A quick tour of R

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The bare essentials

- Everything in R is an object with a name
- Things are nouns
  - Nouns in R are *data objects*, like scalars, matrices, data.frames/tibbles, strings, vectors
- Nouns are acted upon by verbs
  - Verbs in R are *functions*, like `mean(x)`, `nrow(d)`, `dim(d)`, `ggplot` and so on
- You can modify verbs with adverbs
  - Adverbs in R are *function options*, like `mean(x, na.rm=T)`, `geom_point(color='green')`

The bare essentials

- You have to name things to store them
  - This is done with the <- operator, e.g.
    - `mn <- mean(x, na.rm=T)` stores the result of the average
    - `my_theme <- function() theme_bw() + theme(axis.title=element_text(size=14))` stores the function, which you'll call as `my_theme()`

> You can see the objects you have created either by typing `ls()` in the console, or looking in the Environment pane
>
> Note, built-in objects don't show up in the Environment pane or using `ls()`

The bare essentials

There are three kinds of brackets in R

`[]` are used for extracting elements from arrays, matrices, data frames.

- `x[3]` is the 3rd element of an array `x`
- `d[1,3]` is the element in the 1st row and 3rd column of a matrix/data frame `d`
- `d[2,]` is the entire first **row** of a matrix/data frame `d`
- `d[,4]` is the entire 4th **column** of a matrix/data frame `d`

The bare essentials

There are three kinds of brackets in R

`()` are used for specifying arguments to functions

- `mean(x)` gives the mean of an array of numbers `x`
- `summary(d)` gives a summary representation of a data frame `d`

The bare essentials

There are three kinds of brackets in R

`{}` are used to contain groups of commands/statements

A conditional statement

```
if (age < 18){
   person <- 'Minor'
} else if (age > 65) {
  person <- 'Senior'
} else {
  person <- 'Adult'
}
```

A function definition

```
my_mean <- function(x, na.rm = T){
  if(na.rm){
    x <- x[!is.na(x)]
  }
  s <- sum(x)
  n <- length(x)
  mn <- s / n # There is a built-in function mean, sc
  return(mn)
}
```

Data types

A **scalar:**

- `29`
- `"cherry"`
- `TRUE`

Data types

A scalar:

- `29` : *numeric*
- `"cherry"`: *character*
- `TRUE`: *logical*

Data types

Vectors/Arrays

These are constructed using the `c()` function (for *concatenate*).

```
c(1,2,5,6,7,8)
```

```
#>  [1] 1 2 5 6 7 8
```

```
c('apple','berry','melon','citrus')
```

```
#>  [1] "apple"  "berry"  "melon"  "citrus"
```

> Vectors must all contain objects of the same type. Can't mix and match

Data types

Matrices (2-d arrays)

These are typically built from vectors

```
x <- c(1,2,4,5,6,7)
y <- 10:16  # Shortcut for c(10,11,12,13,14,15,16)
```

```
cbind(x, y) # Vectors as columns
```

```
#>       x  y
#>  [1,] 1 10
#>  [2,] 2 11
#>  [3,] 4 12
#>  [4,] 5 13
#>  [5,] 6 14
#>  [6,] 7 15
#>  [7,] 1 16
```

```
rbind(x, y) # Vectors as rows
```

```
#>    [,1] [,2] [,3] [,4] [,5] [,6] [,7]
#>  x    1    2    4    5    6    7    1
#>  y   10   11   12   13   14   15   16
```

Data types

Lists

Lists are basically buckets or containers. Each element of a list can be anything, even other lists

```
my_list <- list('a', c(2,3,5,6), head(ggplot2::mpg))
my_list
```

```
#> [[1]]
#> [1] "a"
#>
#> [[2]]
#> [1] 2 3 5 6
#>
#> [[3]]
#> # A tibble: 6 x 11
#>   manufacturer model displ  year   cyl trans  drv
#>   <chr>        <chr> <dbl> <int> <int> <chr>  <ch
#> 1 audi         a4      1.8  1999     4 auto(… f
#> 2 audi         a4      1.8  1999     4 manua… f
#> 3 audi         a4      2    2008     4 manua… f
#> 4 audi         a4      2    2008     4 auto(… f
#> 5 audi         a4      2.8  1999     6 auto(… f
#> 6 audi         a4      2.8  1999     6 manua… f
```

Data types

data.frame/tibble

This is the typical container for tabular data

- must be rectangular
- each column can be of a different type
- elements within each column have to be of the same type

Data types

data.frame/tibble

```
beaches <- rio::import('data/sydneybeaches3.csv') # use the import function from the package rio
class(beaches)
```

```
#>  [1] "data.frame"
```

```
dim(beaches)
```

```
#>  [1] 344  12
```

```
head(beaches)
```

```
#>          date year month day season rainfall temperature enterococci
#>  1 2013-01-02 2013     1   2      1      0.0        23.4         6.7
#>  2 2013-01-06 2013     1   6      1      0.0        30.3         2.0
#>  3 2013-01-12 2013     1  12      1      0.0        31.4        69.1
#>  4 2013-01-18 2013     1  18      1      0.0        46.4         9.0
#>  5 2013-01-24 2013     1  24      1      0.0        27.5        33.9
#>  6 2013-01-30 2013     1  30      1      0.6        26.6        26.5
#>    day_num month_num month_name season_name
#>  1       2         1    January      Summer
```

Data types

data.frame/tibble

```
library(tidyverse) # Activate the tidyverse package
beaches_t <- as_tibble(beaches)
class(beaches_t)
```

```
#>  [1] "tbl_df"     "tbl"        "data.frame"
```

```
beaches_t
```

```
#>  # A tibble: 344 x 12
#>     date   year month   day season rainfall temperature enterococci day_num
#>     <chr> <int> <int> <int>  <int>    <dbl>       <dbl>       <dbl>   <int>
#>   1 2013…  2013     1     2      1      0          23.4         6.7       2
#>   2 2013…  2013     1     6      1      0          30.3         2         6
#>   3 2013…  2013     1    12      1      0          31.4        69.1      12
#>   4 2013…  2013     1    18      1      0          46.4         9        18
#>   5 2013…  2013     1    24      1      0          27.5        33.9      24
#>   6 2013…  2013     1    30      1      0.6        26.6        26.5      30
#>   7 2013…  2013     2     5      1      0.1        25.7        66.9      36
#>   8 2013…  2013     2    11      1      8          22.2       118.       42
#>   9 2013…  2013     2    17      1     13.6        26.3        75        48
#>  10 2013…  2013     2    23      1      7.2        24.8       311.       54
#>  # … with 334 more rows, and 3 more variables: month_num <int>,
```

Data types

data.frame/tibble

Extracting columns from a data frame:

1. `beaches$temperature`
2. `beaches[,'temperature']`
3. `beaches[['temperature']]`
4. `beaches[,7]`
5. `beaches[[7]]`

Packages in R

R is a modular environment with some base functionality that is augmented by **packages** (think of them as modules)

- Packages can contain *functions* and *data*
- There are over 15K packages on CRAN, the Comprehensive R Archive Network
- There are over 1600 packages on Bioconductor, the main repository for bioinformatics resources
    - Analytic, Annotation, Experimental data and Workflow packages

Finding packages

1. CRAN Task views{target=_blank}
2. Bioconductor BiocViews{target=_blank}
3. GitHub (open source collaboration and version control environment)

Installing packages

From CRAN

```
install.packages("tidyverse")
```

From Bioconductor

```
install.packages("BiocManager") # do once
BioManager::install('limma')
```

From GitHub

```
install.packages('remotes') # do once
remotes::install_github("rstudio/rmarkdown") # usual
```

> GitHub often hosts development version of packages published on CRAN or Bioconductor
>
> Both CRAN and Bioconductor have stringent checks to make sure packages can run properly, with no obvious program flaws. There are typically no guarantees about analytic or theoretical correctness, but most packages have been crowd-validated and there are several reliable developer groups including RStudio

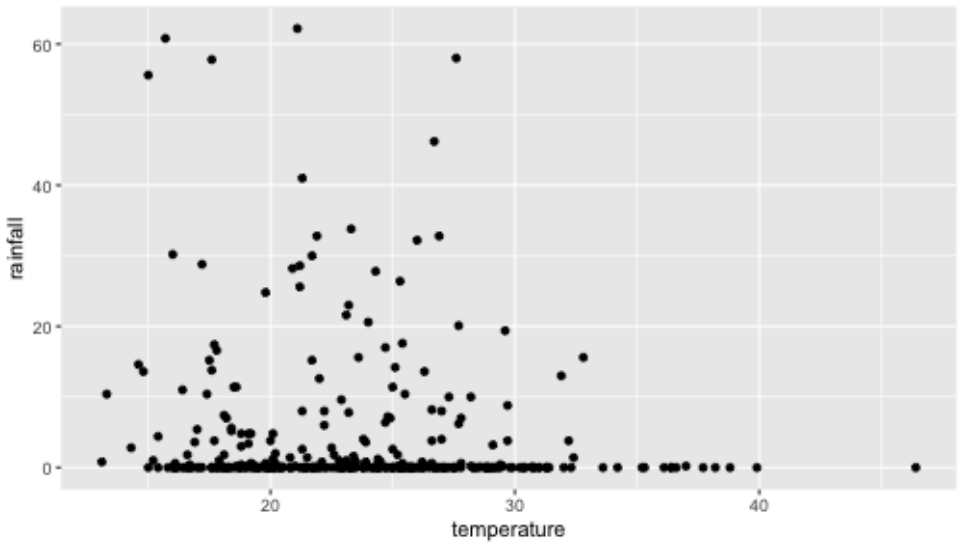
Using packages

You have to first "activate" the package in your current working session using the `library` function.

```
ggplot(beaches, aes(temperature, rainfall)) +
  geom_point()
```

```
#>  Error in ggplot(beaches, aes(temperature, rainfal
```

```
library(ggplot2) # or library(tidyverse)
ggplot(beaches, aes(temperature, rainfall)) +
  geom_point()
```



Tidying data using the tidyverse

What is the "Tidyverse"?

