Linear Regression

Professor Jie Peng, PhD

Department of Statistics

University of California, Davis

Model Ingredients

Key Ingredients

(a) Fixed component: How does the mean of the response variable Y change with the X value(s)?

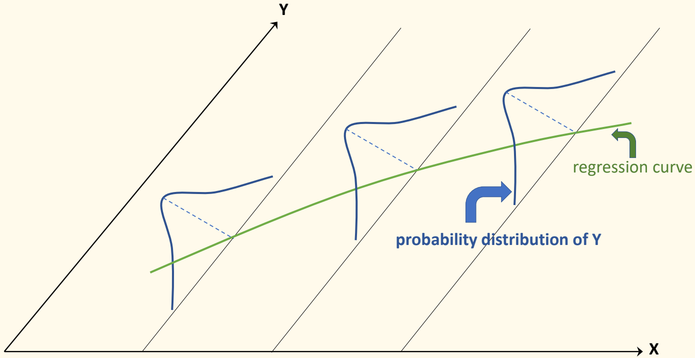
- $E(Y|X = x) = f(x)$: $f(\cdot)$ is called the regression function. What is the functional form of $f(\cdot)$? E.g., $f(x) = \beta_0 + \beta_1 x$, $f(x) = \beta_0 + \beta_1 x + \beta_2 x^2$.

(b) Random component: Given the X value(s), what is the distribution of the response variable Y?

- What is the distribution of Y given $X = x$? E.g., $Y|(X = x) \mid N(f(x), \sigma^2(x))$.

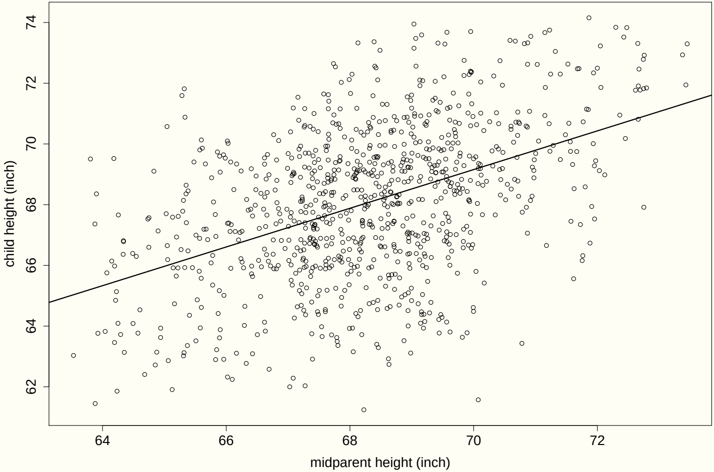
Remark: In this class, we treat X variables as given (and thus non-random).

Figure: Illustration of regression model



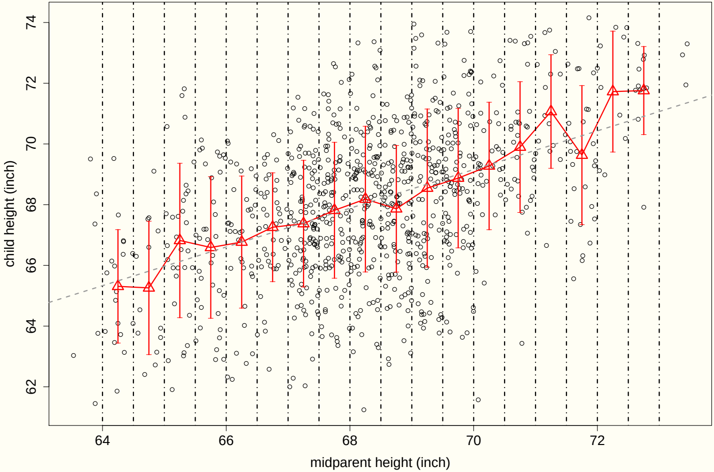
Heights: Scatter Plot

Figure: Child's height versus midparent's height



Heights: Binning

Figure: Child's height versus midparent's height



- bins (indicated by the vertical broken lines) are created by grouping data points with parent's heights within a certain 0.5inch wide interval.
- If we calculate the average of children's heights within each bin (indicated by the red triangles), we can see that they lie approximately on a straight line across the bins (indicated by the red zigzag line).
- The within-bin degree of dispersion of children's heights (indicated by the red vertical segments) is roughly the same across the bins.

