STAT 423/523 Statistical Methods for Engineers and Scientists

Lecture 10: Simple Linear Regression

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Simple Linear Regression

Regression is a statistical method for estimating the relationships among variables. THe simpest form of regression is **simple linear regression**:

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Regression is a statistical method for estimating the relationships among variables. THe simpest form of regression is **simple linear regression**:

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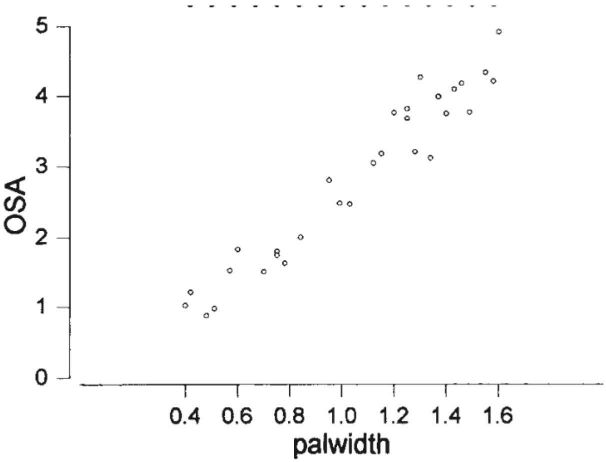
- y_i is the response variable (dependent variable).
- x_i is the predictor variable (independent variable).
- β_0 is the intercept.
- β_1 is the slope.
- ϵ_i is the error term.

Example

- y: ocular surface area
- x: width of the palprebal fissure



Assumptions

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

- Linearity: The relationship between x and y is linear.
- Independence: The errors are independent.
- Normality: The errors are normally distributed.
- Equal variance: The errors have constant variance.

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For short, the LINE assumptions give:

$$y_i = \beta_0 + \beta_1 x_i + N(0, \sigma^2) \quad \forall i$$

Violations of Assumptions

- Linearity: Nonliear regression model.
- Independence: Structural equation model (SEM) in econometrics.
- Normality: ϵ_i could have a heavy-tailed distribution.
- Equal variance: Heteroscedasticity.

Some Statistics

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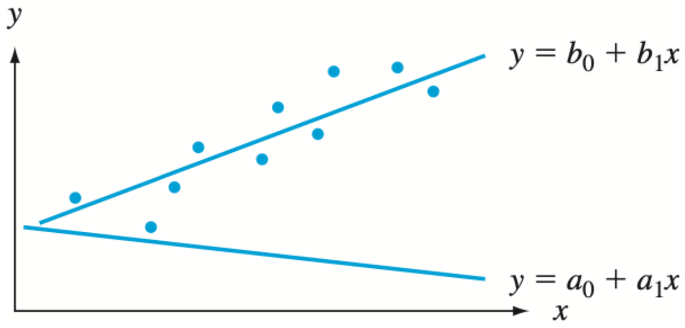
If we get the estimated coefficients $\hat{\beta}_0$ and $\hat{\beta}_1$,

- The **fitted value** for y_i is $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$.
- The **residual** for y_i is $\hat{\epsilon}_i = y_i - \hat{y}_i$.

Estimation

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

Given the data points



we want to find the line that **best fits** the data points.

Ordinary Least Squares

The first approach is **Ordinary Least Squares** (OLS).

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- The OLS estimates are the values of β_0 and β_1 that minimize the RSS:

$$\hat{\beta}_0, \hat{\beta}_1 = \underset{\beta_0, \beta_1}{\arg\min}\ \mathrm{RSS}(\beta_0, \beta_1)$$

Residual Sum of Squares

The residual sum of squares is the sum of the squared distance between the data points and the fitted line.

It is the **vertical** distance, not the orthogonal distance.

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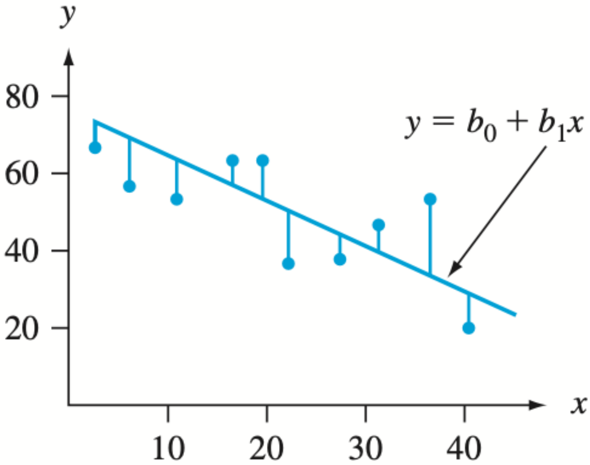