The tidyverse is an opinionated collection of R packages designed for data science. All packages share an underlying design philosophy, grammar, and data structures

What is the "Tidyverse"?

A set of R packages that:

- help make data more computer-friendly
- while making your code more human-friendly

- Most of these packages are (co-)written by Dr. Hadley Wickham, who has rockstar status in the R world
- They are supported by the company RStudio

Tidying data

Tidy data

Tidy datasets are all alike,
but every messy data is messy in its own way

Tidy data

Tidy data is a **computer-friendly** format based on the following characteristics:

- Each row is one observation
- Each column is one variable
- Each set of observational unit forms a table

All other forms of data can be considered **messy data**.

Let us count the ways

There are many ways data can be messy. An incomplete list....

- Column headers are values, not variables
- Multiple variables are stored in a single column
- Variables are stored in both rows and columns
- Multiple types of observational units are saved in the same table
- A single observational unit is stored in multiple tables

Ways to have messy (i.e. not tidy) data

1. Column headers contain values

Country	< $10K	$10-20K	$20-50K	$50-100K	> $100K
India	40	25	25	9	1
USA	20	20	20	30	10

Ways to have messy (i.e. not tidy) data

Column headers contain values

Country	Income	Percentage
India	< $10K	40
USA	< $10K	20

This is a case of reshaping or melting

Ways to have messy (i.e. not tidy) data

Multiple variables in one column

Country	Year	M_0-14	F_0-14	M_ 15-60	F_15-60	M_60+	F_60+
UK	2010						
UK	2011						

Separating columns into different variables

Country	Year	Gender	Age	Count

Tidying data

The typical steps are

- Transforming data from wide to tall (*gather*) and from tall to wide (*spread*)
- Separating columns into different columns
- Putting columns together into new variables

Cleaning data

Some actions on data

- Creating new variables (*mutate*)
- Choose some columns (*select*)
- Selecting rows based on some criteria (*filter*)
- Sort data based on some variables (*arrange*)

Example data

```
head(mtcars, 3)
```

```
#>                mpg cyl disp  hp drat    wt  qsec vs am gear carb
#>  Mazda RX4     21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
#>  Mazda RX4 Wag 21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
#>  Datsun 710    22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
```

- Car names are in an attribute of the data.frame called `rownames`. So it's not in a column
- We might want to convert fuel economy to metric
- We might just want to look at the relationship between displacement and fuel economy based on number of cylinders

Example data (link)

```
link <- 'https://dl.dropboxusercontent.com/s/pqavhcckshqxtjm/brca.csv'
brca_data <- rio::import(link)
```

	id	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean	compactness_mean	concavity_mean	concave.points_mean	sy
1	842302	M	17.990	10.38	122.80	1001.0	0.11840	0.27760	0.300100	0.147100	
2	842517	M	20.570	17.77	132.90	1326.0	0.08474	0.07864	0.086900	0.070170	
3	84300903	M	19.690	21.25	130.00	1203.0	0.10960	0.15990	0.197400	0.127900	
4	84348301	M	11.420	20.38	77.58	386.1	0.14250	0.28390	0.241400	0.105200	
5	84358402	M	20.290	14.34	135.10	1297.0	0.10030	0.13280	0.198000	0.104300	
6	843786	M	12.450	15.70	82.57	477.1	0.12780	0.17000	0.157800	0.080890	
7	844359	M	18.250	19.98	119.60	1040.0	0.09463	0.10900	0.112700	0.074000	

The `tidyverse` package

The `tidyverse` package is a meta-package that installs a set of packages that are useful for data cleaning, data tidying and data munging (manipulating data to get a computationally "attractive" dataset)

The `tidyverse` package

```
# install.packages('tidyverse')
library(tidyverse)
```

> You can specify a function from a particular package as `dplyr::filter`. Note there are two colons there

Core `tidyverse` packages

Package	Description
ggplot2	Data visualization
tibble	data.frame on steroids
tidyr	Data tidying (today)
readr	Reading text files (CSV)
purrr	Applying functions to data iteratively
dplyr	Data cleaning and munging (today)
stringr	String (character) manipulation
forcats	Manipulating categorical variables

Additional `tidyverse` packages

Package	Description
readxl	Read Excel files
haven	Read SAS, SPSS, Stata files
lubridate	Deal with dates and times
magrittr	Provides the pipe operator %>%
glue	Makes pasting text and data easier

Additional useful packages

Package	Description
broom	Turns the results of models or analysis into tidy datasets
fs	Allows directory and file manipulation in OS-agnostic manner
here	Allows robust specification of directory structure in a Project

Pipes

Pipes

Pipes (denoted %>%, spoken as "then") are to analytic pipelines as + is to `ggplot` layers

```
mpg1 <- mpg %>% mutate(id=1:n()) %>% select(id, year, trans, cty, hwy)
mpg_metric <- mpg1 %>%
  mutate_at(vars(cty, hwy), function(x) {x * 1.6/3.8})
```

Original data

id	year	trans	cty	hwy
1	1999	auto(l5)	18	29
2	1999	manual(m5)	21	29
3	2008	manual(m6)	20	31
4	2008	auto(av)	21	30
5	1999	auto(l5)	16	26

Transformed data

id	year	trans	cty	hwy
1	1999	auto(l5)	7.578947	12.21053
2	1999	manual(m5)	8.842105	12.21053
3	2008	manual(m6)	8.421053	13.05263
4	2008	auto(av)	8.842105	12.63158
5	1999	auto(l5)	6.736842	10.94737

> Note I'm assigning a name to the transformed data. Otherwise it'll be lost

Verbs to use in pipes

The verbs in `tidyverse` are specially useful in pipes

Verb	Functionality
mutate	Transform a column with some function
select	Select some columns in the data
arrange	Order the data frame by values of a column(s)
filter	Keep only rows that meet some data criterion
group_by	Group by levels of a variable
gather	Transform a wide dataset to a long dataset
spread	Transform a long dataset to a wide dataset
separate	Separate one column into several columns
unite	Concatenate several columns into 1 column

Pipes almost always start with a data.frame/tibble object, and then "pipes" that data through different transformations (functions)

At each %>%, the results of the previous step are used as input for the next step.

A complicated example

Grab the raw data

```
url <- "http://varianceexplained.org/files/Brauer2008_DataSet1.tds"
raw_data <- read_delim(url, delim='\t')
head(raw_data)
```

```
#>  # A tibble: 6 x 40
#>    GID   YORF  NAME  GWEIGHT G0.05  G0.1 G0.15  G0.2 G0.25  G0.3 N0.05  N0.1
#>    <chr> <chr> <chr>   <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
#>  1 GENE… A_06… SFB2…       1 -0.24 -0.13 -0.21 -0.15 -0.05 -0.05  0.2   0.24
#>  2 GENE… A_06… "   …       1  0.28  0.13 -0.4  -0.48 -0.11  0.17  0.31  0
#>  3 GENE… A_06… QRI7…       1 -0.02 -0.27 -0.27 -0.02  0.24  0.25  0.23  0.06
#>  4 GENE… A_06… CFT2…       1 -0.33 -0.41 -0.24 -0.03 -0.03  0     0.2  -0.25
#>  5 GENE… A_06… SSO2…       1  0.05  0.02  0.4   0.34 -0.13 -0.14 -0.35 -0.09
#>  6 GENE… A_06… PSP2…       1 -0.69 -0.03  0.23  0.2   0    -0.27  0.17 -0.4
#>  # … with 28 more variables: N0.15 <dbl>, N0.2 <dbl>, N0.25 <dbl>,
#>  #   N0.3 <dbl>, P0.05 <dbl>, P0.1 <dbl>, P0.15 <dbl>, P0.2 <dbl>,
#>  #   P0.25 <dbl>, P0.3 <dbl>, S0.05 <dbl>, S0.1 <dbl>, S0.15 <dbl>,
#>  #   S0.2 <dbl>, S0.25 <dbl>, S0.3 <dbl>, L0.05 <dbl>, L0.1 <dbl>,
#>  #   L0.15 <dbl>, L0.2 <dbl>, L0.25 <dbl>, L0.3 <dbl>, U0.05 <dbl>,
#>  #   U0.1 <dbl>, U0.15 <dbl>, U0.2 <dbl>, U0.25 <dbl>, U0.3 <dbl>
```

