

A crash course on R for data analysis

Clemens Schmid



Data recovery

Run the following script to recover the relevant section of your data directory curl -s https://share.eva.mpg.de/index.php/s/dQJe7TKB8iBG6Wc/download | bash If this does not work, please download the file presentation.Rmd from here: https://github.com/nevrome/spaam_r_tidyverse_intro_2h



Getting started for this workshop

Activate the relevant conda environment (don't forget to deactivate it later!)

conda activate r-python

Navigate to

/vol/volume/3b-1-introduction-to-r-and-the-tidyverse/spaam_r_tidyverse_intro_2h

Pull the latest changes in this Git repository

git pull

- Open RStudio
- Load the project with File > Open Project...
- Open this file presentation.Rmd in RStudio



A crash course on R for data analysis



TOC

- The working environment
- Loading data into tibbles
- Plotting data in tibbles
- Conditional queries on tibbles
- Transforming and manipulating tibbles
- Combining tibbles with join operations



The working environment



R, RStudio and the tidyverse

- R is a fully featured programming language, but it excels as an environment for (statistical) data analysis (https://www.r-project.org)
- RStudio is an integrated development environment (IDE) for R (and other languages): (https://www.rstudio.com/products/rstudio)
- The tidyverse is a collection of packages with well-designed and consistent interfaces for the main steps of data analysis: loading, transforming and plotting data (https://www.tidyverse.org)
 - This introduction works with tidyverse ~v1.3.0
 - We will learn about readr, tibble, ggplot2, dplyr, magrittr and tidyr
 - forcats will be briefly mentioned
 - purrr and stringr are left out



Loading data into tibbles



Reading data with readr

- With R we usually operate on data in our computer's memory
- The tidyverse provides the package readr to read data from text files into the memory
- readr can read from our file system or the internet
- It provides functions to read data in almost any (text) format:

```
readr::read_csv()  # .csv files
readr::read_tsv()  # .tsv files
readr::read_delim()  # tabular files with an arbitrary separator
readr::read_fwf()  # fixed width files
readr::read_lines()  # read linewise to parse yourself
```

■ readr automatically detects column types — but you can also define them manually



How does the interface of read_csv work?

- We can learn more about a function with ?. To open a help file: ?readr::read_csv
- readr::read_csv has many options to specify how to read a text file

```
read_csv(
 file,
                          # The path to the file we want to read
 col names = TRUE. # Are there column names?
 col_types = NULL, # Which types do the columns have? NULL -> auto
 locale = default locale(), # How is information encoded in this file?
 na = c("", "NA"),
                       # Which values mean "no data"
 trim ws = TRUE.
                          # Should superfluous white-spaces be removed?
 skip = 0,
                          # Skip X lines at the beginning of the file
 n \max = Inf.
              # Only read X lines
 skip empty rows = TRUE, # Should empty lines be ignored?
 comment = "".
                     # Should comment lines be ignored?
 name repair = "unique". # How should "broken" column names be fixed
  . . .
```



What does readr produce? The tibble!

```
samples <- readr::read_tsv(sample_table_url)</pre>
  ■ The tibble is a "data frame". a tabular data structure with rows and columns
  ■ Unlike a simple array, each column can have another data type
print(samples, n = 3)
## # A tibble: 1.060 x 16
##
     project name publication year publication doi
                                                       site name latitude longitude
##
     <chr>
                            <dbl> <chr>
                                                       <chr>
                                                                   <dbl>
                                                                              <dbl>
## 1 Warinner2014
                              2014 10.1038/ng.2906 Dalheim
                                                                   51.6 8.84
                              2014 10.1038/ng.2906 Dalheim
                                                                   51.6
                                                                              8.84
  2 Warinner2014
  3 Wevrich2017
                              2017 10.1038/nature21674 Gola For~
                                                                    7.66
                                                                             -10 8
  # ... with 1,057 more rows, and 10 more variables: geo loc name <chr>,
## #
       sample_name <chr>, sample_host <chr>, sample age <dbl>.
## #
       sample_age_doi <chr>, community_type <chr>, material <chr>, archive <chr>,
## #
       archive project <chr>, archive accession <chr>
```



