Introduction to Machine Learning

Module 1: Foundations

Tobias Rebholz

University of Tübingen

Fall 2024, SMiP Workshop

Orga

Personal Information

- SMiP alum:
  - April 2023: PhD thesis on statistical modeling in judgment and decision-making (JDM)
- Since July 2023: Postdoc in the Social Cognition and Decision Sciences group in Tübingen
  - I.e., where I also did my PhD
- From April 2025: Visiting research scholar at Duke University
  - Walter-Benjamin grant on advice taking from generative AI
- Contact: tobias.rebholz@uni-tuebingen.de

Research

- My Master's thesis (2019/20!) was about developing and testing machine learning (ML) approaches for ordinal-scaled dependent variables (= "targets" in ML jargon)
  - This is also where most of my "expertise" in this domain is from
- My current ML research covers only a very specific and limited domain
  - Often not directly involves any methodological aspects of ML
  - Instead, mainly from an augmented JDM perspective: Human-computer interaction
- However, like most of you, I'm basically excited about all kinds of methodological research
  - That is also why I ended up giving this workshop on the broad topic of ML in general
- So beware:
  - A) We will mostly stay on a rather conceptual and introductory level
  - B) It is very likely that some of my slides will contain errors, both large and small
  - Please let me know if you find any inconsistencies or mistakes!

Workshop Contents

- Fundamentals of machine learning (ML)
  - Cross validation and hyperparameter tuning
  - Interpretable ML
  - ...
- Various ML methods:
  - Classification and regression trees
  - Cluster analysis
  - Neural networks
  - Large language models
  - ...

Workshop Contents

- Applications in various areas of applied psychology and behavioral economics (due to my own research agenda and interests), such as:
  - Judgment and decision-making (JDM)
  - Management and consumer psychology
- Selected case studies:
  - Analyze the effects of social and informational influences on human JDM processes
  - Identify sentiment or emotion in language
  - Predict consumer behavior, provide personalized recommendations, or cluster brand perceptions

Learning Target

- Develop a basic understanding of ML and its value to applied psychological research
  - Emphasis is on conceptual understanding, rather than (technical) details!
- Gain practical experience in applying specific ML techniques to solve real-world decision problems
  - Extended skills to analyze and interpret complex data sets, such as unstructured text data
- Acquire the competence to critically reflect on the results of ML methods and to evaluate their implications for theory building and psychological research practice
- Prerequisites:
  - Basic understanding of statistics (e.g., linear regression)
  - Familiarity with R

Literature

1. James, G., Witten, D., Hastie, T., & Tibshirani, R. (2021). *An introduction to statistical learning: With applications in R* (2nd ed.). Springer US. https://doi.org/10.1007/978-1-0716-1418-1

- More technical, less related to behavioral science, but more standard
- Available for free at: https://www.statlearning.com/
- Now also available for Python

2. Jacobucci, R., Grimm, K. J., & Zhang, Z. (2023). *Machine Learning for social and behavioral research* (2nd ed.). The Guilford Press.

- Less technical, more related to behavioral science, but less standard
- Should be freely available in Ba-Wü: E.g., via proquest

3. Hastie, T. J., Tibshirani, R., & Friedman, J. H. (2009). *The elements of statistical learning: Data mining, inference, and prediction* (2nd ed). Springer.

- Extremely technical, but basically the bible for ML

Structure

The workshop is divided into two parts:

- Introduction to topics/methods
  - Mainly lectured by me!
- Solving simple programming assignments
  - Mainly hands-on by you!

Material

- Slides, programming assignments etc. will be provided via my personal website: https://tobiasrebholz.github.io/teaching/
  - Password: ...

Tentative Schedule

- Zeitplan gestalten

Questions

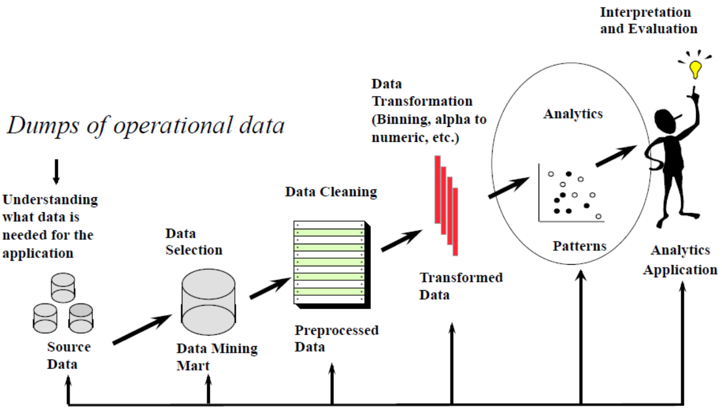
- Any open questions about the organizational details?

Module 1: Foundations

What is Data-Driven Decision-Making?

- Data Science aims to extract and represent knowledge from complex data
  - Machine Learning refers to a vast set of mathematical tools and models which can help to make sense of data
- Techniques from diverse fields, such as:
  - Statistics,
  - Data Mining
  - Visualization
  - ...
- Expertise from different disciplines, such as:
  - Statistics
  - Computer Science
  - Behavioral Science
  - Neuroscience
  - ...

Data Science enables Data-Driven Decision-Making



(https://ebrary.net/168827/computer_science/twitter_s_data_analysis_using_rstudio)

Examples: Medical Diagnosis

AI Now Diagnoses Disease Better Than Your Doctor, Study Finds

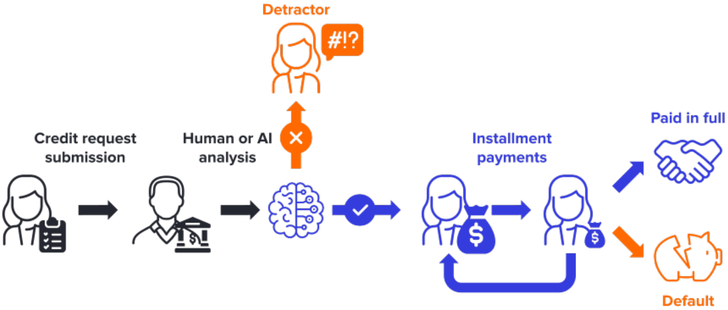
Peer-reviewed study says you'll soon consult Dr. Bot for a second opinion