Look at the annotation data

```
head(raw_data$NAME)
```

```
#>  [1] "SFB2       || ER to Golgi transport || molecular function unknown || YNL049C || 1082129"
#>  [2] "          || biological process unknown || molecular function unknown || YNL095C || 1086222"
#>  [3] "QRI7       || proteolysis and peptidolysis || metalloendopeptidase activity || YDL104C || 1085955"
#>  [4] "CFT2       || mRNA polyadenylylation* || RNA binding || YLR115W || 1081958"
#>  [5] "SSO2       || vesicle fusion* || t-SNARE activity || YMR183C || 1081214"
#>  [6] "PSP2       || biological process unknown || molecular function unknown || YML017W || 1083036"
```

Separate annotation into columns

```
cleaned_data <- raw_data %>%
  separate(NAME, c("name", "BP", "MF", "systematic_name", "number"),
           sep = "\\|\\|")
head(cleaned_data)
```

```
#>  # A tibble: 6 x 44
#>    GID   YORF  name  BP    MF    systematic_name number GWEIGHT G0.05  G0.1
#>    <chr> <chr> <chr> <chr> <chr> <chr>            <chr>    <dbl> <dbl> <dbl>
#>  1 GENE… A_06… "SFB… " ER… " mo… " YNL049C "      " 108…       1 -0.24 -0.13
#>  2 GENE… A_06… "   … " bi… " mo… " YNL095C "      " 108…       1  0.28  0.13
#>  3 GENE… A_06… "QRI… " pr… " me… " YDL104C "      " 108…       1 -0.02 -0.27
#>  4 GENE… A_06… "CFT… " mR… " RN… " YLR115W "      " 108…       1 -0.33 -0.41
#>  5 GENE… A_06… "SSO… " ve… " t-… " YMR183C "      " 108…       1  0.05  0.02
#>  6 GENE… A_06… "PSP… " bi… " mo… " YML017W "      " 108…       1 -0.69 -0.03
#>  # … with 34 more variables: G0.15 <dbl>, G0.2 <dbl>, G0.25 <dbl>,
#>  #   G0.3 <dbl>, N0.05 <dbl>, N0.1 <dbl>, N0.15 <dbl>, N0.2 <dbl>,
#>  #   N0.25 <dbl>, N0.3 <dbl>, P0.05 <dbl>, P0.1 <dbl>, P0.15 <dbl>,
#>  #   P0.2 <dbl>, P0.25 <dbl>, P0.3 <dbl>, S0.05 <dbl>, S0.1 <dbl>,
#>  #   S0.15 <dbl>, S0.2 <dbl>, S0.25 <dbl>, S0.3 <dbl>, L0.05 <dbl>,
#>  #   L0.1 <dbl>, L0.15 <dbl>, L0.2 <dbl>, L0.25 <dbl>, L0.3 <dbl>,
#>  #   U0.05 <dbl>, U0.1 <dbl>, U0.15 <dbl>, U0.2 <dbl>, U0.25 <dbl>,
#>  #   U0.3 <dbl>
```

Get rid of padding in annotation

```
cleaned_data <- raw_data %>%
  separate(NAME, c("name", "BP", "MF", "systematic_name", "number"),
           sep = "\\|\\|") %>%
  mutate_at(vars(name:systematic_name), funs(stringr::str_trim))
head(cleaned_data)
```

```
#>  # A tibble: 6 x 44
#>    GID   YORF  name  BP    MF    systematic_name number GWEIGHT G0.05  G0.1
#>    <chr> <chr> <chr> <chr> <chr> <chr>           <chr>    <dbl> <dbl> <dbl>
#>  1 GENE… A_06… SFB2  ER t… mole… YNL049C         " 108…       1 -0.24 -0.13
#>  2 GENE… A_06… ""    biol… mole… YNL095C         " 108…       1  0.28  0.13
#>  3 GENE… A_06… QRI7  prot… meta… YDL104C         " 108…       1 -0.02 -0.27
#>  4 GENE… A_06… CFT2  mRNA… RNA … YLR115W         " 108…       1 -0.33 -0.41
#>  5 GENE… A_06… SSO2  vesi… t-SN… YMR183C         " 108…       1  0.05  0.02
#>  6 GENE… A_06… PSP2  biol… mole… YML017W         " 108…       1 -0.69 -0.03
#>  # … with 34 more variables: G0.15 <dbl>, G0.2 <dbl>, G0.25 <dbl>,
#>  #   G0.3 <dbl>, N0.05 <dbl>, N0.1 <dbl>, N0.15 <dbl>, N0.2 <dbl>,
#>  #   N0.25 <dbl>, N0.3 <dbl>, P0.05 <dbl>, P0.1 <dbl>, P0.15 <dbl>,
#>  #   P0.2 <dbl>, P0.25 <dbl>, P0.3 <dbl>, S0.05 <dbl>, S0.1 <dbl>,
#>  #   S0.15 <dbl>, S0.2 <dbl>, S0.25 <dbl>, S0.3 <dbl>, L0.05 <dbl>,
#>  #   L0.1 <dbl>, L0.15 <dbl>, L0.2 <dbl>, L0.25 <dbl>, L0.3 <dbl>,
#>  #   U0.05 <dbl>, U0.1 <dbl>, U0.15 <dbl>, U0.2 <dbl>, U0.25 <dbl>,
#>  #   U0.3 <dbl>
```

Get rid of some columns

```
cleaned_data <- raw_data %>%
  separate(NAME, c("name", "BP", "MF", "systematic_name", "number"),
           sep = "\\|\\|") %>%
  mutate_at(vars(name:systematic_name), funs(stringr::str_trim)) %>%
  select(-number, -GID, -YORF, -GWEIGHT)
head(cleaned_data)
```

```
#>  # A tibble: 6 x 40
#>    name  BP    MF    systematic_name G0.05  G0.1 G0.15  G0.2 G0.25  G0.3
#>    <chr> <chr> <chr> <chr>           <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
#>  1 SFB2  ER t… mole… YNL049C         -0.24 -0.13 -0.21 -0.15 -0.05 -0.05
#>  2 ""    biol… mole… YNL095C          0.28  0.13 -0.4  -0.48 -0.11  0.17
#>  3 QRI7  prot… meta… YDL104C         -0.02 -0.27 -0.27 -0.02  0.24  0.25
#>  4 CFT2  mRNA… RNA … YLR115W         -0.33 -0.41 -0.24 -0.03 -0.03  0
#>  5 SSO2  vesi… t-SN… YMR183C          0.05  0.02  0.4   0.34 -0.13 -0.14
#>  6 PSP2  biol… mole… YML017W         -0.69 -0.03  0.23  0.2   0    -0.27
#>  # … with 30 more variables: N0.05 <dbl>, N0.1 <dbl>, N0.15 <dbl>,
#>  #   N0.2 <dbl>, N0.25 <dbl>, N0.3 <dbl>, P0.05 <dbl>, P0.1 <dbl>,
#>  #   P0.15 <dbl>, P0.2 <dbl>, P0.25 <dbl>, P0.3 <dbl>, S0.05 <dbl>,
#>  #   S0.1 <dbl>, S0.15 <dbl>, S0.2 <dbl>, S0.25 <dbl>, S0.3 <dbl>,
#>  #   L0.05 <dbl>, L0.1 <dbl>, L0.15 <dbl>, L0.2 <dbl>, L0.25 <dbl>,
#>  #   L0.3 <dbl>, U0.05 <dbl>, U0.1 <dbl>, U0.15 <dbl>, U0.2 <dbl>,
#>  #   U0.25 <dbl>, U0.3 <dbl>
```

Make data tidy

```
cleaned_data <- raw_data %>%
  separate(NAME, c("name", "BP", "MF", "systematic_name", "number"),
           sep = "\\|\\|") %>%
  mutate_at(vars(name:systematic_name), funs(stringr::str_trim)) %>%
  select(-number, -GID, -YORF, -GWEIGHT) %>%
  tidyr::gather(sample, expression, G0.05:U0.3)
head(cleaned_data)
```

```
#>  # A tibble: 6 x 6
#>    name  BP               MF               systematic_name sample expression
#>    <chr> <chr>            <chr>            <chr>           <chr>       <dbl>
#>  1 SFB2  ER to Golgi tra… molecular funct… YNL049C         G0.05       -0.24
#>  2 ""    biological proc… molecular funct… YNL095C         G0.05        0.28
#>  3 QRI7  proteolysis and… metalloendopept… YDL104C         G0.05       -0.02
#>  4 CFT2  mRNA polyadenyl… RNA binding      YLR115W         G0.05       -0.33
#>  5 SSO2  vesicle fusion*  t-SNARE activity YMR183C         G0.05        0.05
#>  6 PSP2  biological proc… molecular funct… YML017W         G0.05       -0.69
```

