# R-eproducible workflows

1-day workshop
Morning overview





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#### Disclaimer

- Hadley Wickham and David Robinson are the go-to resources for most of the content in this session



**HADLEY WICKHAM** 

TEACHING CODE PERSONAL

I also teach in person workshops from time-to-time; see the RStudio workshops page for more details.

#### CODE

Most of my work is in the form of open source R code, which you can find on my github. You can roughly divide my work into three categories: tools for data science, tools for data import, and software engineering tools.

#### **DATA SCIENCE**

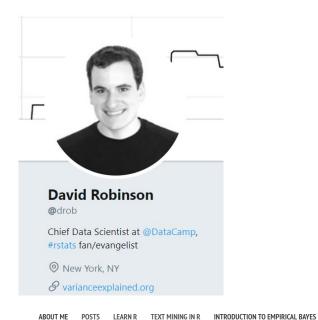
- ggplot2 for visualising data.
- dplyr for manipulating data.
- tidyr for tidying data.
- stringr for working with strings.
- lubridate for working with date/times.

#### **DATA IMPORT**

- readr for reading .csv and fwf files.
- readxl for reading .xls and .xlsx files.
- haven for SAS, SPSS, and Stata files.
- httr for talking to web APIs. • rvest for scraping websites.
- xml2 for importing XML files.

#### SOFTWARE ENGINEERING

- devtools for general package development.
- roxygen2 for in-line documentation.
- testthat for unit testing



VARIANCE EXPLAINED

**David Robinson** 

Chief Data Scientist at DataCamp, works in R and

Python

■ Email

☑ Twitter

Github

Stack Overflow

DataCamp. For more about me, see here.

This is the homepage and blog of David Robinson, Chief Data Scientist at

A live screencast of an exploratory data analysis from the Tidy Tuesday series. This one explores college major and income data from 538.

Who wrote the anti-Trump New York Times op-ed? Using tidytext to find September 06, 2018

October 16, 2018

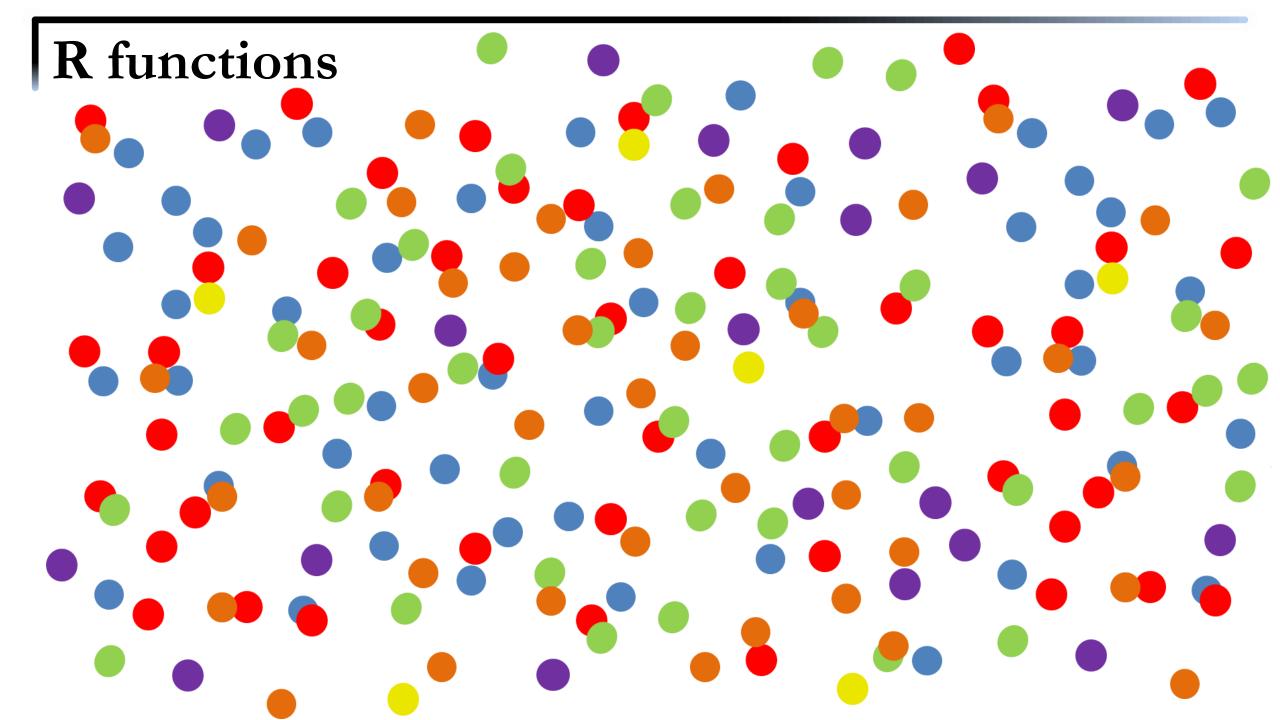
An analysis of an anonymous op-ed in the New York Times, using document similarity metrics to match it to Twitter accounts.

