# Data Structures and Data Wrangling

# TRR259 seminar Session 1

JS

29.10.2025

# Goal: Empower you to perform your own data analysis

- 1. Develop skills in data handling and visualisation
- 2. Speed up data processing and analysis of repeated projects
- 3. Dive into Sequencing data and RNA Seq analysis
- 4. Underline domain-specific statistics

#### Outline for the first Session

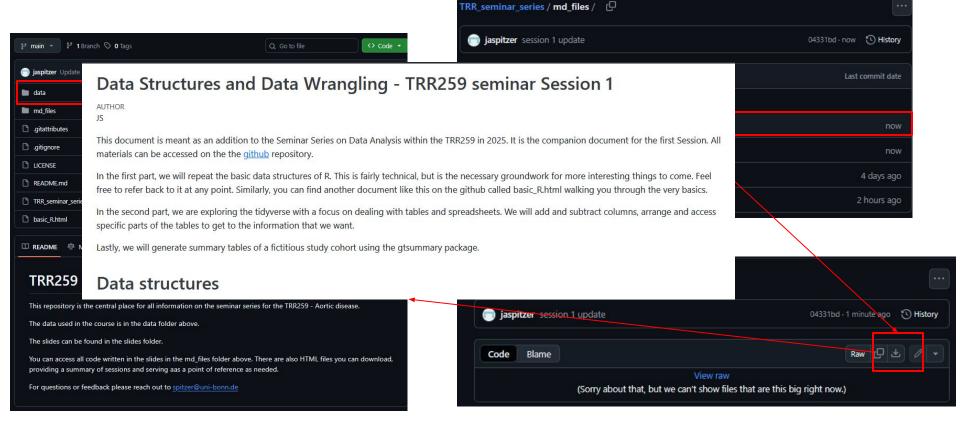
- 1. General introduction, expectations, goals
- 2. Data structures in R
- 3. Data wrangling using the tidyverse
- 4. Summary of survey data using gtsummary
- 5. Practice Problems

#### Course structure and materials

- 4 sessions with one session every two weeks, each session 2 to 2.5 h
- 1-1.5 h will be lecture-style presentation, the rest will be practical
- Material will be deposited on the github page:
  - Slides
  - All code written here, compiled with an in-depth explanation
  - questions and problems
- for questions, suggestions and complaints, feel free to contact me under spitzer@uni-bonn.de



#### **Quick Github tutorial**



#### Go with the flow!

- you are learning a new coding language
- you are learning how to think differently about your data
- you are learning new statistics
- you are going to learn new biology

This stuff is not easy, understanding takes time

#### Data structures in R

- vector
- factor
- matrix
- data frame
- list

#### Data structures in R - Vector

```
c(120,360,600,840)
                                                           Creates a vector
ages <- c(120,360,600,840)
                                                           Saves the vector with the name "ages"
length(ages)
                                                           How many values are in "ages"?
ages[3]
                                                            Third value in ages
ages[3:4] | ages[c(3,4)]
                                                           First two values of the vector
ages[-3]
                                                           Everything but the third value
ages + 5
                                                           Adds 5 to every age in ages
ages / 60
                                                           Divides all ages by 60
ages > 480
                                                           Is an age larger than 480?
sum(ages > 480)
                                                           How many ages are over 480?
mean(ages)
                                                           What is the mean age?
```

#### Data structures in R - Vector

```
c(120,360,600,840)
ages <- c(120,360,600,840)
length(ages)
ages[3]
ages[3:4] \mid ages[c(3,4)]
ages[-3]
ages + 5
ages / 60
ages > 480
sum(ages > 480)
mean(ages)
```

```
[1] 120 360 600 840
[1]
[1] 600
[1] 600 840
[1] 600 840
[1] 120 360 840
[1] 125 365 605 845
[1] 2 6 10 14
[1] FALSE FALSE TRUE TRUE
[1] 2
[1] 480
```

#### Data structures in R - Factor

Creates a factor with 2 levels, A and C

By default, levels are alphabetical

sort f

Relevel f with C as the default

sort f

Access the levels of f

#### Data structures in R - Factor

```
[1] A A A C C C
Levels: A C
[1] C C C A A A
Levels: C A
[1] "C" "A"
```

#### Data structures in R - two dimensional data

- most commonly used data format
- we'll use both matrix and dataframe, but mostly dataframes
- both forms are organised in rows and columns

#### Data structures in R - Matrix

```
m <- matrix(1:20, nrow = 5)
m[1, ]
m[ ,1]
colnames(m) <- c("a", "b", "c", "d")
rownames(m) <- c("v", "w", "x", "y", "z")
m["x", "a"]</pre>
```

Creates a matrix, here a simple 4 by 5 matrix

retrieves the first row of the *m* 

retrieves the first column of the *m* 

Sets column names for m

sets row names for *m* 

Accesses a single value using the names

#### Data structures in R - Matrix

```
m <- matrix(1:20, nrow = 5)
m[1, ]
m[ ,1]
colnames(m) <- c("a", "b", "c", "d")
rownames(m) <- c("v", "w", "x", "y", "z")
m["x", "a"]</pre>
```

```
[,1] [,2] [,3] [,4]
[1,]
     2 7 12
3 8 13
4 9 14
                      17
                      18
                     19
                      20
    1 6 11 16
[1] 1 2 3 4 5
 a b c d
     6 11 16
  2 7 12 17
  3 8 13 18
    9 14 19
z 5 10 15 20
```

#### Data structures in R - Data Frame

```
df <- data.frame(diagnosis = rep(c("CTRL",</pre>
                                                            Generates a data frame df with 3 variables
                                          "AAA"),
                                                                  diagnosis - CTRL or AAA
                                        each = 5),
                    diameter = c(rnorm(5, 5, 0.5),
                                                                  diameter, here randomly generated
                                    rnorm(5, 2, 0.1)),
                    age = round(runif(10, 45, 80)))
                                                                  age, randomly generated
df
                                                            returns the data frame df
df[ ,1]
                                                            Returns the first column of df
df$diameter
                                                            Returns the column of df called diameter
summary(df)
                                                            Quick statistical overview for df
df$diagnosis <- as.factor(df$diagnosis)</pre>
                                                            Replace diagnosis with a factor version
summary(df)
                                                            Results from summary() changes now
```

