

# Advanced R Day 2

Sereina Herzog

Institute for Medical Informatics, Statistics and Documentation Medical University of Graz

05.03.2024

05.03.2024



# Course Content - Advanced R (Day 2)

► Statistical tests & models



# **Course Content - Advanced R (Day 2)**

- ► Statistical tests & models
- ► Simple linear regression



# Course Content - Advanced R (Day 2)

- ► Statistical tests & models
- ► Simple linear regression
- ► Data import & preparation



Statistical tests & models 05.03.2024



Which statistical tests and models are suitable for your research questions?

Statistical tests & models 05.03.2024



Which statistical tests and models are suitable for your research questions?

- measuring level
  - nominal, ordinal, . . .



Which statistical tests and models are suitable for your research questions?

- measuring level
  - nominal, ordinal, . . .
- number of variables
  - types: independent (predictor), dependent (outcome)



Which statistical tests and models are suitable for your research questions?

- measuring level
  - nominal, ordinal, . . .
- number of variables
  - types: independent (predictor), dependent (outcome)
- ▶ type of relationship between variables
  - e.g., difference between . . .



Which statistical tests and models are suitable for your research questions?

- measuring level
  - nominal, ordinal, . . .
- number of variables
  - types: independent (predictor), dependent (outcome)
- type of relationship between variables
  - e.g., difference between . . .
- ▶ study design, ...



Which statistical tests and models are suitable for your research questions?

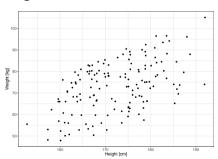
 $\Rightarrow$  not easy to give an answer





# Example - Height & Weight

What is the relationship between height and weight, respectively can height explain weight?

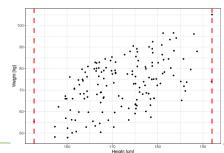




► Regression analysis is used to describe the nature of a relationship using a mathematical equation



- ► Regression analysis is used to describe the nature of a relationship using a mathematical equation
- ► Possibility of prognosis/prediction for an individual patient (incl. CI) within the value range of the predictor



Simple Linear Regression



- ► Dependent variable
  - target variable, response, outcome
  - this variable is to be calculated from the other variable (y-axis)



- ► Dependent variable
  - target variable, response, outcome
  - this variable is to be calculated from the other variable (y-axis)
- ► Independent variable(s)
  - explanatory variable(s), predictor
  - x-axis



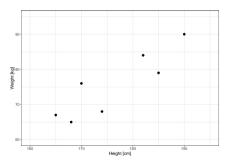
- ► Dependent variable
  - target variable, response, outcome
  - this variable is to be calculated from the other variable (y-axis)
- ► Independent variable(s)
  - explanatory variable(s), predictor
  - x-axis
- ► Aim of the regression analysis
  - $\bullet$  prediction, inference of  $x \to y$



- ► Dependent variable
  - target variable, response, outcome
  - this variable is to be calculated from the other variable (y-axis)
- ► Independent variable(s)
  - explanatory variable(s), predictor
  - x-axis
- ► Aim of the regression analysis
  - prediction, inference of  $x \rightarrow y$
- method
  - e.g. minimize deviation squares of the observed values from the regression line

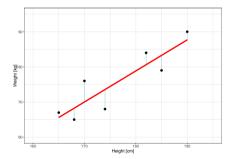


### Find a straight line





- ▶ Problem: Find a straight line so that the vertical distance (residuals) between the data points and the straight line is minimized.
- ► Method, e.g., least squares method





As a statistical model

$$Y = \beta_0 + \beta_1 * X$$



As a statistical model

$$Y = \beta_0 + \beta_1 * X$$

As an empirical model with data

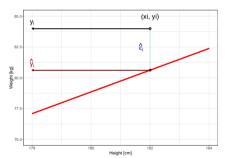
$$y_i = \beta_0 + \beta_1 * x_i + \epsilon_i$$

where  $\epsilon_i$  describes the error (residual)



$$\hat{y}_i = \hat{eta}_0 + \hat{eta}_1 * x_i$$
 are the predicted values of the regression

$$\hat{\epsilon}_i = \hat{y}_i - y_i$$
 are the residuals of the regression





1) Independence - Observations are independent of each other.



- 1) **Independence** Observations are independent of each other.
- 2) **Linearity** The relationship between X and the mean of Y is linear.