May 10, 2018

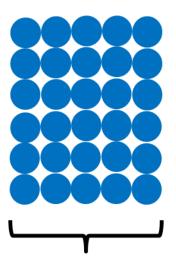
Introducing an analogy to 'technical debt' for data scientists.

**Recent Posts** 

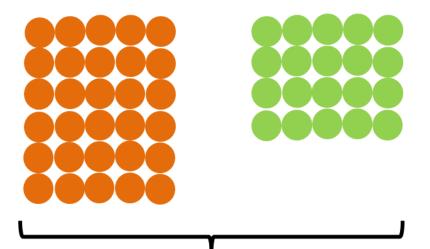
Exploring college major and income: a live data analysis in R



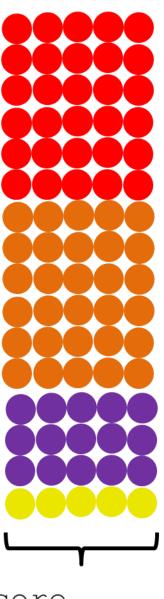
# R packages



Base R: Comes preloaded

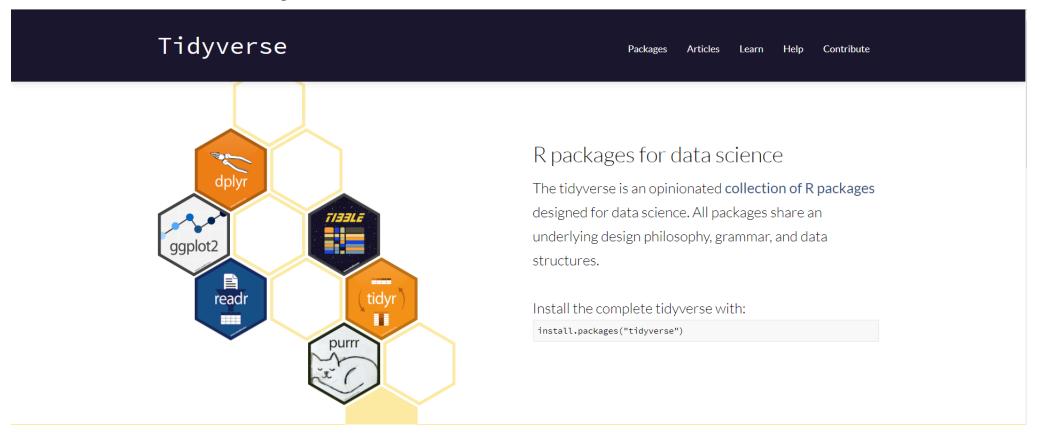


Other packages:
Install once
Update regularly
Load each session



core
tidyverse

# What is the tidyverse?



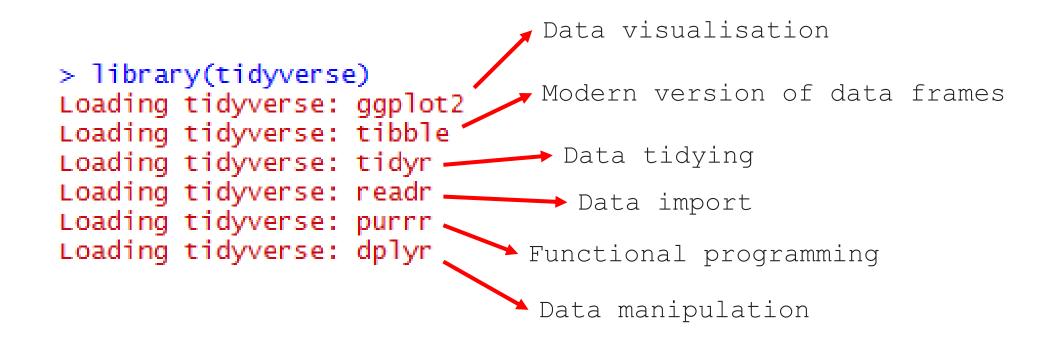
- Joined up collection of packages for data analysis
  - Consistent functions
  - Uses (tidy) data
  - Supports end-to-end workflows

