Course 02402 Introduction to Statistics

Lecture 8: Simple linear regression

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## Overview

1. Example: Height-Weight
2. Linear regression model
3. Least squares method
4. Statistics and linear regression?
5. Hypothesis tests and confidence intervals for β_0 and β_1
6. Confidence and prediction intervals for the line
7. Summary of 'summary(lm(y$\sim$x))'
8. Correlation
9. Residual Analysis: Model validation

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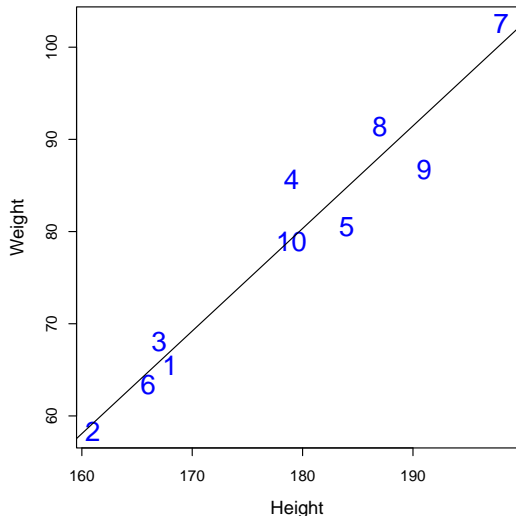
8. Correlation

9. Residual Analysis: Model validation

Example: Height-Weight

Heights (x_i)	168	161	167	179	184	166	198	187	191	179
Weights (y_i)	65.5	58.3	68.1	85.7	80.5	63.4	102.6	91.4	86.7	78.9
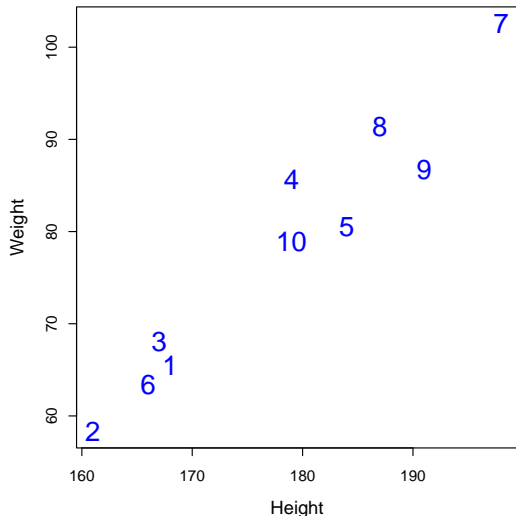
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```
summary(lm(y ~ x))

