#### Course 02402 Introduction to Statistics

## Lecture 8: Simple linear regression

DTU Compute Technical University of Denmark 2800 Lyngby – Denmark

#### Overview

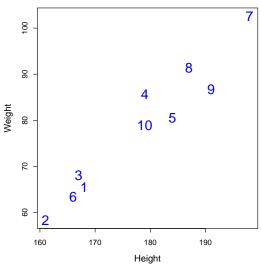
- Example: Height-Weight
- Linear regression model
- Least squares method
- Statistics and linear regression?
- ullet Hypothesis tests and confidence intervals for  $eta_0$  and  $eta_1$
- Confidence and prediction intervals for the line
- Summary of 'summary( $Im(y \sim x)$ )'
- Correlation
- Residual Analysis: Model validation

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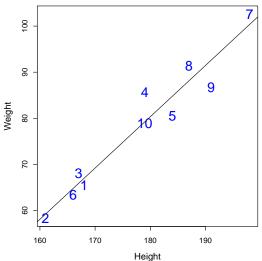
## Example: Height-Weight

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



## Example: Height-Weight

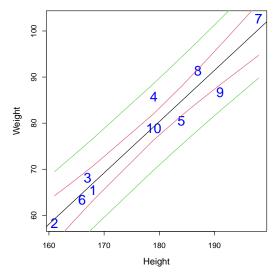
Heights  $(x_i)$ 168 161 167 179 184 166 198 187 191 179 Weights  $(y_i)$ 65.5 58.3 68.1 85.7 80.5 63.4 102.6 91.4 86.7 78.9



```
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
summary(lm(v ~ x))
##
## Call:
## lm(formula = y ~ x)
##
## Residuals:
    Min 10 Median 30 Max
##
## -5.876 -1.451 -0.608 2.234 6.477
##
## Coefficients:
##
            Estimate Std. Error t value Pr(>|t|)
## x
               ## ---
## 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

| 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 |

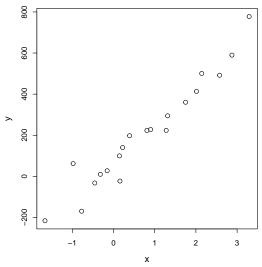


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## A scatter plot of some data

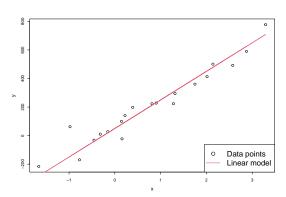
• We have n pairs of data points  $(x_i, y_i)$ .



## Express a linear model

• Express a linear model:

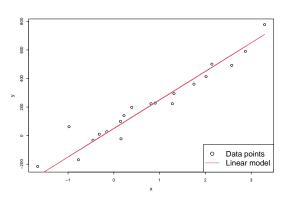
$$y_i = \beta_0 + \beta_1 x_i + ?$$



## Express a linear model

• Express a linear model:

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



• Something is missing: Description of the random variation.

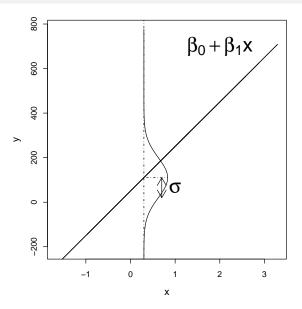
## Express a linear regression model

• Express the linear regression model:

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

- $Y_i$  is the dependent/outcome variable. A random variable.
- $x_i$  is an independent/explanatory variable. Deterministic numbers.
- $\varepsilon_i$  is the deviation/error. A random variable.
- We assume that the  $\varepsilon_i$ ,  $i=1,\ldots,n$ , are independent and identically distributed (i.i.d.), with  $\varepsilon_i \sim N(0,\sigma^2)$ .

### Illustration of statistical model



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• How can we estimate the parameters  $\beta_0$  and  $\beta_1$ ?

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- Good idea: Minimize the variance  $\sigma^2$  of the residuals.

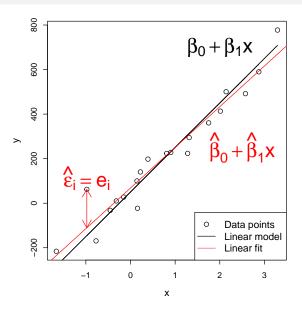
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- But how?

- How can we estimate the parameters  $\beta_0$  and  $\beta_1$ ?
- Good idea: Minimize the variance  $\sigma^2$  of the residuals.
- But how?
- Minimize the Residual Sum of Squares (RSS),

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

 $\hat{eta}_0$  and  $\hat{eta}_1$  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  $\beta_0$  and  $\beta_1$  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

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

## R example