David Leibowitz · Follow

Published in Towards Data Science · 7 min read · Sep 29, 2020

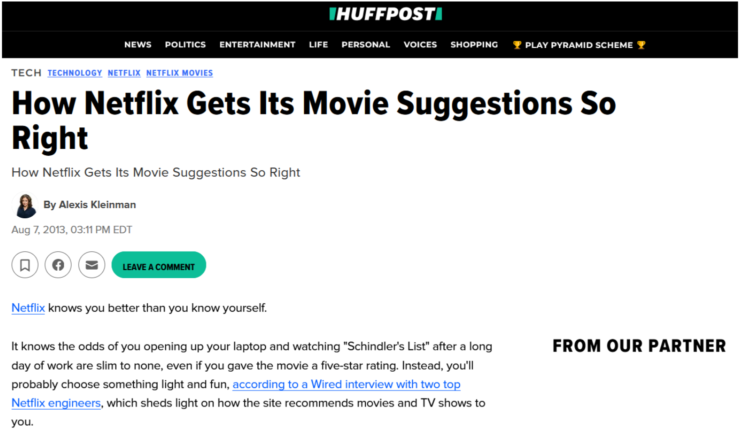
- "In the peer-reviewed study, authored by researchers from Babylon Health and University College London, the new model scored higher than 72% of general practitioner doctors when tasked with diagnosing written test cases of realistic illnesses." (https://towardsdatascience.com/ai-diagnoses-disease-better-than-your-doctor-study-finds-a5cc0ffbf32)

Examples: Credit Scoring in FinTech Industry



https://nilg.ai/202107/insights-in-ai-applied-to-credit-scoring/

Examples: Recommender Systems



HUFFPOST

NEWS POLITICS ENTERTAINMENT LIFE PERSONAL VOICES SHOPPING PLAY PYRAMID SCHEME

TECH TECHNOLOGY NETFLIX NETFLIX MOVIES

How Netflix Gets Its Movie Suggestions So Right

How Netflix Gets Its Movie Suggestions So Right

By Alexis Kleinman

Aug 7, 2013, 03:11 PM EDT

LEAVE A COMMENT

Netflix knows you better than you know yourself.

It knows the odds of you opening up your laptop and watching "Schindler's List" after a long day of work are slim to none, even if you gave the movie a five-star rating. Instead, you'll probably choose something light and fun, according to a Wired interview with two top Netflix engineers, which sheds light on how the site recommends movies and TV shows to you.

FROM OUR PARTNER

https://nilg.ai/202107/insights-in-ai-applied-to-credit-scoring/

Examples: Political Elections

nature

Explore content About the journal Publish with us Subscribe

nature > world view > article

WORLD VIEW | 09 April 2024

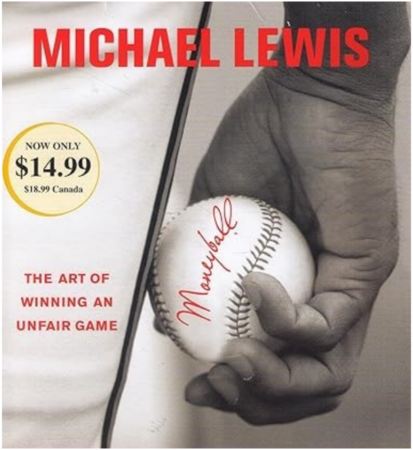
AI-fuelled election campaigns are here — where are the rules?

Political candidates are increasingly using AI-generated 'softfakes' to boost their campaigns. This raises deep ethical concerns.

By Rumman Chowdhury

- "Softfakes … are images, videos or audio clips that are doctored to make a political candidate seem more appealing. Whereas deepfakes (digitally altered visual media) and cheap fakes (low-quality altered media) are associated with malicious actors, softfakes are often made by the candidate's campaign team itself." (https://www.nature.com/articles/d41586-024-00995-9)

Examples: Sports

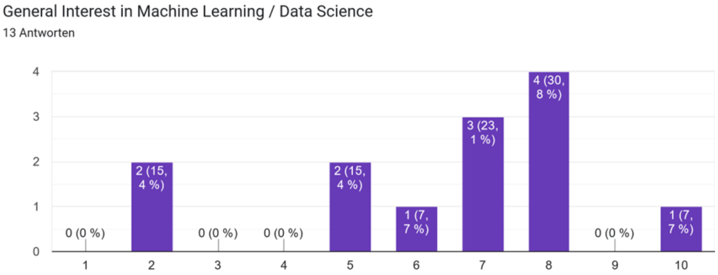


https://en.wikipedia.org/wiki/Moneyball

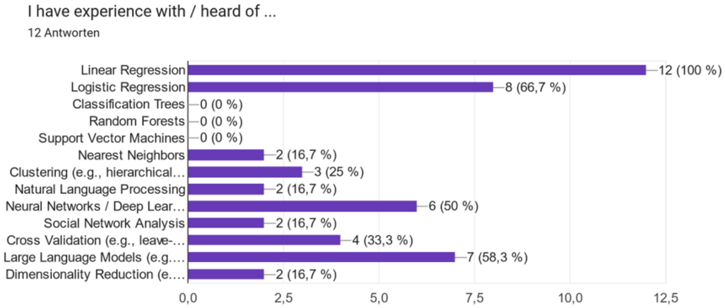
A Brief History of ML

- Early 19th century: Method of least squares was developed
  - Precursor to linear regression
- 1940s: Introduction of logistic regression for predicting qualitative values
- Early 1970s: Coining of the term "generalized linear models", encompassing linear and logistic regression
- 1980s: Improvement in computing technology allows for nonlinear methods
- Mid-1980s: Development of classification and regression trees
- 1980s: Early neural networks (e.g., perceptron)
- 1990s: Emergence of support vector machines
- 2001: Random Forests (i.e., ensample methods)
- 2010s: Deep Learning (i.e., advanced neural networks)
- 2017: Transformer models (e.g., large language models)
  - Enabled high-performance chatbots, such as OpenAI's ChatGPT

Your interests



Your experience



Analytics

- Supervised Learning: Predicting/estimating an output based on one or more inputs
- Unsupervised Learning: Learning relationships/structure from inputs only
  - I.e., there is no supervising output
- Visualization: Visual representation of predictions, relationships, but also raw data