OLS

In order to minimize the RSS, we first compute its partial derivatives.

$$\mathrm{RSS}(\beta_0, \beta_1) = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

$$\frac{\partial \mathrm{RSS}}{\partial \beta_0} = -2 \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i) = -2 \sum_{i=1}^{n} y_i + 2N\beta_0 + 2\beta_1 \sum_{i=1}^{n} x_i$$

$$\frac{\partial \mathrm{RSS}}{\partial \beta_1} = -2 \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i) x_i = -2 \sum_{i=1}^{n} y_i x_i + 2\beta_0 \sum_{i=1}^{n} x_i + 2\beta_1 \sum_{i=1}^{n} x_i^2$$

To find the minimum, we set the partial derivatives to zero.

OLS

The **estimating equations** for OLS are:

$$0 = -2\sum_{i=1}^{n} y_i + 2n\beta_0 + 2\beta_1 \sum_{i=1}^{n} x_i \tag{1}$$

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Compute $(1) \times \sum_i x_i - (2) \times n$:

$$0 = 2n\sum_i x_i y_i - 2\sum_i x_i \sum_i y_i + \left(\left(\sum_i x_i\right)^2 - n\sum_i x_i^2\right)\beta_1.$$

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$$\implies \hat{\beta}_1 = \frac{\sum_i x_i y_i - n^{-1}\sum_i x_i \sum_i y_i}{\sum_i x_i^2 - n^{-1}\left(\sum_i x_i\right)^2}.$$

OLS

$$\hat{\beta}_1 = \frac{\sum_i x_i y_i - n^{-1} \sum_i x_i \sum_i y_i}{\sum_i x_i^2 - n^{-1} \left(\sum_i x_i\right)^2}.$$

- The numerator is

$$\sum_i x_i y_i - n^{-1} \sum_i x_i \sum_i y_i = S_{xy} = \sum_i (y_i - \bar{y})(x_i - \bar{x})$$

- The denominator is

$$\sum_i x_i^2 - n^{-1} \left(\sum_i x_i\right)^2 = S_{xx} = \sum_i (x_i - \bar{x})^2$$

OLS

Therefore,

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}} = \frac{\mathrm{Cov}(X,Y)}{\mathrm{Var}(X)}$$

with

$$S_{xy} = \sum_i (y_i - \bar{y})(x_i - \bar{x}) = \sum_i y_i x_i - n^{-1} \sum_i x_i \sum_i y_i$$

$$S_{xx} = \sum_i (x_i - \bar{x})^2 = \sum_i x_i^2 - n^{-1} \left(\sum_i x_i \right)^2$$

OLS

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From Eq. (1), we can get $\hat{\beta}_0$:

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}.$$

OLS

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- $n-2$ is the degrees of freedom.

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- $n-2$ is the degrees of freedom.

A quick formula in computing $\mathrm{RSS}(\hat{\beta}_0, \hat{\beta}_1)$ is

$$\mathrm{RSS}(\hat{\beta}_0, \hat{\beta}_1) = S_{yy} - \hat{\beta}_1 S_{xy} = S_{yy} - \hat{\beta}_1^2 S_{xx},$$

where

$$S_{yy} = \sum_i (y_i - \bar{y})^2 = \sum_i y_i^2 - n^{-1}\left(\sum_i y_i\right)^2.$$

OLS

Summary for OLS estimators:

$$
\begin{aligned}
\hat{\beta}_1 &= \frac{S_{xy}}{S_{xx}} = \frac{\mathrm{Cov}(X, Y)}{\mathrm{Var}(X)} \\
\hat{\beta}_0 &= \bar{y} - \hat{\beta}_1 \bar{x} \\
\hat{\sigma}^2 &= \frac{\mathrm{RSS}(\hat{\beta}_0, \hat{\beta}_1)}{n-2} = \frac{S_{yy} - \hat{\beta}_1 S_{xy}}{n-2}
\end{aligned}
$$

Example (Textbook Example 12.8)

x	12	30	36	40	45	57	62	67	71	78	93	94	100	105
y	3.3	3.2	3.4	3.0	2.8	2.9	2.7	2.6	2.5	2.6	2.2	2.0	2.3	2.1

Some statistics:

$$n = 14 \qquad \sum x_i = 890 \qquad \sum x_i^2 = 67182$$

$$\sum y_i = 37.6 \qquad \sum y_i^2 = 103.54 \qquad \sum x_i y_i = 2234.30$$

Example (Textbook Example 12.8)