How to look at a tibble?

```
samples # Typing the name of an object will print it to the console
str(samples) # A structural overview of an object
summary(samples) # A human-readable summary of an object
View(samples) # RStudio's interactive data browser
```

R provides a very flexible indexing operation for data.frames and tibbles

```
samples[1,1]  # Access the first row and column
samples[1,]  # Access the first row
samples[,1]  # Access the first column
samples[c(1,2,3),c(2,3,4)]  # Access a selection of rows and columns
samples[,-c(1,2)]  # Remove the first two columns
samples[,c("site_name", "material")]  # Columns can be selected by name
```

■ tibbles are mutable data structures, so their content can be overwritten

```
samples[1,1] \leftarrow "Cheesecake2015" # replace the first value in the first column
```



Plotting data in tibbles



ggplot2 and the "grammar of graphics"

ggplot2 offers an unusual, but powerful and logical interface

library(ggplot2) # Loading a library to use its functions without ::

■ The following example describes a stacked bar chart

■ geom_*: data + geometry + statistical transformation + repositioning

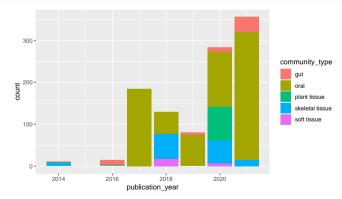
fill = community_type # publication_year -> fill color



ggplot2 and the "grammar of graphics"

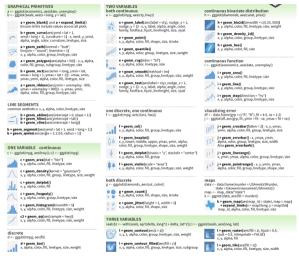
■ This is the plot described above: number of samples per community type through time

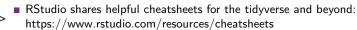
```
ggplot(samples) +
geom_bar(aes(x = publication_year, fill = community_type))
```





ggplot2 features many geoms

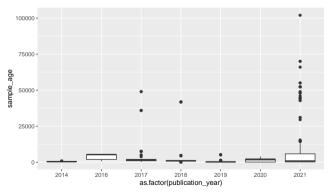


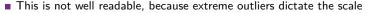


scales control the behaviour of visual elements

■ Another plot: Boxplots of sample age through time

```
ggplot(samples) +
geom_boxplot(aes(x = as.factor(publication_year), y = sample_age))
```



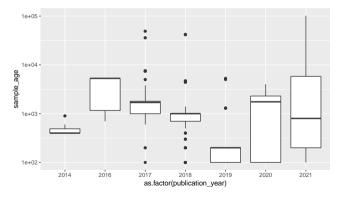




scales control the behaviour of visual elements

■ We can change the **scale** of different visual elements - e.g. the y-axis

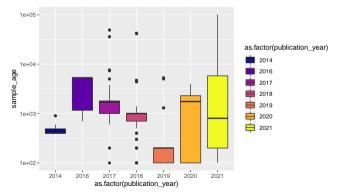
```
ggplot(samples) +
geom_boxplot(aes(x = as.factor(publication_year), y = sample_age)) +
scale_y_log10()
```





scales control the behaviour of visual elements

■ (Fill) color is a visual element of the plot and its scaling can be adjusted

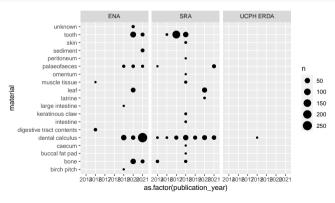




Defining plot matrices via facets

■ Splitting up the plot by categories into facets is another way to visualize more variables at once

```
ggplot(samples) +
geom_count(aes(x = as.factor(publication_year), y = material)) +
facet_wrap(~archive)
```

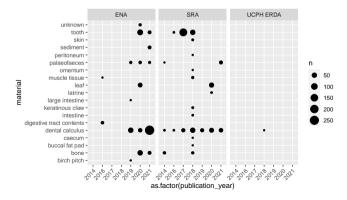




Setting purely aesthetic settings with theme

■ Aesthetic changes like this can be applied as part of the theme

```
ggplot(samples) +
geom_count(aes(x = as.factor(publication_year), y = material)) +
facet_wrap(~archive) +
theme(axis.text.x = element_text(angle = 45, hjust = 1, vjust = 1))
```