#### Data structures in R - Data Frame

```
diagnosis
                              diameter
 CTRL
                              5.348054
                                                       64
CTRL
                                                        70
                              4.206326
 CTRL
                              4.765926
                                                       55
 CTRL
                              4.408508
                                                       69
CTRL
                              4.438945
                                                        59
 AAA
                                                        59
                              2.154448
 AAA
                              2.146144
                                                       73
 AAA
                              2.187224
                                                       67
 AAA
                              2.210580
                                                       51
AAA
                              2.000905
1-10 of 10 rows
```

```
df[ ,1]
df$diameter
summary(df)
df$diagnosis <- as.factor(df$diagnosis)
summary(df)</pre>
```

```
[1] "CTRL" "CTRL" "CTRL" "CTRL" "AAA" "AAA" "AAA"
[1] 5.348054 4.206326 4.765926 4.408508 4.438945 2.154448 2.146144 2.187224 2.210580
2.000905
 diagnosis
                      diameter
Length:10
                   Min.
                         :2.001
                                  Min. :49.0
Class :character
                   1st Qu.:2.163
                                  1st Qu.:56.0
 Mode :character
                   Median :3,208
                                   Median:61.5
                         :3.387
                                         :61.6
                   3rd Qu.:4.431
                                   3rd Ou.:68.5
                         :5.348
                                  Max.
                                         :73.0
diagnosis
             diameter
                               age
 AAA :5
                 :2.001
                          Min. :49.0
                         1st Qu.:56.0
 CTRL:5
          1st Qu.:2.163
          Median:3.208
                          Median:61.5
                 :3.387
                          Mean
                               :61.6
           3rd Ou.:4.431
                          3rd Ou.:68.5
                 :5.348
                          Max.
                                 :73.0
```

#### Data structures in R - list

examples <- list("a", c("c", "example"), df))	generates a <i>list</i> and stores it in <i>examples</i>
examples[[1]]	accesses the first element of <i>examples</i> , note the double brackets
examples[1:2]	accesses the first elements of examples, but returns a list
length(examples)	How many elements are in examples?
str(examples)	Gives a summary of examples and its elements

#### Data structures in R - list

```
examples <- list("a", c("c", "example"), df))
examples[[1]]

examples[1:2]

[1] "a"
[[1]] "a"

length(examples)

str(examples)

[1] "c" "examples</pre>
```

```
[[1]]
Г1] "a"
[[2]]
[1] "c"
             "example"
[1] 3
List of 3
 $ : chr "a"
 $ : chr [1:2] "c" "example"
 $:'data.frame': 10 obs. of 3 variables:
  ..$ diagnosis: Factor w/ 2 levels "AAA", "CTRL": 2 2 2 2 2 1 1 1 1 1
  ..$ diameter : num [1:10] 4.71 5.2 5.36 4.51 4.65 ...
              : num [1:10] 73 77 53 47 64 66 80 73 47 64
  ..$ age
```

#### Data structures in R - named vectors and lists

#### Data structures in R - named vectors and lists

```
[1] 3
[1] "Tick" "Trick" "Track"
```

diagnosis <fctr></fctr>	diameter <dbl></dbl>	age <dbl></dbl>	
CTRL	4.709629	73	
CTRL	5.204867	77	
CTRL	5.355331	53	
CTRL	4.513321	47	
CTRL	4.650572	64	
AAA	2.034768	66	
AAA	2.019956	80	
AAA	2.052112	73	
AAA	2.159436	47	
AAA	1.974188	64	

# Data wrangling in the *tidyverse*

- group of packages designed for data science
- most of the work will take place in data frames or the tidyverse version, tibble
- assumed structure: each row is an observation, each column is a variable

Individual packages in this family have specialised purpose

- dplyr and tidyr for data cleaning and wrangling
- stringr and forcats for character and factor manipulation

# Data used throughout the course - aneurysm data

- generated by me (not real data!)
- contains 900 patients, their aortic diameters as well as some additional information on comorbidities, age, etc.
- this data set is meant as an exercise tool

diagnosis <chr></chr>	abdominal <dbl></dbl>	thoracic_dia <dbl></dbl>	age <dbl></dbl>	male <dbl></dbl>	hypertension <dbl></dbl>	cad <dbl></dbl>	artherioscle <dbl></dbl>	bmi <dbl></dbl>
CTRL	1.903918	1.918242	64	0	0	0	0	25.20
CTRL	2.050726	2.033109	49	1	0	0	1	22.95
CTRL	1.780361	1.868136	55	0	0	0	1	23.34
CTRL	1.799354	1.641936	52	1	0	1	0	22.26
CTRL	1.950962	1.588081	52	1	1	0	0	23.07
CTRL	2.081565	2.117073	69	1	0	0	1	23.57
CTRL	1.783003	1.670469	74	1	1	0	0	24.23
CTRL	2.144597	2.048529	47	0	Ī	0	1	22.75
CTRL	1.975882	1.762458	52	0	0	0	1	22.75
CTRL	2.075961	2.249491	76	0	0	0	1	27.66

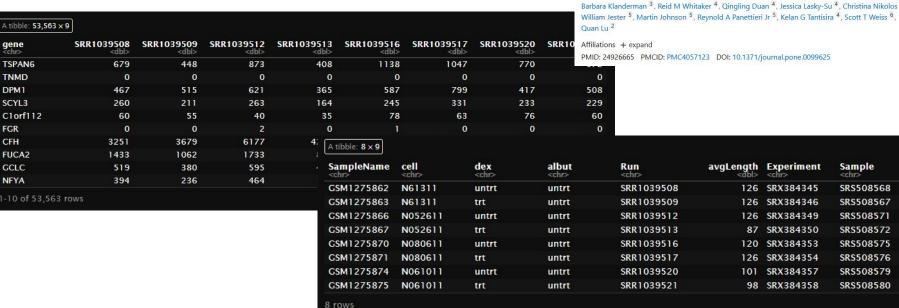
# Data used throughout the course - airway data