We can compute the following statistics:

$$S_{xx} = 10603.43, \quad S_{xy} = -155.99, \quad S_{yy} = 2.557$$

The estimators are

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}} = \frac{-155.99}{10603.43} = -0.0147$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} = \frac{37.6}{14} - (-0.0147) \times \frac{890}{14} = 3.62$$

$$\hat{\sigma}^2 = \frac{S_{yy} - \hat{\beta}_1 S_{xy}}{n-2} = \frac{2.557 - (-0.0147) \times (-155.99)}{14-2} = 0.022$$

Properties of OLS Estimators

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- S_{xy} can be written as

$$S_{xy} = \sum x_i y_i - n^{-1} \sum x_i \sum y_i = \sum_i \left[(x_i - \bar{x}) \, y_i \right]$$

The highlighted y_i's are the only random variables and we have

$$y_i \sim N(\beta_0 + \beta_1 x_i, \sigma^2),$$

where β_0 and β_1 are the true parameters.

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- Now we have

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}} \sim N(\beta_1, \sigma^2 S_{xx}^{-1})$$

Properties of OLS Estimators

- For the intercept estimator, we have

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \sim N(\beta_0, (n^{-1} + \bar{x}^2 S_{xx}^{-1})\sigma^2)$$

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- For the variance estimator, we have

$$E(\hat{\sigma}^2) = \sigma^2.$$

Properties of OLS Estimators

Summary:

- All OLS estimators are **unbiased**:

$$E(\hat{\beta}_0) = \beta_0$$
$$E(\hat{\beta}_1) = \beta_1$$
$$E(\hat{\sigma}^2) = \sigma^2$$

- The estimated **standard errors (se)** of the estimators are:

$$s_{\hat{\beta}_0} = \sqrt{(n^{-1} + \bar{x}^2 S_{xx}^{-1})\hat{\sigma}^2}$$
$$s_{\hat{\beta}_1} = \sqrt{S_{xx}^{-1}\hat{\sigma}^2}$$
$$s_{\hat{\sigma}^2} = \sqrt{\frac{2\hat{\sigma}^4}{n-2}}$$

Confidence Interval

The $(1-\alpha)$ confidence interval for β_1 is

$$\hat{\beta}_1 \pm t_{\alpha/2,n-2} s_{\hat{\beta}_1}.$$

- Confidence interval uses two-sided t-distribution with $n-2$ degrees of freedom.
- It is t-distributed because we are estimating σ^2 from the data.

Hypothesis Testing

Consider the following hypothesis testing:

$$H_0 : \beta_1 = 0 \quad H_a : \beta_1 \neq 0.$$

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Method 1: reject null if the CI does not cover 0:

$$\text{reject null if } 0 \notin (\hat{\beta}_1 - t_{\alpha/2,n-2} s_{\hat{\beta}_1}, \hat{\beta}_1 + t_{\alpha/2,n-2} s_{\hat{\beta}_1})$$

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Method 2: reject null if the test statistic

$$t = \frac{\hat{\beta}_1}{s_{\hat{\beta}_1}}$$

is greater than $t_{\alpha/2,n-2}$ in absolute value.

Hypothesis Testing

$$H_0 : \beta_1 = 0 \quad H_a : \beta_1 \neq 0.$$

Method 3: reject null if the p-value

$$p = 2\left(1 - F_{t,n-2}(|\hat{\beta}_1 / s_{\hat{\beta}_1}|)\right)$$

is less than α.

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- To test $H_0 : \beta_1 > 0$, we should use one-sided t-test.

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is less than α.

- To test $H_0 : \beta_1 > 0$, we should use one-sided t-test.
- Same process for testing $\beta_0 = 0$.

Goodness of Fit

The variation in the response variable y_i is

$$SST = \sum_i (y_i - \bar{y})^2$$

The variation explained by the regression model is

$$SSR = \sum_i (\hat{y}_i - \bar{y})^2$$

The variation not explained by the regression model is

$$SSE = \sum_i (y_i - \hat{y}_i)^2$$

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The variation not explained by the regression model is

$$SSE = \sum_i (y_i - \hat{y}_i)^2$$

We have

$$SST = SSR + SSE$$

Goodness of Fit

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$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}.$$

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$$R^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}.$$

- R^2 is the proportion of the variation in the response variable that is explained by the regression model.
- R^2 is between 0 and 1.
- R^2 is a measure of the goodness of fit of the regression model.