Split columns

```
cleaned_data <- raw_data %>%
  separate(NAME, c("name", "BP", "MF", "systematic_name", "number"),
           sep = "\\|\\|") %>%
  mutate_at(vars(name:systematic_name), funs(stringr::str_trim)) %>%
  select(-number, -GID, -YORF, -GWEIGHT) %>%
  tidyr::gather(sample, expression, G0.05:U0.3) %>%
  separate(sample, c("nutrient", "rate"), sep=1, convert = TRUE)
head(cleaned_data)
```

```
#>  # A tibble: 6 x 7
#>    name  BP           MF           systematic_name nutrient  rate expression
#>    <chr> <chr>        <chr>        <chr>           <chr>    <dbl>      <dbl>
#>  1 SFB2  ER to Golgi… molecular f… YNL049C         G         0.05      -0.24
#>  2 ""    biological … molecular f… YNL095C         G         0.05       0.28
#>  3 QRI7  proteolysis… metalloendo… YDL104C         G         0.05      -0.02
#>  4 CFT2  mRNA polyad… RNA binding  YLR115W         G         0.05      -0.33
#>  5 SSO2  vesicle fus… t-SNARE act… YMR183C         G         0.05       0.05
#>  6 PSP2  biological … molecular f… YML017W         G         0.05      -0.69
```

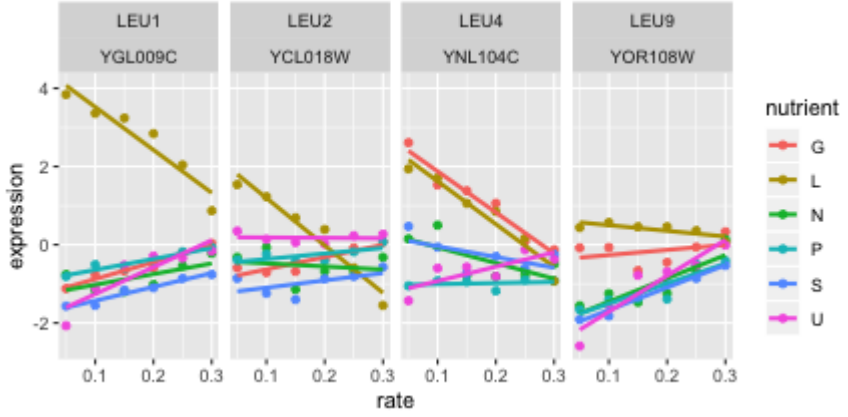
Get rid of rows with missing expression or name

```
cleaned_data <- raw_data %>%
  separate(NAME, c("name", "BP", "MF", "systematic_name", "number"),
           sep = "\\|\\|") %>%
  mutate_at(vars(name:systematic_name), funs(stringr::str_trim)) %>%
  select(-number, -GID, -YORF, -GWEIGHT) %>%
  tidyr::gather(sample, expression, G0.05:U0.3) %>%
  separate(sample, c("nutrient", "rate"), sep=1, convert = TRUE) %>%
  filter(!is.na(expression), systematic_name != '')
head(cleaned_data)
```

```
#>  # A tibble: 6 x 7
#>    name  BP           MF           systematic_name nutrient  rate expression
#>    <chr> <chr>        <chr>        <chr>           <chr>    <dbl>      <dbl>
#>  1 SFB2  ER to Golgi… molecular f… YNL049C         G         0.05      -0.24
#>  2 ""    biological … molecular f… YNL095C         G         0.05       0.28
#>  3 QRI7  proteolysis… metalloendo… YDL104C         G         0.05      -0.02
#>  4 CFT2  mRNA polyad… RNA binding  YLR115W         G         0.05      -0.33
#>  5 SSO2  vesicle fus… t-SNARE act… YMR183C         G         0.05       0.05
#>  6 PSP2  biological … molecular f… YML017W         G         0.05      -0.69
```

Visualize

```
cleaned_data %>%
  filter(BP == "leucine biosynthesis") %>%
  ggplot(aes(rate, expression, color = nutrient)) +
  geom_point() +
  geom_smooth(method = "lm", se = FALSE) +
  facet_wrap(~name + systematic_name, nrow=1) +
  theme(legend.position='right')
```



Modeling and the broom package

Representing model relationships

In R, there is a particularly convenient way to express models, where you have

- one dependent variable
- one or more independent variables, with possible transformations and interactions

```
y ~ x1 + x2 + x1:x2 + I(x3^2) + x4*x5
```

`y` depends on ...

- `x1` and `x2` linearly
- the interaction of `x1` and `x2` (represented as `x1:x2`)
- the square of `x3` (the `I()` notation ensures that the `^` symbol is interpreted correctly)
- `x4`, `x5` and their interaction (same as `x4 + x5 + x4:x5`)

Representing model relationships

```
y ~ x1 + x2 + x1:x2 + I(x3^2) + x4*x5
```

This interpretation holds for the vast majority of statistical models in R

- For decision trees and random forests and neural networks, don't add interactions or transformations, since the model will try to figure those out on their own

Our first model

```
library(survival)
data(pbc)
myLinearModel <- lm(chol ~ bili, data = pbc)
```

Note that everything in R is an **object**, so you can store a model in a variable name.

This statement runs the model and stored the fitted model in `myLinearModel`

R does not interpret the model, evaluate the adequacy or appropriateness of the model, or comment on whether looking at the relationship between cholesterol and bilirubin makes any kind of sense.

Our first model

```
myLinearModel
```

```
#>
#>  Call:
#>  lm(formula = chol ~ bili, data = pbc)
#>
#>  Coefficients:
#>  (Intercept)         bili
#>       303.20        20.24
```

> Not very informative, is it?

Our first model

```
summary(myLinearModel)
```

```
#>
#>  Call:
#>  lm(formula = chol ~ bili, data = pbc)
#>
#>  Residuals:
#>      Min       1Q   Median       3Q      Max
#>  -565.39  -89.90  -35.36   44.92 1285.33
#>
#>  Coefficients:
#>              Estimate Std. Error t value Pr(>|t|)
#>  (Intercept)  303.204     15.601  19.435  < 2e-16 ***
#>  bili          20.240      2.785   7.267 3.63e-12 ***
#>  ---
#>  Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
#>
#>  Residual standard error: 213.2 on 282 degrees of freedom
#>    (134 observations deleted due to missingness)
#>  Multiple R-squared:  0.1577,    Adjusted R-squared:  0.1547
#>  F-statistic:  52.8 on 1 and 282 DF,  p-value: 3.628e-12
```

> A little better

Our first model

```
broom::tidy(myLinearModel)
```

```
#>  # A tibble: 2 x 5
#>    term        estimate std.error statistic  p.value
#>    <chr>          <dbl>     <dbl>     <dbl>    <dbl>
#>  1 (Intercept)    303.      15.6      19.4  5.65e-54
#>  2 bili            20.2      2.79      7.27 3.63e-12
```

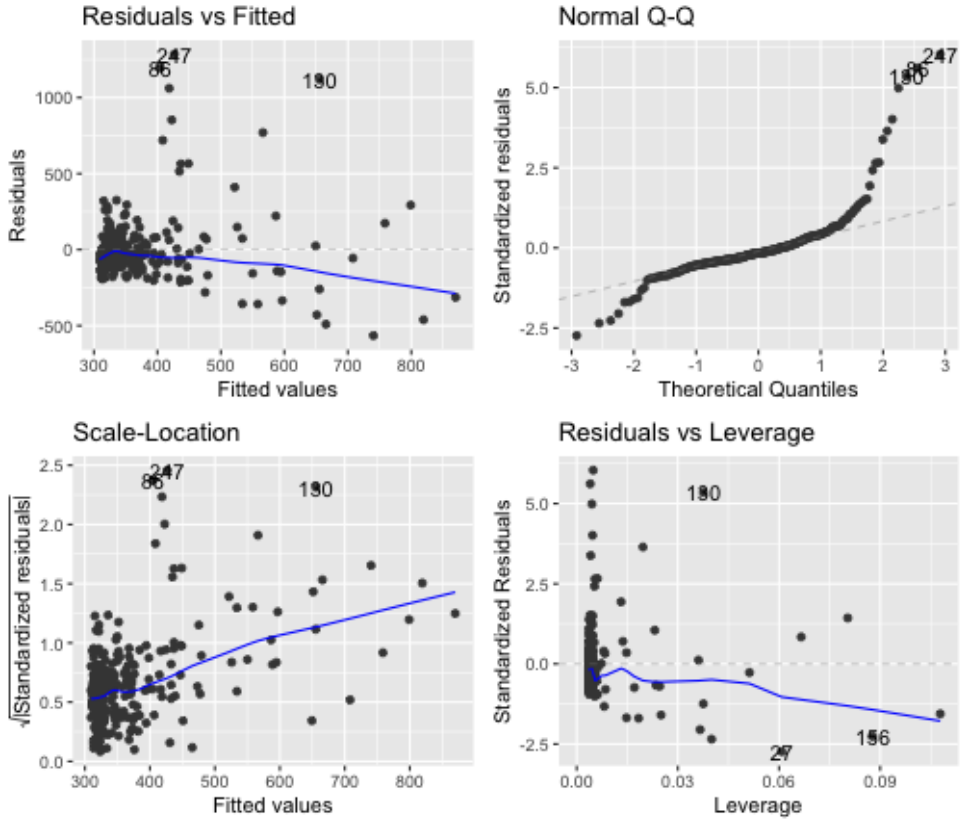
```
broom::glance(myLinearModel)
```

```
#>  # A tibble: 1 x 11
#>    r.squared adj.r.squared sigma statistic  p.value    df logLik   AIC   BIC
#>        <dbl>         <dbl> <dbl>     <dbl>    <dbl> <int>  <dbl> <dbl> <dbl>
#>  1     0.158         0.155  213.      52.8 3.63e-12     2 -1925. 3856. 3867.
#>  # … with 2 more variables: deviance <dbl>, df.residual <int>
```