Important Topics

- Overfitting
- Imbalance
- Sparseness
- Robustness
- Hyperparameters

Data Types

- Continuous data
  - E.g., age, income, . . .
  - Can be discretized (e.g., age categories)
- Binary data
  - E.g., yes vs. no response
  - Usually coded as a 0-1 dummy variable
- Categorical data
  - E.g., gender, group membership, . . .
  - Sometimes converted into dummies: One dummy variable per category
- Ordinal data
  - E.g., highest educational degree
  - Must be treated with caution, as they are neither continuous nor categorical

Complex Data: Multivariate

- Data on demographics and Big Five personality trait scores:

```
head(dat, 15)
##         CASE gender education      age agree conscientious extra neuro open
## 652  63116      1         3 40.55747   5.8          3.40   3.6   1.5 3.80
## 999  63967      1         4 35.37340   4.6          3.60   4.0   1.0 3.60
## 991  63955      2         4 21.55923   3.0          3.20   4.0   3.8 4.40
## 392  62547      2         1 22.80091   4.8          5.20   4.4   2.0 4.80
## 788  63493      2         2 23.07484   5.2          3.40   4.4   2.6 4.60
## 330  62419      2         3 30.08120   5.4          4.00   4.4   4.0 3.80
## 2231 66716      2         5 37.61331   3.8          4.80   4.4   4.2 5.00
## 1128 64275      1         4 37.76547   5.0          5.00   4.6   3.6 4.60
## 1061 64101      1         3 17.58908   4.6          4.00   4.6   1.8 3.60
## 1474 65080      2         4 22.49090   2.8          3.80   4.0   3.0 3.00
## 1949 66088      1         2 58.15496   5.0          4.75   5.0   4.8 5.00
## 1005 63983      1         3 23.31878   3.6          4.60   3.2   2.6 3.40
## 261  62266      1         3 30.89218   3.0          3.40   3.6   4.0 4.00
## 2024 66264      2         3 24.58253   4.8          3.40   4.2   2.0 4.75
## 2441 67257      2         5 18.87679   4.8          4.40   4.0   4.6 4.00
```

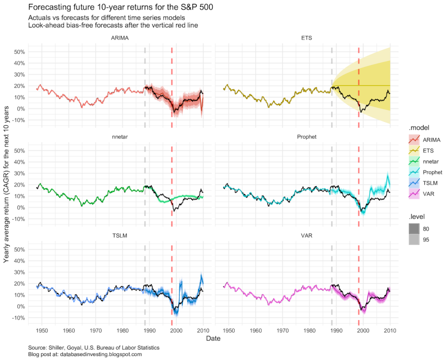
Complex Data: Spatial

- Traffic data:

https://unece.org/traffic-census-map

Complex Data: Time-stamped

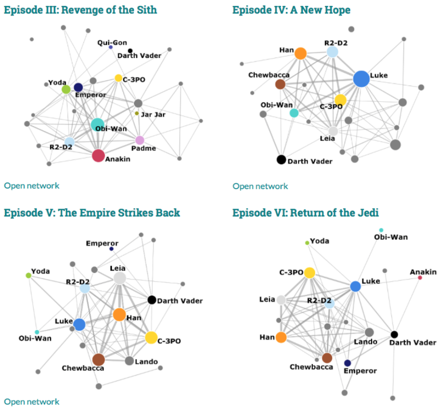
- Stock market data:



https://www.r-bloggers.com/2020/05/forecasting-the-next-decade-in-the-stock-market-using-time-series-models/

Complex Data: Relational

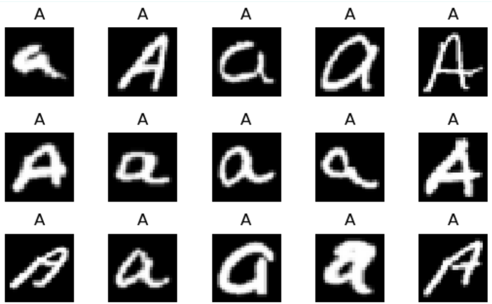
- Network data:



https://www.martingrandjean.ch/star-wars-data-visualization/

Complex Data: Unstructured

- Image data:



https://github.com/zandreika/letters-recognition

- Further unstructured data: Videos, audios, text, health records, ...

Statistics of Data

- Mean: $\mu = \frac{1}{N}\sum_{i=1}^{N} x_i$
- Variance: $\sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2$
- Standard deviation: $\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2}$
- Minimum: $\min = \text{minimize}_{i \in N}\{x_i\}$
- Maximum: $\max = \text{maximize}_{i \in N}\{x_i\}$

- Bringing variables to the same range (very useful for multivariate data):
  - Standarizing:
    $$\frac{x-\mu}{\sigma} \tag{1}$$
  - Normalizing:
    $$\frac{x-\min}{\max-\min} \tag{2}$$

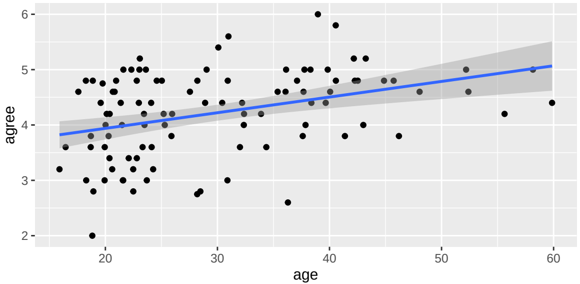
Summary

- Data Science builds mathematical models to extract and represent knowledge
- Data-Driven Decision-Making can be relevant to any setting in:
  - Psychology
  - Economics
  - Medicine
  - Physics
  - ...
- Prior to building the models, data often needs some preprocessing

Linear Regression

Linear Regression

```
library(tidyverse)

ggplot(dat, aes(y = agree, x = age)) +
  geom_point() +
  stat_smooth(method = "lm")
## `geom_smooth()` using formula = 'y ~ x'
```



Research Goal

- **Description:** Research with the aim of describing relationships or distributions

vs.

- **Explanation:** Research with the aim of understanding the underlying mechanisms

vs.