Residual Plot

The **residual** is defined as the difference between the observed value and the fitted value:

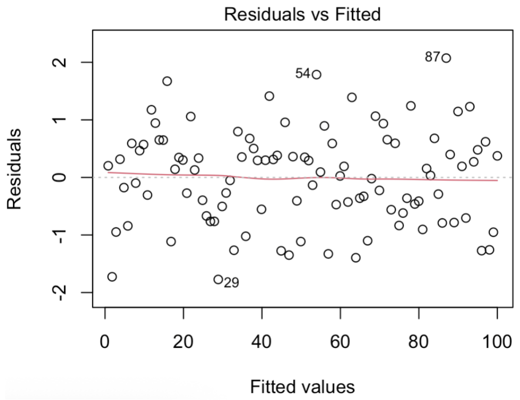
$$\hat{\epsilon}_i = y_i - \hat{y}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i.$$

Residual Plot

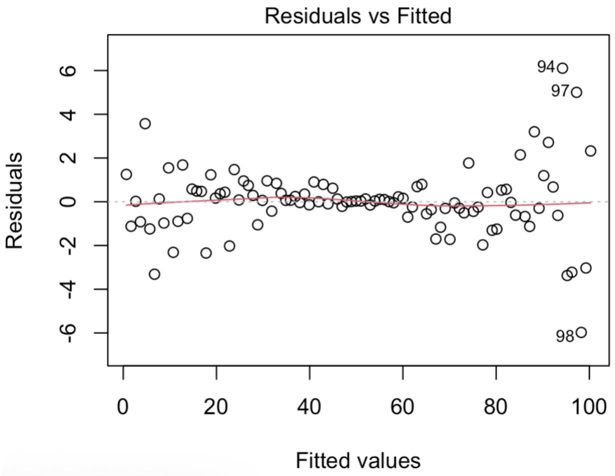
The **residual** is defined as the difference between the observed value and the fitted value:

$$\hat{\epsilon}_i = y_i - \hat{y}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i.$$

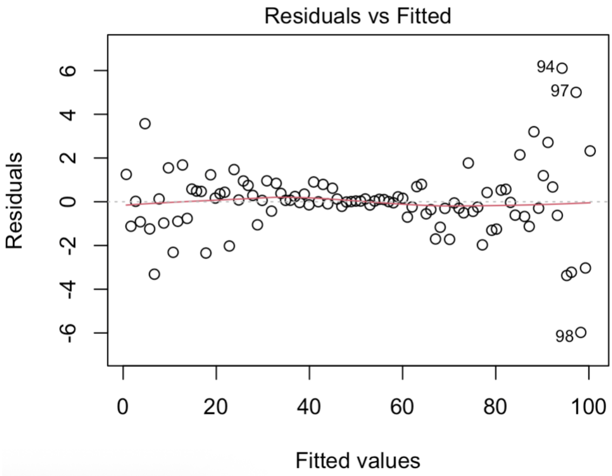
The **residual plot** is a scatter plot of the residuals against the fitted values.



Residual Plot

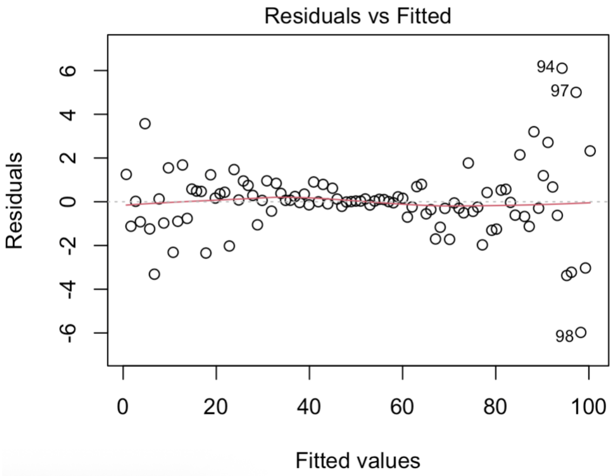


Residual Plot



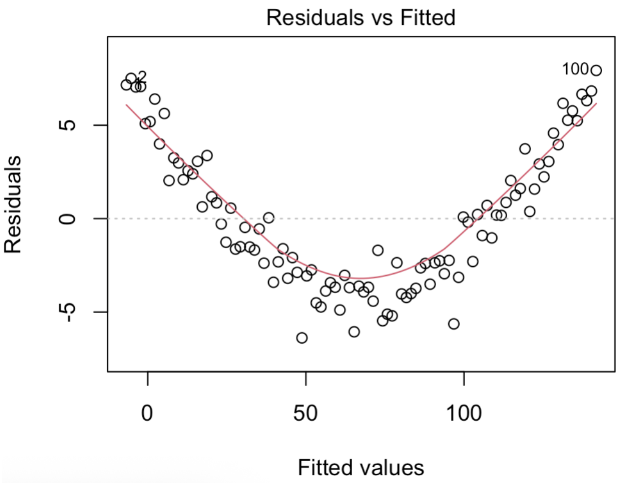
The variance is not equal for all ϵ_i's.