- data from the <u>airway</u> R package
- split into expression and annotation

modulates cytokine function in airway smooth muscle cells Blanca E Himes 1, Xiaofeng Jiang 2, Peter Wagner 2, Ruoxi Hu 2, Qiyu Wang 2 Barbara Klanderman 3, Reid M Whitaker 4, Qingling Duan 4, Jessica Lasky-Su 4, Christina Nikolos 5, William Jester 5, Martin Johnson 5, Reynold A Panettieri Jr 5, Kelan G Tantisira 4, Scott T Weiss 6 Quan Lu 2 Affiliations + expand PMID: 24926665 PMCID: PMC4057123 DOI: 10.1371/journal.pone.0099625 0 508 229 60 0 Run avgLength Experiment Sample <chr> <chr> SRR1039508 126 SRX384345 SRS508568 SRR1039509 126 SRX384346 SRS508567 SRR1039512 126 SRX384349 SRS508571 SRR1039513 87 SRX384350 SRS508572 120 SRX384353 SRS508575 SRR1039516 126 SRX384354 SRS508576 SRR1039517 SRR1039520 SRX384357 SRS508579 SRR1039521 98 SRX384358 SRS508580

> PLoS One. 2014 Jun 13;9(6):e99625. doi: 10.1371/journal.pone.0099625. eCollection 2014. RNA-Seq transcriptome profiling identifies

CRISPLD2 as a glucocorticoid responsive gene that





#### readr and readxl

```
library(tidyverse)

df <- read_tsv("example_data.txt")

df <- read_csv("example_data.csv")

df <- read_csv2("example_data2.csv")

readxl::read_xlsx("example_data.xlsx", sheet = 1)</pre>
```

activating the tidyverse packages

reading in a tab separated .txt file, saving it in df

read in a comma separated .csv file, saving it in df

read in the same file as above, using a totally not annoying german convention of .csv files, where the separator is ";", and the decimal point is ","

read in the same date from an excel file readxl is a little discouraged, so you need to specify its use

or un *library(readxl)* 



#### readr and readxl

```
library(tidyverse)
df <- read_tsv("example_data.txt")</pre>
df <- read_csv("example_data.csv")</pre>
df <- read_csv2("example_data2.csv")</pre>
readxl::read_xlsx("example_data.xlsx", sheet = 1)
```

diagnosis <chr></chr>	abdominal <dbl></dbl>	thoracic_dia <dbl></dbl>	age <dbl></dbl>	male <dbl></dbl>	hypertension <dbl></dbl>	cad <dbl></dbl>	artherioscle <dbl></dbl>	<b>bm</b> <dbl:< th=""></dbl:<>
CTRL	1.903918	1.918242	64	0	0	0	0	25.20
CTRL	2.050726	2.033109	49			0		22.9
CTRL	1.780361	1.868136	55	0		0		23.3
CTRL	1.799354	1.641936	52		0			22.20
CTRL	1.950962	1.588081	52			0	0	23.0
CTRL	2.081565	2.117073	69			0		23.5
CTRL	1.783003	1.670469	74			0	0	24.2
CTRL	2.144597	2.048529	47	0				22.7
CTRL	1.975882	1.762458	52	0	0	0		22.7
CTRL	2.075961	2.249491	76	0	0	0		27.6

# dplyr - grammar for data manipulation

- mutate creating a new column
- filter filter the observation based on a TRUE/FALSE criterium
- select select (or de-select) columns by name, position, class
- summarise perform summary calculations like mean, median, sum, ...

 group\_by - group observations by a variable and apply following calculations group-wise







```
df <- aa_data
df <- mutate(df,</pre>
           patient = paste("Pat", 1:900, sep="_"))
df <- mutate(df, age_months = age * 12)</pre>
                                                          adds a new column, multiplying age by 12
df <- mutate(df,severe_AAA = ifelse(</pre>
                            abdominal_diameter > 5,
                            "severe",
                            "non_severe"))
df <- mutate(df, diameter_ratio =</pre>
           abdominal_diameter / thoracic_diameter)
df <- mutate(df, diameter_ratio =</pre>
           round(diameter_ratio, 2))
```

save the aneurysm data in df adds a new column called patient to df

returns a classification of severe AAA based on diameter

Calculates the ratio of diameters

Round the previous ratio



```
delyr
```

```
df <- aa data
df <- mutate(df.</pre>
           patient = paste("Pat", 1:900, sep="_"))
df <- mutate(df, age_months = age * 12)</pre>
df <- mutate(df,severe_AAA = ifelse(diameter > 5,
                                    "severe".
                                    "non_severe"))
df <- mutate(df, diameter_ratio =</pre>
           abdominal_diameter / thoracic_diameter)
df <- mutate(df, diameter_ratio =</pre>
           thoracic_diameter / abdominal_diameter)
df <- mutate(df, diameter_ratio =</pre>
           round(diameter_ratio, 2))
```

### mutate() examples



```
Rows: 900
Columns: 13
$ diagnosis
                                                               <chr> "CTRL", "CT
 "CTRL", "CTRL", "CTRL", "CTRL", "CTRL", "CT...
$ abdominal_diameter <dbl> 1.903918, 2.050726, 1.780361, 1.799354, 1.950962, 2.081565, 1.783003, 2.144597, 1.975882,
2.075961, 2.197370, 1.883413, 1.864002, 2...
$ thoracic diameter <db/>
<db/>
1.918242, 2.033109, 1.868136, 1.641936, 1.588081, 2.117073, 1.670469, 2.048529, 1.762458,
2.249491, 2.157571, 1.946155, 1.762742, 1...
$ age
                                                                <db1> 64, 49, 55, 52, 52, 69, 74, 47, 52, 76, 48, 71, 61, 46, 60, 76, 65, 72, 59, 58, 72, 72, 50,
61. 77. 74. 69. 63. 66. 75. 63. 57. 63....
                                                                <db1> 0, 1, 0, 1, 1, 1, 1, 0, 0, 0, 1, 1, 0, 0, 0, 1, 1, 1, 1, 1, 0, 1, 0, 0, 0, 0, 1, 1, 1, 1, 0,
$ male
0, 0, 0, 0, 1, 1, 1, 0, 1, 1, 0, 1, 0,...
                                                               <db1> 0, 0, 0, 0, 1, 0, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0
$ hypertension
$ cad
                                                                0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, ...
$ artheriosclerosis <db1> 0, 1, 1, 0, 0, 1, 0, 1, 1, 1, 1, 1, 0, 1, 0, 0, 0, 1, 0, 0, 1, 0, 0, 1, 1, 1, 1, 1, 0, 1, 0, 1,
1, 1, 0, 0, 0, 1, 1, 1, 1, 0, 0, 0, 0, ...
$ bmi
                                                                <db1> 25.20, 22.95, 23.34, 22.26, 23.07, 23.57, 24.23, 22.75, 22.75, 27.66, 20.97, 22.94, 26.49,
21.74, 25.72, 24.90, 22.32, 25.91, 25.94...
                                                                <chr> "Pat_1", "Pat_2", "Pat_3", "Pat_4", "Pat_5", "Pat_6", "Pat_7", "Pat_8", "Pat_9", "Pat_10",
$ patient
 "Pat_11", "Pat_12", "Pat_13", "Pat_14", ...
$ age_months
                                                                <db1> 768, 588, 660, 624, 624, 828, 888, 564, 624, 912, 576, 852, 732, 552, 720, 912, 780, 864,
708, 696, 864, 864, 600, 732, 924, 888, 8...
$ severe AAA
                                                                <chr> "non_severe", "non_
 "non_severe", "non_severe", "non_severe", "non_...
$ diameter ratio
                                                               <db/>
| 1.01, 0.99, 1.05, 0.91, 0.81, 1.02, 0.94, 0.96, 0.89, 1.08, 0.98, 1.03, 0.95, 0.80, 0.81,
0.83, 1.00, 1.01, 1.02, 0.90, 1.09, 1.14,...
```





