

A crash course on R for data analysis

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The working environment



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



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
- The following example describes a stacked bar chart

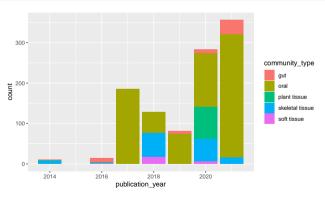
■ geom_*: data + geometry + statistical transformation + repositioning



ggplot2 and the "grammar of graphics"

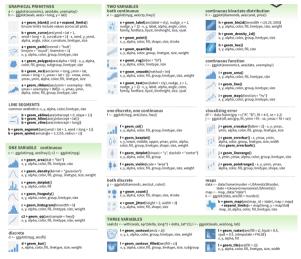
■ This is the plot described above: number of samples per community type through time

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





ggplot2 features many geoms



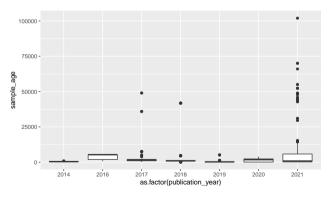


 RStudio shares helpful cheatsheets for the tidyverse and beyond: https://www.rstudio.com/resources/cheatsheets

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))
```



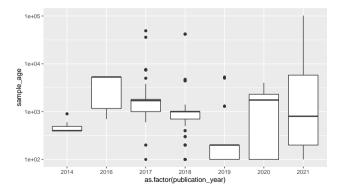


This is not well readable, because extreme outliers dictate the scale

scales control the behaviour of visual elements

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

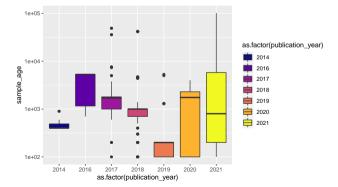
```
ggplot(samples) +
geom_boxplot(aes(x = as.factor(publication_year), y = sample_age)) +
scale_y_log10()
```





scales control the behaviour of visual elements

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

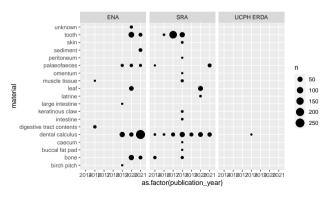




Defining plot matrices via facets

■ 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)
```

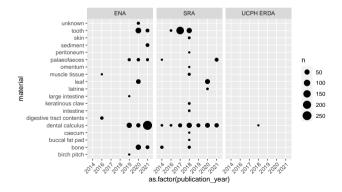




Setting purely aesthetic settings with theme

■ 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
- 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

 \blacksquare Visualize the relationship between *Gross horsepower* and 1/4 *mile time*

```
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
```

 \blacksquare 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

lacktriangle 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
)
```

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

```
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

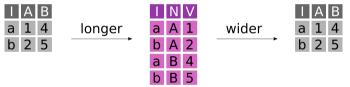
```
samples %>% dplyr::mutate(hemi = ifelse(latitude >= 0, "North", "South")) %$% hemi
samples %>% dplyr::mutate(
  hemi = ifelse(is.na(latitude), "unknown", ifelse(latitude >= 0, "North", "South"))
) %$% hemi
```

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

<chr> <dbl> <dbl> <dbl> <dbl> <dbl>

25

40

30

120

45

55

20

67

```
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`
```

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

Sound 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
 - Right join: Take observations from v 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
- - Semi join: Keep every observation in x that is in v
 - 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}

```
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 C D
b u 2 2
c v 3
```



■ 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 + a t 3 b u 2 = a t 1 3
b u 2 d w 1 = d w - 1
```

```
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>
  1 Warinner2014 B61
                                      900 S1-Shot-B61-calc
                                                              13228381
## # ... with 1,819 more rows
```



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

Inner join

Join the overlapping observations from \boldsymbol{x} and \boldsymbol{y}

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

```
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

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

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

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

```
full <- dplvr::full join(</pre>
      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 x that is in y

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



■ 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 1 b u 2 b u 2 c v 3 A B D a c v 3
```



■ 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")
```