Residual Plot

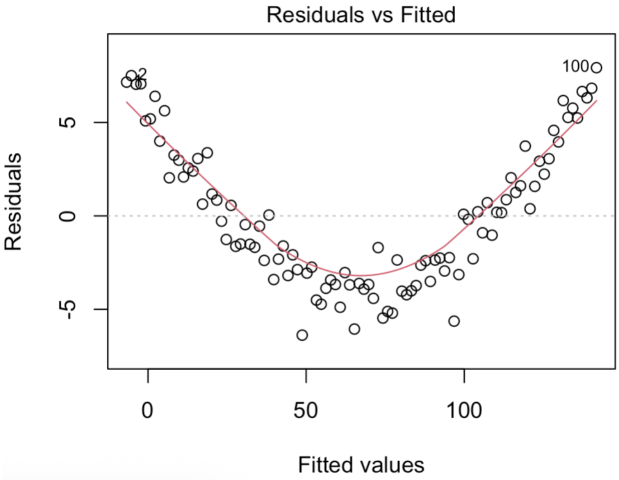


The variance is not equal for all ϵ_i's. **Solution**: data need to be transformed.

Residual Plot

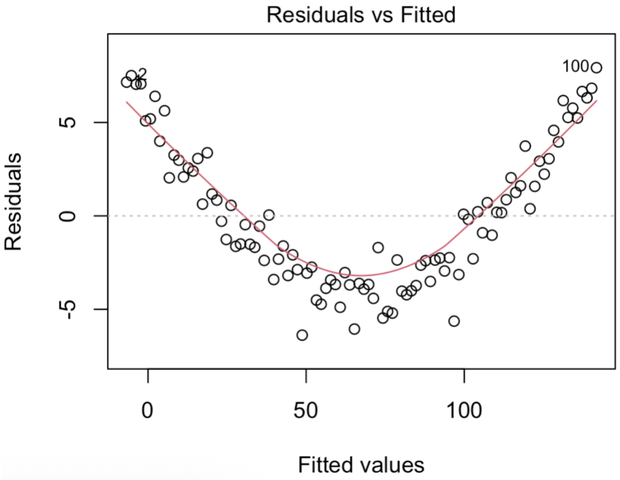


Residual Plot



The residual is not independent with the fitted value.

Residual Plot



The residual is not independent with the fitted value. **Solution**: add more predictors.

QQ Plot

The **QQ plot** is a scatter plot of the quantiles of the residuals against the quantiles of the normal distribution.

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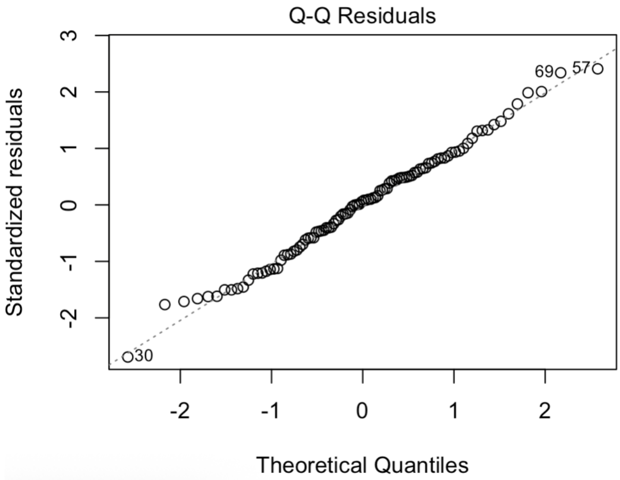
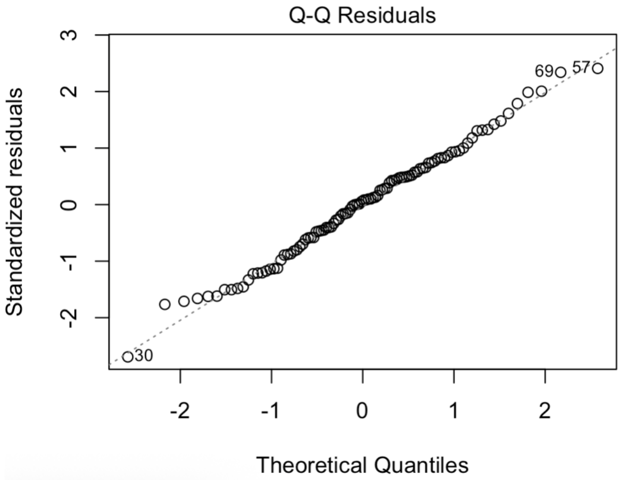
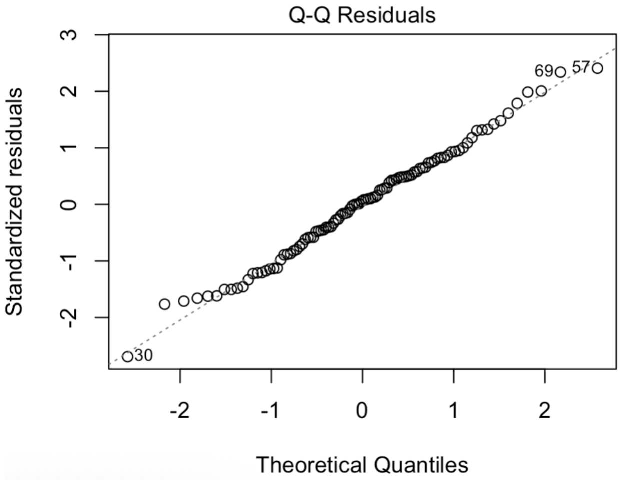


