Stat 206: Linear Models

Lecture 2

Sept. 30, 2015

ReCap: Least Squares Principle

For a given line: $y = b_0 + b_1 x$, the *sum of squared vertical deviations* of the observations $\{(X_i, Y_i)\}_{i=1}^n$ from the corresponding points on the line is:

$$Q(b_0, b_1) = \sum_{i=1}^{n} (Y_i - (b_0 + b_1 X_i))^2 .$$

- $(X_i, b_0 + b_1 X_i)$ is the point on the line with the same x-coordinate as the ith observation point (X_i, Y_i).
- The *least squares (LS) principle* is to fit the observed data by minimizing the sum of squared vertical deviations.

LS line has the smallest sum of squared vertical deviations among all straight lines.

ReCap: Least Squares Estimators

LS estimators of β_0, β_1 are the pair of values b_0, b_1 that minimize the function $Q(\cdot, \cdot)$:

$$(\hat{\beta}_0, \hat{\beta}_1) = \mathrm{argmin}_{b_0, b_1} Q(b_0, b_1).$$

- LS estimators:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (X_i - \overline{X})(Y_i - \overline{Y})}{\sum_{i=1}^n (X_i - \overline{X})^2} = r_{XY} \frac{s_Y}{s_X}, \qquad \hat{\beta}_0 = \overline{Y} - \hat{\beta}_1 \overline{X} \quad (1)$$

- $\overline{X} = 1/n \sum_{i=1}^n X_i$, $\overline{Y} = 1/n \sum_{i=1}^n Y_i$ are the sample means.
- *Is there a situation such that the LS estimators are not defined?*

- If X_is are all equal , then LS estimators do not exist! Though this is rare in practice.
- If the data are centered such that $\overline{X} = 0, \overline{Y} = 0$, then $\hat{\beta}_0 = 0$ and the LS line passes the origin $(0, 0)$. (Recall the "exam score" example.)
- Useful identities:

$$\sum_{i=1}^{n}(X_i - \overline{X})^2 = \sum_{i=1}^{n} X_i^2 - n(\overline{X})^2,$$

$$\sum_{i=1}^{n}(X_i - \overline{X})(Y_i - \overline{Y}) = \sum_{i=1}^{n}(X_i - \overline{X})Y_i = \sum_{i=1}^{n} X_i Y_i - n\overline{X}\,\overline{Y}.$$

Could you write down the formulae for sample correlation r_{XY} and sample standard deviations s_Y, s_X?

How to derive the LS Estimators?

The values of b_0, b_1 that minimize the function Q satisfy:

$$\frac{\partial Q(b_0, b_1)}{\partial b_0} = 0, \quad \frac{\partial Q(b_0, b_1)}{\partial b_1} = 0.$$

This leads to the **normal equations**:

$$\begin{aligned} nb_0 + b_1 \sum_{i=1}^{n} X_i &= \sum_{i=1}^{n} Y_i \\ b_0 \sum_{i=1}^{n} X_i + b_1 \sum_{i=1}^{n} X_i^2 &= \sum_{i=1}^{n} X_i Y_i \end{aligned}$$

Can you solve these two equations with respect to b_0, b_1?

Fitted Values

- The **fitted regression line (LS line)**:

$$y = \hat{\beta}_0 + \hat{\beta}_1 x = \overline{Y} + \hat{\beta}_1 (x - \overline{X}). \tag{2}$$

  - The fitted regression line passes through the point $(\overline{X}, \overline{Y})$ – the center of the data.

- The **fitted value** for the *ith* case:

$$\widehat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_i = \overline{Y} + \hat{\beta}_1 (X_i - \overline{X}), \quad i = 1, \cdots n.$$

Residuals

Residuals are differences between the observed values Y_i and their respective fitted values $\widehat{Y}_i$:

$$\begin{aligned} e_i &= Y_i - \widehat{Y}_i = Y_i - (\hat{\beta}_0 + \hat{\beta}_1 X_i), \quad i = 1, \cdots n. \\ &= (Y_i - \overline{Y}) - \hat{\beta}_1 (X_i - \overline{X}). \end{aligned}$$