### What is the tidyverse?

```
> install.packages(c("broom", "cli2", "crayon",
"dbplyr", "dplyr", "forcats", "ggplot2", "haven",
"hms", "httr", "jsonlite", "lubridate",
"magrittr", "modelr", "pillar", "purrr", "readr",
"readxl", "reprex", "rlang", "rstudioapi",
"rvest", "stringr", "tibble", "tidyr", "xml2")
```

> install.packages("tidyverse")

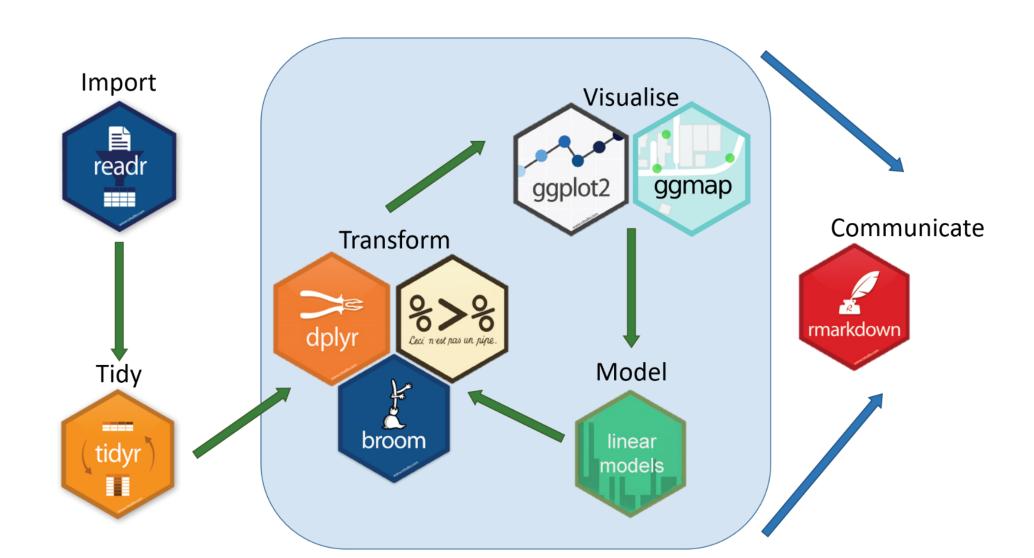
# The tidyverse Oct 2017



### The tidyverse Oct 2018

### Putting the pieces together

- Data analysis in a tidyverse nutshell



#### Tidyverse works best with tidy data

- Each variable forms a column
- Each observation forms a row

#### Problems with Brauer et al., data...

Column headers contain values

Multiple variables are stored in one column

```
e.g. column "NAME" contains values such as;
SFB2 || ER to Golgi transport || molecular function unknown || YNL049C || 1082129
```

These need to be split up

- G0.05 letter identifies a compound
  - number is the concentration of that compound

#### Code structure v1

```
separated_gene <- separate(raw_gene, NAME, c("name", "BP", "MF", "systematic_name", "number"), sep = "\\|\\|")
```

```
separated_gene
                          - the new tibble you will create
                          - the assign operator
<-
                          - the function you are calling on
separate

    the tibble to be used

(raw_gene,
                          - the column to be altered
NAME,
c("name", "BP", "MF", "systematic_name", "number"),
                          - new columns IDs for the new columns
```