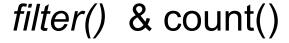
```
df <- aa data
                                                              save the aneurysm data in df
filter(df, diagnosis == "AAA")
                                                              filters df for only the AAA diagnosis
filter(df, diameter > 4.5)
                                                              filters df for a diameter > 4.5
filter(df, age < 75, abdominal_diameter > 4.5)
                                                              filters for both age and the diameter
filter(df, abdominal_diameter > 4 |
                                                              filter if either abdominal or thoracic diameter > 4. The
             thoracic_diameter > 4)
                                                              indicates the or
df <- mutate(df,</pre>
                                                              the same patient column as before
            patient = paste("Pat", 1:900, sep="_"))
filter(df, patient %in% c("Pat_2", "Pat_6"))
                                                              filters df for two patients using their ID
```



```
dplur
```

```
df <- aa data
filter(df, diagnosis == "AAA")
filter(df, diameter > 4.5)
filter(df, age < 75, abdominal_diameter > 4.5)
filter(df, abdominal_diameter > 4 |
           thoracic_diameter > 4)
df <- mutate(df,</pre>
          patient = paste("Pat", 1:900, sep="_"))
filter(df, patient %in% c("Pat_2", "Pat_6"))
```

```
$ there is calcelered in the combination of the com
```



```
dplyr
```

save the aneurysm data in df

filter only male patients without hypertensions with coronary artery disease

counts the patients with different diagnosis filtered from the original data drame







```
df <- aa data
                                                             save the aneurysm data in df
select(df, diagnosis, age, abdomninal_diameter)
                                                             select 3 columns from df
select(df, -age)
                                                             select all but one column from df
select(df, 1:3)
                                                             selects the first three columns
select(df, -c(1:2))
                                                             de-selects the first and second column from df
select(df, where(is.character))
                                                             only selects character columns from df
select(df, where(is.numeric))
                                                             only selects numeric columns from df
select(df, diagnosis, where(is.numeric))
                                                             selects a specific column and all numeric columns
```

# select() examples

```
dplyr
```

```
df <- aa_data
select(df, diagnosis, age, abdominal_diameter)
select(df, -age)
select(df, 1:3)
select(df, -c(1:2))
select(df, where(is.character))
select(df, where(is.numeric)) __
select(df, diagnosis, where(is.numeric))
```

diagnosis schr>	age <dbl></dbl>	abdominal_diameter
CTRL	64	1.903918
CTRL	49	2.050726
CTRL	55	1.780361
CTRL	52	1.799354
CTRL	52	1.950962
CTRL	69	2.081565
CTRL	74	1.783003
CTRL	47	2.144597
CTRL	52	1.975882
CTRL	76	2.075961

A tibble: 900 x 8							
abdominal_di	thoracic_dia <dbl></dbl>	age <dd>&gt;</dd>	male <dbi></dbi>	hypertension «dbl»	cad <dbl></dbl>	artherioscler	bmi <dbl></dbl>
1.903918	1.918242	64	0	0	.0	0	25.20
2.050726	2.033109	49		0			22.95
1.780361	1.868136	55		0	0		23.34
1.799354	1.641936	52					22.26
1.950962	1.588081	52			0	0	23.07
2.081565	2.117073	69		0	0		23.57
1.783003	1.670469	74			0	0	24.23
2.144597	2.048529	47					22.75
1.975882	1.762458	52	0	0	0		22.75
2.075961	2.249491	76	0	0	0		27.66
1-10 of 900 rows					Previous 1	] 2 3 4 5	6 90 Next

# The Pipe: %>% and |>



Some R code can be rather wonky and illegible

this code performs exactly the same operations, but it is formatted a different way. The pipe '%>%' passes on the output to the next operation.





```
df <- aa data
summarise(df, mean_diameter = mean(diameter))
summarise(df, median_age = median(age),
              mean\_age = mean(age),
              sd_age = sd(age)
df %>%
     group_by(diagnosis) %>%
     summarise(median_age = mean(age),
               sd_age = sd(age)
df %>%
     filter(diagnosis == "AAA") %>%
     group_by(abdominal_diameter > 4.5) %>%
     summarise(mean_bmi = mean(bmi),
               sd_bmi = sd(bmi))
```

saving the data in df

get the overall mean of diameter

get the median *age* of the data and the mean and the standard deviation

pipes *df*groups the *df* by *diagnosis*summarise (per group), generate mean *age*generate standard deviation of *age* 

pipes df filter on only AAA patients group them by their abdominal diameter calculate summary statistics