Exercise 1

- Look at the mtcars dataset and read up on the meaning of its variables
- ${f 2}$ Visualize the relationship between *Gross horsepower* and 1/4 *mile time*
- Integrate the Number of cylinders into your plot



Possible solutions 1

Look at the mtcars dataset and read up on the meaning of its variables

?mtcars

```
ggplot(mtcars) + geom_point(aes(x = hp, y = qsec))
```

Integrate the Number of cylinders into your plot

```
ggplot(mtcars) + geom_point(aes(x = hp, y = qsec, color = as.factor(cyl)))
```



Conditional queries on tibbles



Selecting columns and filtering rows with select and filter

The dplyr package includes powerful functions to subset data in tibbles based on conditions
 dplyr::select allows to select columns



Chaining functions together with the pipe %>%

■ The pipe %>% in the magrittr package is a clever infix operator to chain data and operations

```
library(magrittr)
samples %>% dplyr::filter(publication_year == 2014)
```

- It pipes the LHS in as the first argument of the function appearing on the RHS
- That allows for sequences of functions ("tidyverse style")

```
samples %>%
  dplyr::select(sample_host, community_type) %>%
  dplyr::filter(sample_host == "Homo sapiens" & community_type == "oral") %>%
  nrow() # count the rows
```

■ magrittr also offers some more operators, among which the extraction %\$% is particularly useful

```
samples %>%
  dplyr::filter(material == "tooth") %$%
  sample_age %>% # extract the sample_age column as a vector
  max() # get the maximum of said vector
```



Summary statistics in base R

 Summarising and counting data is indispensable and R offers all operations you would expect in its base package

```
nrow(samples)
                           # number of rows in a tibble
length(samples$site_name)
                           # length/size of a vector
unique(samples$material)
                           # unique elements of a vector
min(samples$sample_age)
                           # mi.n.i.mu.m
max(samples$sample_age)
                           # maximum
mean(samples$sample_age)
                           # mean
median(samples$sample_age) # median
var(samples$sample age)
                           # nariance
sd(samples$sample age) # standard deviation
quantile(samples$sample age, probs = 0.75) # sample quantiles for the given probs
```

■ many of these functions can ignore missing values with an option na.rm = TRUE



Group-wise summaries with group_by and summarise

- These summary statistics are particular useful when applied to conditional subsets of a dataset
- dplyr allows such summary operations with a combination of group_by and summarise

```
samples %>%
  dplyr::group_by(material) %>% # group the tibble by the material column
  dplyr::summarise(
    min_age = min(sample_age), # a new column: min age for each group
    median_age = median(sample_age), # a new column: median age for each group
    max_age = max(sample_age) # a new column: max age for each group
)
```

grouping can be applied across multiple columns

```
samples %>%
dplyr::group_by(material, sample_host) %>% # group by material and host
dplyr::summarise(
   n = dplyr::n(), # a new column: number of samples for each group
   .groups = "drop" # drop the grouping after this summary operation
)
```



Sorting and slicing tibbles with arrange and slice

dplyr allows to arrange tibbles by one or multiple columns

■ Sorting also works within groups and can be paired with slice to extract extreme values per group

```
samples %>%
  dplyr::group_by(publication_year) %>%  # group by publication year
  dplyr::arrange(dplyr::desc(sample_age)) %>% # sort by age within (!) groups
  dplyr::slice_head(n = 2) %>%  # keep the first two samples per group
  dplyr::ungroup()  # remove the still lingering grouping
```

■ Slicing is also the relevant operation to take random samples from the observations in a tibble

```
samples \%>% dplyr::slice_sample(n = 20)
```



Exercise 2

- Determine the number of cars with four *forward gears* (gear) in the mtcars dataset
- \blacksquare Determine the mean 1/4 mile time (qsec) per Number of cylinders (cyl) group
- Identify the least efficient cars for both transmission types (am)