##
## Call:
## lm(formula = y ~ x)
##
## Residuals:
##    Min     1Q Median    3Q    Max
## -5.876 -1.451 -0.608  2.234  6.477
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -119.958     18.897   -6.35  0.00022 ***
## x              1.113      0.106   10.50  5.9e-06 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3.88 on 8 degrees of freedom
## Multiple R-squared:  0.932,Adjusted R-squared:  0.924
## F-statistic:  110 on 1 and 8 DF,  p-value: 5.87e-06
```

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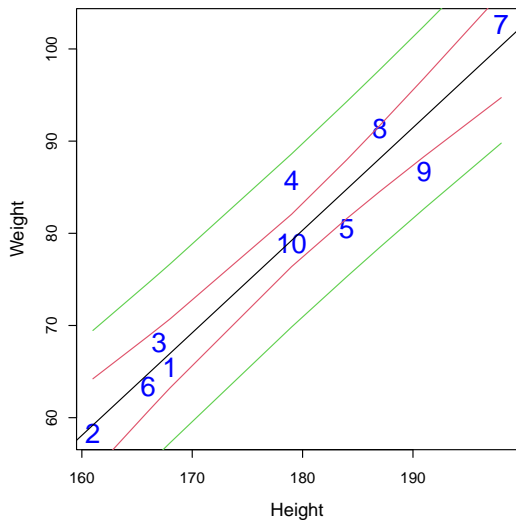
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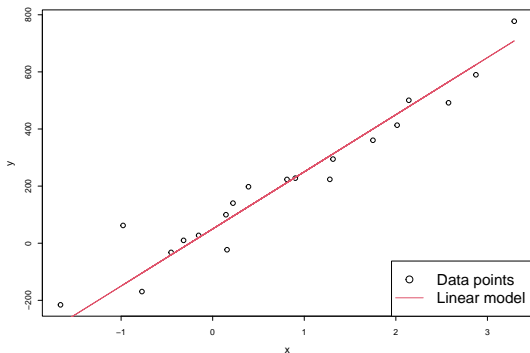
A scatter plot of some data

- We have n pairs of data points (x_i, y_i).
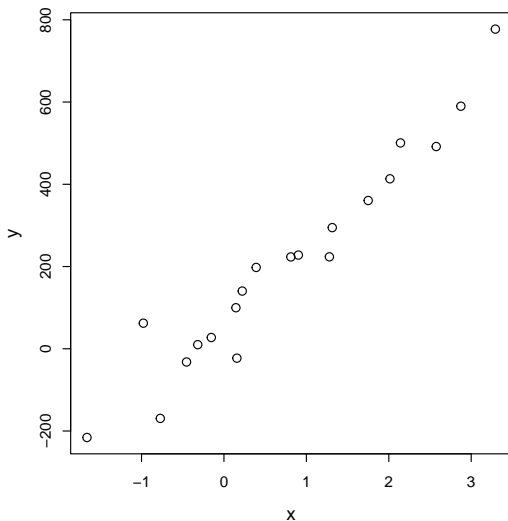
Express a linear model

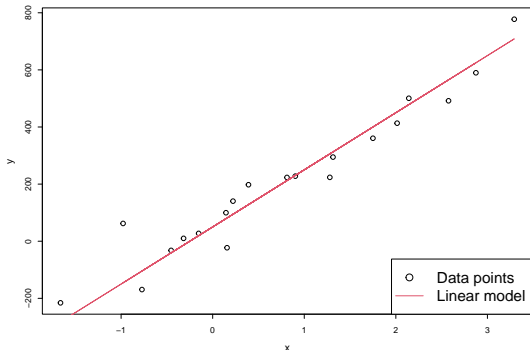- Express a linear model:

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

Express a linear model

- Express a linear model:

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

- Something is missing: Description of the *random variation*.

Express a linear regression model

- Express the *linear regression model*:

$$Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad i = 1, \ldots, n.$$

- Y_i is the *dependent/outcome variable*. A random variable.

- x_i is an *independent/explanatory variable*. Deterministic numbers.

- ε_i is the deviation/error. A random variable.