## summarise() examples

```
df <- aa data
summarise(df, mean_diameter = mean(diameter))
summarise(df, median_age = median(age),
              mean\_age = mean(age),
              sd_age = sd(age)
df %>%
     group_by(diagnosis) %>%
     summarise(median_age = mean(age),
               sd_age = sd(age)
df %>%
     filter(diagnosis == "AAA") %>%
     group_by(abdominal_diameter > 4.5) %>%
     summarise(mean_bmi = mean(bmi),
               sd_bmi = sd(bmi))
```



diagnosis <chr></chr>	median_age <dbl></dbl>	sd_age <dbl></dbl>
AAA	62	10.16246
CTRL	62	10.01787
TAA	62	10.01206

abdominal_diameter > 4.5 < g >	mean_bmi <dbl></dbl>	sd_bmi <dbl></dbl>
FALSE	27.71643	5.793834
TRUE	27.37563	5.992346





```
df <- aa_data
arrange(df, bmi)
arrange(df, -bmi)
slice_max(df, abdominal_diameter, n = 3)
slice_min(df, bmi, n = 10)</pre>
```

diagnosis <chr></chr>	abdominal <dbl></dbl>	thoracic_di	age <dbl></dbl>	male <dbl></dbl>	hypertension «dbl»	cad <dbl></dbl>	artherioscl	bmi <dbl></dbl>
TAA	1.417867	3.313813	63	0	1	0	0	20.13
CTRL	1.434809	1.857863	77	0	0	0	0	21.95
TAA	1.472359	4.125879	76	1	0	0	0	25.27
CTRL	1.474740	2.082274	67	0	0	0	0	24.93
TAA	1.498853	3.795084	75	0	0	0	0	24.25
CTRL	1.503340	1.643513	76	0	0	0	0	24.19
TAA	1.518932	3.893461	68	1	0	0	0	25.84
TAA	1.532775	4.091640	68	1	0	0	0	22.50
TAA	1.538799	3.861082	72	1	0	0	0	18.99
TAA	1.561262	3.621747	52	1	1	0	0	23.84

saving the data in *df*arrange the *data frame* by the *bmi* column, ascending

arrange the *data frame* by the *bmi* column, descending

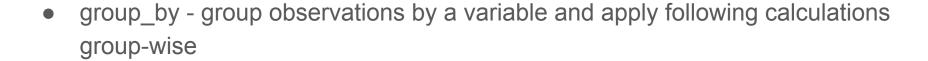
get the top 3 observations by abdominal diameter

get the bottom 10 observations by *bmi* 

diagnosis	abdominal	thoracic_di	age <dbl></dbl>	male <dbi></dbi>	hypertension «dbl»	cad <dbl></dbl>	artherioscl	bmi <dbl></dbl>
AAA	6.025393	2.169723	46	1	0	0	0	36.33
AAA	5.740262	1.952531	62	1	0	0		25.34
AAA	5.712208	2.109896	78	- 1	1	0	0	35.38

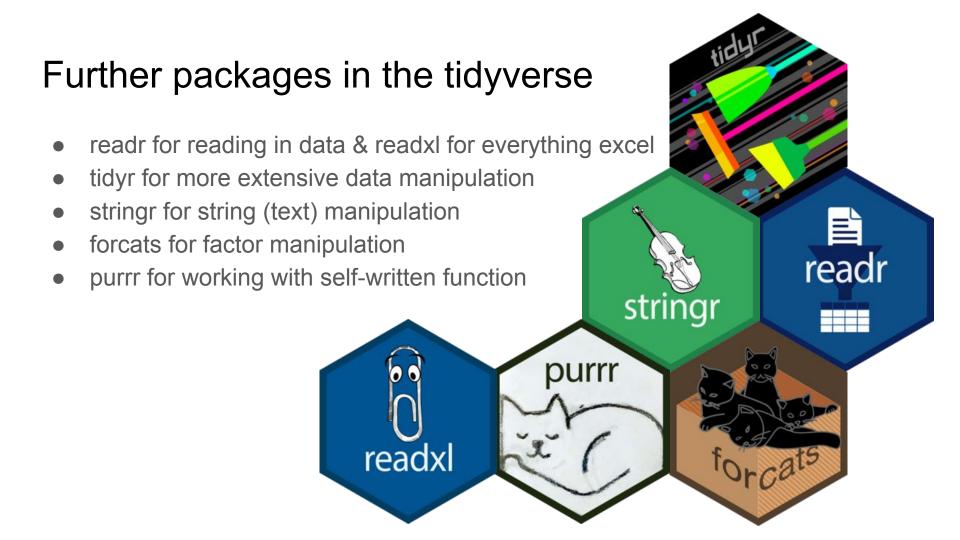
## dplyr - grammar for data manipulation

- mutate creating a new column
- filter filter the observation based on a TRUE/FALSE criterium
- select select (or de-select) columns by name, position, class
- summarise perform summary calculations like mean, median, sum, ...



chain together operations using the pipe





## Some practise for you after the break



Use the Github to get to the html doc for this session: practise on the bottom:

### Easy

E1: Use the code below to generate a vector called words. Access the third value of words.

```
words <- c("This", "is", "so", "great")
```

E2: Use the length() function to get to the length of the vector. What is its length?

E3: What class is words?

Refer to the github and download the data from the data folder. As a help you can check out the the basic\_R.html file, download and open it.

E3: Read in the aneurysm survey data. How many rows does it have? How many columns? Use the colnames() function to receive the column names.

E4: Add a column to the data frame containing a specific label for each patient. Which patient is the oldest? Which patient has the smallest thoracic diameter? Does that patient also have hypertension?

E5: Using the same data, how many patients have a thoracic diameter larger than 3.5 cm? Hint: use the filter() function

E6: We do not need that much precision in the diameters we have. Round them to two decimal points.

## Data used throughout the course - airway data

data from the <u>airway</u> R package

A tibble: 53,563 x 9

SRR1039508

679

467

260

60

3251

1433

519

394

0

0

SRR1039509

448

515

55

0

3679

1062

380

236

0

gene <chr>

TSPAN6

TNMD

DPM1

SCYL3

**FGR** 

CFH

FUCA2

GCLC

**NFYA** 

1-10 of 53,563 rows

Clorf112

split into expression and annotation

SRR1039512

873

621

263

40

6177

1733

595

464

0

muscle cells Blanca E Himes 1, Xiaofeng Jiang 2, Peter Wagner 2, Ruoxi Hu 2, Qiyu Wang 2 William Jester 5, Martin Johnson 5, Reynold A Panettieri Jr 5, Kelan G Tantisira 4, Scott T Weiss 6 Quan Lu 2 SRR10 Affiliations + expand PMID: 24926665 PMCID: PMC4057123 DOI: 10.1371/journal.pone.0099625 0 508 229 60 0 albut Run avgLength Experiment Sample <chr> <chr> <chr> SRR1039508 126 SRX384345 SRS508568 untrt SRR1039509 126 SRX384346 SRS508567 untrt SRR1039512 126 SRX384349 SRS508571 untrt untrt SRR1039513 87 SRX384350 SRS508572 120 SRX384353 SRS508575 SRR1039516 untrt SRS508576 SRR1039517 126 SRX384354 untrt SRR1039520 SRX384357 SRS508579 untrt untrt SRR1039521 98 SRX384358 SRS508580

RNA-Seq transcriptome profiling identifies CRISPLD2 as a glucocorticoid responsive gene that modulates cytokine function in airway smooth

> PLoS One. 2014 Jun 13;9(6):e99625. doi: 10.1371/journal.pone.0099625. eCollection 2014.