- **Prediction:** Research with the aim of maximally explaining the variability in an outcome
  - ML, and therefore this course, is mainly devoted to predictive analytics

Predictive Analytics

- There is a dependent variable or "target", y
- There is a set of p explanatory variables or "features", $x_1, x_2, \ldots, x_p$
- We build a model that predicts y using the information in $X = (x_1, x_2, \ldots, x_p)$
- The model differs depending on the nature of the target
  - Regression task: The target is continuous
  - Classification task: The target is discrete

Simple Linear Regression

- For each instance i in a population, we have:
  - **One** feature, x_i
  - Continuous target, $y_i \in \mathbb{R}$
- Goal: Predict the target for new instances for whom we know the value of the feature, but not the value of the target:

$$x_{new} \rightarrow \hat{y}_{new} \in \mathbb{R} \tag{3}$$

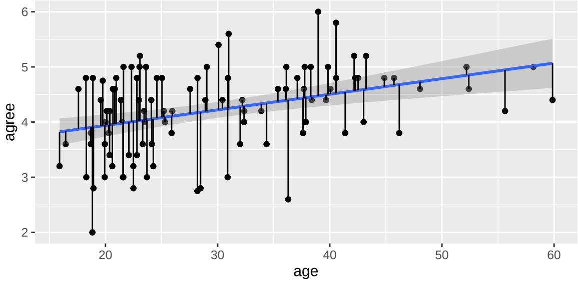
Simple Linear Regression

- We assume that there is a linear relationship between the (single) feature and the target: $y = \beta_0 + \beta_1 x$
- As β_0 and β_1 are unknown, we have to estimate them from the data
  - Goal: Ensuring low errors ("residuals"), $e_i = y_i - \hat{y}_i$
    - Where the target value predicted by the model is: $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$
  - Note: The residuals are assumed to be normally distributed
- In other words, we want to find the values of β_0 and β_1 that minimize the difference between the predicted and observed target values for the entire sample
  - Mean squared (prediction) error:

$$MSE = \sum_{i=1}^{N} e_i^2 = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2 \tag{4}$$

Simple Linear Regression

```
mdl <- lm(agree ~ age, data = dat)

mdl %>%
  ggplot(aes(y = agree, x = age)) +
  geom_point() +
  geom_smooth(method = "lm") +
  geom_segment(aes(xend = age, yend = .fitted))
## `geom_smooth()` using formula = 'y ~ x'
```



Simple Linear Regression in base R

```
summary(mdl)
##
## Call:
## lm(formula = agree ~ age, data = dat)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -1.9057 -0.5915  0.1043  0.5542  1.5251
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 3.373290   0.223798  15.073  < 2e-16 ***
## age         0.028270   0.007092   3.986 0.000129 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7274 on 98 degrees of freedom
## Multiple R-squared:  0.1395, Adjusted R-squared:  0.1307
## F-statistic: 15.89 on 1 and 98 DF,  p-value: 0.0001292
```

- Fitted model: $ag\hat{r}ee = \hat{\beta}_0 + \hat{\beta}_1 * age = 3.37 + 0.03 * age$
  - Prediction for a new participant with $age = 30$: $ag\hat{r}ee = 3.37 + 0.03 * 30 = 4.22$

Prediction "Out-of-Sample"

1. Use a subset of the sample to fit the model:

```
N <- nrow(dat)
train <- sample(1:N, N*0.9)

df_subset <- dat[train,]

mdl_subset <- lm(agree ~ age, data = df_subset)
summary(mdl_subset)
##
## Call:
## lm(formula = agree ~ age, data = df_subset)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.9365 -0.6068  0.1003  0.5975  1.5335
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 3.440593   0.246566  13.954  < 2e-16 ***
## age         0.026329   0.007975   3.301  0.00139 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7449 on 88 degrees of freedom
## Multiple R-squared:  0.1102, Adjusted R-squared:  0.1001
```

Prediction "Out-of-Sample"

2. Test the model on the remaining, held-out data

```
df_rest <- dat[-train,]

df_rest$agree_predicted <- predict(mdl_subset, df_rest)

df_rest %>% select(agree, agree_predicted)
##      agree agree_predicted
## 1949   5.0        4.971744
## 274    2.8        3.939006
## 2378   4.8        4.560227
## 1672   5.0        4.204977
## 1000   4.2        3.970284
## 737    4.8        4.644516
## 1754   4.8        4.621869
## 2550   4.0        4.106741
## 816    3.2        4.079394
## 744    4.0        4.437448
```

- We will expand on this idea over the weeks

Simple Linear Regression in mlr3

1. Define a (prediction) task, which is mlr3's way to store the raw data along with some meta-information for modeling
2. Specify which ML model to apply later for prediction
   - `mlr3` does not implement its own ML models but links to available implementations in other R packages (e.g., "regr.lm" links to the ordinary `lm()` function in the stats package)
3. Train the linear regression model
   - In `mlr3`, objects have "abilities" (or "methods") that can be applied with the following $-syntax (here, the train method of the learner object is used to train the learner from step 2 on the task specified in step 1)

```
library(mlr3verse)
tsk = as_task_regr(agree ~ age, data = dat) #1.
mdl = lrn("regr.lm") #2.
mdl$train(tsk) #3.
```

Simple Linear Regression in mlr3

- The estimated model output is exactly the same as with using base R
  - Not surprising, as `lrn("regr.lm")` is simply applying the `lm()` function to estimate the model, which is exactly equivalent to what we did a couple of slides ago

```
summary(mdl$model)
##
## Call:
## stats::lm(formula = task$formula(), data = task$data())
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -1.9057 -0.5915  0.1043  0.5542  1.5251
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 3.373290   0.223798  15.073  < 2e-16 ***
## age         0.028270   0.007092   3.986 0.000129 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7274 on 98 degrees of freedom
## Multiple R-squared:  0.1395, Adjusted R-squared:  0.1307
## F-statistic: 15.89 on 1 and 98 DF,  p-value: 0.0001292
```

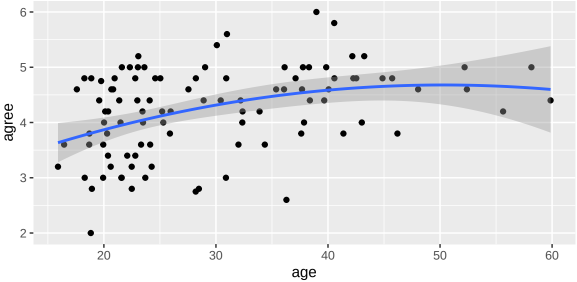
Excurse: Why `mlr3`?