- We assume that the ε_i, $i = 1, \ldots, n$, are *independent and identically distributed (i.i.d.)*, with $\varepsilon_i \sim N(0, \sigma^2)$.

Illustration of statistical model
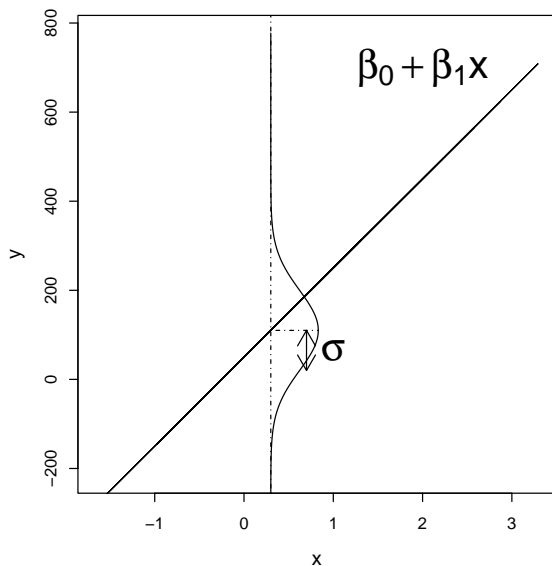
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Least squares method

- How can we estimate the parameters β_0 and β_1?

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- Good idea: Minimize the variance σ^2 of the residuals.

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- But how?

Least squares method

- How can we estimate the parameters β_0 and β_1?
- Good idea: Minimize the variance σ^2 of the residuals.
- But how?
- Minimize the Residual Sum of Squares (RSS),

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

$\hat{\beta}_0$ and $\hat{\beta}_1$ minimize the RSS.

Illustration of model, data and fit
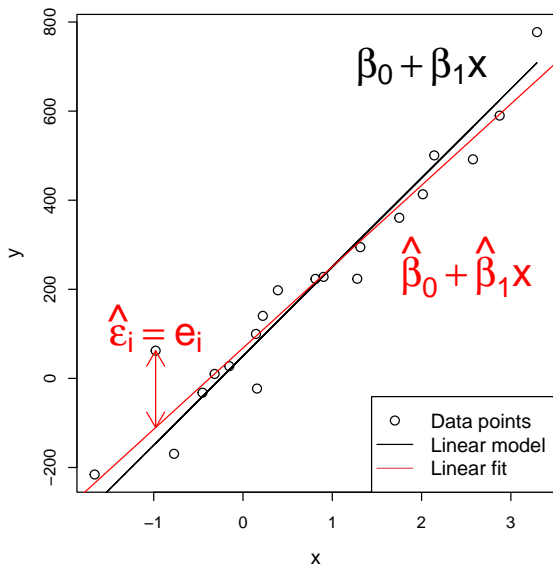
Least squares estimator

Theorem 5.4 (here as estimators, as in the book)

The least squares estimators of β_0 and β_1 are given by

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(Y_i - \bar{Y})(x_i - \bar{x})}{S_{xx}}$$

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

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

Least squares estimates

Theorem 5.4 (here as *estimates*)

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

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

R example