SRR1039516 SRR1039517 SRR1039520 <dhl> <dbl> 1138 1047 770 0 0 0 587 799 417 245 331 233 78 63 76 0 0

dex

<chr>

untrt

untrt

untrt

untrt

trt

trt

trt

trt

363
164
35
0
4: A tibb
1 400
Sam <chr></chr>
GSM

SRR1039513

<dbl>

408

0

8×9

leName

275862

275863

275866

275867

275870

GSM1275875 N061011

GSM1275871

GSM1275874

8 rows

cell

<chr>

N61311

N61311

N052611

N052611

N080611

N080611

N061011



## tidyr for extensive data manipulation

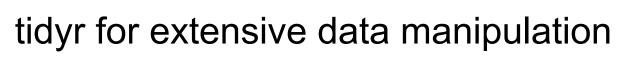
activating the tidyverse packages

reading in a tab separated .txt file, saving it in df

piping *df* select the cols to pivot longer, here de-selecting *gene* put the column names to *sample* put the values in a new column named *count* 

gene <chr></chr>	SRR1039508 <dbl></dbl>	SRR1039509 <dbl></dbl>	SRR1039512 <dbl></dbl>	SRR1039513 <dbl></dbl>	SRR1039516 <dbl></dbl>	SRR1039517 <dbl></dbl>	SRR1039520 <dbl></dbl>	SRR1039521 <dbl></dbl>
TSPAN6	679	448	873	408	1138	1047	770	572
TNMD	0	0	0	0	0	0	0	0
DPM1	467	515	621	365	587	799	417	508
SCYL3	260	211	263	164	245	331	233	229
Clorf112	60	55	40	35	78	63	76	60
FGR	0	0	2	0	1	0	0	0
CFH	3251	3679	6177	4252	6721	11027	5176	7995
FUCA2	1433	1062	1733	881	1424	1439	1359	1109
GCLC	519	380	595	493	820	714	696	704
NEYA	394	236	464	175	658	584	360	269

gene <chr></chr>	sample <chr></chr>	count <dbl></dbl>
TSPAN6	SRR1039508	679
TSPAN6	SRR1039509	448
TSPAN6	SRR1039512	873
TSPAN6	SRR1039513	408
TSPAN6	SRR1039516	1138
TSPAN6	SRR1039517	1047





```
library(tidyverse)
anno <- read_tsv("annotation.txt")</pre>
anno_filtered <- anno %>%
     select(Run, dex, cell)
df_long <- df_long %>%
     inner_join(anno_filtered,
                by = join_by(sample == Run))
df_long %>%
     filter(gene == "IL6") %>%
     group_by(dex) %>%
     summarise(mean_expression = mean(count))
```

activating the tidyverse packages

reading in a tab separated .txt file, saving it in anno

piping *anno*select only columns of interest, here *Run*, *dex*, and *cell* 

takes the *df\_long* from the previous slides joins in the annotation created above observations are "sorted", where *sample* in *df\_long* is equivalent to *Run* from *anno\_filtered* 

take *df\_long*filter on only *IL6*group by dexa treatment
get the mean expression per group

tidyr for extensive data manipulation

```
A tibble: 8 x 3
                                                                                          Run
                                                                                                               dex
<chr>
library(tidyverse)
                                                                                                                                   N61311
                                                                                          SRR1039508
                                                                                                               untrt
                                                                                          SRR1039509
                                                                                                                                   N61311
                                                                                                               trt
anno <- read_tsv("annotation.txt")</pre>
                                                                                          SRR1039512
                                                                                                               untrt
                                                                                                                                   N052611
                                                                                          SRR1039513
                                                                                                                                   N052611
                                                                                                               trt
                                                                                          SRR1039516
                                                                                                                                   N080611
                                                                                                               untrt
anno_filtered <- anno %>%
                                                                                          SRR1039517
                                                                                                                                   N08061
                                                                                                               trt
                                                                                          SRR1039520
                                                                                                                                   N06101
                                                                                                               untrt
       select(Run, dex, cell)
                                                                                          SRR1039521
                                                                                                               trt
                                                                                                                                   N061011
                                                                                          8 rows
df_long <- df_long %>%
                                                                          A tibble: 6 x 5
       inner_join(anno_filtered,
                                                                                         sample
                       by = join_by(sample == Run)
                                                                          TSPAN6
                                                                          TSPAN6
                                                                                         SRR1039509
                                                                                                                                       N61311
                                                                          TSPAN6
                                                                                                                                       N052611
                                                                                         SRR1039512
                                                                          TSPAN6
                                                                                         SRR1039513
                                                                                                                                       N052611
                                                                          TSPAN6
                                                                          TSPAN6
                                                                                         SRR1039517
                                                                                                                    1047 trt
                                                                                                                                       N080611
df_long %>%
                                                                         6 rows
       filter(gene == "IL6") %>%
       group_by(dex) %>%
                                                                                   A tibble: 2 x 2
       summarise(mean_expression = mean(count))
```

dex

trt

untrt 2 rows mean expression

98.5 146.0



## tidyr for extensive data manipulation

```
df_wide <- df_long %>%
    pivot_wider(
        names_from = "gene",
        values_from = "count")
```

take the data from the previous slide in long format pivot wider

taking the new column names from the *gene* column taking the values for the new columns from the *count* column

Colombia	parameter and the second secon	200000	and the same of th	
gene	sample kohr>	count	cho-	cell i
TSPAN6	SRR1039508	679	untrt	N61311
TSPAN6	SRR1039509	448	trt	N61311
TSPAN6	SRR1039512	873	untrt	N052611
TSPAN6	SRR1039513	408	trt	N052611
TSPAN6	SRR1039516	1138	untrt	N080611
TSPAN6	SRR1039517	1047	trt	N080611
TSPAN6	SRR1039520	770	untrt	N061011
TSPAN6	SRR1039521	572	trt	N061011
TNMD	SRR1039508	0	untrt	N61311
TNMD				