- The residual e_i is an "estimator" of the respective error term: $\epsilon_i = Y_i - (\beta_0 + \beta_1 X_i)$.
- Properties of residuals: (i) $\sum_{i=1}^n e_i = 0$; (ii) $\sum_{i=1}^n X_i e_i = 0$; (iii) $\sum_{i=1}^n \widehat{Y}_i e_i = 0$. *What are geometric interpretation of these properties?*

A Simulation Example

This is a simulated data set with $n = 5$ cases and

$$Y_i = 2 + X_i + \epsilon_i, \quad i = 1, \cdots, 5,$$

where ϵ_i are generated as i.i.d. $N(0, 1)$. *What is the true regression function and what is the true error variance σ^2?*

case i	X_i	Y_i	$X_i - \overline{X}$	$Y_i - \overline{Y}$	$(X_i - \overline{X})^2$	$(X_i - \overline{X})(Y_i - \overline{Y})$
1	1.86	3.34	-0.17	-0.94	0.03	0.16
2	0.22	1.79	-1.81	-2.48	3.29	4.50
3	3.55	5.66	1.52	1.39	2.30	2.11
4	3.29	5.83	1.26	1.56	1.58	1.96
5	1.25	4.74	-0.78	0.47	0.61	-0.36
Column Sum	10.17	21.36	0.00	0.00	7.81	8.37

$$\overline{X} = 10.17/5 = 2.03, \quad \overline{Y} = 21.36/5 = 4.27, \quad \sum_{i=1}^{5}(X_i - \overline{X})^2 = 7.81, \quad \sum_{i=1}^{5}(X_i - \overline{X})(Y_i - \overline{Y}) = 8.37.$$

$$\hat{\beta}_1 = 8.37/7.81 = 1.07, \quad \hat{\beta}_0 = 4.27 - 1.07 \times 2.03 = 2.09.$$

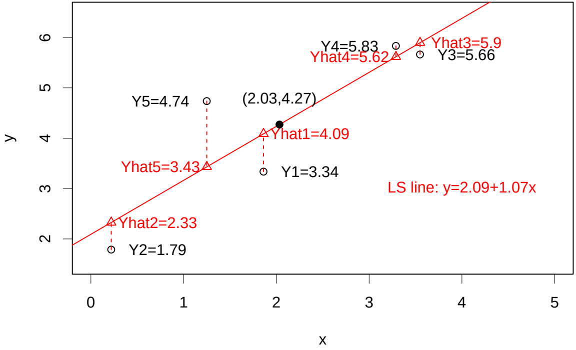
LS line: $y = 2.09 + 1.07x$.

Case i	X_i	Y_i	$\widehat{Y}_i$	e_i
1	1.86	3.34	4.09	-0.75
2	0.22	1.79	2.33	-0.54
3	3.55	5.66	5.90	-0.23
4	3.29	5.83	5.62	0.22
5	1.25	4.74	3.43	1.31

Example. $X_1 = 1.86$, $\widehat{Y}_1 = 2.09 + 1.07 \times 1.86 = 4.09$
and $e_1 = Y_1 - \widehat{Y}_1 = 3.34 - 4.09 = -0.75$.

Check the three properties of residuals.

Figure: LS line and fitted values



more example

Estimation of Error Variance by MSE

- Recall $\sigma^2 = \mathrm{Var}(\epsilon_i)$, so it is reasonable to estimate σ^2 by the "variance" of the residuals e_i.
- **Error sum of squares (SSE)**:

$$
\begin{aligned}
SSE := \sum_{i=1}^{n} e_i^2 &= \sum_{i=1}^{n} (Y_i - \widehat{Y}_i)^2 \\
&= \sum_{i=1}^{n} (Y_i - \overline{Y})^2 - \hat{\beta}_1^2 \sum_{i=1}^{n} (X_i - \overline{X})^2.
\end{aligned}
$$

  - $E(SSE) = (n-2)\sigma^2$.
  - The **degrees of freedom** of SSE is $n-2$

- **Mean squared error (MSE)**:

$$s^2 = MSE = \frac{SSE}{n-2}, \quad E(MSE) = \sigma^2. \tag{3}$$

So MSE is an ubiased estimator of σ^2.