QQ Plot



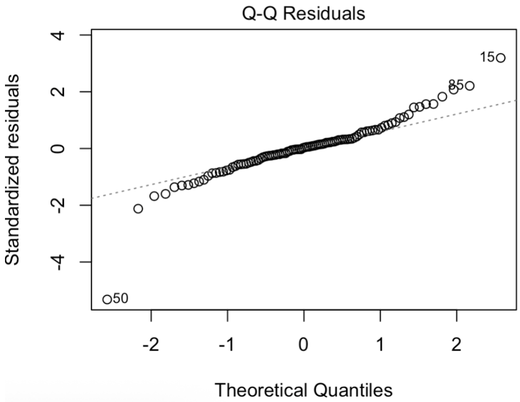
Q-Q Residuals
Standardized residuals
Theoretical Quantiles
-2
-1
0
1
2
3
69
57
30

QQ Plot



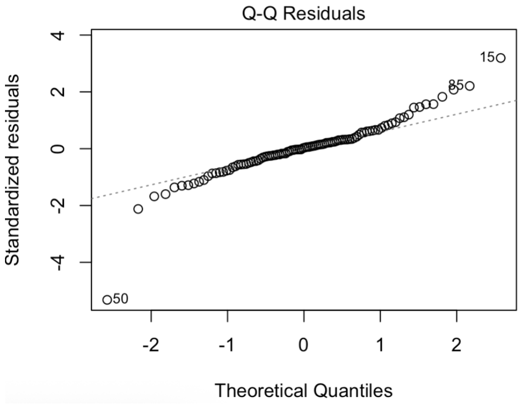
If all the points are on the line, then the residuals are normally distributed.

QQ Plot



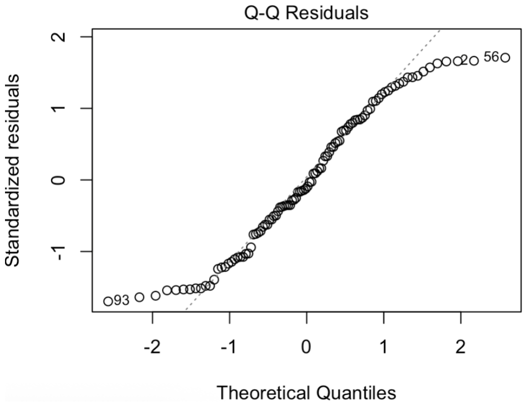
Q-Q Residuals
Standardized residuals
Theoretical Quantiles
-4
-2
0
2
4
-2
-1
0
1
2
15
85
50

QQ Plot

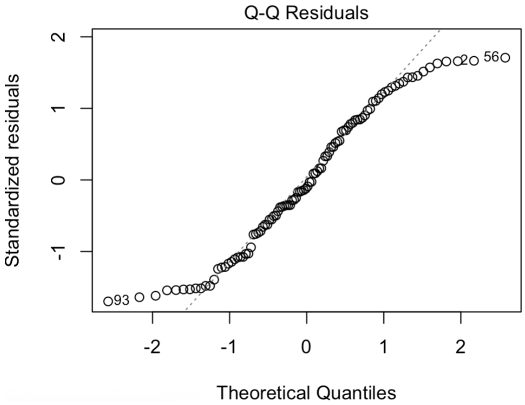


If the left tail is bended down and the right tail is bended up, then the residuals are **heavy-tailed**.