```r
set.seed(100)

# Generate x
x <- runif(n = 20, min = -2, max = 4)

# Simulate y
beta0 <- 50; beta1 <- 200; sigma <- 90
y <- beta0 + beta1 * x + rnorm(n = length(x), mean = 0, sd = sigma)

# From here: like for the analysis of 'real data', we have data in x and y:

# Scatter plot of y against x
plot(x, y)

# Find the least squares estimates, use Theorem 5.4
(beta1hat <- sum( (y - mean(y))*(x-mean(x)) ) / sum( (x-mean(x))^2 ))
(bet0hat <- mean(y) - beta1hat*mean(x))

# Use lm() to find the estimates
lm(y ~ x)

# Plot the fitted  line
abline(lm(y ~ x), col="red")
```

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The parameter estimates are random variables

What if we took a new sample?

Would the values of $\hat{\beta}_0$ and $\hat{\beta}_1$ be the same?

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No, they are random variables!

If we took a new sample, we would get another realisation.

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What are the (sampling) distributions of the parameter estimates ...

... in a linear regression model w. normal distributed errors?

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What are the (sampling) distributions of the parameter estimates ...

... in a linear regression model w. normal distributed errors?

This may be investigated using simulation ...

Let's go to R!

The distribution of $\hat{\beta}_0$ and $\hat{\beta}_1$

- $\hat{\beta}_0$ and $\hat{\beta}_1$ are normal distributed and their variance can be estimated:

Theorem 5.8 (first part)

$$V[\hat{\beta}_0] = \frac{\sigma^2}{n} + \frac{\bar{x}^2 \sigma^2}{S_{xx}}$$

$$V[\hat{\beta}_1] = \frac{\sigma^2}{S_{xx}}$$

$$Cov[\hat{\beta}_0, \hat{\beta}_1] = -\frac{\bar{x} \sigma^2}{S_{xx}}$$

- We won't use the covariance $Cov[\hat{\beta}_0, \hat{\beta}_1]$ for now.

Estimates of standard deviations of $\hat{\beta}_0$ and $\hat{\beta}_1$

Theorem 5.8 (second part)

σ^2 is usually replaced by its estimate, $\hat{\sigma}^2$, the *central estimator of* σ^2:

$$\hat{\sigma}^2 = \frac{RSS(\hat{\beta}_0, \hat{\beta}_1)}{n-2} = \frac{\sum_{i=1}^{n} e_i^2}{n-2}.$$

When the estimate of σ^2 is used, the variances also become estimates.
We'll refer to them as $\hat{\sigma}_{\beta_0}^2$ and $\hat{\sigma}_{\beta_1}^2$.

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When the estimate of σ^2 is used, the variances also become estimates.
We'll refer to them as $\hat{\sigma}_{\beta_0}^2$ and $\hat{\sigma}_{\beta_1}^2$.

Estimates of standard deviations of $\hat{\beta}_0$ and $\hat{\beta}_1$ (equations 5-43 and 5-44):

$$\hat{\sigma}_{\beta_0} = \hat{\sigma}\sqrt{\frac{1}{n} + \frac{\bar{x}^2}{S_{xx}}}; \quad \hat{\sigma}_{\beta_1} = \hat{\sigma}\sqrt{\frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2}}$$

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Hypothesis tests for β_0 and β_1

We can carry out hypothesis tests for the parameters in a linear regression model:

$$
\begin{aligned}
H_{0,i} : & \quad \beta_i = \beta_{0,i} \\
H_{1,i} : & \quad \beta_i \neq \beta_{1,i}
\end{aligned}
$$

Hypothesis tests for β_0 and β_1

We can carry out hypothesis tests for the parameters in a linear regression model:

$$H_{0,i}: \quad \beta_i = \beta_{0,i}$$
$$H_{1,i}: \quad \beta_i \neq \beta_{1,i}$$

Theorem 5.12

Under the null-hypotheses ($\beta_0 = \beta_{0,0}$ and $\beta_1 = \beta_{0,1}$) the statistics

$$T_{\beta_0} = \frac{\hat{\beta}_0 - \beta_{0,0}}{\hat{\sigma}_{\beta_0}}; \quad T_{\beta_1} = \frac{\hat{\beta}_1 - \beta_{0,1}}{\hat{\sigma}_{\beta_1}},$$

are t-distributed with $n-2$ degrees of freedom, and inference should be based on this distribution.

Hypothesis tests for β_0 and β_1

- See Example 5.13 for an example of a hypothesis test.

- Test if the parameters are significantly different from 0:

$$H_{0,i} : \beta_i = 0, \quad H_{1,i} : \beta_i \neq 0$$

```r
# Read data into R

x <- c(168, 161, 167, 179, 184, 166, 198, 187, 191, 179)
y <- c(65.5, 58.3, 68.1, 85.7, 80.5, 63.4, 102.6, 91.4, 86.7, 78.9)

# Fit model to data
fit <- lm(y ~ x)

# Look at model summary to find Tobs-values and p-values
summary(fit)
```

Confidence intervals for β_0 and β_1

Method 5.15

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

$$\hat{\beta}_0 \pm t_{1-\alpha/2}\, \hat{\sigma}_{\beta_0}$$

$$\hat{\beta}_1 \pm t_{1-\alpha/2}\, \hat{\sigma}_{\beta_1}$$

where $t_{1-\alpha/2}$ is the $(1-\alpha/2)$-quantile of a t-distribution with $n-2$ degrees of freedom.

- Remember that $\hat{\sigma}_{\beta_0}$ and $\hat{\sigma}_{\beta_1}$ may be found using equations 5-43 and 5-44.

- In R, we can find $\hat{\sigma}_{\beta_0}$ and $\hat{\sigma}_{\beta_1}$ under "Std. Error" from summary(fit).

Illustration of CIs by simulation

```r
# Number of repetitions (here: CIs)
nRepeat <- 1000

# Empty logical vector of length nRepeat
TrueValInCI <- logical(nRepeat)

# Repeat the simulation and estimation nRepeat times:
for(i in 1:nRepeat){
  # Generate x
  x <- runif(n = 20, min = -2, max = 4)
  # Simulate y
  beta0 = 50; beta1 = 200; sigma = 90
  y <- beta0 + beta1 * x + rnorm(n = length(x), mean = 0, sd = sigma)
  # Use lm() to fit model
  fit <- lm(y ~ x)
  # Use confint() to compute 95% CI for intercept
  ci <- confint(fit, "(Intercept)", level=0.95)
  # Was the 'true' intercept included in the interval? (covered)
  (TrueValInCI[i] <-  ci[1] < beta0  &  beta0 < ci[2])
}