Possible solutions 2

Determine the number of cars with four forward gears (gear) in the mtcars dataset
mtcars %>% dplyr::filter(gear == 4) %>% nrow()

```
Determine the mean 1/4 mile time (qsec) per Number of cylinders (cyl) group
mtcars %>% dplyr::group_by(cyl) %>% dplyr::summarise(qsec_mean = mean(qsec))
```

Identify the least efficient cars for both transmission types (am)

```
#mtcars3 <- tibble::rownames_to_column(mtcars, var = "car") %>% tibble::as_tibble()
mtcars %>% dplyr::group_by(am) %>% dplyr::arrange(mpg) %>% dplyr::slice_head()
```



Transforming and manipulating tibbles



Renaming and reordering columns and values with rename, relocate and recode

■ Columns in tibbles can be renamed with dplyr::rename and reordered with dplyr::relocate

```
samples %>% dplyr::rename(country = geo_loc_name) # rename a column
samples %>% dplyr::relocate(site_name, .before = project_name) # reorder columns
```

■ Values in columns can also be changed with dplyr::recode

```
samples$sample_host %>% dplyr::recode(`Homo sapiens` = "modern human")
```

- R supports explicitly ordinal data with factors, which can be reordered as well
- factors can be handeld more easily with the forcats package

```
ggplot(samples) + geom_bar(aes(x = community_type)) # bars are alphabetically ordered
sa2 <- samples
sa2$cto <- forcats::fct_reorder(sa2$community_type, sa2$community_type, length)
# fct_reorder: reorder the input factor by a summary statistic on an other vector
ggplot(sa2) + geom_bar(aes(x = community_type)) # bars are ordered by size</pre>
```



Adding columns to tibbles with mutate and transmute

A common application of data manipulation is adding derived columns. dplyr offers that with mutate

dplyr::transmute removes all columns but the newly created ones

```
samples %>%
  dplyr::transmute(
    sample_name = tolower(sample_name), # overwrite this columns
    publication_doi # select this column
)
```

 $\blacksquare \ \, \texttt{tibble::add_column} \ \, \texttt{behaves as dplyr::mutate}, \ \, \texttt{but gives more control over column position}$

```
samples %>% tibble::add_column(., id = 1:nrow(.), .before = "project_name")
```



Conditional operations with ifelse and case_when

ifelse allows to implement conditional mutate operations, that consider information from other columns, but that gets cumbersome easily

```
samples %>% dplyr::mutate(hemi = ifelse(latitude >= 0, "North", "South")) %$% hemi
samples %>% dplyr::mutate(
  hemi = ifelse(is.na(latitude), "unknown", ifelse(latitude >= 0, "North", "South"))
) %$% hemi
```

dplyr::case_when is a much more readable solution for this application



Long and wide data formats

■ For different applications or to simplify certain analysis or plotting operations data often has to be transformed from a **wide** to a **long** format or vice versa



- A table in wide format has N key columns and N value columns
- A table in long format has N key columns, one descriptor column and one value column



A wide dataset

```
carsales <- tibble::tribble(
 ~brand, ~`2014`, ~`2015`, ~`2016`, ~`2017`,
 "BMW", 20, 25, 30, 45,
                             55
 "VW". 67. 40. 120.
## # A tibble: 2 \times 5
    brand `2014` `2015` `2016` `2017`
##
    <chr> <dbl> <dbl> <dbl>
##
                             <dbl>
## 1 BMW
             20
                    25
                          30
                                45
## 2 VW
             67
                    40
                         120
                                55
```

- Wide format becomes a problem, when the columns are semantically identical. This dataset is in wide format and we can not easily plot it
- We generally prefer data in long format, although it is more verbose with more duplication. "Long" format data is more "tidy"



Making a wide dataset long with pivot_longer

```
carsales_long <- carsales %>% tidyr::pivot_longer(
  cols = tidyselect::num range("", range = 2014:2017), # set of columns to transform
 names to = "vear".
                     # the name of the descriptor column we want
 names transform = as.integer, # a transformation function to apply to the names
 values_to = "sales"
                         # the name of the value column we want
## # A tibble: 8 x 3
##
   brand vear sales
    <chr> <int> <dbl>
##
## 1 BMW
           2014
                   20
## 2 BMW
           2015
                25
## 3 BMW
           2016
                   30
## 4 RMW
           2017
                   45
                   67
## 5 VW
           2014
## 6 VW
                   40
           2015
## 7 VW
           2016
                  120
                   55
## 8 VW
           2017
```