- 1) **Independence** Observations are independent of each other.
- 2) **Linearity** The relationship between X and the mean of Y is linear.
- 3) **Normality** For any fixed value of X, Y is normally distributed.



- 1) **Independence** Observations are independent of each other.
- 2) **Linearity** The relationship between X and the mean of Y is linear.
- 3) **Normality** For any fixed value of X, Y is normally distributed.
- 4) Homoscedasticity The variance of residual is the same for any value of X.



- 1) **Independence** Observations are independent of each other.
- 2) Linearity The relationship between X and the mean of Y is linear.
- 3) **Normality** For any fixed value of X, Y is normally distributed.
- 4) **Homoscedasticity** The variance of residual is the same for any value of X.

► For 1) study design question



- 1) Independence Observations are independent of each other.
- 2) **Linearity** The relationship between X and the mean of Y is linear.
- 3) Normality For any fixed value of X, Y is normally distributed.
- 4) Homoscedasticity The variance of residual is the same for any value of X.
- ► For 1) study design question
- For 2) scatter plot



- 1) **Independence** Observations are independent of each other.
- 2) Linearity The relationship between X and the mean of Y is linear.
- 3) Normality For any fixed value of X, Y is normally distributed.
- 4) Homoscedasticity The variance of residual is the same for any value of X.
- ► For 1) study design question
- For 2) scatter plot
- ► For 3) & 4) looking at residuals



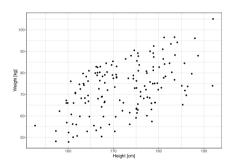
### Coefficient of Determination $R^2$

 $R^2$  specifies the proportion of variance in the data that is explained by the model

$$R^2=rac{\sum(\hat{y}_i-ar{y})^2}{\sum(y_i-ar{y})^2}$$
 and  $0\leq R^2\leq 1$ 



# **Example - Height & Weight**



- 1) Independence ✓
- 2) Linearity ✓



### **Example - Height & Weight (Residuals)**

```
res_model <- lm(weight ~ height, data = dt_regression)
```

```
## 'stat_bin()' using 'bins = 30'. Pick better value with 'binwidth'.
```

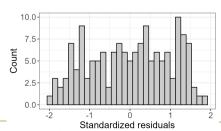


### **Example - Height & Weight (Residuals)**

```
res_model <- lm(weight ~ height, data = dt_regression)
```

```
## 'stat_bin()' using 'bins = 30'. Pick better value with 'binwidth'.
```

### Normality √?

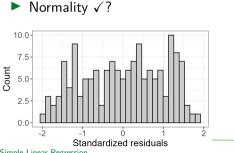


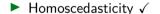


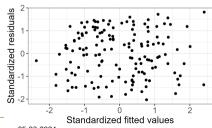
### Example - Height & Weight (Residuals)

```
res_model <- lm(weight ~ height, data = dt_regression)
```

## 'stat\_bin()' using 'bins = 30'. Pick better value with 'binwidth'.







05.03.2024



## **Example - Height & Weight (Residuals)**

▶ If a model accurately captures the structure in the data, then all that should remain after the model is through making its predictions is random noise!

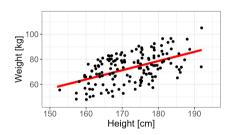


## **Example - Height & Weight (Residuals)**

- ▶ If a model accurately captures the structure in the data, then all that should remain after the model is through making its predictions is random noise!
- Why plot residuals vs. fitted values, and not observations?
  - Because residuals and fitted values are uncorrelated by construction
  - Residuals and observations may be correlated—they both depend on observations which would make such plots harder to interpret

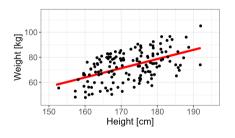


## **Example - Height & Weight**





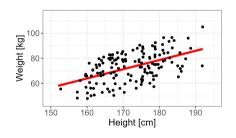
## Example - Height & Weight



- ► intercept -53.49 (95% CI -87.3 to -19.69)
- ► slope 0.73 (95% CI 0.54 to 0.93)
- $R^2 = 0.27$
- $R_{adj}^2 = 0.265$



### Example - Height & Weight



- ► intercept -53.49 (95% CI -87.3 to -19.69)
- ► slope 0.73 (95% CI 0.54 to 0.93)
- $R^2 = 0.27$
- $R_{adj}^2 = 0.265$

What weight can you expect from a 1.75 m tall person?