# How often was the true intercept included in the CI?
sum(TrueValInCI) / nRepeat
```

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Method 5.18 Confidence interval for $\beta_0 + \beta_1 x_0$

- The confidence interval for $\beta_0 + \beta_1 x_0$ corresponds to a confidence interval for the line at the point x_0.

- The $100(1-\alpha)\%$ CI is computed by

$$(\hat{\beta}_0 + \hat{\beta}_1 x_0) \pm t_{\alpha/2} \cdot \hat{\sigma} \sqrt{\frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}}} \, .$$

Method 5.18 Prediction interval for $\beta_0 + \beta_1 x_0 + \varepsilon_0$

- The prediction interval for Y_0 is found using a value x_0.

- This is done *before* Y_0 is observed, using

$$(\hat{\beta}_0 + \hat{\beta}_1 x_0) \pm t_{\alpha/2} \cdot \hat{\sigma} \sqrt{1 + \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{S_{xx}}} \, .$$

- In $100(1 - \alpha)\%$ of cases, the prediction interval will contain the observed y_0.

- For a given α, a prediction interval is wider than a confidence interval.

Example of confidence intervals for the line

```r
# Generate x
x <- runif(n = 20, min = -2, max = 4)

# Simulate y
beta0 = 50; beta1 = 200; sigma = 90
y <- beta0 + beta1 * x + rnorm(n = length(x), sd = sigma)

# Use lm() to fit model
fit <- lm(y ~ x)

# Make a sequence of 100 x-values
xval <- seq(from = -2, to = 6, length.out = 100)

# Use the predict function
CI <- predict(fit, newdata = data.frame(x = xval),
              interval = "confidence",
              level = 0.95)

# Check what we got
head(CI)

# Plot the data, model fit and intervals
plot(x, y, pch = 20)
abline(fit)
lines(xval, CI[, "lwr"], lty=2, col = "red", lwd = 2)
lines(xval, CI[, "upr"], lty=2, col = "red", lwd = 2)
```
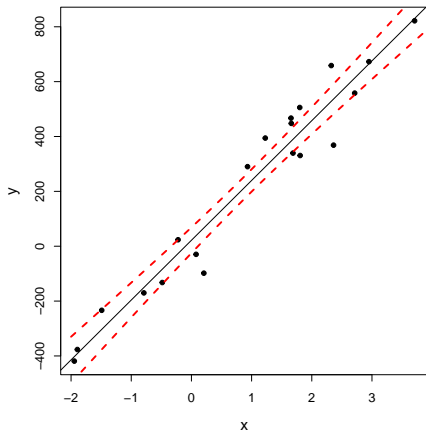
Example of prediction intervals for the line

```
# Generate x
x <- runif(n = 20, min = -2, max = 4)

# Simulate y
beta0 = 50; beta1 = 200; sigma = 90
y <- beta0 + beta1 * x + rnorm(n = length(x), sd = sigma)

# Use lm() to fit model
fit <- lm(y ~ x)

# Make a sequence of 100 x-values
xval <- seq(from = -2, to = 6, length.out = 100)

# Use the predict function
PI <- predict(fit, newdata = data.frame(x = xval),
              interval = "prediction",
              level = 0.95)

# Check what we got
head(CI)

# Plot the data, model fit and intervals
plot(x, y, pch = 20)
abline(fit)
lines(xval, PI[, "lwr"], lty = 2, col = "blue", lwd = 2)
lines(xval, PI[, "upr"], lty = 2, col = "blue", lwd = 2)
```
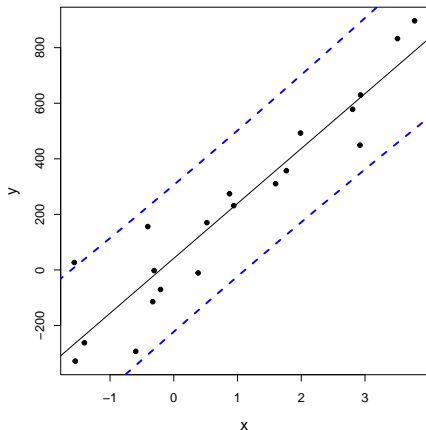
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What more do we get from `summary()`?