*How are these observations related to the regression model? Can you think another application of **binning**?*

Heights

- Model the mean of children's heights as a linear function of the midparent's height (X):

$$f(x) = E(Y|X = x) = \beta_0 + \beta_1 x$$

- Model the distribution of children's heights as having a constant variance (i.e., not depending on the X-value):

$$Var(Y|X = x) \equiv \sigma^2$$

Simple Regression Model

Simple Linear Regression Model

The model contains **only one X variable**:

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \qquad i = 1, \ldots, n.$$

- Y_i : value of the response variable in the *ith* case; X_i : value of the X variable in the *ith* case.
- **Random errors/fluctuations**: ϵ_i – random variables: zero-mean; equal-variance; uncorrelated;
- **Unknown parameters**: β_0 – **regression intercept**; β_1 – **regression slope**; σ^2 – **error variance**

Given X_i, the response Y_i is the sum of two terms:

- Non-random (deterministic) term:

$$E(Y_i) = \beta_0 + \beta_1 X_i$$

- Random term:

$$\epsilon_i \sim \text{zero mean, common variance, uncorrelated}$$

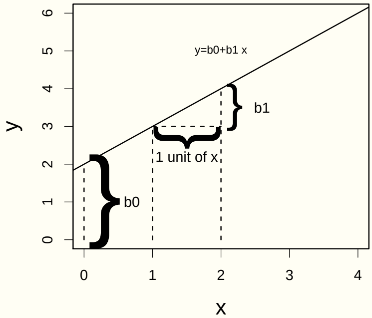
The simple linear regression model says:

- The response variable Y_i is a random variable.
- Its mean is linearly related to X_i.
- Its variance is a constant (i.e., not depending on X_i).
- Two responses Y_i and Y_j ($i \neq j$) are uncorrelated.

Regression Line

The fixed component: $y = \beta_0 + \beta_1 x$

- β_1 – regression slope: the change in $E(Y)$ per unit change of X.
- β_0 – regression intercept: the value of $E(Y)$ when $X = 0$.

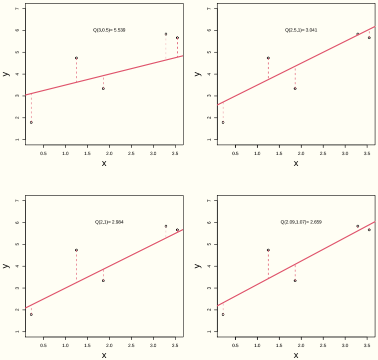


Least-Squares Estimator

Which Line is the “Best” Fit?

The answer depends on how the *goodness of fit to the data* is evaluated.

Figure: A data set with 5 data points



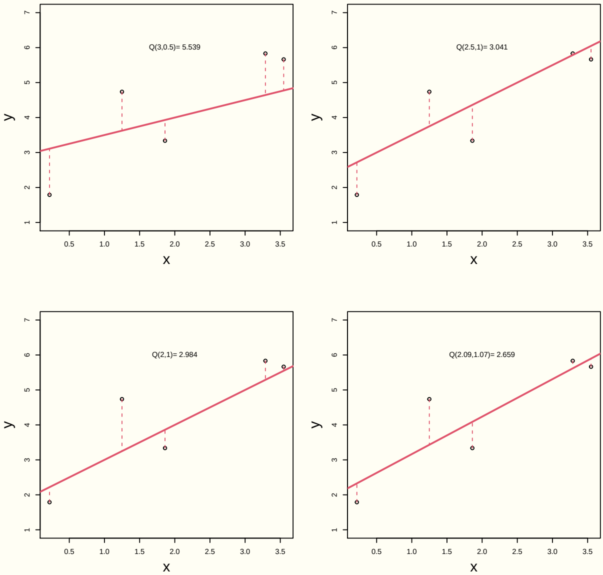
Least-Squares Principle

Given the observations $\{(X_i, Y_i)\}_{i=1}^n$ and a line $y = b_0 + b_1 x$, we can calculate the *sum of squared vertical deviations* of the observations from this line:

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

- The **least squares (LS) principle** is to find the line that minimizes the sum of squared vertical deviations.

Figure: A data set with 5 data points: $Q(b_0, b_1)$ for four different lines.



Least-Squares Estimator

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

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

- $\overline{X} = \frac{1}{n} \sum_{i=1}^n X_i, \quad \overline{Y} = \frac{1}{n} \sum_{i=1}^n Y_i$, are the **sample means**.
- $s_X = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (X_i - \overline{X})^2}, \quad s_Y = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (Y_i - \overline{Y})^2}$, are the **sample standard deviations**.
- r_{XY} is the **sample correlation** between X and Y.

What happens if X_is are all equal?