A tibble: 8 × 53,566									
sample	dex	cell	TSPAN6	TNMD <dbl></dbl>	DPM1	SCYL3	Clorf112	FGR <dbi></dbi>	CFH ,
SRR1039508	untrt	N61311	679	0	467	260	60	0	3251
SRR1039509	trt	N61311	448	0	515	211	55	0	3679
SRR1039512	untrt	N052611	873	0	621	263	40	2	6177
SRR1039513	trt	N052611	408	0	365	164	35	0	4252
SRR1039516	untrt	N080611	1138	0	587	245	78	1	6721
SRR1039517	trt	N080611	1047	0	799	331	63	0	11027
SRR1039520	untrt	N061011	770	0	417	233	76	0	5176
SRR1039521	trt	N061011	572	0	508	229	60	0	7995

## stringr - text manipulation

package designed for manipulation of strings (text)



- we'll be mainly using 3 different functions:
  - str\_detect(string, pattern) → detect a certain pattern in a string
  - str\_replace(string, pattern, replacement) → replaces a certain pattern in a string
  - str\_remove(string, pattern) → removes a certain pattern in a string

this becomes a lot more powerful when working with regular expressions,
 <u>regex</u>

## stringr - str\_detect()



```
test_string <- "Hello, this is some writing"</pre>
str_detect(test_string, "Hello")
str_detect(test_string, "Howdy")
df_long %>%
     filter(str_detect(gene, "MT-")) %>%
     group_by(gene, dex) %>%
     summarise(mean_expression = mean(count))
df_long %>% filter(!str_detect(gene, "-AS"))
```

an example text bit

Detecting whether or not "Hello" is present in the string

Detecting whether or not "Howdy" is present in the string

starting with the long expression data from before filter to only genes containing "MT-" → mitochondrial group by gene and treatment generate a mean per group and gene

filter expression data to exclude antisense RNAs ("-AS")

## stringr - str detect()

```
test_string <- "Hello, this is some writing"</pre>
                                                                    [1] TRUE
                                                                    [1] FALSE
str_detect(test_string, "Hello")
str_detect(test_string, "Howdy")
df_long %>%
     filter(str_detect(gene, "MT-")) %>%
     group_by(gene, dex) %>%
     summarise(mean_expression = mean(count))
df_long %>% filter(str_detect(gene, "IL"))
df_long %>% filter(!str_detect(gene, "-AS"))
```

gene <chr></chr>	dex <chr></chr>	mean_count <dbl></dbl>
MT-CO3	trt	52225.25
MT-CO3	untrt	53137.25
MT-CYB	trt	61816.75
MT-CYB	untrt	56403.25
MT-ND1	trt	31134.75
MT-ND1	untrt	30542.50
MT-ND2	trt	32005.25
MT-ND2	untrt	31839.25
MT-ND3	trt	5399.75
MT-ND3	untrt	5685.00

## stringr - str\_replace()



the aneurysma survey data

take the data replace the AAA in diagnosis with BAA

expression data annotation

replace the "trt" in the dex column with "treated

Run	dex	cell
SRR1039508	untrt	N61311
SRR1039509	trt	N61311
SRR1039512	untrt	N052611
SRR1039513	trt	N052611
SRR1039516	untrt	N080611
SRR1039517	trt	N080611
SRR1039520	untrt	N061011
SRR1039521	trt	N061011

A tibble: 8 x 3		
Run	dex «chr»	cell
SRR1039508	untreated	N61311
SRR1039509	treated	N61311
SRR1039512	untreated	N052611
SRR1039513	treated	N052611
SRR1039516	untreated	N080611
SRR1039517	treated	N080611
SRR1039520	untreated	N061011
SRR1039521	treated	N061011
The second secon		

## gtsummary - a tool for summary tables

- package designed for summary tables
- high customizability
- ideal for a supplementary figure / table to give you an overview over your study cohort

Characteristic	$\mathbf{CTRL}$ $N = 300^{1}$	<b>AAA</b> $N = 300^{1}$	<b>TAA</b> N = 300 <sup>1</sup>	p-value
Abdominal diameter	2.00 (1.88, 2.11)	3.95 (3.44, 4.59)	1.98 (1.83, 2.11)	<0.001
Thoracic diameter	2.00 (1.84, 2.12)	2.02 (1.94, 2.09)	4.02 (3.79, 4.18)	<0.001
Age	62 (52, 71)	62 (53, 71)	62 (54, 71)	0.8
Male	148 (49%)	229 (76%)	231 (77%)	<0.001
Hypertension	67 (22%)	150 (50%)	129 (43%)	< 0.001
Coronary artery disease	25 (8.3%)	53 (18%)	31 (10%)	0.001
Artheriosclerosis	157 (52%)	91 (30%)	112 (37%)	< 0.001

Median (Q1, Q3); n (%)

<sup>2</sup> Kruskal-Wallis rank sum test; Pearson's Chi-squared test

library(gtsummary)

aa\_data %>%
 select(-bmi) %>%
 tbl\_summary()

Characteristic	$N = 900^{1}$	
diagnosis		
AAA	300 (33%)	
CTRL	300 (33%)	
TAA	300 (33%)	
abdominal_diameter	2.11 (1.94, 3.44)	
thoracic_diameter	2.10 (1.96, 3.79)	
age	62 (53, 71)	
male	608 (68%)	
hypertension	346 (38%)	
cad	109 (12%)	
artheriosclerosis	360 (40%)	
n (%); Median (Q1, Q3	)	



```
aa_data %>%
  select(-bmi) %>%
  tbl_summary(label = list(
    abdominal_diameter ~ "Abdominal diameter",
    thoracic_diameter ~ "Thoracic diameter",
    age ~ "Age",
    male ~ "Male",
    hypertension ~ "Hypertension",
    cad ~ "Coronary artery disease",
    artheriosclerosis ~ "Artheriosclerosis"))
```