```
summary(fit)

##
## Call:
## lm(formula = y ~ x)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -216.86  -66.09   -7.16   58.48  293.37
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)     41.8       30.9    1.35     0.19
## x              197.6       16.4   12.05  4.7e-10 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 122 on 18 degrees of freedom
## Multiple R-squared:  0.89,Adjusted R-squared:  0.884
## F-statistic:  145 on 1 and 18 DF,  p-value: 4.73e-10
```

summary(lm(y~x))

- Residuals: Min   1Q   Median   3Q   Max

summary(lm(y∼x))

- ```
  Residuals:        Min        1Q    Median        3Q       Max
  ```
  The residuals': minimum, 1st quartile, median, 3rd quartile, maximum

summary(lm(y~x))

- Residuals: Min   1Q   Median   3Q   Max
  The residuals': minimum, 1st quartile, median, 3rd quartile, maximum

- Coefficients:
                Estimate Std. Error t value Pr(>|t|) "stars"

summary(lm(y∼x))

- Residuals: Min   1Q   Median   3Q   Max

  The residuals': minimum, 1st quartile, median, 3rd quartile, maximum

- Coefficients:

               Estimate Std. Error t value Pr(>|t|) "stars"

  The coefficients':

  $$\hat{\beta}_i \qquad\qquad \hat{\sigma}_{\beta_i} \qquad\qquad t_{\text{obs}} \qquad\qquad p\text{-value}$$

  - The test is $H_{0,i} : \beta_i = 0$ vs. $H_{1,i} : \beta_i \neq 0$
  - The stars indicate which size category the p-value belongs to.

summary(lm(y~x))

- Residuals: Min   1Q   Median   3Q   Max

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- Residual standard error: XXX on XXX degrees of freedom

summary(lm(y∼x))

- `Residuals:        Min       1Q    Median       3Q      Max`
  The residuals': minimum, 1st quartile, median, 3rd quartile, maximum

- `Coefficients:`
  `            Estimate Std. Error t value Pr(>|t|) "stars"`
  The coefficients':

  $$\hat{\beta}_i \qquad \hat{\sigma}_{\beta_i} \qquad t_{\text{obs}} \qquad p\text{-value}$$

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  - The stars indicate which size category the p-value belongs to.

- `Residual standard error: XXX on XXX degrees of freedom`
  $\varepsilon_i \sim N(0, \sigma^2)$, the output shows $\hat{\sigma}$ and ν degrees of freedom (used for hypothesis tests, CIs, PIs etc.)

summary(lm(y~x))

- `Residuals:          Min      1Q   Median       3Q      Max`
  The residuals': minimum, 1st quartile, median, 3rd quartile, maximum

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  The coefficients':
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- `Residual standard error: XXX on XXX degrees of freedom`
  $\varepsilon_i \sim N(0, \sigma^2)$, the output shows $\hat{\sigma}$ and ν degrees of freedom (used for hypothesis tests, CIs, PIs etc.)

- `Multiple R-squared:  XXX`

summary(lm(y~x))

- Residuals: Min   1Q   Median   3Q   Max

  The residuals': minimum, 1st quartile, median, 3rd quartile, maximum

- Coefficients:

                Estimate Std. Error t value Pr(>|t|) "stars"

  The coefficients':

  $$\hat{\beta}_i \qquad \hat{\sigma}_{\beta_i} \qquad t_{\mathrm{obs}} \qquad p\text{-value}$$

  - The test is $H_{0,i} : \beta_i = 0$ vs. $H_{1,i} : \beta_i \neq 0$
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- Residual standard error: XXX on XXX degrees of freedom

  $\varepsilon_i \sim N(0, \sigma^2)$, the output shows $\hat{\sigma}$ and ν degrees of freedom (used for hypothesis tests, CIs, PIs etc.)

- Multiple R-squared: XXX

  Explained variation r^2.

summary(lm(y∼x))

- ```
  Residuals:        Min       1Q   Median       3Q      Max
  ```
  The residuals': minimum, 1st quartile, median, 3rd quartile, maximum

- ```
  Coefficients:
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  ```
  The coefficients':
  $$\hat{\beta}_i \qquad \hat{\sigma}_{\beta_i} \qquad t_{\text{obs}} \qquad p\text{-value}$$
  - The test is $H_{0,i} : \beta_i = 0$ vs. $H_{1,i} : \beta_i \neq 0$
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  Residual standard error: XXX on XXX degrees of freedom
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  $\varepsilon_i \sim N(0, \sigma^2)$, the output shows $\hat{\sigma}$ and ν degrees of freedom (used for hypothesis tests, CIs, PIs etc.)

- ```
  Multiple R-squared:   XXX
  ```
  Explained variation r^2.