- If the end result (i.e., fitted model) is exactly the same as with `base` R, why use `mlr3` at all?
- In `mlr3`, the model fitting procedure (i.e., steps 1-3) is exactly the same **no matter what ML method we're using** to model the data
  - It merely provides a **unified framework/syntax** (cf. `tidyverse`) to fit different ML models
    - The ML models themselves, however, stem from other, established R packages (e.g., "regr.lm" links to the ordinary `lm()` function in the stats package), which are also described in detail in, e.g., James et al. (2021)
  - Allows us to **focus more on the concepts** and less on the specific programming in R
- `mlr3` is **the state-of-the-art framework for ML in R** (cf. `scikit-learn` in Python)

Excurse: Nonlinear Regression

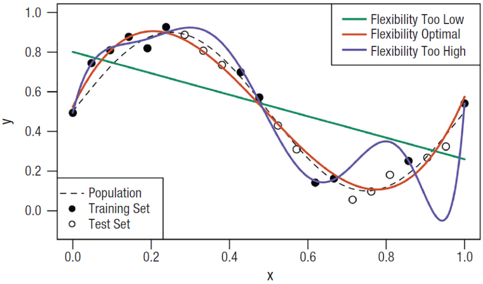
- Using linear modeling, we can even build nonlinear models
  - E.g., by including polynomial transformations of features (i.e., quadratic age): $a\hat{gree} = \hat{\beta}_0 + \hat{\beta}_1 * age + \hat{\beta}_2 * age^2$

```
ggplot(dat, aes(y = agree, x = age)) +
  geom_point() +
  stat_smooth(method = "lm", formula = y ~ x + I(x^2))
```



Bias-Variance Trade-Off

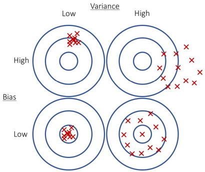
- Bias-variance trade-off: Good out-of-sample performance requires low variance as well as low squared bias
  - Why "trade-off"? – "Inflexible" model with low variance but high bias *vs.* "flexible" model with low bias but high variance
  - The challenge lies in finding a model for which both the variance and the (squared) bias are low



(Pargent et al., 2023, Figure 3a)

Bias-Variance Trade-Off

- Darts metaphor:
  - Bullseye = True value (i.e., expected target value for a given combination of feature values)
  - Each cross is the prediction made by a concrete ML model (trained on a randomly drawn training set, all from the same population and with the same sample size)



(Pargent et al., 2023, ESM, Figure 2)

- Optimal model: Low bias and low variance (bottom left)
  - Noise = Irreducible error of the true model: Reason why predictions (across different samples) are not similar, even when hitting the bullseye

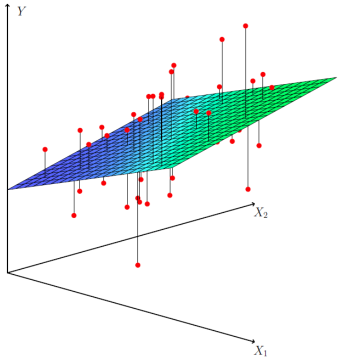
Multiple Linear Regression

- Everything is the same as in simple regression, except that we have multiple features (incl. polynomial transformations of features to build nonlinear models)
  - Note: Higher dimensionality (i.e., more features) = More flexibility
- For each instance i in a population, we have:
  - A **vector** of features, $X_i = (x_{i1}, x_{i2}, \ldots, x_{ip})$
  - Continuous target, $y_i \in \mathbb{R}$
- Goal: Predict the target for new instances for whom we know the vector of features but not the value of the target:

$$X_{new} \rightarrow \hat{y}_{new} \in \mathbb{R} \tag{5}$$

Multiple Linear Regression

- E.g., vector of features of size 2:



(James et al., 2021, Figure 3.4)

Multiple Linear Regression in base R

```
mdl <- lm(agree ~ age + gender, data = dat)
summary(mdl)
##
## Call:
## lm(formula = agree ~ age + gender, data = dat)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.86767 -0.49583  0.07832  0.53912  1.45493
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 3.040273   0.351015   8.661 1.04e-13 ***
## age         0.028927   0.007093   4.078 9.31e-05 ***
## gender      0.188803   0.153585   1.229    0.222
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7255 on 97 degrees of freedom
## Multiple R-squared:  0.1527, Adjusted R-squared:  0.1353
## F-statistic: 8.743 on 2 and 97 DF,  p-value: 0.0003229
```

Multiple Linear Regression in mlr3

```r
tsk = as_task_regr(agree ~ age + gender, data = dat)
mdl = lrn("regr.lm")
mdl$train(tsk)
summary(mdl$model)
##
## Call:
## stats::lm(formula = task$formula(), data = task$data())
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.86767 -0.49583  0.07832  0.53912  1.45493
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 3.040273   0.351015   8.661 1.04e-13 ***
## age         0.028927   0.007093   4.078 9.31e-05 ***
## gender      0.188803   0.153585   1.229    0.222
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7255 on 97 degrees of freedom
## Multiple R-squared:  0.1527, Adjusted R-squared:  0.1353
## F-statistic: 8.743 on 2 and 97 DF,  p-value: 0.0003229
```

Hands-on Practical Tutorial

- Now it's your turn:
  - Go to ILIAS
  - Navigate to the "Tutorials" folder
  - Download the "Module 1" folder
  - Work on the tutorial "module1-linear_regression"