```
set.seed(100)
# Generate x
x \leftarrow runif(n = 20, min = -2, max = 4)
# Simulate y
beta0 <- 50; beta1 <- 200; sigma <- 90
y \leftarrow 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 \leftarrow 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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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 $\hat{eta}_0$ and $\hat{eta}_1$

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

## Theorem 5.8 (first part)

$$\begin{split} V[\hat{\beta}_0] &= \frac{\sigma^2}{n} + \frac{\bar{x}^2 \sigma^2}{S_{xx}} \\ V[\hat{\beta}_1] &= \frac{\sigma^2}{S_{xx}} \\ Cov[\hat{\beta}_0, \hat{\beta}_1] &= -\frac{\bar{x}\sigma^2}{S_{xx}} \end{split}$$

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

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

#### Theorem 5.8 (second part)

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

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

When the estimate of  $\sigma^2$  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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Estimates of standard deviations of  $\hat{\beta}_0$  and  $\hat{\beta}_1$  (equations 5-43 and 5-44):

$$\hat{\sigma}_{eta_0} = \hat{\sigma}\sqrt{rac{1}{n} + rac{ar{x}^2}{S_{xx}}}; \quad \hat{\sigma}_{eta_1} = \hat{\sigma}\sqrt{rac{1}{\sum_{i=1}^n (x_i - ar{x})^2}}$$

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## Hypothesis tests for $\beta_0$ and $\beta_1$

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

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

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

## Hypothesis tests for $\beta_0$ and $\beta_1$

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

#### Theorem 5.12

Under the null-hypotheses  $(eta_0 = eta_{0,0} \ {\sf and} \ eta_1 = eta_{0,1})$  the statistics

$$T_{eta_0} = rac{\hat{eta}_0 - eta_{0,0}}{\hat{oldsymbol{\sigma}}_{eta_0}}; \quad T_{eta_1} = rac{\hat{eta}_1 - eta_{0,1}}{\hat{oldsymbol{\sigma}}_{eta_1}},$$

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

## Hypothesis tests for $\beta_0$ and $\beta_1$

- See Example 5.13 for an example of a hypothesis test.
- Test if the parameters are significantly different from 0:

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

```
# 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 $\beta_0$ and $\beta_1$

#### Method 5.15

(1-lpha) confidence intervals for  $eta_0$  and  $eta_1$  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.
- ullet In R, we can find  $\hat{\sigma}_{eta_0}$  and  $\hat{\sigma}_{eta_1}$  under "Std. Error"from summary(fit).

## Illustration of CIs by simulation

```
# Number of repetitions (here: CIs)
nRepeat <- 1000
# Empty logical vector of length nRepeat
TrueValInCI <- logical(nRepeat)</pre>
# Repeat the simulation and estimation nRepeat times:
for(i in 1:nRepeat){
  # Generate x
 x \leftarrow runif(n = 20, min = -2, max = 4)
  # Simulate u
  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)</pre>
  # 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 $\beta_0 + \beta_1 x_0 + \varepsilon_0$

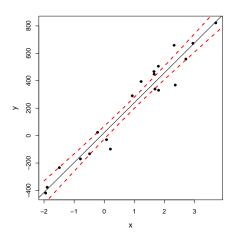
- The prediction interval for  $Y_0$  is found using a value  $x_0$ .
- This is done *before*  $Y_0$  is observed, using

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

- In  $100(1-\alpha)\%$  of cases, the prediction interval will contain the observed  $y_0$ .
- ullet For a given lpha, a prediction interval is wider than a confidence interval.

