

# A crash course on R for data analysis

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#### 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 content of the following Git repository: 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 the 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 R 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  $\sim v1.3.0$
  - 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_yea:	publication_doi	site_name	latitude	longitude
##		<chr> <dbl:< th=""><th><chr></chr></th><th><chr></chr></th><th><dbl></dbl></th><th><dbl></dbl></th></dbl:<></chr>	<chr></chr>	<chr></chr>	<dbl></dbl>	<dbl></dbl>
##	1	Warinner2014 2014	l 10.1038/ng.2906	Dalheim	51.6	8.84
##	2	Warinner2014 2014	l 10.1038/ng.2906	Dalheim	51.6	8.84
##	3	Weyrich2017 201	' 10.1038/nature21674	Gola For~	7.66	-10.8
##	#	with 1,057 more rows, and	1 10 more variables:	geo_loc_nam	e <chr>,</chr>	
##	#	<pre>sample_name <chr>, sample_l</chr></pre>	nost <chr>, sample_ag</chr>	e <dbl>,</dbl>		
##	#	<pre>sample_age_doi <chr>, community_type <chr>, material <chr>, archive <chr>,</chr></chr></chr></chr></pre>				
##	#	archive_project <chr>, arc</chr>	nive_accession <chr></chr>			



## How to look at a tibble?

samples	# Typing the name of an object will print it to the console					
<pre>str(samples)</pre>	# A structural overview of an object					
<pre>summary(samples)</pre>	# 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 values from 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] <- "Cheesecake2015" # replace the first value in the first column</pre>



# 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

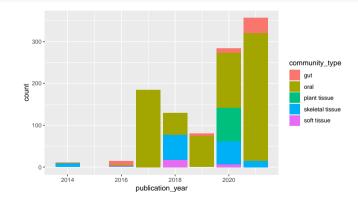
```
library(ggplot2) # Loading a library to use its functions without ::
```

■ geom\_\*: data + geometry (bars) + statistical transformation (sum)



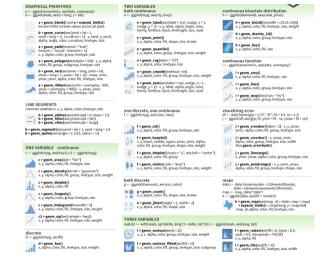
# ggplot2 and the "grammar of graphics"

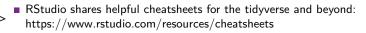
This is the plot described above: number of samples per community type through time
ggplot(samples) +
geom\_bar(aes(x = publication\_year, fill = community\_type))





#### ggplot2 features many geoms

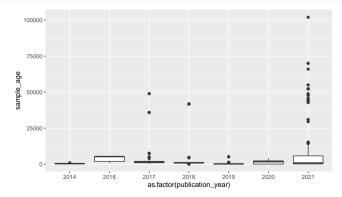




#### scales control the behaviour of visual elements

Another plot: Boxplots of sample age through time

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

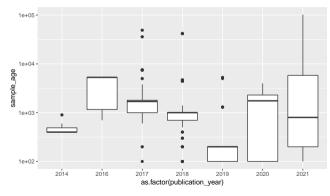


This is not well readable, because extreme outliers dictate the scale

# scales control the behaviour of visual elements

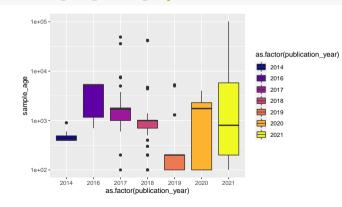
We can change the scale of different visual elements - e.g. the y-axis

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



The log-scale improves readability

#### scales control the behaviour of visual elements

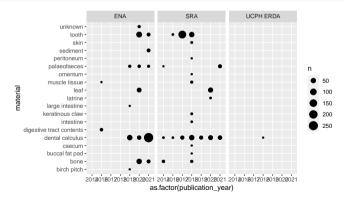




#### Defining plot matrices via facets

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)
```

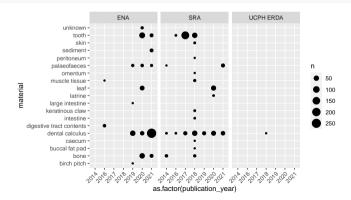


Unfortunately the x-axis became unreadable

#### 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
- **2** Visualize the relationship between Gross horsepower and 1/4 mile time
- **I**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

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

dplyr::select(samples, project\_name, sample\_age) # reduce to two columns
dplyr::select(samples, -project\_name, -sample\_age) # remove two columns

dplyr::filter allows for conditional filtering of rows



# 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 forwards the LHS 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$sample_age)
                           # min.i.mum
max(samples$sample_age)
                           # maximum
mean(samples$sample_age)
                           # mean
median(samples$sample_age) # median
var(samples$sample_age)
                           # variance
sd(samples$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  $\gg d plyr::slice_sample(n = 20)$ 



Exercise 2

- I Determine the number of cars with four forward gears (gear) in the mtcars dataset
- **2** Determine the mean 1/4 mile time (qsec) per Number of cylinders (cyl) group
- **3** 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))

**3** 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")

 $\blacksquare$  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

tibble::add\_column behaves as dplyr::mutate, 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

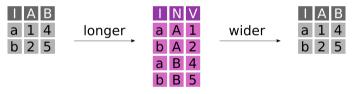
```
samples %>% dplyr::mutate(
    hemi = ifelse(is.na(latitude), "unknown", ifelse(latitude >= 0, "North", "South"))
) %$% hemi
```