Our first model

We do need some sense as to how well this model fit the data

```
# install.packages('ggfortify')
library(ggfortify)
autoplot(myLinearModel)
```



Displaying model results

Let's start with this model:

```
myModel <- lm(log10(enterococci) ~ rainfall + temperature + season_name + factor(year), data = beaches)
broom::tidy(myModel)
```

```
#>  # A tibble: 11 x 5
#>     term              estimate std.error statistic  p.value
#>     <chr>                <dbl>     <dbl>     <dbl>    <dbl>
#>   1 (Intercept)        1.23      0.208       5.92  8.39e- 9
#>   2 rainfall           0.0284    0.00296     9.58  2.72e-19
#>   3 temperature       -0.00830   0.00769    -1.08  2.81e- 1
#>   4 season_nameSpring -0.325     0.0840     -3.87  1.31e- 4
#>   5 season_nameSummer  0.0862    0.0909      0.948 3.44e- 1
#>   6 season_nameWinter -0.332     0.0889     -3.74  2.22e- 4
#>   7 factor(year)2014   0.0498    0.102       0.486 6.27e- 1
#>   8 factor(year)2015   0.0807    0.100       0.804 4.22e- 1
#>   9 factor(year)2016   0.0815    0.0975      0.836 4.04e- 1
#>  10 factor(year)2017  -0.0676    0.0972     -0.696 4.87e- 1
#>  11 factor(year)2018   0.0440    0.107       0.411 6.81e- 1
```

Displaying model results

Let's start with this model:

```
plt_data <- broom::tidy(myModel)
plt_data <- plt_data %>% filter(term != '(Intercept)') %>%
  mutate(term = str_replace(term, 'season_name',''))
plt_data
```

```
#>  # A tibble: 10 x 5
#>     term              estimate std.error statistic  p.value
#>     <chr>                <dbl>     <dbl>     <dbl>    <dbl>
#>   1 rainfall           0.0284    0.00296     9.58  2.72e-19
#>   2 temperature       -0.00830   0.00769    -1.08  2.81e- 1
#>   3 Spring            -0.325     0.0840     -3.87  1.31e- 4
#>   4 Summer             0.0862    0.0909      0.948 3.44e- 1
#>   5 Winter            -0.332     0.0889     -3.74  2.22e- 4
#>   6 factor(year)2014   0.0498    0.102       0.486 6.27e- 1
#>   7 factor(year)2015   0.0807    0.100       0.804 4.22e- 1
#>   8 factor(year)2016   0.0815    0.0975      0.836 4.04e- 1
#>   9 factor(year)2017  -0.0676    0.0972     -0.696 4.87e- 1
#>  10 factor(year)2018   0.0440    0.107       0.411 6.81e- 1
```

Displaying model results

Let's start with this model:

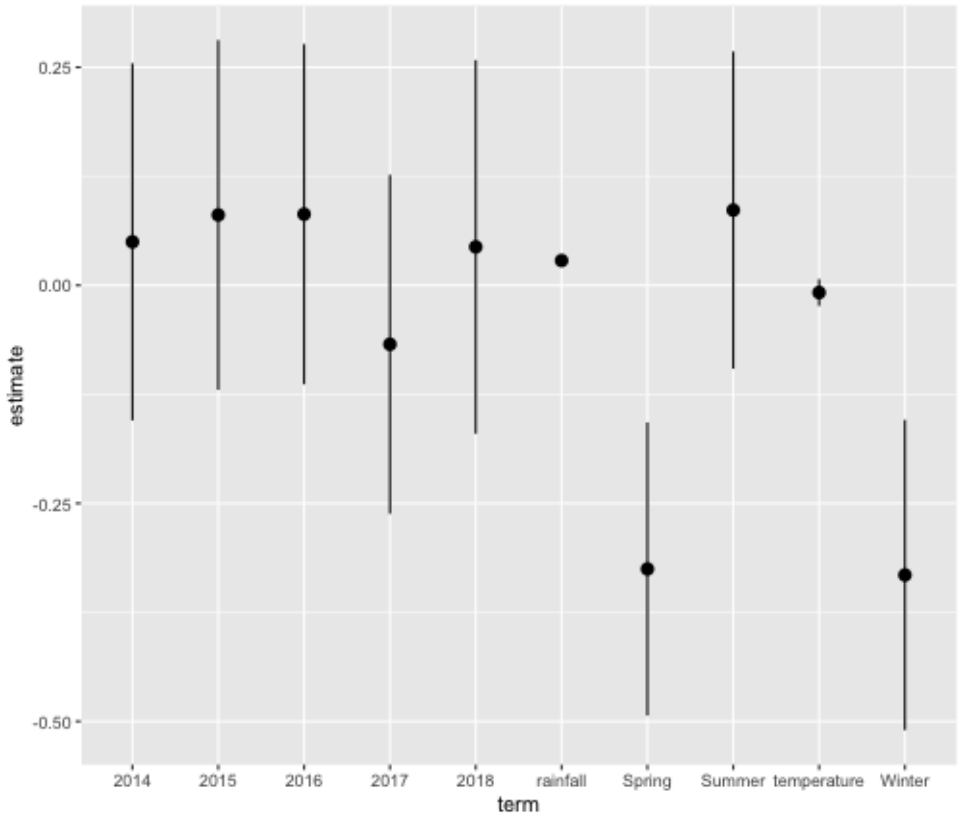
```
plt_data <- broom::tidy(myModel)
plt_data <- plt_data %>% filter(term != '(Intercept)') %>%
  mutate(term = str_replace(term, 'season_name','')) %>%
  mutate(term = str_replace(term, 'factor\\(year\\)','')) # Brackets are "escaped" using \\
plt_data
```

```
#>  # A tibble: 10 x 5
#>    term        estimate std.error statistic  p.value
#>    <chr>          <dbl>     <dbl>     <dbl>    <dbl>
#>  1 rainfall     0.0284    0.00296     9.58  2.72e-19
#>  2 temperature -0.00830   0.00769    -1.08  2.81e- 1
#>  3 Spring      -0.325     0.0840     -3.87  1.31e- 4
#>  4 Summer       0.0862    0.0909      0.948 3.44e- 1
#>  5 Winter      -0.332     0.0889     -3.74  2.22e- 4
#>  6 2014         0.0498    0.102       0.486 6.27e- 1
#>  7 2015         0.0807    0.100       0.804 4.22e- 1
#>  8 2016         0.0815    0.0975      0.836 4.04e- 1
#>  9 2017        -0.0676    0.0972     -0.696 4.87e- 1
#> 10 2018         0.0440    0.107       0.411 6.81e- 1
```

Displaying model results

Let's start with this model:

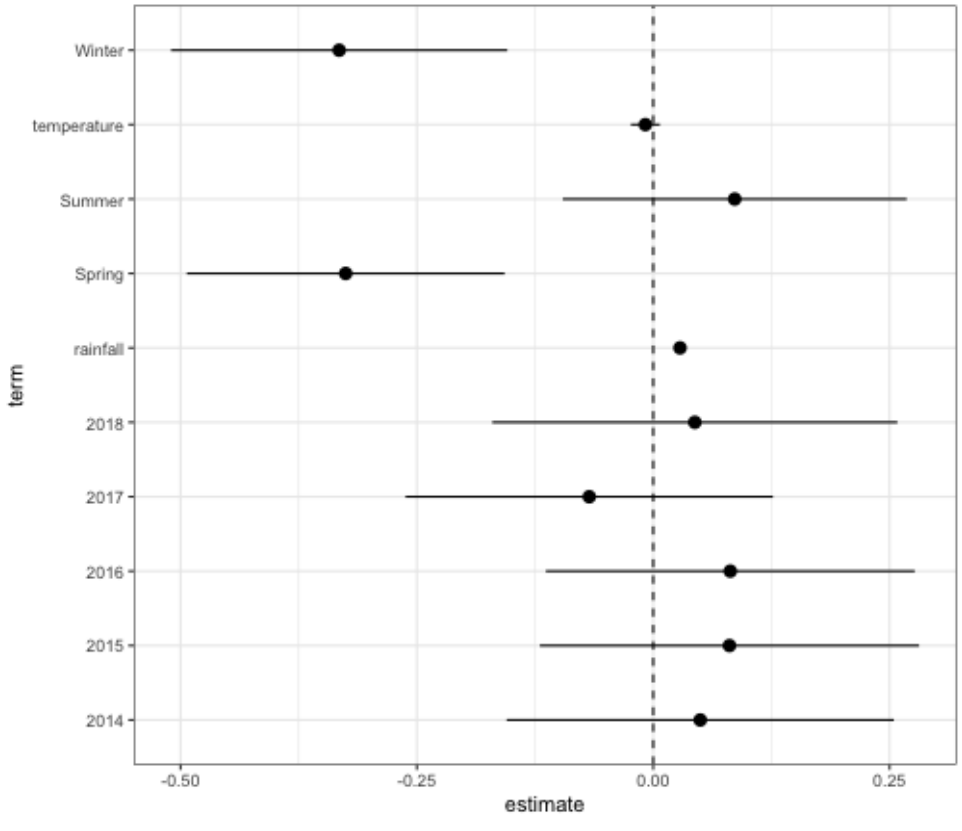
```
plt_data <- broom::tidy(myModel)
plt_data %>% filter(term != '(Intercept)') %>%
  mutate(term = str_replace(term, 'season_name',''))
  mutate(term = str_replace(term, 'factor\\(year\\)',
  ggplot(aes(x = term, y = estimate,
             ymin = estimate - 2 * std.error,
             ymax = estimate + 2 * std.error))+
    geom_pointrange()
```



Displaying model results

Let's start with this model:

```
plt_data <- broom::tidy(myModel)
plt_data %>% filter(term != '(Intercept)') %>%
  mutate(term = str_replace(term, 'season_name',''))
  mutate(term = str_replace(term, 'factor\\(year\\)',
  ggplot(aes(x = term, y = estimate,
             ymin = estimate - 2 * std.error,
             ymax = estimate + 2 * std.error))+
    geom_pointrange() +
    geom_hline(yintercept = 0, linetype=2) +
    theme_bw() +
    coord_flip()
```

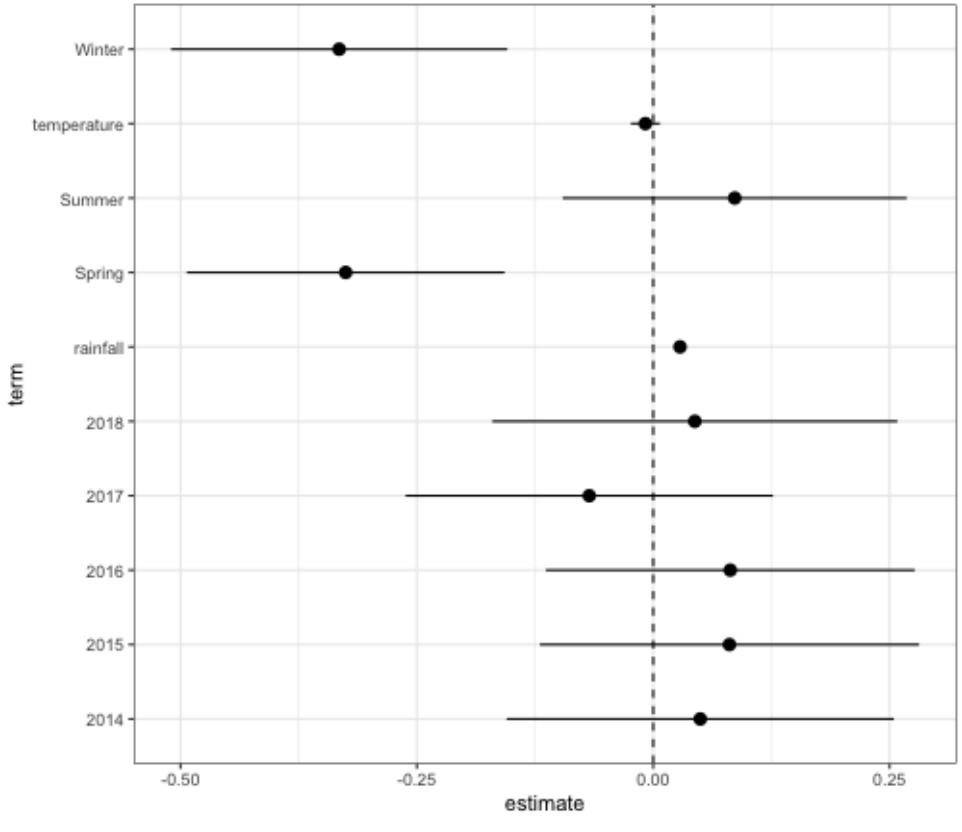


Displaying model results

Let's start with this model:

```
plt_data <- broom::tidy(myModel)
plt_data %>% filter(term != '(Intercept)') %>%
  mutate(term = str_replace(term, 'season_name',''))
  mutate(term = str_replace(term, 'factor\\(year\\)',
  ggplot(aes(x = term, y = estimate,
             ymin = estimate - 2 * std.error,
             ymax = estimate + 2 * std.error))+
    geom_pointrange() +
    geom_hline(yintercept = 0, linetype=2) +
    theme_bw() +
    coord_flip()

ggsave('results.png') # ggsave knows format from file
```



You can also save the graph from the RStudio Plots pane, but coding it using `ggsave` is more reproducible

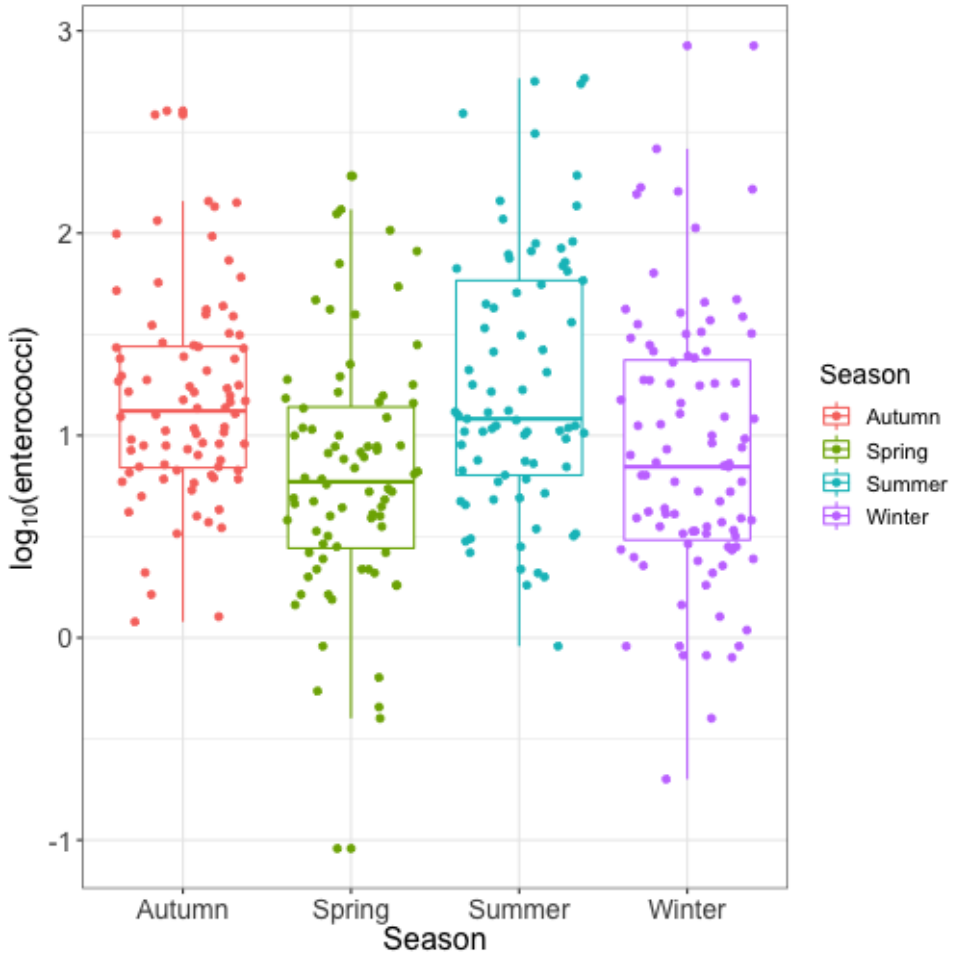
If you need to get a high-definition TIFF, your best bet is to save your graph as a PDF and then convert

Showing group differences ("Figure 1")

The package `ggpubr`, which extends `ggplot2`, makes this very easy. It provides the function `stat_compare_means`