Logistic Regression

Logistic Regression

- Everything is the same as in linear regression, except that we have a discrete target
- For each instance i in a population, we have:
  - A vector of features, $X_i = (x_{i1}, x_{i2}, \ldots, x_{ip})$
  - **Binary** class membership, $y_i \in \{0, 1\}$
    - E.g., buying vs. not buying a specific product
- Goal: Predict the target (i.e., class membership) for new instances for whom we know the vector of features but not the value of the target:

$$X_{new} \to \hat{y}_{new} \in \mathbb{R} \quad (6)$$

Logistic Regression

- Auxiliary target: Probability of membership in class 1, p
  - Counter probability $1 - p$: Membership in class 0
  - **Continuous, but bounded** target
- Auxiliary goal: Predict the auxiliary target (i.e., probability) for new instances for whom we know the vector of features but not the value of the target:

$$X_{new} \rightarrow \hat{p}_{new} \in (0, 1) \tag{7}$$

- Predicted class:

$$\hat{y}_{new} = \begin{cases} 1 \text{ if } \hat{p}_{new} > 0.5 \\ 0 \text{ else} \end{cases} \tag{8}$$

Logistic Regression

- Fitting a logistic function to the probability of class 1:

$$p = \frac{e^{\beta_0+\beta_1 x_1+\cdots+\beta_p x_p}}{1+e^{\beta_0+\beta_1 x_1+\cdots+\beta_p x_p}} \tag{9}$$

... is equivalent to fitting a linear function to the logarithm of the odds

$$\log\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p \tag{10}$$

- In general, "odds" is defined as the probability of an event occurring relative to the probability of the event not occurring
  - Here, the odds are the probability for membership in class 1 relative to the probability for membership in class 0
- As $\beta_0, \beta_1, \ldots, \beta_p$ are unknown, we have to estimate them from the data
  - E.g., by maximizing the log likelihood function $\Rightarrow \hat{\beta}_p$ is called the "maximum likelihood estimate" (MLE)

Logistic Regression in mlr3

- Data preparation:

```
dat$agree_high <- ifelse(dat$agree > 4, 1, 0)
dat %>% select(agree, agree_high) %>% tail(., 10)
##      agree agree_high
## 442    4.8          1
## 2270   5.0          1
## 1133   5.2          1
## 1210   4.8          1
## 1912   4.6          1
## 744    4.0          0
## 1485   5.0          1
## 9      4.0          0
## 866    3.6          0
## 1591   4.4          1
```

Logistic Regression in mlr3

- Model fitting:

```
tsk = as_task_classif(agree_high ~ age, data = dat, positive = "1")
mdl = lrn("classif.log_reg")
mdl$train(tsk)
summary(mdl$model)
##
## Call:
## stats::glm(formula = task$formula(), family = "binomial", data = data,
##     model = FALSE)
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept) -1.83118    0.73681  -2.485  0.01294 *
## age          0.07940    0.02561   3.100  0.00193 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 133.75  on 99  degrees of freedom
## Residual deviance: 121.83  on 98  degrees of freedom
## AIC: 125.83
##
## Number of Fisher Scoring iterations: 4
```

Logistic Regression in `mlr3`

- Fitted model: $\hat{p}_{agree>4} = \frac{e^{\hat{\beta}_0+\hat{\beta}_1*age}}{1+e^{\hat{\beta}_0+\hat{\beta}_1*age}} = \frac{e^{-1.83+0.08*age}}{1+e^{-1.83+0.08*age}}$
  - Prediction for a new participant with $age = 30$:
    $\hat{p}_{agree>4} = \frac{e^{-1.83+0.08*30}}{1+e^{-1.83+0.08*30}} = 0.63$

```
summary(mdl$model)$coefficients
##                Estimate Std. Error   z value    Pr(>|z|)
## (Intercept) -1.83118304 0.73680914 -2.485288 0.012944661
## age          0.07940429 0.02561037  3.100474 0.001932111
```

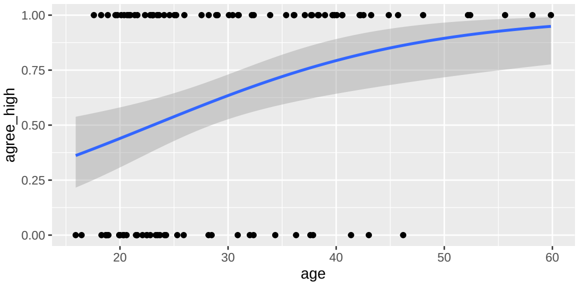
- Odds ratios:

```
exp(coefficients(mdl$model))
## (Intercept)         age
##   0.1602239   1.0826419
```

Logistic Regression in mlr3

- We can plot the estimated probability of class 1 membership as a function of age:

```
ggplot(dat, aes(y = agree_high, x = age)) +
  geom_point() +
  geom_smooth(method = "glm", method.args = list(family = binomial(link = "logit")))
## `geom_smooth()` using formula = 'y ~ x'
```



Classification Performance

- Main goal: Correct classification
  - E.g., minimizing the mean misclassification error:

$$MMCE = \frac{1}{N} \sum_{i=1}^{N} I\{y_i \neq \hat{y}_i\} \tag{11}$$

    - Where $I\{\cdot\}$ is the indicator function taking the value 1 if the condition in the parentheses is true and 0 otherwise
  - This is equivalent to maximizing classification accuracy:

$$Acc = 1 - MMCE = \frac{N_{0,0} + N_{1,1}}{N} \tag{12}$$

- Confusion matrix:

	$\hat{y} = 0$	$\hat{y} = 1$	
$y = 0$	$N_{0,0}$ (TN)	$N_{0,1}$ (FP)	$N_{0,\cdot}$
$y = 1$	$N_{1,0}$ (FN)	$N_{1,1}$ (TP)	$N_{1,\cdot}$
	$N_{\cdot,0}$	$N_{\cdot,1}$	N

Classification Performance

- Other important metrics:
  - Sensitivity (or true positive rate, recall):

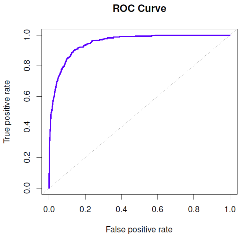
$$Sens = \frac{TP}{TP + FN} \tag{13}$$

  - Specificity (or true negative rate):

$$Spec = \frac{TN}{TN + FP} \tag{14}$$

Classification Performance

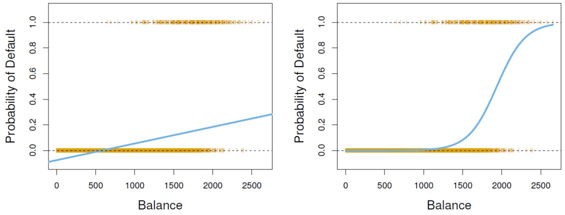
- Predicted class: $\hat{y} = \begin{cases} 1 \text{ if } \hat{p} > 0.5 \\ 0 \text{ else} \end{cases}$
  - Other thresholds than 0.5 can lead to better performance
- Area under the (receiver operating) curve (AUC):
  - The probability that an observation randomly drawn from class 1 has a higher predicted probability to belong to class 1 than an observation randomly drawn from class 0
  - The ROC traces out $Sens$ and $Spec$ for varying classification thresholds