- The rest we don't use in this course.

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8. **Correlation**

9. Residual Analysis: Model validation

Explained variation and correlation

- Explained variation in a model is r^2, in summary "Multiple R-squared".

- Found as

$$r^2 = 1 - \frac{\sum_i(y_i - \hat{y}_i)^2}{\sum_i(y_i - \bar{y})^2} \, ,$$

where $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$.

- The proportion of the total variability explained by the model.

Explained variation and correlation

- The correlationen ρ is a measure of *linear relation* between two random variables.

- Estimated (i.e. empirical) correlation satisfies that

$$\hat{\rho} = r = \sqrt{r^2}\, sgn(\hat{\beta}_1)$$

where $sgn(\hat{\beta}_1)$ is: -1 for $\hat{\beta}_1 \leq 0$ and 1 for $\hat{\beta}_1 > 0$

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- Hence:
  - Positive correlation when positive slope.
  - Negative correlation when negative slope.

Test for significance of correlation

- Test for significance of correlation (linear relation) between two variables

$$H_0 : \rho = 0$$
$$H_1 : \rho \neq 0$$

is equivalent to

$$H_0 : \beta_1 = 0$$
$$H_1 : \beta_1 \neq 0$$

where $\hat{\beta}_1$ is the estimated slope in a simple linear regression model

Example: Correlation and R^2 for height-weight data

```r
# Read data into R

x <- c(168, 161, 167, 179, 184, 166, 198, 187, 191, 179)
y <- c(65.5, 58.3, 68.1, 85.7, 80.5, 63.4, 102.6, 91.4, 86.7, 78.9)

# Fit model to data
fit <- lm(y ~ x)

# Scatter plot of data with fitted line
plot(x,y, xlab = "Height", ylab = "Weight")
abline(fit, col="red")

# See summary
summary(fit)

# Correlation between  x and y
cor(x,y)

# Squared correlation is the "Multiple R-squared" from summary(fit)
cor(x,y)^2
```

Overview

1. Example: Height-Weight

2. Linear regression model

3. Least squares method

4. Statistics and linear regression?

5. Hypothesis tests and confidence intervals for β_0 and β_1

6. Confidence and prediction intervals for the line

7. Summary of 'summary(lm(y~x))'

8. Correlation

9. **Residual Analysis: Model validation**

Residual Analysis

Method 5.28

- Check normality assumptions with a qq-plot.

- Check (non-)systematic behavior by plotting the residuals, e_i, as a function of the fitted values $\hat{y}_i$.

(Method 5.29)

- Is the independence assumption reasonable?

Residual analysis in R

```
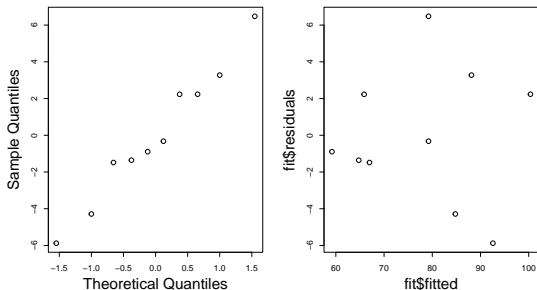x <- c(168, 161, 167, 179, 184, 166, 198, 187, 191, 179)
y <- c(65.5, 58.3, 68.1, 85.7, 80.5, 63.4, 102.6, 91.4, 86.7, 78.9)
fit <- lm(y ~ x)

par(mfrow = c(1, 2))
qqnorm(fit$residuals, main = "", cex.lab = 1.5)
plot(fit$fitted, fit$residuals, cex.lab = 1.5)
```

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