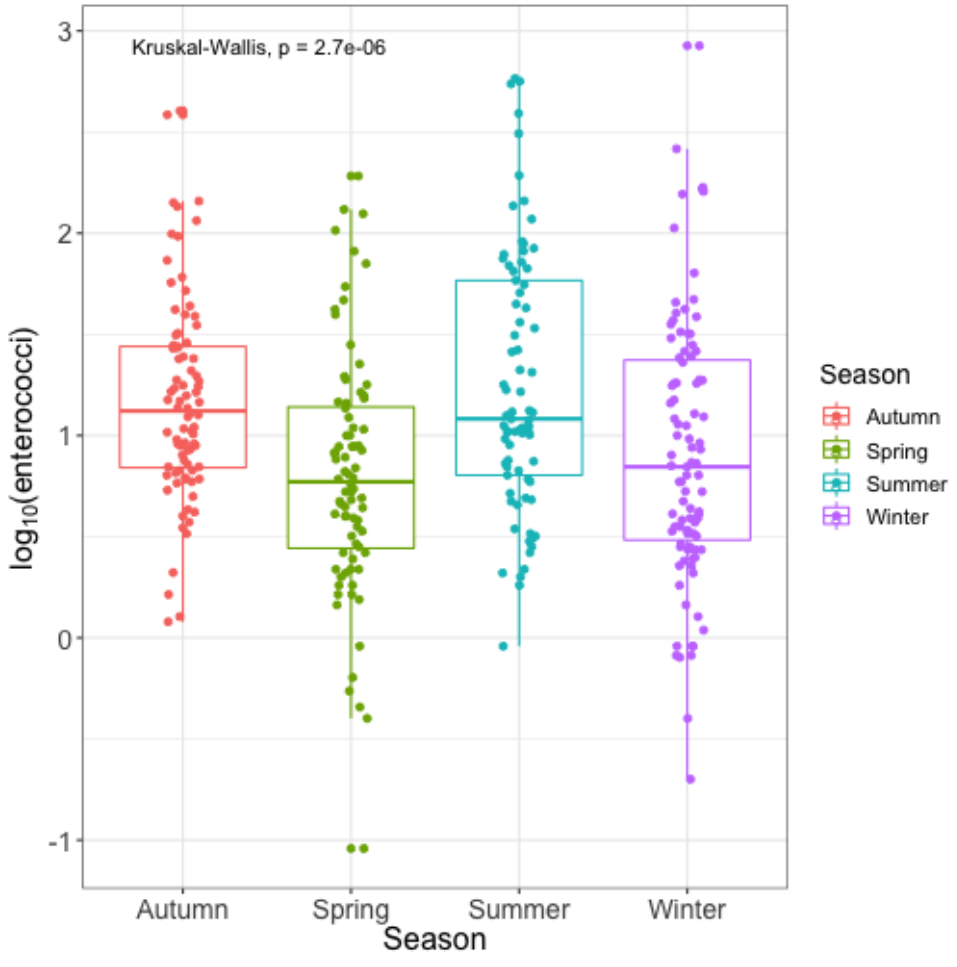
Showing group differences ("Figure 1")

```
library(ggpubr)
theme_viz <- function(){
  theme_bw() +
    theme(axis.title = element_text(size=16),
          axis.text = element_text(size=14),
          text = element_text(size = 14))
}
ggplot(
  data=beaches,
  mapping= aes(x = season_name, y = log10(enterococci
  geom_boxplot()+geom_jitter()+
  labs(x = 'Season', y = expression(paste('log'['10']
  theme_viz()
```



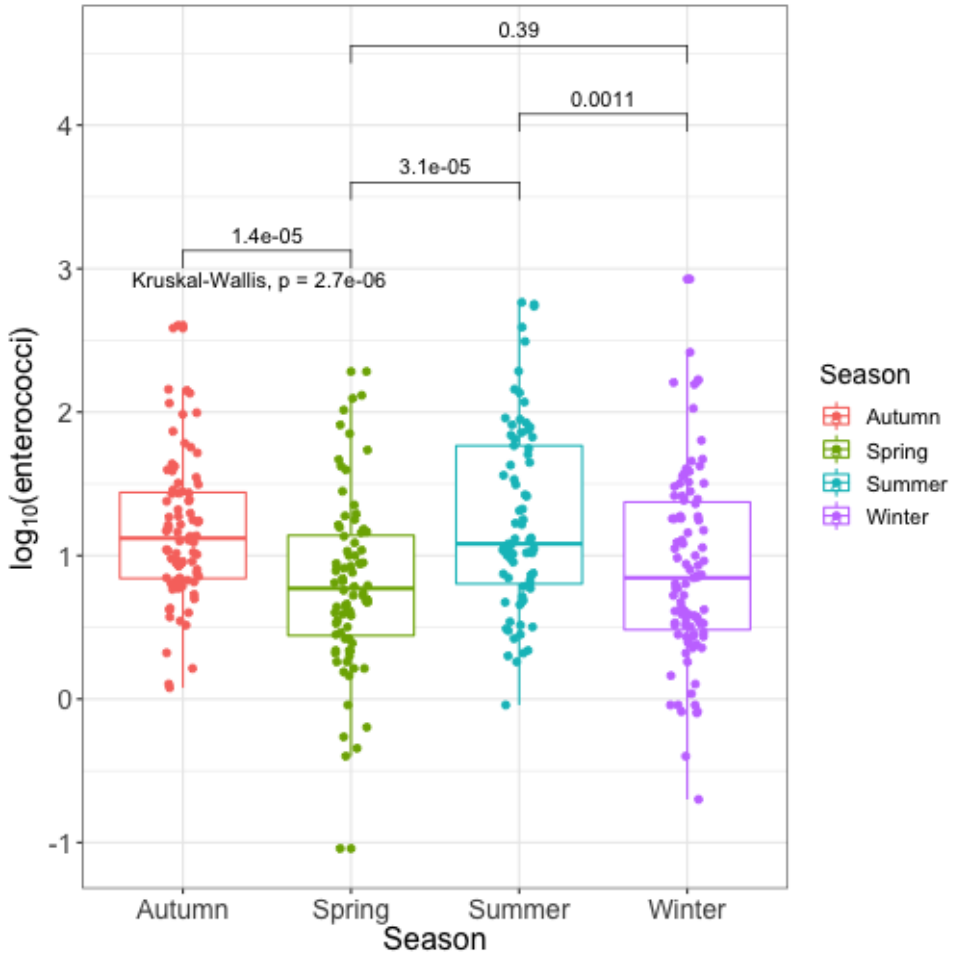
Showing group differences ("Figure 1")

```
library(ggpubr)
plt <- ggplot(
  data=beaches,
  mapping= aes(x = season_name, y = log10(enterococci
  geom_boxplot() +
  geom_jitter(width=0.1) +
  labs(x = 'Season', y = expression(paste('log'['10']
  theme_viz()
my_comparisons <- list(c('Autumn','Spring'),
                       c('Spring','Summer'),
                       c('Summer','Winter'),
                       c('Spring','Winter'))
plt + stat_compare_means()
```



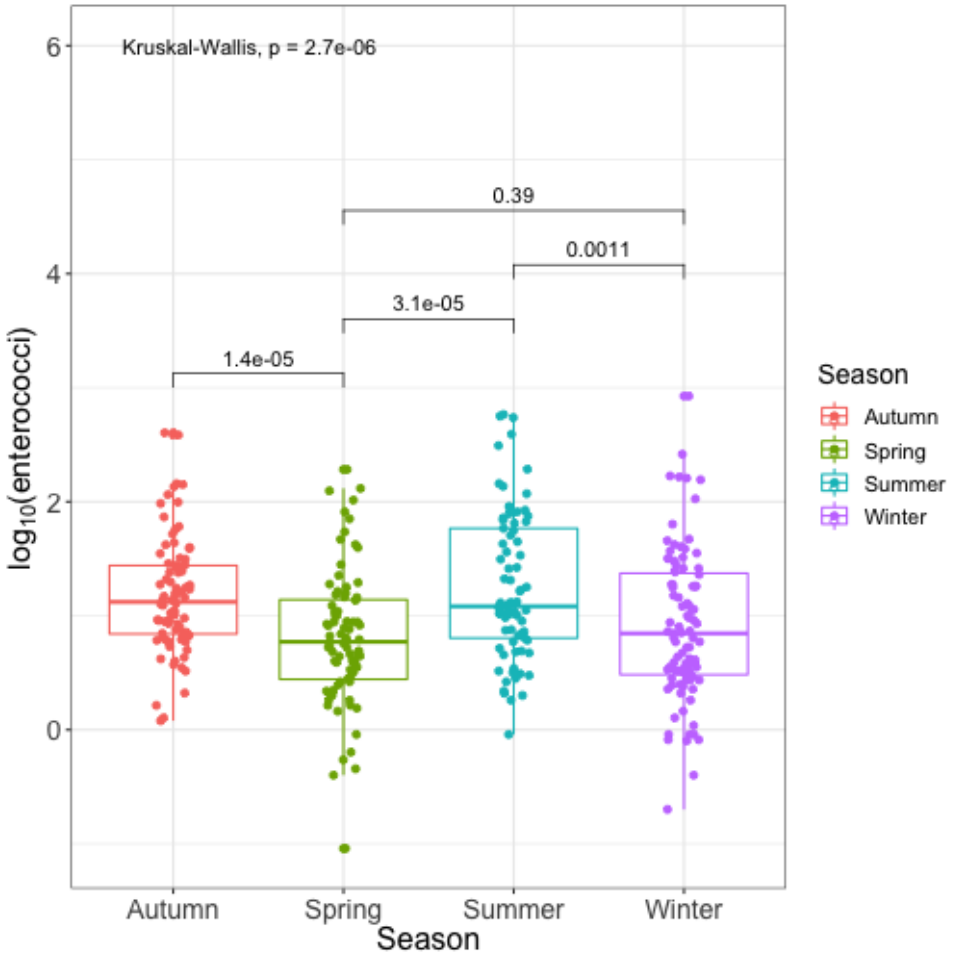
Showing group differences ("Figure 1")

```
library(ggpubr)
plt <- ggplot(
  data=beaches,
  mapping= aes(x = season_name, y = log10(enterococci
  geom_boxplot() +
  geom_jitter(width=0.1)+
    labs(x = 'Season', y = expression(paste('log'['10
         color='Season') +
  theme_viz()
my_comparisons <- list(c('Autumn','Spring'),
                       c('Spring','Summer'),
                       c('Summer','Winter'),
                       c('Spring','Winter'))
plt + stat_compare_means() +
  stat_compare_means(comparisons = my_comparisons)
```