Making a long dataset wide with pivot_wider

20

67

25

40

30

120

```
carsales_wide <- carsales_long %>% tidyr::pivot_wider(
  id_cols = "brand", # the set of id columns that should not be changed
  names_from = year, # the descriptor column with the names of the new columns
  values_from = sales # the value column from which the values should be extracted
)

## # A tibble: 2 x 5

## brand `2014` `2015` `2016` `2017`

## <chr> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> </dbl>
```

 Applications of wide datasets are adjacency matrices to represent graphs, covariance matrices or other pairwise statistics

45

55

■ When data gets big, then wide formats can be significantly more efficient (e.g. for spatial data)



<ch:

2 VW

Exercise 3

- Move the column gear to the first position of the mtcars dataset
- Make a new dataset mtcars2 with the column mpg and an additional column am_v, which encodes the transmission type (am) as either "manual" or "automatic"
- © Count the number of cars per transmission type (am_v) and number of gears (gear). Then transform the result to a wide format, with one column per transmission type.



Possible solutions 3

■ Move the column gear to the first position of the mtcars dataset

```
mtcars %>% dplyr::relocate(gear, .before = mpg)
```

Make a new dataset mtcars2 with the column gear and an additional column am_v, which encodes the transmission type (am) as either "manual" or "automatic"

```
mtcars2 <- mtcars %>% dplyr::mutate(
  gear, am_v = dplyr::case_when(am == 0 ~ "automatic", am == 1 ~ "manual")
)
```

© Count the number of cars in mtcars2 per transmission type (am_v) and number of gears (gear). Then transform the result to a wide format, with one column per transmission type.

```
mtcars2 %>% dplyr::group_by(am_v, gear) %>% dplyr::tally() %>%
   tidyr::pivot_wider(names_from = am_v, values_from = n)
```



Combining tibbles with join operations



Types of joins

Joins combine two datasets x and y based on key columns

- Mutating joins add columns from one dataset to the other
 - Left join: Take observations from x and add fitting information from y
 - \blacksquare Right join: Take observations from y and add fitting information from x
 - Inner join: Join the overlapping observations from x and y
 - Full join: Join all observations from x and y, even if information is missing
- Filtering joins remove observations from x based on their presence in y
 - lacktriangle Semi join: Keep every observation in x that is in y
 - Anti join: Keep every observation in x that is not in y



A second dataset

```
libraries <- readr::read_tsv(library_table_url)</pre>
print(libraries, n = 3)
## # A tibble: 1.657 x 20
##
     project name publication year data publication doi sample name archive
                                                        <chr>
##
     <chr>>
                             <dbl> <chr>
                                                                     <chr>>
## 1 Warinner2014
                              2014 10.1038/ng.2906
                                                        B61
                                                                     SRA
  2 Warinner2014
                              2014 10.1038/ng.2906
                                                        B61
                                                                     SRA
## 3 Warinner2014
                              2014 10.1038/ng.2906
                                                        B61
                                                                     SR.A
  # ... with 1,654 more rows, and 15 more variables: archive project <chr>,
## #
       archive sample accession <chr>, library name <chr>, strand type <chr>,
## #
       library polymerase <chr>, library treatment <chr>,
## #
       library concentration <dbl>, instrument model <chr>, library layout <chr>,
       library strategy <chr>, read count <dbl>, archive data accession <chr>,
## #
## #
       download links <chr>, download md5s <chr>, download sizes <chr>
```

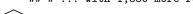


Meaningful subsets

```
print(samsub, n = 3)
## # A tibble: 1,060 x 3
##
     project_name sample_name sample_age
##
     <chr>>
                  <chr>>
                                   <db1>
## 1 Warinner2014 B61
                                     900
## 2 Warinner2014 G12
                                     900
  3 Wevrich2017 Chimp
                                     100
## # ... with 1,057 more rows
print(libsub, n = 3)
## # A tibble: 1.657 x 4
##
     project name sample name library name
                                               read_count
##
     <chr>
                  <chr>
                              <chr>
                                                     <db1>
                                                 13228381
## 1 Warinner2014 B61
                              S1-Shot-B61-calc
  2 Warinner2014 B61
                              S2-Shot-B61-calc
                                                  13260566
  3 Warinner2014 B61
                              S3-Shot-B61-calc
                                                 8869866
  # ... with 1.654 more rows
```