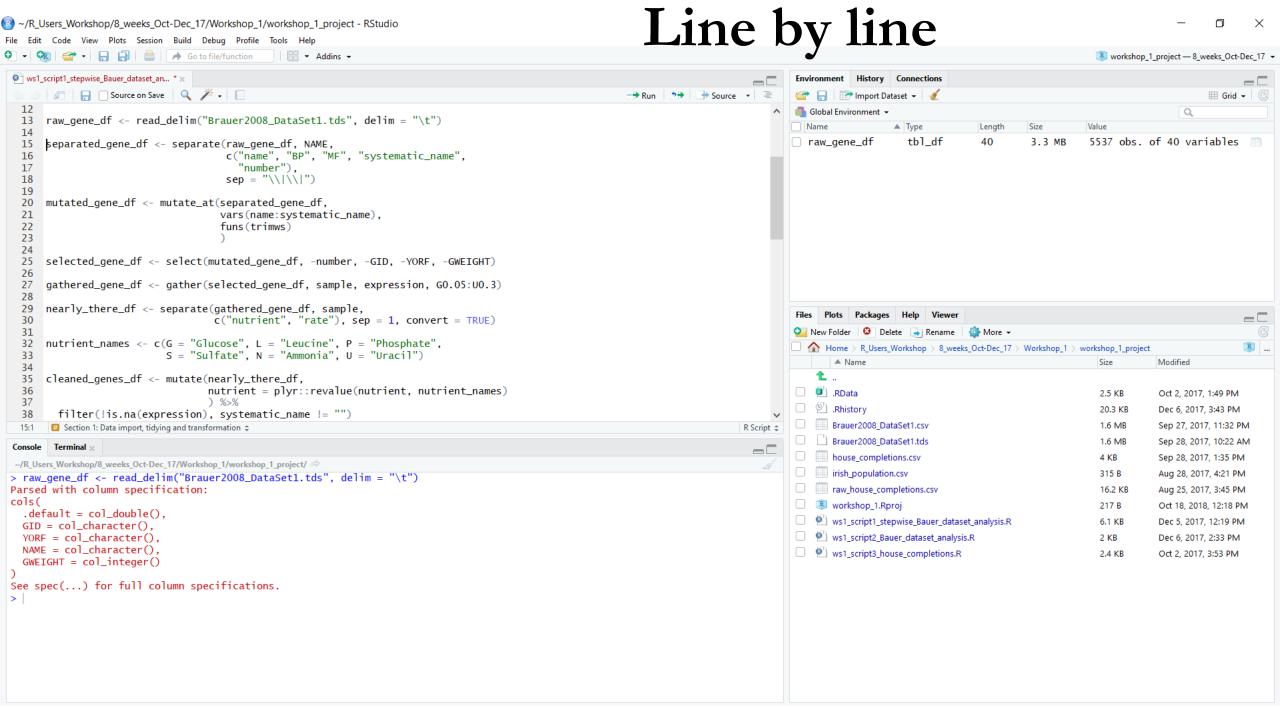
sep = "\\|\\|") - identify the separator to be used