Showing group differences ("Figure 1")

```
library(ggpubr)
plt <- ggplot(
  data=beaches,
  mapping= aes(x = season_name, y = log10(enterococci
  geom_boxplot() +
  geom_jitter(width=0.1)+
  labs(x = 'Season', y = expression(paste('log'['10']
  theme_viz()
my_comparisons <- list(c('Autumn','Spring'),
                       c('Spring','Summer'),
                       c('Summer','Winter'),
                       c('Spring','Winter'))
plt + stat_compare_means(label.y = 6) +
  stat_compare_means(comparisons = my_comparisons)
```



Manipulating data for plotting

We would like to get density plots of all the variables

```
dat_spine <- rio::import('data/Dataset_spine.csv', ch
head(dat_spine)
```

```
#>    Pelvic.incidence Pelvic.tilt Lumbar.lordosis.an
#>  1         63.02782   22.552586              39.60
#>  2         39.05695   10.060991              25.01
#>  3         68.83202   22.218482              50.09
#>  4         69.29701   24.652878              44.31
#>  5         49.71286    9.652075              28.31
#>  6         40.25020   13.921907              25.12
#>    Pelvic.radius Degree.spondylolisthesis Pelvic.s
#>  1      98.67292                -0.254400    0.744
#>  2     114.40543                 4.564259    0.415
#>  3     105.98514                -3.530317    0.474
#>  4     101.86850                11.211523    0.369
#>  5     108.16872                 7.918501    0.543
#>  6     130.32787                 2.230652    0.789
#>    Thoracic.slope Cervical.tilt Sacrum.angle Scoli
#>  1        14.5386       15.30468   -28.658501
#>  2        17.5323       16.78486   -25.530607
#>  3        17.4861       16.65897   -29.031888
#>  4        12.7074       11.42447   -30.470246
#>  5        15.9546        8.87237   -16.378376
#>  6        12.0036       10.40462    -1.512209
```

Facets only work by grouping on a variable. Here we have data in several columns

Manipulating data for plotting

We would like to get density plots of all the variables.

```
dat_spine %>%
  tidyr::gather(variable, value, everything())
```

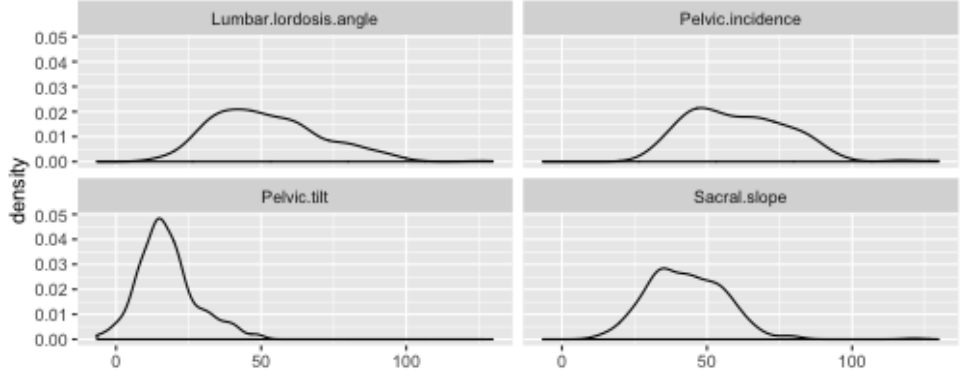
```
#>                      variable       value
#>  1           Pelvic.incidence   63.0278175
#>  2           Pelvic.incidence  39.05695098
#>  3           Pelvic.incidence  68.83202098
#>  4           Pelvic.incidence  69.29700807
#>  5           Pelvic.incidence  49.71285934
#>  6           Pelvic.incidence  40.25019968
#>  7           Pelvic.incidence  53.43292815
#>  8           Pelvic.incidence  45.36675362
#>  9           Pelvic.incidence  43.79019026
#>  10          Pelvic.incidence  36.68635286
#>  11          Pelvic.incidence  49.70660953
#>  12          Pelvic.incidence  31.23238734
#>  13          Pelvic.incidence  48.91555137
#>  14          Pelvic.incidence   53.5721702
#>  15          Pelvic.incidence  57.30022656
#>  16          Pelvic.incidence  44.31890674
#>  17          Pelvic.incidence  63.83498162
#>  18          Pelvic.incidence  31.27601184
#>  19          Pelvic.incidence  38.69791243
#>  20          Pelvic.incidence  41.72996308
```

The `gather` function turns this wide dataset to a long dataset, stacking all the variables on top of each other

Manipulating data for plotting

We would like to get density plots of all the variables.

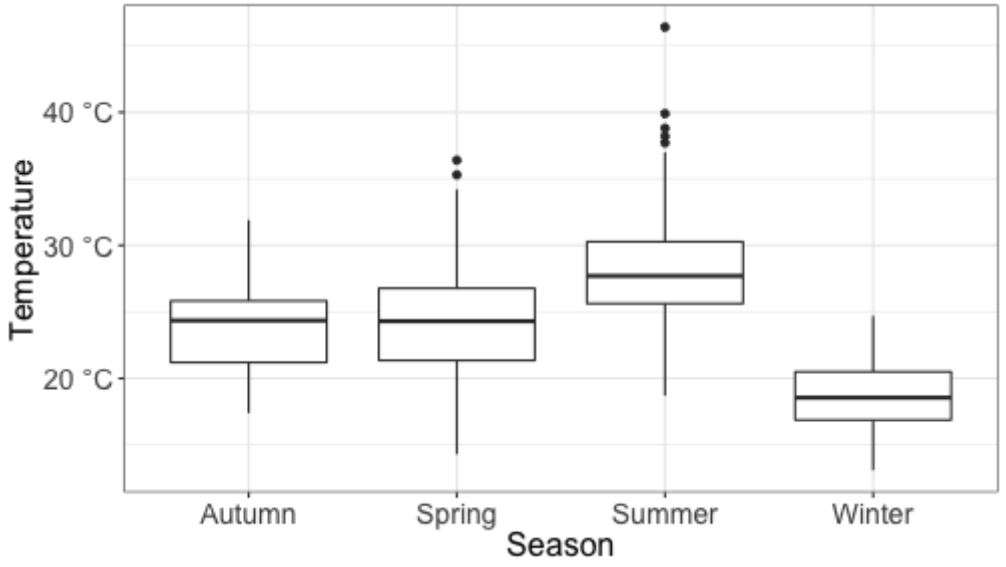
```
dat_spine %>%
  select(Pelvic.incidence:Sacral.slope) %>%
  tidyr::gather(variable, value) %>%
  ggplot(aes(x = value)) +
  geom_density() +
  facet_wrap(~variable) +
  labs(x = '')
```



This is one of my most used tricks for getting facetted plots from wide data

Re-ordering factors

```
beaches %>%
  ggplot(aes(x = season_name, y = temperature)) +
  geom_boxplot() +
  scale_y_continuous(labels = scales::unit_format(unit = "\u00B0C")) +
  labs(x = 'Season', y = 'Temperature') +
  theme_bw() +
  theme(axis.title = element_text(size = 16),
        axis.text = element_text(size = 14))
```



Re-ordering factors

```
beaches %>%
  mutate(season_name = fct_relevel(season_name, 'Autumn','Winter','Spring','Summer')) %>%
  ggplot(aes(x = season_name, y = temperature)) +
  geom_boxplot() +
  scale_y_continuous(labels = scales::unit_format(unit = "\u00B0C")) +
  labs(x = 'Season', y = 'Temperature') +
  theme_bw() +
  theme(axis.title = element_text(size = 16),
        axis.text = element_text(size = 14))
```