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STAT2008/STAT6038

Simple linear regression in matrix notation

Simple Linear Regression in matrix notation

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$$Y_1, \ldots Y_n \Rightarrow Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

$$\begin{bmatrix} Y_1 \\ \cdot \\ \cdot \\ \cdot \\ Y_n \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & X_1 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ 1 & X_n \end{bmatrix}}_{\text{Design matrix}} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \cdot \\ \cdot \\ \cdot \\ \varepsilon_n \end{bmatrix}$$

Matrix Multiplication

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$$\begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \\ 1 & X_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} \beta_0 + \beta_1 X_1 \\ \beta_0 + \beta_1 X_2 \\ \vdots \\ \beta_0 + \beta_1 X_n \end{bmatrix}$$

Key elements of SLR in matrix notation

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$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix}, \quad \mathbf{X} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \\ 1 & X_n \end{bmatrix}, \quad \beta = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \quad \mathcal{E} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

SLR in matrix notation

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$$\begin{aligned} Y_1 &= \beta_0 + \beta_1 X_1 + \varepsilon_1, \\ Y_2 &= \beta_0 + \beta_1 X_2 + \varepsilon_2, \\ &\vdots \\ Y_n &= \beta_0 + \beta_1 X_n + \varepsilon_n \end{aligned}$$

- Can be written as:

$$\mathbf{Y} = \mathbf{X}\beta + \mathcal{E}$$

Error variance-covariance matrix

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- An error covariance matrix shows the covariances amongst the different error terms.
- By definition, error covariance matrices are symmetric (the number in the i^{th} row and j^{th} column is the same as the number in the j^{th} row and i^{th} column).
- The number, or "element", in the i^{th} row and j^{th} column is the covariance between the i^{th} and j^{th} errors.

Error Covariance Matrix

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$$\varepsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

$$Var(\varepsilon) = \begin{bmatrix} \text{cov}(\varepsilon_1, \varepsilon_1) & \text{cov}(\varepsilon_1, \varepsilon_2) & \dots & \text{cov}(\varepsilon_1, \varepsilon_n) \\ \text{cov}(\varepsilon_1, \varepsilon_2) & \text{cov}(\varepsilon_2, \varepsilon_2) & & \\ & \vdots & \ddots & \\ \text{cov}(\varepsilon_1, \varepsilon_n) & & & \text{cov}(\varepsilon_n, \varepsilon_n) \end{bmatrix}$$

The errors have common variance and are uncorrelated :

$$\text{cov}(\varepsilon_i, \varepsilon_j) = \begin{cases} \sigma^2 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{cases}$$

So $Var(\varepsilon) = \sigma^2 I$ where I is the n × n identity matrix

Fitted Values and Residuals

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$$\hat{\mathbf{Y}} = \begin{bmatrix} \hat{Y}_1 \\ \hat{Y}_2 \\ \vdots \\ \hat{Y}_n \end{bmatrix} = \begin{bmatrix} b_0 + b_1 X_1 \\ b_0 + b_1 X_2 \\ \vdots \\ b_0 + b_1 X_n \end{bmatrix} = \mathbf{X}\mathbf{b}$$

$$\mathbf{e} = \mathbf{Y} - \hat{\mathbf{Y}} = \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix}$$

Example – Section 1

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x	y	$\hat{y}_i = 1 + 1.3x_i$	$r_i = y_i - \hat{y}_i$	$(y_i - \hat{y}_i)^2$
1	3	2.3	0.7	0.49
2	3	3.6	-0.6	0.36
4	7	6.2	0.8	0.64
5	6	7.5	-1.5	2.25
8	12	11.4	0.6	0.36

Fitted Values and Residuals

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$$\hat{\mathbf{Y}} = \begin{bmatrix} 2.3 \\ 3.6 \\ 6.2 \\ 7.5 \\ 11.4 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 4 \\ 1 & 5 \\ 1 & 8 \end{bmatrix} \begin{bmatrix} 1 \\ 1.3 \end{bmatrix} = \begin{bmatrix} 1+1.3\times1 \\ 1+1.3\times2 \\ 1+1.3\times4 \\ 1+1.3\times5 \\ 1+1.3\times8 \end{bmatrix}$$

$$\mathbf{e} = \mathbf{Y} - \hat{\mathbf{Y}} = \begin{bmatrix} 0.7 \\ -0.6 \\ 0.8 \\ -1.5 \\ 0.6 \end{bmatrix}$$

Least Squares Estimates in matrix notation

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$$Define \quad b = \begin{bmatrix} b_0 \\ b_1 \end{bmatrix}$$