- *What are the similarities with and differences from the estimation of the variance of a single population based on an i.i.d. sample?*
- Simulation example.

$$SSE = (-0.75)^2 + (-0.54)^2 + (-0.23)^2 + 0.22^2 + 1.31^2 = 2.6715$$

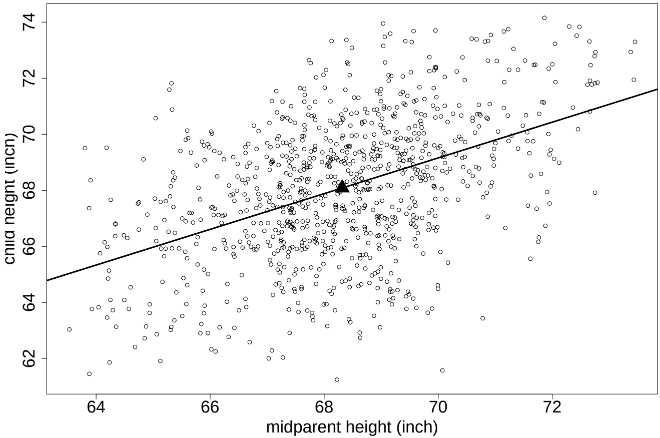
and $n = 5$, so $MSE = = \frac{2.6715}{5-2} = 0.8905$.

Heights

Summary statistics:
$n = 928$, $\overline{X} = 68.316$, $\overline{Y} = 68.082$, $\sum_i X_i^2 = 4334058$, $\sum_i Y_i^2 = 4307355$, $\sum_i X_i Y_i = 4318152$. Thus

$$\begin{aligned}
\sum_{i=1}^{n}(X_i - \overline{X})(Y_i - \overline{Y}) &= \sum_{i=1}^{n} X_i Y_i - n\overline{X}\,\overline{Y} \\
&= 4318152 - 928 \times 68.316 \times 68.082 = 1936.738 \\
\sum_{i=1}^{n}(X_i - \overline{X})^2 &= \sum_{i=1}^{n} X_i^2 - n(\overline{X})^2 \\
&= 4334058 - 928 \times 68.316^2 = 3038.761. \\
\hat{\beta}_1 &= 1936.738/3038.761 = 0.637 \\
\hat{\beta}_0 &= 68.082 - 0.637 \times 68.316 = 24.54.
\end{aligned}$$

Figure: LS line of the heights data: $y = 24.54 + 0.637x$



```
Child Midparent
1 61.57220  70.07404
2 61.24382  68.22505
3 61.90968  65.12639
4 61.85769  64.23529
5 61.44986  63.88177
6 62.00005  67.02702
......
```

$X_1 = 70.07404$, $Y_1 = 61.57220$, $\widehat{Y}_1 = 24.54 + 0.637 \times 70.07404 = 69.17716$, $e_1 = 61.57220 - 69.17716 = -7.60496$.
$SSE = \sum_i e_i^2 = 4658.966$, $\quad n = 928$ so $MSE = \frac{4658.966}{928-2} = 5.031$.

back

Properties of LS Estimators

- **LS estimators are linear functions of the responses Y_is.**

$$\hat{\beta}_1 = \sum_{i=1}^{n} \frac{X_i - \overline{X}}{\sum_{j=1}^{n}(X_j - \overline{X})^2} Y_i = \sum_{i=1}^{n} k_i Y_i$$

$$\hat{\beta}_0 = \sum_{i=1}^{n} (\frac{1}{n} - \bar{X} k_i) Y_i.$$

- The fitted values $\widehat{Y}_i$ and the residuals e_i are also linear functions of the responses Y_is.

Can you write down their respective coefficients?

- **LS estimators are unbiased**: For **all** values of β_0, β_1,

$$E(\hat{\beta}_0) = \beta_0, \quad E(\hat{\beta}_1) = \beta_1.$$

Notes: Use the fact $E(Y_i) = \beta_0 + \beta_1 X_i, \quad i = 1, \cdots n.$

- Variances of $\hat{\beta}_0, \hat{\beta}_1$:

$$\begin{aligned} \sigma^2\{\hat{\beta}_0\} &= \sigma^2\left[\frac{1}{n} + \frac{\overline{X}^2}{\sum_{i=1}^n (X_i - \overline{X})^2}\right] \\ \sigma^2\{\hat{\beta}_1\} &= \frac{\sigma^2}{\sum_{i=1}^n (X_i - \overline{X})^2}. \end{aligned}$$

Notes: Use the fact that Y_i*s are uncorrelated.*