```
dplyr::case_when is a much more readable solution for this application
samples %>% dplyr::mutate(
    hemi = dplyr::case_when(
    latitude >= 0 ~ "North",
    latitude < 0 ~ "South",
    TRUE ~ "unknown" # TRUE catches all remaining cases
    )
) %$% hemi</pre>
```



# 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,
    "VW", 67, 40, 120, 55
)</pre>
```

##	#	A tibb	ole: 2 x	: 5		
##		brand	`2014`	2015	2016	2017
##		< chr >	<dbl></dbl>	<dbl></dbl>	<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

##	#	A tibl	ble: 8	х З	
##		brand	year	sales	
##		< chr >	<int></int>	<dbl></dbl>	
##	1	BMW	2014	20	
##	2	BMW	2015	25	
##	3	BMW	2016	30	
##	4	BMW	2017	45	
##	5	VW	2014	67	
##	6	VW	2015	40	
##	7	VW	2016	120	
##	8	VW	2017	55	
$\sim$					

#### Making a long dataset wide with pivot\_wider

```
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>
## 1 BMW 20 25 30 45
## 2 VW 67 40 120 55
```

- 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)



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")
)
```

I 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
  - 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
  - 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)
print(libraries, n = 3)</pre>
```

##	#	A tibble: 1,657 x 20						
##		<pre>project_name publication_ye</pre>	ar	data_publication_doi	<pre>sample_name</pre>	archive		
##		<chr> <dt <dt<="" td=""><td>1&gt;</td><td><chr></chr></td><td><chr></chr></td><td><chr></chr></td></dt></chr>	1>	<chr></chr>	<chr></chr>	<chr></chr>		
##	1	Warinner2014 20	14	10.1038/ng.2906	B61	SRA		
##	2	Warinner2014 20	14	10.1038/ng.2906	B61	SRA		
##	3	Warinner2014 20	14	10.1038/ng.2906	B61	SRA		
##	#	with 1,654 more rows, and 15 more variables: archive_project <chr>,</chr>						
##	#	archive_sample_accession <chr>, library_name <chr>, strand_type <chr>,</chr></chr></chr>						
##	#	<pre>library_polymerase <chr>, library_treatment <chr>,</chr></chr></pre>						
##	#	<pre>library_concentration <dbl>, instrument_model <chr>, library_layout <chr>,</chr></chr></dbl></pre>						
##	#	library_strategy <chr>, read_count <dbl>, archive_data_accession <chr>,</chr></dbl></chr>						

## # download\_links <chr>, download\_md5s <chr>, download\_sizes <chr>



### Meaningful subsets

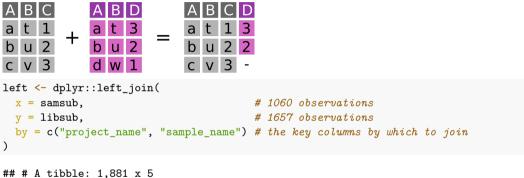
```
print(samsub, n = 3)
```

```
## # A tibble: 1,060 x 3
##
     project_name sample_name sample_age
##
     <chr>
                  <chr>>
                                    < dbl >
## 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>
                                                    <dbl>
                                                 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  $\boldsymbol{y}$ 

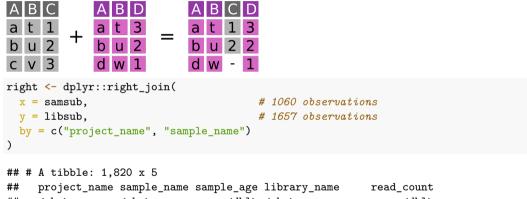


## project\_name sample\_name sample\_age library\_name read\_count
## <chr> <chr> <chr> <chr> <chr> <chr> <dbl> <chr> <chr> in uniner2014 B61 in the sample\_age library\_name read\_count
## 1 Warinner2014 B61 in the sample\_age library\_name read\_count
## ... with 1,880 more rows

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

## Right join

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

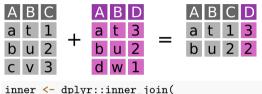


## project\_name sample\_name sample\_age library\_name read\_count
## <chr> <chr> <chr> <chr> <chr> <chr> <dbl> <chr> <dbl> <chr> <dbl> = 1 Warinner2014 B61 900 S1-Shot-B61-calc 13228381
## # ... with 1,819 more rows

 $\blacksquare$  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  $\boldsymbol{y}$ 



```
x = samsub,  # 1060 observations
y = libsub,  # 1657 observations
by = c("project_name", "sample_name")
```

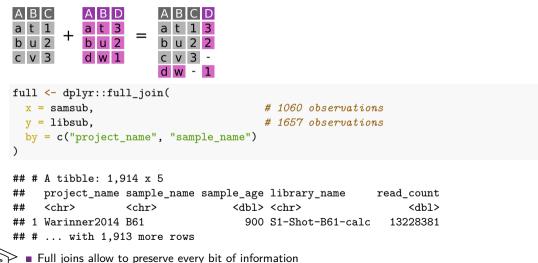
## # A tibble: 1,787 x 5
## project\_name sample\_name sample\_age library\_name read\_count
## <chr> <chr> <chr> <chr> <chr> <chr> <chr> <chr> minimized minimized

## 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

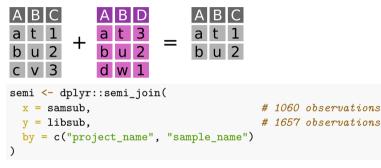
## Full join

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



## Semi join

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



## # A tibble: 966 x 3
## project\_name sample\_name sample\_age
## <chr> <chr> <chr> <chr> <dbl>
## 1 Warinner2014 B61 900
## # ... with 965 more rows

Semi joins are underused operations to filter datasets

### Anti join

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



## # ... with 93 more rows

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

2 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")