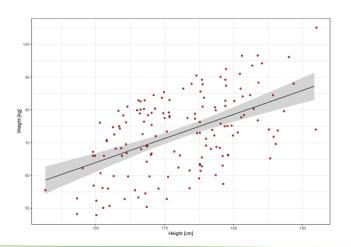
#### **Example - Prediction**

```
predict(res_model, newdata = tibble(height = 175),
    interval = "confidence", level = 0.95)
```

```
## fit lwr upr
## 1 74.95 73.25 76.65
```



## **Example - Uncertainty**





ightharpoonup mathematical relationship  $\neq$  causality



- ightharpoonup mathematical relationship  $\neq$  causality
- $ightharpoonup R^2$  vs.  $R_{adj}^2$



- ▶ mathematical relationship ≠ causality
- $ightharpoonup R^2$  vs.  $R_{adi}^2$
- $ightharpoonup R^2$  tends to increase as more variables are added to the model (even if they don't improve the model significantly)
  - $R_{adi}^2$  penalizes the addition of unnecessary variables:
    - $R_{adj}^2 = 1 \frac{(1-R^2)(n-1)}{n-p-1}$
    - n = number of samples
    - ightharpoonup p = number of predictors



- ▶ mathematical relationship ≠ causality
- $ightharpoonup R^2$  vs.  $R_{adj}^2$
- $ightharpoonup R^2$  tends to increase as more variables are added to the model (even if they don't improve the model significantly)
  - $R_{adj}^2$  penalizes the addition of unnecessary variables:
    - $ightharpoonup R_{adj}^2 = 1 \frac{(1-R^2)(n-1)}{n-p-1}$
    - n = number of samples
    - ightharpoonup p = number of predictors
- $ightharpoonup R^2$ ,  $R_{adj}^2$ 
  - does not indicate whether the model was specified correctly
  - low/high coefficient of determination ≠ bad/good model



Assumptions not fulfilled - What then?



Assumptions not fulfilled - What then?

- ▶ Transform X (e.g.  $Z = X^2$ ,  $Y = \beta_0 + \beta_1 * Z$ )
  - if linearity condition is violated



Assumptions not fulfilled - What then?

- ► Transform X (e.g.  $Z = X^2$ ,  $Y = \beta_0 + \beta_1 * Z$ )
  - · if linearity condition is violated
- ► Transform Y (e.g. log-transformation of Y)
  - in case of violation of variance homogeneity and/or normal distribution



Assumptions not fulfilled - What then?

- ▶ Transform X (e.g.  $Z = X^2$ ,  $Y = \beta_0 + \beta_1 * Z$ )
  - if linearity condition is violated
- ► Transform Y (e.g. log-transformation of Y)
  - in case of violation of variance homogeneity and/or normal distribution
- Apply more complex or robust estimation methods
  - e.g. weighted least squares estimation, sandwich estimator, bootstrapping,...



#### Assumptions not fulfilled - What then?

- ▶ Transform X (e.g.  $Z = X^2$ ,  $Y = \beta_0 + \beta_1 * Z$ )
  - if linearity condition is violated
- ightharpoonup Transform Y (e.g. log-transformation of Y)
  - in case of violation of variance homogeneity and/or normal distribution
- Apply more complex or robust estimation methods
  - $\bullet$  e.g. weighted least squares estimation, sandwich estimator, bootstrapping,  $\ldots$
- Multiple regression: further conditions must be checked (multicollinearity).



## Data import



#### R packages for import

#### readr

- to read rectangular data (like csv, tsv, and fwf)
- is a core package
- https://readr.tidyverse.org/



#### R packages for import

#### readr

- to read rectangular data (like csv, tsv, and fwf)
- is a core package
- https://readr.tidyverse.org/

#### readxl

- to read data from Excel (xls, xlsx)
- is not a core package
- https://readxl.tidyverse.org/



#### R packages for import

#### readr

- to read rectangular data (like csv, tsv, and fwf)
- is a core package
- https://readr.tidyverse.org/

#### readxl

- to read data from Excel (xls, xlsx)
- is not a core package
- https://readxl.tidyverse.org/
- ▶ ... just search, e.g., import to R dat



### **Data import**

ightharpoonup file type ightarrow R package and function



#### **Data import**

- ightharpoonup file type ightarrow R package and function
- work with arguments in functions
  - e.g., first row contains column headers
  - e.g., type of parameters
  - e.g., which strings to interpret as missing values
  - ...