- The distance or squared error loss function

$$e'e = d(b) = (Y - Xb)^T (Y - Xb)$$

- Taking the derivative wrt b and setting to zero yields the normal equations

$$\frac{\partial d}{\partial b} = -2X^T(Y - Xb) = 0.$$

Least Squares Estimates in matrix notation

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- We can then see that:

$$X^T X b = X^T Y$$

$$b = (X^T X)^{-1} X^T Y.$$

Some important linear algebra

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$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ X_1 & X_2 & \cdots & X_n \end{bmatrix} \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \\ 1 & X_n \end{bmatrix} = \begin{bmatrix} n & \sum_{i=1}^n X_i \\ \sum_{i=1}^n X_i & \sum_{i=1}^n X_i^2 \end{bmatrix}$$

$$\mathbf{X}'\mathbf{Y} = \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ \vdots & \\ 1 & X_n \end{bmatrix}' \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n Y_i \\ \sum_{i=1}^n X_i Y_i \end{bmatrix}$$

Some important relationships

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$$S_{xx} = \sum_{i=1}^n (x_i - \bar{x})^2 = \sum_{i=1}^n (x_i - \bar{x}) x_i = \sum_{i=1}^n x_i^2 - n\bar{x}^2$$

$$S_{xy} = \sum_{i=1}^n (x_i - \bar{x}) Y_i = \sum_{i=1}^n (x_i - \bar{x})(Y_i - \bar{Y}) = \sum_{i=1}^n x_i Y_i - n\bar{x}\bar{Y}$$

Using the results on the previous slides

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$$X^T X = \begin{pmatrix} n & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{pmatrix}$$

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad \text{then} \quad A^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

$$(X^T X)^{-1} = \frac{1}{nS_{xx}} \begin{pmatrix} \sum_{i=1}^n x_i^2 & -\sum_{i=1}^n x_i \\ -\sum_{i=1}^n x_i & n \end{pmatrix}$$

Solving to find *b*

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$$b = (X^T X)^{-1} X^T Y = \frac{1}{nS_{xx}} \begin{pmatrix} \sum_{i=1}^n x_i^2 & -\sum_{i=1}^n x_i \\ -\sum_{i=1}^n x_i & n \end{pmatrix} \begin{pmatrix} \sum_{j=1}^n Y_j \\ \sum_{j=1}^n x_j Y_j \end{pmatrix}$$

$$= \frac{1}{nS_{xx}} \begin{pmatrix} \sum_{i=1}^n x_i^2 \sum_{j=1}^n Y_j - \sum_{i=1}^n x_i \sum_{j=1}^n x_j Y_j \\ n\sum_{j=1}^n x_j Y_j - \sum_{i=1}^n x_i \sum_{j=1}^n Y_j \end{pmatrix}$$

$$= \frac{1}{S_{xx}} \begin{pmatrix} \overline{Y} \sum_{i=1}^n x_i^2 - \overline{x} \sum_{j=1}^n x_j Y_j \\ \sum_{j=1}^n x_j Y_j - n\overline{x}\overline{Y} \end{pmatrix}$$

Solving to find *b* continued

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$$= \frac{1}{S_{xx}} \begin{pmatrix} \overline{Y} \sum_{i=1}^n x_i^2 - n\overline{Y}\overline{x}^2 + n\overline{Y}\overline{x}^2 - \overline{x} \sum_{j=1}^n x_j Y_j \\ S_{xy} \end{pmatrix}$$

$$= \frac{1}{S_{xx}} \begin{pmatrix} \overline{Y} S_{xx} - \overline{x} S_{xy} \\ S_{xy} \end{pmatrix}$$

$$= \begin{pmatrix} \overline{Y} - \overline{x}\frac{S_{xy}}{S_{xx}} \\ \frac{S_{xy}}{S_{xx}} \end{pmatrix}.$$

The "hat matrix"

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This form of the least-squares estimator leads to another useful matrix, since we may write

$$\hat{Y} = Xb = X(X^T X)^{-1} X^T Y = HY,$$

where $H = X(X^T X)^{-1} X^T$ is called the "hat matrix" since multiplying the response vector, Y, by H yields $\hat{Y}$. Similarly, the vector of residuals can be written as

$$e = Y - \hat{Y} = Y - HY = (I - H)Y.$$

Leverage

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The diagonal elements of H are a measure of the *influence* of each data point. It turns out that the i^{th} diagonal element of H is:

$$h_{ii} = \frac{\sum_{j=1}^{n}(x_j - x_i)^2}{nS_{xx}},$$

and the value h_{ii} is referred to as the *leverage* of the i^{th} data point. The leverage h_{ii} quantifies how far away the i^{th} x value is from the rest of the x values. If the i^{th} x value is far away, the leverage h_{ii} will be large; and otherwise not.

We see that this is a measure of how far from the main body of the data each point is in the horizontal (or predictor) direction.

The leverage h_{ii} is a number between 0 and 1

Leverage example

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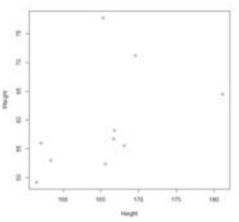

- Data on women from R worksheet 2 (available in the file: worksheet2_women.csv on Wattle)
- Which observation do we think may have high leverage?