Least-Squares Line

$$y = \hat{\beta}_0 + \hat{\beta}_1 x = \overline{Y} + r_{XY}\frac{s_Y}{s_X}(x - \overline{X}).$$

- The LS line passes through the **center of the data** – $(\overline{X}, \overline{Y})$.
- If the data are **centered** (i.e., $\overline{X} = 0$, $\overline{Y} = 0$), then $\hat{\beta}_0 = 0$ and the LS line must pass the origin $(0, 0)$.
- If the data are **standardized** (i.e., $\overline{X} = 0, s_X = 1; \overline{Y} = 0, s_Y = 1$), then $\hat{\beta}_0 = 0$ and $\hat{\beta}_1 = r_{XY}$.
- **Regression effect**: One standard deviation change in X leads to r_{XY} standard deviation change in $E(Y)$. (Recall $|r_{XY}| \leq 1$)

Reading: Derive the LS Estimator

The pair (b_0, b_1) that minimizes the function $Q(\cdot, \cdot)$ satisfies:

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

This leads to the **normal equations**:

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

The solution is the LS estimator.

Fitted Values and Residuals

Fitted Values and Residuals

- **Fitted values** (one for each case) are predictions by the LS line :

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

- **Residuals** (one for each case) are differences between the observed values and their respective fitted values, i.e, they are the vertical deviations of the observations to the LS line:

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

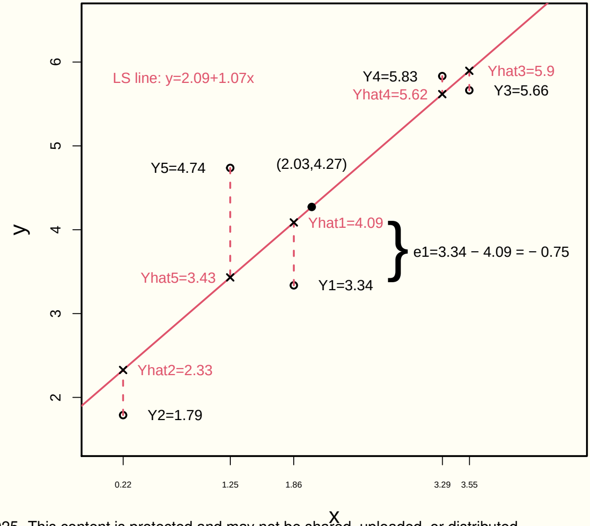
Residuals e_i and error terms ϵ_i are NOT the same thing!

Example

Case	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
Col. Sum	10.17	21.36	0.00	0.00	7.81	8.37
Col. Mean	2.03	4.27				

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

Figure: LS line, fitted values and residuals



Properties of Residuals

The residuals e_is satisfy the following constraints (two independent constraints):

(i) $\sum_{i=1}^{n} e_i = 0$; (ii) $\sum_{i=1}^{n} X_i e_i = 0$; (iii) $\sum_{i=1}^{n} \widehat{Y}_i e_i = 0$

Case	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

Mean Squared Error

Estimation of Error Variance

- Error variance $\sigma^2 = \mathrm{Var}(\epsilon_i)$.
- Idea: Estimate σ^2 by the "variance" of residuals. (Recall residual $e_i = Y_i - \hat{Y}_i = Y_i - (\hat{\beta}_0 + \hat{\beta}_1 X_i)$ and $\epsilon_i = Y_i - (\beta_0 + \beta_1 X_i)$)
- **Error sum of squares (SSE)**:

$$SSE := \sum_{i=1}^{n} e_i^2 \quad = \quad \sum_{i=1}^{n} (Y_i - \widehat{Y}_i)^2$$

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

$$MSE = \frac{SSE}{\color{red}{n-2}}$$

Degrees of Freedom

- The **degrees of freedom** of a random vector is the number of its components that are free to vary.
- Recall $\sum_{i=1}^{n} e_i = 0, \ \sum_{i=1}^{n} X_i e_i = 0 \rightarrow$ degrees of freedom of $(e_1, \cdots, e_n)$ is $n - 2$.
- $d.f.(SSE) = n - 2$.
- Indeed, it can be shown that $E(SSE) = (n-2)\sigma^2$; thus $E(MSE) = \sigma^2$, i.e, MSE is an **unbiased estimator** of σ^2.

Example (Cont'd)

Case	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

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

$$MSE = \frac{2.6715}{5-2} = 0.8905.$$

LS Estimator: Properties

Mean and Variance

Given that the simple regression model holds:

- **LS estimators are unbiased**:

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

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

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

Standard Errors (SE)

These are calculated by replacing σ^2 by MSE and then taking the square-root of the variance formulae:

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

- SE decreases with the increase of the sample size n or the sample variance s_X^2. (Recall $\sum_{i=1}^{n}(X_i - \overline{X})^2 = (n-1)s_X^2$)
- SE tends to increase with the increase of the error variance σ^2.