(James et al., 2021, Figure 4.8)

Excurse: Logistic vs. Linear Regression

- Linear regression: Some estimated probabilities are negative
- Logistic regression: All estimated probabilities lie between 0 and 1 (i.e., are well-defined)



(James et al., 2021, Figure 4.2)

Hands-on Practical Tutorial

- Your turn:
  - Work on the tutorial “module1-logistic_regression”

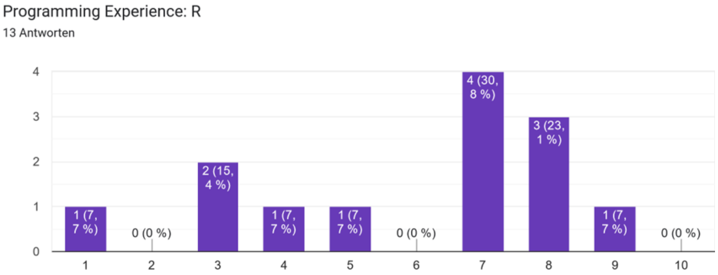
Summary

Summary

- Machine Learning (ML) is as easy and straightforward as:
  - Linear regression: Building models to estimate the (linear) relationship between a continuous target variable and a set of features
  - Logistic regression: Building models to estimate the probability of class membership based on a set of features
- Before building the model, the data may need to be preprocessed
  - E.g., normalized or standardized features, transformed targets, ...
- To expand:
  - Other, more advanced Supervised Learning algorithms
  - Variable selection
  - Cross validation

Appendix

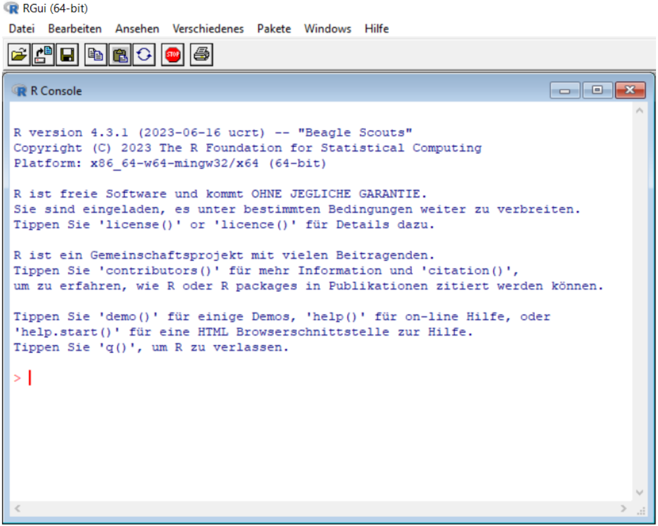
Your experiences



Quick Facts about R

- It is a programming language
- It contains tools from Statistics, Data Mining, Machine Learning, Visualization, ...
- It has good graphical facilities
- It includes cutting-edge technology
- It is Open Source
- It runs on different platforms (Windows, MacOS, UNIX)
- It has extensive documentation for help

R Console

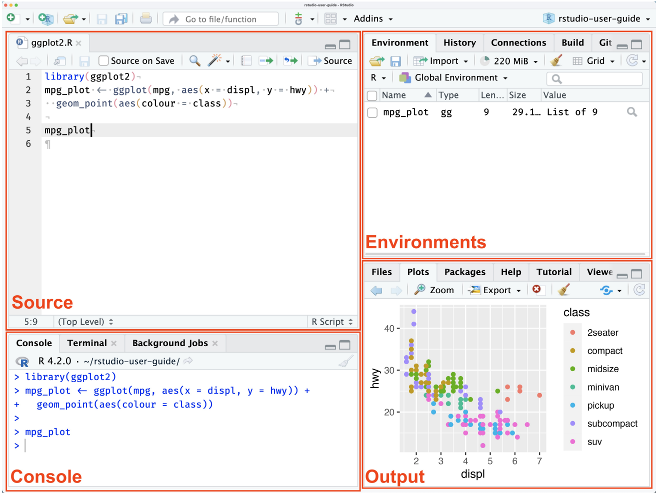

RGui (64-bit)
Datei Bearbeiten Ansehen Verschiedenes Pakete Windows Hilfe
R Console
R version 4.3.1 (2023-06-16 ucrt) -- "Beagle Scouts"
Copyright (C) 2023 The R Foundation for Statistical Computing
Platform: x86_64-w64-mingw32/x64 (64-bit)
R ist freie Software und kommt OHNE JEGLICHE GARANTIE.
Sie sind eingeladen, es unter bestimmten Bedingungen weiter zu verbreiten.
Tippen Sie 'license()' or 'licence()' für Details dazu.
R ist ein Gemeinschaftsprojekt mit vielen Beitragenden.
Tippen Sie 'contributors()' für mehr Information und 'citation()',
um zu erfahren, wie R oder R packages in Publikationen zitiert werden können.
Tippen Sie 'demo()' für einige Demos, 'help()' für on-line Hilfe, oder
'help.start()' für eine HTML Browserschnittstelle zur Hilfe.
Tippen Sie 'q()', um R zu verlassen.
>

Installation

- Go to http://www.r-project.org
- Click on the download link on the main page
- Choose your preferred CRAN mirror
- Navigate to "Download and Install R"
- Choose your platform

- Important: We will be working with R Version 4.3.3
  - Same version makes troubleshooting much easier
  - You can check your installed version by executing `R.Version()` in your console

RStudio Editor



Installation

- Before starting, make sure that R is installed correctly
- Go to https://posit.co/downloads/
- Click on the download link on the main page
- Navigate to “Install RStudio”
- Choose your platform

Coding in R

- Command lines start with ">"
- Comment lines start with "#"
- Use "<-" or "=" to assign a value to a variable
- Use "==", "<", ">", and "!=" to check logical conditions

Variables, Vectors, Matrices, ...