Example continued

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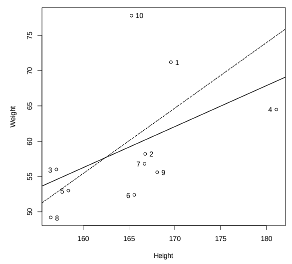
```
>abline(lsfit(Height,Weight))
>abline(lsfit(Height[-4],Weight[-4]),lty=2)
```



Leverage and Influence

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A point is highly influential if its removal from the dataset causes a dramatic change in the estimated parameters of the regression line.

One useful way of flagging the potentially influential data points is through the use of the *leverages*, h_{ii}

In order to see whether points with high leverage truly are influential, we examine how the fitted regression line would change once that flagged point is deleted from the data set.

Leverage

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It turns out that the sum of all the leverages in a simple linear regression is equal to 2:

$$\sum_{i=1}^{n} h_{ii} = 2.$$

If all the data points had the same leverage, each of the h_{ii}'s should be equal to 2/n.

So, any point which exceeds this value, and more particularly, any point which exceeds twice this value is a potentially influential point.

We will see this again later!

Example – Leverage Bar Plot

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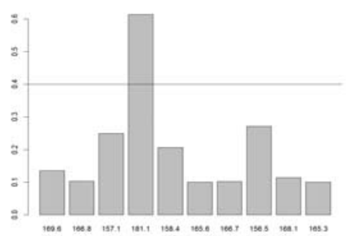
```
barplot(hat(Height),names.arg=Height)
abline(h=4/length(Height))
```



Properties of Least Squares Estimators

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The estimates b_0 and b_1 are unbiased:

$$E(b_1) = E(\frac{S_{xy}}{S_{xx}})$$

$$= E(\sum_{i=1}^{n} \frac{(x_i - \bar{x})(Y_i - \bar{Y})}{S_{xx}})$$

$$= E(\sum_{i=1}^{n} \frac{x_i Y_i - x_i \bar{Y} - \bar{x} Y_i + \bar{x}\bar{Y}}{S_{xx}})$$

$$= \sum_{i=1}^{n} \frac{(x_i - \bar{x}) E(Y_i)}{S_{xx}}$$

$$= \frac{\sum_{i=1}^{n} (x_i - \bar{x})(\beta_0 + \beta_1 x_i)}{S_{xx}}$$

$$= \frac{\beta_0 \sum_{i=1}^{n} (x_i - \bar{x}) + \beta_1 S_{xx}}{S_{xx}}$$

$$= \beta_1$$

x_i is an independent (or predictor) variable which is known exactly, while y is a dependent (or response) random variable.

Properties of Least-Squares Estimators

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The estimates b_0 and b_1 are unbiased:

$$E(b_0) = E(\bar{Y} - b_1 \bar{x}) = \frac{1}{n} \sum_{i=1}^{n} E(Y_i) - \beta_1 \bar{x} = \frac{1}{n} \sum_{i=1}^{n} (\beta_0 + \beta_1 x_i) - \beta_1 \bar{x} = \beta_0.$$

Matrix Notation is easier!

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since $Y = X\beta + \epsilon$ implies that the least-squares estimator, $b = (X^T X)^{-1} X^T Y$, may be written as:

$$(X^T X)^{-1} X^T (X\beta + \epsilon)$$

$$= (X^T X)^{-1} X^T X \beta + (X^T X)^{-1} X^T \epsilon$$

$$= \beta + (X^T X)^{-1} X^T \epsilon,$$

which implies that $E(b) = E\{\beta + (X^T X)^{-1} X^T \epsilon\} = \beta + (X^T X)^{-1} X^T E(\epsilon) = \beta$, since $E(\epsilon) = 0$.

Variance – Matrix Notation

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We know the least squares estimator $b = (X^T X)^{-1} X^T Y$

$$Var(b) = Var\{\beta + (X^T X)^{-1} X^T \epsilon\}$$

employing the rule $Var(AZ) = A Var(Z) A^T$

$$= (X^T X)^{-1} X^T Var(\epsilon) \{(X^T X)^{-1} X^T\}^T$$

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

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

employing the rule $(A^{-1})^T = (A^T)^{-1}$

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

Properties of the Least-Squares Estimators

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- Using $(X^T X)^{-1} = \frac{1}{n S_{xx}} \begin{pmatrix} \sum_{i=1}^{n} x_i^2 & -\sum_{i=1}^{n} x_i \\ -\sum_{i=1}^{n} x_i & n \end{pmatrix}$

and using $\sum_{i=1}^{n} x_i^2 = S_{xx} + n\bar{x}^2$

$$Var(b) = \sigma^2 (X^T X)^{-1},$$

We can see that:

$$Var(b_1) = \frac{\sigma^2}{S_{xx}}$$

and

$$Var(b_0) = \sigma^2 \left(\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}} \right)$$

Properties of our Estimators

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$$E\left(\hat{\beta}_0\right) = \beta_0$$

$$E\left(\hat{\beta}_1\right) = \beta_1$$

unbiased

$$\text{Var}\left(\hat{\beta}_0\right) \downarrow 0 \quad as \quad n \uparrow \infty$$

$$\text{Var}\left(\hat{\beta}_1\right) \downarrow 0 \quad as \quad n \uparrow \infty$$