Illustration by Simulation

Simulation

- $n = 5$ cases with the X values

$$X_1 = 1.86, \quad X_2 = 0.22, \quad X_3 = 3.55, \quad X_4 = 3.29, \quad X_5 = 1.25,$$

  fixed throughout.
- The responses:
  - First generate $\epsilon_1, \cdots, \epsilon_5$ i.i.d. from $N(0, 1)$.
  - Then set the response variable as:

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

- Repeat 100 times $\rightarrow$ 100 data sets.

''data set 1"

case	X	Y
1	1.86	3.08
2	0.22	2.27
3	3.55	4.38
4	3.29	5.12
5	1.25	1.38

$\hat{\beta}_0 = 1.34,\ \hat{\beta}_1 = 0.94,\ MSE = 0.79.$

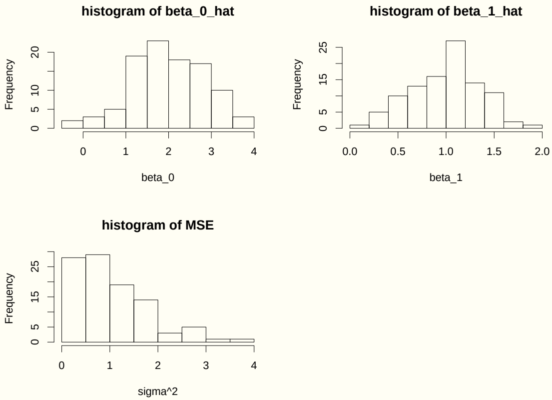
$\cdots,\cdots$

''data set 100"

case	X	Y
1	1.86	3.36
2	0.22	2.50
3	3.55	5.93
4	3.29	5.36
5	1.25	2.67

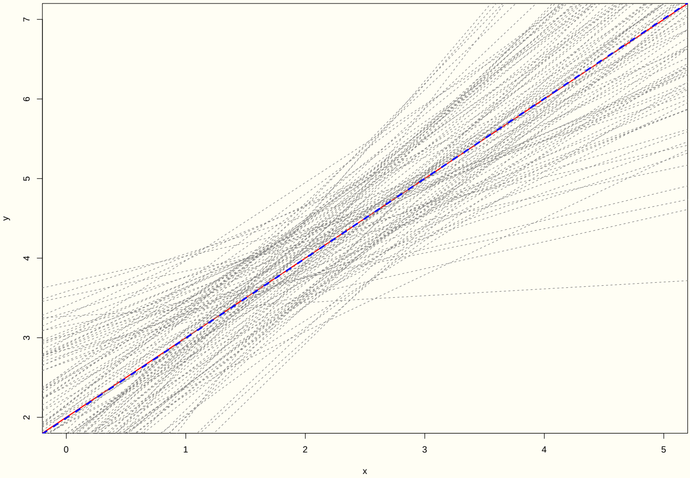
$\hat{\beta}_0 = 1.75,\ \hat{\beta}_1 = 1.09,\ MSE = 0.24.$

Figure: Sampling distributions of $\hat{\beta}_0, \hat{\beta}_1$ and MSE



Sample means are 1.99, 1.02, 1.04, respectively. True parameters are 2, 1, 1, respectively.

Figure: True: red solid; LS lines: grey broken; mean LS line: blue broken



Compare sample mean and sample standard deviation of these 100 realizations of $\hat{\beta}_0, \hat{\beta}_1$ to the respective theoretical values.

- $\hat{\beta}_0$: Theoretical mean and standard deviation:

$$E(\hat{\beta}_0) = \beta_0 = 2, \quad \sigma\{\hat{\beta}_0\} = \sqrt{\sigma^2 \left[\frac{1}{n} + \frac{\overline{X}^2}{\sum_{i=1}^n (X_i - \overline{X})^2}\right]} = 0.854$$

  Sample mean and sample standard deviation: $1.99, 0.847$.

- $\hat{\beta}_1$: Theoretical mean and standard deviation:

$$E(\hat{\beta}_1) = \beta_1 = 1, \quad \sigma\{\hat{\beta}_0\} = \sqrt{\frac{\sigma^2}{\sum_{i=1}^n (X_i - \overline{X})^2}} = 0.358$$

  Sample mean and sample standard deviation: $1.002, 0.36$.