## Data preparation with tidyverse



#### What is tibble?

"A **tibble**, or **tbl\_df**, is a modern reimagining of the data.frame, keeping what time has proven to be effective, and throwing out what is not. Tibbles are data."

https://tibble.tidyverse.org/



▶ tidyverse is a collection of R packages designed for data science



- ▶ tidyverse is a collection of R packages designed for data science
  - they share an underlying design philosophy, grammar, and data structure



- ▶ tidyverse is a collection of R packages designed for data science
  - they share an underlying design philosophy, grammar, and data structure
    - ggplot2 for data visualization



- ▶ tidyverse is a collection of R packages designed for data science
  - they share an underlying design philosophy, grammar, and data structure
    - ▶ ggplot2 for data visualization
    - readr for data importation from various file sources



- ▶ tidyverse is a collection of R packages designed for data science
  - they share an underlying design philosophy, grammar, and data structure
    - ▶ ggplot2 for data visualization
    - readr for data importation from various file sources
    - tidyr and dplyr useful for data cleaning



- ▶ tidyverse is a collection of R packages designed for data science
  - they share an underlying design philosophy, grammar, and data structure
    - ggplot2 for data visualization
    - readr for data importation from various file sources
    - tidyr and dplyr useful for data cleaning
    - **.** . . .
  - all core packages can be loaded at once: library(tidyverse)



- ▶ tidyverse is a collection of R packages designed for data science
  - they share an underlying design philosophy, grammar, and data structure
    - ▶ ggplot2 for data visualization
    - readr for data importation from various file sources
    - tidyr and dplyr useful for data cleaning
    - **.** . . .
  - all core packages can be loaded at once: library(tidyverse)
  - 'R for Data Science' (see slide with links)



▶ select() extracts columns and returns a tibble



- select() extracts columns and returns a tibble
- ► arrange() changes the ordering of the rows



- select() extracts columns and returns a tibble
- arrange() changes the ordering of the rows
- ▶ filter() picks cases based on their values



- select() extracts columns and returns a tibble
- arrange() changes the ordering of the rows
- filter() picks cases based on their values
- mutate() adds new variables that are functions of existing variables



### What is %>% in Tidyverse?

%>% is used to emphasis a sequence of actions, rather than the object that the actions are being performed on



### What is %>% in Tidyverse?

%>% is used to emphasis a sequence of actions, rather than the object that the actions are being performed on

```
dt_example %>%
  mutate(bmi = weight/(height^2)) %>%
  select(pat_id, sex, bmi)
```



#### What will we cover

- ▶ We will look at
  - importing data (example: .xlsx)
  - useful function for data preparation
  - save R environment (.Rdata)
- ▶ Data import and preparation in R file (.R)
  - input: dataset (e.g., .xlsx)
  - output: .Rdata
- ▶ We will work with .Rdata in a Rmarkdown file



#### **Example supraclavicular**

This data set contains 103 patients who were scheduled to undergo an upper extremity procedure suitable for supraclavicular anesthesia. Patients were randomly assigned to either

- (1) combined group-ropivacaine and mepivacaine mixture; or
- (2) sequential group-mepivacaine followed by ropivacaine.

A number of demographic and post-op pain medication variables (fentanyl, alfentanil, midazolam) were collected. The primary outcome is time to 4-nerve sensory block onset.

[Source: R package medicaldata]



## Links



## Links (I)

- ▶ Introduction to R
  - R for Data Science (https://r4ds.hadley.nz/)
- ► Plots using ggplot
  - Overview with further links to course material: https://ggplot2.tidyverse.org/
- Display tables using flextable
  - flextable bool https://ardata-fr.github.io/flextable-book/
  - Function references https://davidgohel.github.io/flextable/reference/index.html
- knit\_child()
  - link (https://bookdown.org/yihui/rmarkdown-cookbook/child-document.html)



# Links (II)

- ▶ Download R
  - CRAN (https://cran.r-project.org/)
- ► Download RStudio
  - RStudio Desktop (https://posit.co/download/rstudio-desktop/)