QQ Plot


Q-Q Residuals
Standardized residuals
Theoretical Quantiles
-2
-1
0
1
2
93
2
56

QQ Plot



If the left tail is bended up and the right tail is bended down, then the residuals are **light-tailed**.

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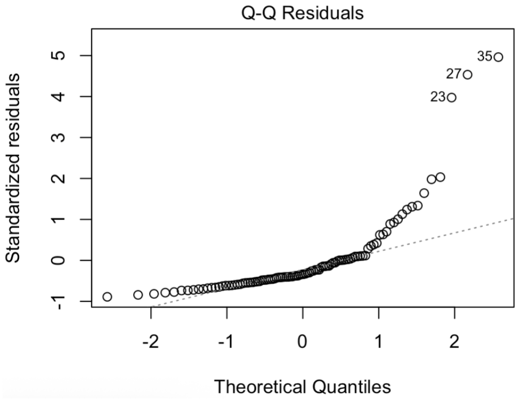
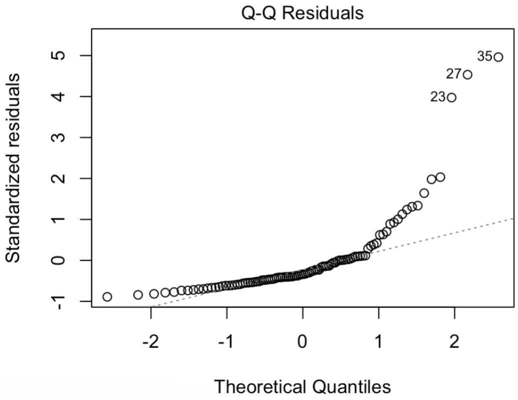

Q-Q Residuals
Standardized residuals
Theoretical Quantiles
-1
0
1
2
3
4
5
-2
-1
0
1
2
35
27
23

QQ Plot



If the two tails are bended to the same direction, then the residuals are **skewed**.

QQ Plot

- If the points are on the line, then the residuals are normally distributed.
- If the points are not on the line, then the residuals are not normally distributed.

QQ Plot

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- If the points are not on the line, then the residuals are not normally distributed.
- Light tails is usually not a problem.
- But heavy tails is a problem.

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The hypothesis testing of $H_0 : \beta_1 = 0$ can be done by the F-test:

$$\text{reject null when } F > F_{\alpha,n-2}$$

T-test vs. F-test

$$H_0 : \beta_1 = 0 \quad \text{v.s.} \quad H_a : \beta_1 \neq 0.$$

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For t-test, we have

$$t = \frac{\hat{\beta}_1}{s_{\hat{\beta}_1}} = \frac{S_{xy}/S_{xx}}{\sqrt{S_{xx}^{-1}\hat{\sigma}^2}} = \frac{S_{xy}}{\sqrt{S_{xx} \cdot \mathrm{MSE}}}$$

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Therefore, the t-test and F-test for β_1 are equivalent.

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- $\hat{y}_*$ is a random variable
  because $\hat{\beta}_0$ and $\hat{\beta}_1$ are random variables depending on the data.

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$$E(\hat{y}_*) = E(\hat{\beta}_0) + E(\hat{\beta}_1)x_* = \beta_0 + \beta_1 x_* = \bar{y}_*$$

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- An estimate of the variance is

$$\hat{\sigma}^2 \left(\frac{1}{n} + \frac{(x_* - \bar{x})^2}{S_{xx}} \right).$$

Prediction

The $(1-\alpha)$ **confidence interval for the mean response** is

$$\hat{y}_* \pm t_{\alpha/2,n-2}\sqrt{\hat{\sigma}^2\left(\frac{1}{n}+\frac{(x_*-\bar{x})^2}{S_{xx}}\right)}$$

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- y_* is more noisy than $\bar{y}_*$.
- Above CI has a less coverage for y_* than $\bar{y}_*$.
- We need a wider CI for y_*.

Prediction

The $(1-\alpha)$ **prediction interval for the response** is

$$\hat{y}_* \pm t_{\alpha/2,n-2}\sqrt{\hat{\sigma}^2\left(1+\frac{1}{n}+\frac{(x_*-\bar{x})^2}{S_{xx}}\right)}$$

Prediction

The $(1-\alpha)$ **prediction interval for the response** is

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The interpretation is:
The probability that this PI covers the **response** y_* is $1-\alpha$.