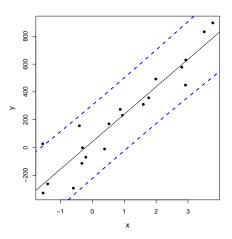
### Example of confidence intervals for the line

```
# Generate x
x \leftarrow runif(n = 20, min = -2, max = 4)
# Simulate v
beta0 = 50; beta1 = 200; sigma = 90
y <- beta0 + beta1 * x + rnorm(n = length(x), sd = sigma)
fit <- lm(v ~ x)
# Make a sequence of 100 x-values
xval \leftarrow 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
# 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 \leftarrow runif(n = 20, min = -2, max = 4)
# Simulate v
beta0 = 50; beta1 = 200; sigma = 90
y <- beta0 + beta1 * x + rnorm(n = length(x), sd = sigma)
fit <- lm(v ~ x)
# Make a sequence of 100 x-values
xval \leftarrow 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
# 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"], ltv = 2, col = "blue", lwd = 2)
```



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## What more do we get from summary()?

```
summary(fit)
##
## Call:
## lm(formula = v ~ 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
      197.6 16.4 12.05 4.7e-10 ***
## x
## ---
## Signif. codes: 0 '***' 0.001 '**' 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
```

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

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

$$\hat{eta}_i$$
  $\hat{oldsymbol{\sigma}}_{eta_i}$   $t_{
m obs}$   $p$ -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.

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- Residual standard error: XXX on XXX degrees of freedom

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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 v degrees of freedom (used for hypothesis tests, CIs, PIs etc.)

- Residuals: Min 1Q Median 3Q Max The residuals': minimum, 1st quartile, median, 3rd quartile, maximum
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m obs}$   $p$ -value

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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 v degrees of freedom (used for hypothesis tests, Cls, Pls etc.)
- Multiple R-squared: XXX

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- 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.
- Residual standard error: XXX on XXX degrees of freedom  $\varepsilon_i \sim N(0, \sigma^2)$ , the output shows  $\hat{\sigma}$  and v degrees of freedom (used for hypothesis tests, Cls, Pls etc.)
- Multiple R-squared: XXX Explained variation  $r^2$ .

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

$$\hat{eta}_i \qquad \hat{oldsymbol{\sigma}}_{eta_i} \qquad t_{
m obs} \qquad p$$
-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.
- Residual standard error: XXX on XXX degrees of freedom  $\varepsilon_i \sim N(0, \sigma^2)$ , the output shows  $\hat{\sigma}$  and v degrees of freedom (used for hypothesis tests, Cls, Pls etc.)
- Multiple R-squared: XXX Explained variation  $r^2$ .
- The rest we don't use in this course.

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

### Explained variation and correlation

- The correlationen  $\rho$  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  $\hat{\beta}_1 > 0$ 

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

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

```
# Read data into R
x \leftarrow c(168, 161, 167, 179, 184, 166, 198, 187, 191, 179)
y \leftarrow 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 \leftarrow lm(y \sim 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

- Example: Height-Weight
- 2 Linear regression model
- Least squares method
- Statistics and linear regression?
- ullet Hypothesis tests and confidence intervals for  $eta_0$  and  $eta_1$
- © Confidence and prediction intervals for the line
- Summary of 'summary( $Im(y \sim x)$ )'
- Correlation
- 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  $\hat{y}_i$ .

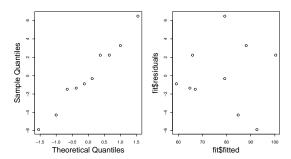
#### (Method 5.29)

• 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)</pre>
```



#### Overview

- Example: Height-Weight
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