{\beta}_1) = \frac{\sigma_\epsilon^2}{(\text{n}-1)\text{S}_\text{X}^2}$, we see that the sampling variance of the slope estimate will be small when

    - The error variance σ_ϵ^2 is small

    - The sample size n is large

    - The explanatory-variable values are spread out (i.e. have a large variance, S_X^2)

- (Gauss-Markov theorem) Under the assumptions of linearity, constant variance, and independence, the least-squares estimators are BLUE (Best Linear Unbiased Estimator), that is they have the smallest sampling variance and are unbiased. (show this)
  Proof:

- Under the full suite of assumptions, the least-squares coefficients $\hat{\beta}_0$ and $\hat{\beta}_1$ are the maximum-likelihood estimators of β_0 and β_1. (show this)
  Proof:

- Under the assumption of normality, the least-squares coefficients are themselves normally distributed. Summing up,

$$\hat{\beta}_0 \sim N(\beta_0, \frac{\sigma_\epsilon^2 \sum x_i^2}{n \sum (x_i - \bar{x})^2})$$
$$\hat{\beta}_1 \sim N(\beta_1, \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2})$$

Statistical inference of the SLR model

Now we have the distribution of $\hat{\beta}_0$ and $\hat{\beta}_1$

$$\hat{\beta}_0 \sim N(\beta_0, \frac{\sigma_\epsilon^2 \sum x_i^2}{n \sum (x_i - \bar{x})^2})$$
$$\hat{\beta}_1 \sim N(\beta_1, \frac{\sigma_\epsilon^2}{\sum (x_i - \bar{x})^2}).$$

However, σ_ϵ is never known in practice. Instead, an *unbiased* estimator of σ_ϵ^2 is given by

$$\hat{\sigma_\epsilon}^2 = MS[E] = \frac{SS[E]}{n-2}.$$

Proof:

Confidence intervals

Now we substitute $\hat{\sigma}_\epsilon^2$ into the distribution of $\hat{\beta}_0$ and $\hat{\beta}_1$

$$\hat{\beta}_1 \sim N(\beta_1, \frac{\sigma_\epsilon^2}{\sum(x_i - \bar{x})^2})$$

$$\hat{\beta}_0 \sim N(\beta_0, \frac{\sigma_\epsilon^2 \sum x_i^2}{n \sum(x_i - \bar{x})^2})$$

to get the estimated standard errors:

$$\widehat{SE}(\hat{\beta}_1) = \sqrt{\frac{MS[E]}{\sum(x_i - \bar{x})^2}}$$

$$\widehat{SE}(\hat{\beta}_0) = \sqrt{MS[E] \left(\frac{1}{n} + \frac{\bar{x}^2}{\sum(x_i - \bar{x})^2}\right)}$$

And the $100(1 - \alpha)\%$ confidence intervals for β_1 and β_0 are given by

$$\hat{\beta}_1 \pm t(n - 2, \alpha/2)\sqrt{\frac{MS[E]}{S_{xx}}}$$

$$\hat{\beta}_0 \pm t(n - 2, \alpha/2)\sqrt{MS[E] \left(\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}}\right)}$$

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

Confidence interval for $\mathbf{E}\,(Y|X = x_0)$

The conditional mean $\mathbf{E}\,(Y|X = x_0)$ can be estimated by evaluating the regression function $\mu(x_0)$ at the estimates $\hat{\beta}_0$, $\hat{\beta}_1$. The conditional variance of the expression isn't too difficult (already shown):

$$\mathrm{Var}(\hat{\beta}_0 + \hat{\beta}_1 x_0 | X = x_0) = \sigma^2 (\frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}})$$

This leads to a confidence interval of the form

$$\hat{\beta}_0 + \hat{\beta}_1 x_0 \pm t(n - 2, \alpha/2)\sqrt{MS[E] \left(\frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}}\right)}$$

Prediction interval

Often, prediction of the response variable Y for a given value, say x_0, of the independent variable of interest. In order to make statements about future values of Y, we need to take into account

- the sampling distribution of $\hat{\beta}_0$ and $\hat{\beta}_1$

- the randomness of a future value Y.

We have seen the <u>predicted value</u> of Y based on the linear regression is given by $\hat{Y}_0 = \hat{\beta}_0 + \hat{\beta}_1 x_0$.

The <u>95% prediction interval</u> has the form

$$\hat{Y}_0 \pm t(n-2, \alpha/2)\sqrt{MS[E]\left(1 + \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}}\right)}.$$

Hypothesis test

To test the hypothesis $\boxed{H_0 : \beta_1 = \beta_{slope_0}}$ that the population slope is equal to a specific value β_{slope_0} (most commonly, the null hypothesis has $\beta_{slope_0} = 0$), we calculate the test statistic (T-statistics) with $df = n - 2$

$$t_0 = \frac{\hat{\beta}_1 - \beta_{slope_0}}{\widehat{SE}(\hat{\beta}_1)} \sim t_{n-2}$$