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The $(1-\alpha)$ **prediction interval for the response** is

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The interpreation is:
The probability that this PI covers the **response** y_* is $1-\alpha$.

- The constant 1 in the above formula accounts for the variance of the error term ϵ_*.
- The prediction interval is wider than the confidence interval for the mean response.

Example (textbook example 12.13)

x = carbonation depth (mm) and y = strength (MPa).

x	8.0	15.0	16.5	20.0	20.0	27.5	30.0	30.0	35.0
y	22.8	27.2	23.7	17.1	21.5	18.6	16.1	23.4	13.4

x	38.0	40.0	45.0	50.0	50.0	55.0	55.0	59.0	65.0
y	19.5	12.4	13.2	11.4	10.3	14.1	9.7	12.0	6.8

Summary statistics:

$$n = 18 \qquad \sum_i x_i = 659.0 \qquad \sum_i x_i^2 = 28967.50$$

$$\sum_i y_i = 293.2 \qquad \sum_i y_i^2 = 5335.76 \qquad \sum_i x_i y_i = 9293.95$$

Example (textbook example 12.13)

We first compute:

$$S_{xx} = 28967.50 - \frac{659^2}{18} = 4840.778$$
$$S_{xy} = 9293.95 - \frac{659 \times 293.2}{18} = -1440.428$$
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The estimators are:

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}} = -0.2976$$
$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} = 27.183$$
$$\hat{\sigma}^2 = \frac{S_{yy} - \hat{\beta}_1 S_{xy}}{n-2} = 8.203$$

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The 95% confidence interval for the mean response is

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The 95% prediction interval for the response is

$$13.79 \pm t_{0.025,16}\sqrt{8.203\left(1 + \frac{1}{18} + \frac{(45 - 36.611)^2}{4840.778}\right)} = (7.50, 20.08)$$

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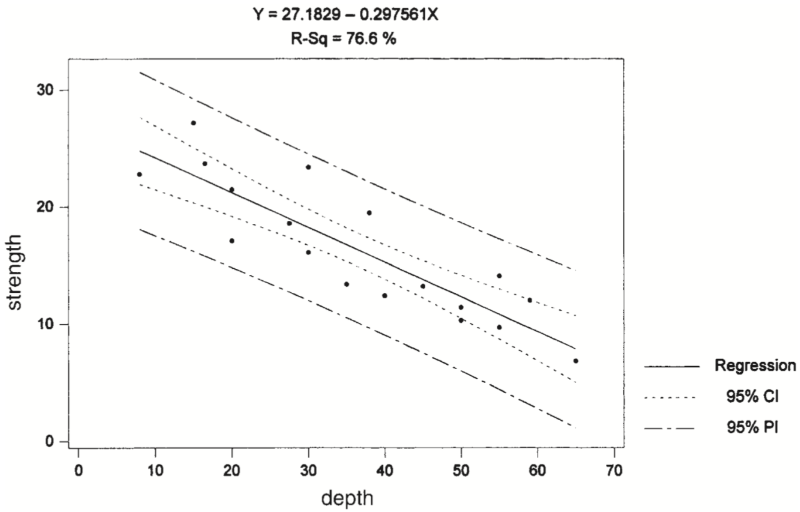

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- The **pointwise confidence band for the mean response** is the region that

$$|y - (\hat{\beta}_0 + \hat{\beta}_1 x)| < t_{\alpha/2,n-2}\sqrt{\hat{\sigma}^2\left(\frac{1}{n} + \frac{(x_* - \bar{x})^2}{S_{xx}}\right)}$$

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- Interpreation: for any given x, the probability that the mean response at x is in the band is $1 - \alpha$.

Confidence Band

The **Working-Hotelling simultaneous confidence band** is the region that

$$|y - (\hat{\beta}_0 + \hat{\beta}_1 x)| < \sqrt{2F_{\alpha,2,n-2}}\sqrt{\hat{\sigma}^2\left(1 + \frac{1}{n} + \frac{(x_* - \bar{x})^2}{S_{xx}}\right)}$$

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- Interpreation: the probability that the confidence band covers the whole mean response curve is $1 - \alpha$.
- The simultaneous confidence band is wider than the pointwise confidence band.

$$2F_{\alpha,2,n-2} > F_{\alpha,1,n-2} = t^2_{\alpha/2,n-2}$$