Left join

Take observations from \boldsymbol{x} and add fitting information from \boldsymbol{y}



■ Left joins are the most common join operation: Add information from another dataset

Right join

Take observations from y and add fitting information from \boldsymbol{x}

```
A B C A B D A B C D
a t 1
b u 2
c v 3
A B D a t 1
b u 2
d w 1
A B C D
a t 1 3
b u 2 2
d w 1
```

1 Warinner2014 B61

... with 1,819 more rows

```
right <- dplvr::right join(
      samsub,
                                         # 1060 observations
 x =
  v = libsub.
                                         # 1657 observations
 by = c("project name", "sample name")
## # A tibble: 1,820 x 5
##
     project_name sample_name sample_age library_name
                                                            read count
##
     <chr>>
                  <chr>>
                                    <dbl> <chr>
                                                                 <dbl>
```

900 S1-Shot-B61-calc

13228381

(i)

■ Right joins are almost identical to left joins – only x and y have reversed roles

Inner join

Join the overlapping observations from x and y

```
A B C A B D A B C D
a t 1
b u 2 + a t 3
b u 2 d w 1

A B D a t 1 3
b u 2 2
```

```
inner <- dplvr::inner join(</pre>
      samsub,
                                          # 1060 observations
  x =
  v = libsub.
                                          # 1657 observations
  by = c("project name", "sample name")
## # A tibble: 1,787 x 5
     project_name sample_name sample_age library_name
##
                                                             read count
##
     <chr>>
                   <chr>>
                                    <dbl> <chr>
                                                                  <dbl>
   1 Warinner2014 B61
                                       900 S1-Shot-B61-calc
                                                               13228381
## # ... with 1,786 more rows
```



■ Inner joins are a fast and easy way to check, to which degree two dataset overlap

Full join

Join all observations from \boldsymbol{x} and \boldsymbol{y} , even if information is missing

```
ABC a t 1 b u 2 + a t 3 b u 2 c v 3 - d w - 1

full <- dplyr::full join(
```

```
samsub,
                                         # 1060 observations
 x =
  v = libsub.
                                         # 1657 observations
 by = c("project name", "sample name")
## # A tibble: 1,914 x 5
    project_name sample_name sample_age library_name
##
                                                            read count
##
     <chr>>
                  <chr>>
                                    <dbl> <chr>
                                                                 <dbl>
  1 Warinner2014 B61
                                      900 S1-Shot-B61-calc
                                                              13228381
## # ... with 1,913 more rows
```



■ Full joins allow to preserve every bit of information

Semi join

Keep every observation in \boldsymbol{x} that is in \boldsymbol{y}

1 Warinner2014 B61

... with 965 more rows

```
A B C A B D A B C a t 1 b u 2 = A B C c v 3
```

900

■ Semi joins are underused operations to filter datasets

Anti join

Keep every observation in \boldsymbol{x} that is not in \boldsymbol{y}

```
A B C A B D A B C a t 3 b u 2 c v 3 = A B C
```

```
anti <- dplyr::anti_join(
    x = samsub,  # 1060 observations
    y = libsub,  # 1657 observations
    by = c("project_name", "sample_name")
)</pre>
```



■ Anti joins allow to quickly specify incomplete datasets and missing information

Exercise 4

Consider the following additional dataset:

```
gear_opinions <- tibble::tibble(gear = c(3, 5), opinion = c("boring", "wow"))</pre>
```

- Add my opinions about gears to the mtcars dataset
- Remove all cars from the dataset for which I don't have an opinion



Possible Solutions 4

Add my opinions about gears to the mtcars dataset

```
dplyr::left_join(mtcars, gear_opinions, by = "gear")
```

Remove all cars from the dataset for which I don't have an opinion

```
dplyr::anti_join(mtcars, gear_opinions, by = "gear")
```