- Variables: Define a variable, `x`, assign it the value 1, print `x`, add 5 to `x`, print `x` again

```
x <- 1
print(x)
## [1] 1

x <- x + 5
print(x)
## [1] 6
```

- Vectors: Define two vectors, `u = (1, 4, 10, -1)` and `v = (10, -4, 3, 0)`, print `u + v`

```
u <- c(1, 4, 10, -1)
v <- c(10, -4, 3, 0)

z = u + v
print(z)
## [1] 11  0 13 -1
```

Variables, Vectors, Matrices, ...

- Matrices: Define a 4×2 matrix with columns `u` and `v`, print the matrix

```
mtrx <- cbind(u, v)
print(mtrx)
##       u  v
## [1,]  1 10
## [2,]  4 -4
## [3,] 10  3
## [4,] -1  0
```

- Data frame: Closely related to the concept of a matrix
  - The rows represent individual observations or “instances” (lines 1-4) and the columns represent variables (`u` and `v`)

```
as.data.frame(mtrx)
##    u  v
## 1  1 10
## 2  4 -4
## 3 10  3
## 4 -1  0
```

Arithmetics

- Mathematical operations:

```
x <- 10
y <- 7

x + y
## [1] 17

x - y
## [1] 3

x * y
## [1] 70

x / y
## [1] 1.428571

x %% y
## [1] 3
```

Functions

- Mathematical functions:

```
x
## [1] 10

sqrt(x)
## [1] 3.162278

v
## [1] 10 -4  3  0

abs(v)
## [1] 10  4  3  0
```

- Logical functions:

```
if (x >= 1) {
  print(TRUE)
} else {
  print(FALSE)
}
## [1] TRUE
```

Functions

- Statistical functions:

```
u
## [1]  1  4 10 -1

mean(u)
## [1] 3.5

sd(u)
## [1] 4.795832

median(u)
## [1] 2.5

summary(u)
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##    -1.0     0.5     2.5     3.5     5.5    10.0
```

Dataset Handling

- Reading from/writing to a file:

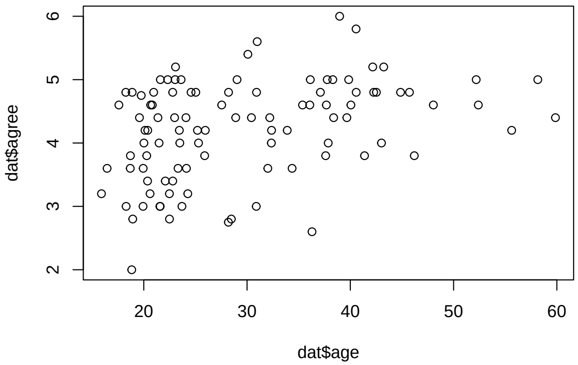
```
#reading data from drive
dat <- read.csv('subfiles/data/bfi.csv', header = TRUE)
head(dat)
##    CASE gender education      age agree conscientious extra neuro open
## 1 63116      1         3 40.55747   5.8           3.4   3.6   1.5  3.8
## 2 63967      1         4 35.37340   4.6           3.6   4.0   1.0  3.6
## 3 63955      2         4 21.55923   3.0           3.2   4.0   3.8  4.4
## 4 62547      2         1 22.80091   4.8           5.2   4.4   2.0  4.8
## 5 63493      2         2 23.07484   5.2           3.4   4.4   2.6  4.6
## 6 62419      2         3 30.08120   5.4           4.0   4.4   4.0  3.8

# writing data to drive
write.csv(dat, file = 'subfiles/data/bfi.csv', row.names = FALSE)
```

- Well-known data repositories for research purposes:
  - http://archive.ics.uci.edu/ml/
  - https://www.kaggle.com/datasets

Plotting

- Scatterplot:

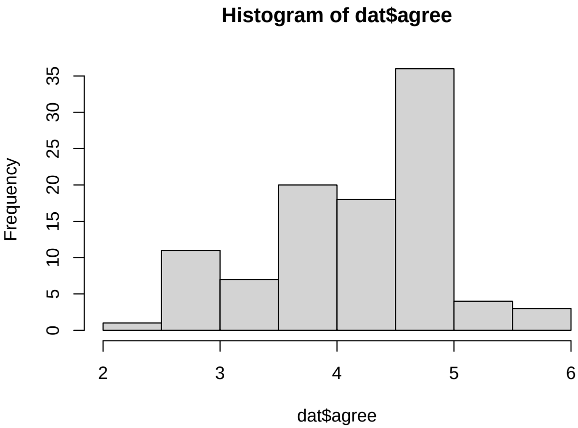
```
plot(dat$agree ~ dat$age)
```



Plotting

- Histogram:

```r
hist(dat$agree)
```



Packages

- Some packages are included by default, such as `stats` and `graphics`
  - Use `installed.packages()` to find out which ones
- Other packages can be installed using `install.packages("name")`
  - Packages provide extended functionality for R
    - Most important package for data handling: `tidyverse`
    - Most important package for ML: `mlr3verse`
  - Ideally, install packages with `dependencies = TRUE` to also include any packages that might be used in the package `name` you are installing
- You have to load new packages with `library("name")` every time you start a new session
  - Alternatively, you can access individual functions from installed packages without loading the entire package (cf. Python) with `name::function()`

Packages

- Caution: Different packages can have the same names for different functions
  - The last loaded package overwrites any functions with the same name in previously loaded packages
- Recommendations:
  - Load all packages needed for the analysis in one section at the beginning of the script
  - Usually it is best to load `tidyverse` and `mlr3verse` last
  - Pay attention to warnings when loading packages
    - If certain functions are overwritten, you can still access them with `name::function()`
  - Always start a new R session when you start your analysis to avoid unexpected behavior from packages loaded from previous sessions

More to come

- You can access the internal help with `?command`
- Google (and recently also GPT) are your best friends for solving programming issues
- With the practical tutorials, we will get more familiar with R