Characteristic	N = 900 <sup>†</sup>	
diagnosis		
AAA	300 (33%)	
CTRL	300 (33%)	
TAA	300 (33%)	
Abdominal diameter	2.11 (1.94, 3.44)	
Thoracic diameter	2.10 (1.96, 3.79)	
Age	62 (53, 71)	
Male	608 (68%)	
Hypertension	346 (38%)	
Coronary artery disease	109 (12%)	
Artheriosclerosis	360 (40%)	
<sup>1</sup> n (%); Median (Q1, Q3)		



columns

```
atsummary 30 00
```

```
aa_data %>%
  select(-bmi) %>%
  tbl_summary(by = diagnosis,
    label = list(
    abdominal_diameter ~ "Abdominal diameter",
    thoracic_diameter ~ "Thoracic diameter",
    age ~ "Age",
    male ~ "Male",
    hypertension ~ "Hypertension",
    cad ~ "Coronary artery disease",
    artheriosclerosis ~ "Artheriosclerosis"))
```

pipe the aneurysm survey data deselect bmi get the table & split by diagnosis supply custom labels for the columns

Characteristic	<b>AAA</b> N = 300 <sup>†</sup>	CTRL $N = 300^{\circ}$	<b>TAA</b> N = 300 <sup>1</sup>
Abdominal diameter	3.95 (3.44, 4.59)	2.00 (1.88, 2.11)	1.98 (1.83, 2.11)
Thoracic diameter	2.02 (1.94, 2.09)	2.00 (1.84, 2.12)	4.02 (3.79, 4.18)
Age	62 (53, 71)	62 (52, 71)	62 (54, 71)
Male	229 (76%)	148 (49%)	231 (77%)
Hypertension	150 (50%)	67 (22%)	129 (43%)
Coronary artery disease	53 (18%)	25 (8.3%)	31 (10%)
Artheriosclerosis	91 (30%)	157 (52%)	112 (37%)
Median (Q1, Q3); n (%)			

```
aa data %>%
  select(-bmi) %>%
     mutate(diagnosis =
          fct_relevel(diagnosis, "CTRL")) %>%
  tbl_summary(by = diagnosis,
     label = list(
     abdominal_diameter ~ "Abdominal diameter",
     thoracic_diameter ~ "Thoracic diameter",
     age ~ "Age",
     male ~ "Male",
     hypertension ~ "Hypertension",
     cad ~ "Coronary artery disease",
     artheriosclerosis ~ "Artheriosclerosis"))
```



pipe the aneurysm survey data deselect bmi relevel using the forcats package (focussed on next session)

get the table & split by diagnosis supply custom labels for the columns

CTRL	AAA	TAA
$N = 300^{7}$	$N = 300^{7}$	$N = 300^{7}$
2.00 (1.88, 2.11)	3.95 (3.44, 4.59)	1.98 (1.83, 2.11)
2.00 (1.84, 2.12)	2.02 (1.94, 2.09)	4.02 (3.79, 4.18)
62 (52, 71)	62 (53, 71)	62 (54, 71)
148 (49%)	229 (76%)	231 (77%)
67 (22%)	150 (50%)	129 (43%)
25 (8.3%)	53 (18%)	31 (10%)
157 (52%)	91 (30%)	112 (37%)
	N = 300 <sup>†</sup> 2.00 (1.88, 2.11) 2.00 (1.84, 2.12) 62 (52, 71) 148 (49%) 67 (22%) 25 (8.3%)	N = 300 <sup>1</sup> N = 300 <sup>1</sup> 2.00 (1.88, 2.11) 3.95 (3.44, 4.59)  2.00 (1.84, 2.12) 2.02 (1.94, 2.09)  62 (52, 71) 62 (53, 71)  148 (49%) 229 (76%)  67 (22%) 150 (50%)  25 (8.3%) 53 (18%)

```
gtsumman est
```

```
aa data %>%
  select(-bmi) %>%
     mutate(diagnosis =
          fct_relevel(diagnosis, "CTRL")) %>%
  tbl_summary(by = diagnosis,
     label = list(
     abdominal_diameter ~ "Abdominal diameter",
     thoracic_diameter ~ "Thoracic diameter",
     age ~ "Age",
     male ~ "Male",
     hypertension ~ "Hypertension",
     cad ~ "Coronary artery disease",
     artheriosclerosis ~ "Artheriosclerosis"))%>%
  italisize_labels() %>%
  add_p()
```

pipe the aneurysm survey data deselect bmi relevel using the forcats package (focussed on next session) get the table & split by diagnosis

supply custom labels for the columns

Characteristic	N = 300 <sup>†</sup>	<b>AAA</b> N = 300 <sup>1</sup>	<b>TAA</b> N = 300 <sup>1</sup>	p-value <sup>2</sup>
Abdominal diameter	2.00 (1.88, 2.11)	3.95 (3.44, 4.59)	1.98 (1.83, 2.11)	<0.001
Thoracic diameter	2.00 (1.84, 2.12)	2.02 (1.94, 2.09)	4.02 (3.79, 4.18)	<0.001
Age	62 (52, 71)	62 (53, 71)	62 (54, 71)	0.8
Male	148 (49%)	229 (76%)	231 (77%)	<0.001
Hypertension	67 (22%)	150 (50%)	129 (43%)	<0.001
Coronary artery disease	25 (8.3%)	53 (18%)	31 (10%)	0.001
Artheriosclerosis	157 (52%)	91 (30%)	112 (37%)	<0.001

Median (Q1, Q3); n (%)

<sup>&</sup>lt;sup>2</sup> Kruskal-Wallis rank sum test; Pearson's Chi-squared test

## Summary

- Reading in data with readr
- data wrangling and manipulation with dplyr
- grouping and piping
- summary calculations
- string manipulation with stringr
- building summary tables using gtsummary

### Practise Practise

For practise purposes, I have compiled some questions in the github.

Please work through them and ask any questions you might encounter!

I'll be happy to answer questions and receive feedback!



## More practise questions!

#### Medium

M1: What is the minimal aortic diameter in the AAA condition?

M2: What is the mean abdominal diameter in the data set?

M3: What is the mean abdominal diameter by diagnosis? Considering only patients older than 60, how does this change?

M4: If you consider the median instead of mean and thoracic diameter instead of abdominal, what are the results?

### Hard

H1: Refer back to the github and read in the expression data set. Merge them in the same fashion as above.

H2: Consider the gene CXCL8. What is the mean expression in the data set? What is the mean expression per treatment? What is the mean expression by treatment and cell line? Which sample shows the highest expression of CXCL8?

H2a: CXCL8 is the gene name coding for the protein IL8. For your table, you want to replace the gene name with the protein name. Hint: use str\_replace() and mutate()

H3: Generate an overview table of the aneurysm survey data using gtsummary.

H4: Split the table by diagnosis.

H5: Subset your study data to only include patients over the age of 50 and with a BMI larger than 22.