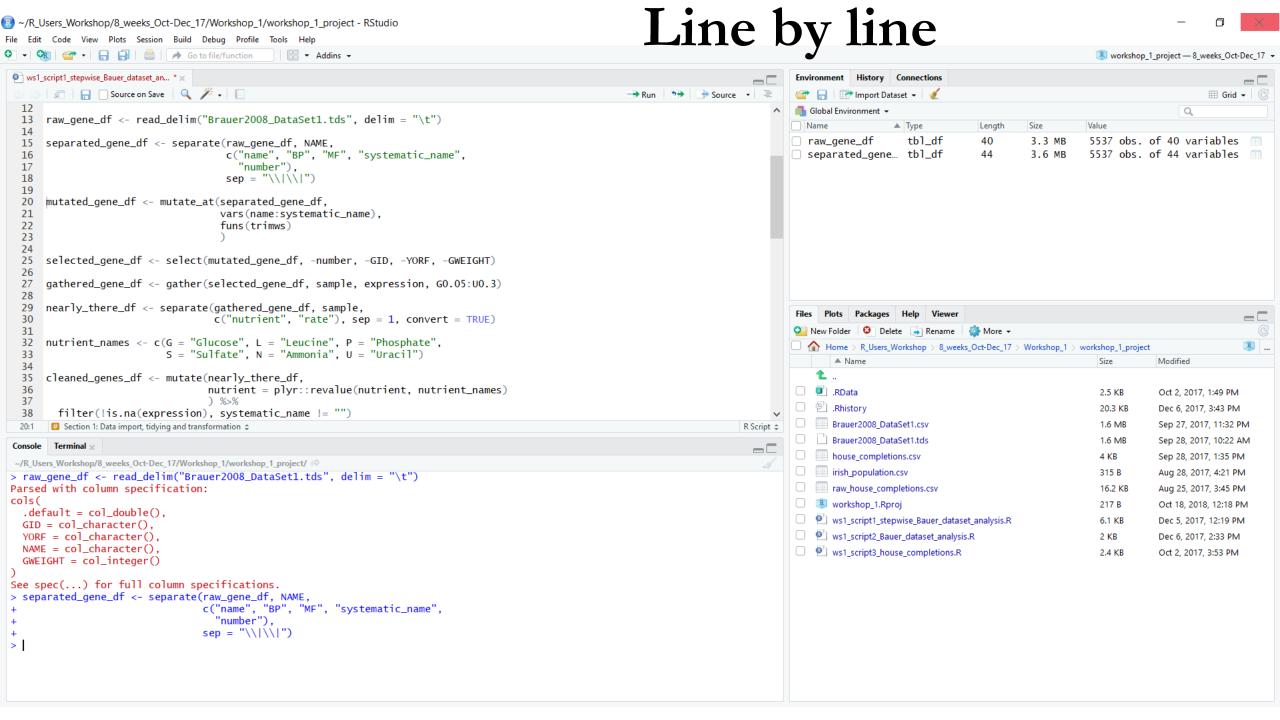
<b>(</b>		▽ Filter							(	C,
•	GID <sup>‡</sup>	YORF <sup>‡</sup>	NAME ÷	GWEIGHT <sup>‡</sup>	G0.05 <sup>‡</sup>	G0.1 <sup>‡</sup>	G0.15 <sup>‡</sup>	G0.2 <sup>‡</sup>	G0.25 <sup>‡</sup>	G0.3 <sup>‡</sup> I
1	GENE1331X	A_06_P5820	SFB2    ER to Golgi transport    molecular function unknown    YNL049C    108	1	-0.24	-0.13	-0.21	-0.15	-0.05	-0.05
2	GENE4924X	A_06_P5866	biological process unknown    molecular function unknown    YNL095C    1	1	0.28	0.13	-0.40	-0.48	-0.11	0.17
3	GENE4690X	A_06_P1834	QRI7    proteolysis and peptidolysis    metalloendopeptidase activity    YDL104	1	-0.02	-0.27	-0.27	-0.02	0.24	0.25
4	GENE1177X	A_06_P4928	CFT2    mRNA polyadenylylation*    RNA binding    YLR115W    1081958	1	-0.33	-0.41	-0.24	-0.03	-0.03	0.00
5	GENE511X	A_06_P5620	SSO2    vesicle fusion*    t-SNARE activity    YMR183C    1081214	1	0.05	0.02	0.40	0.34	-0.13	-0.14
6	GENE2133X	A_06_P5307	PSP2    biological process unknown    molecular function unknown    YML01	1	-0.69	-0.03	0.23	0.20	0.00	-0.27
7	GENE1002X	A_06_P6258	RIB2    riboflavin biosynthesis    pseudouridylate synthase activity*    YOL066C	1	-0.55	-0.30	-0.12	-0.03	-0.16	-0.11
8	GENE5478X	A_06_P7082	VMA13    vacuolar acidification    hydrogen-transporting ATPase activity, rota	1	-0.75	-0.12	-0.07	0.02	-0.32	-0.41
9	GENE2065X	A_06_P2554	EDC3    deadenylylation-independent decapping    molecular function unkno	1	-0.24	-0.22	0.14	0.06	0.00	-0.13
10	GENE2440X	A_06_P6431	VPS5    protein retention in Golgi*    protein transporter activity    YOR069W	1	-0.16	-0.38	0.05	0.14	-0.04	-0.01
11	GENE4180X	A_06_P6220	biological process unknown    molecular function unknown    YOL029C    1	1	-0.22	-0.18	0.27	0.18	0.03	-0.04
12	GENE5247X	A_06_P1410	AMN1    negative regulation of exit from mitosis*    protein binding    YBR158	1	0.18	0.61	1.55	1.34	0.23	-0.03
13	GENE2121X	A_06_P2983	SCW11    cytokinesis, completion of separation    glucan 1,3-beta-glucosidas	1	-0.67	-0.47	1.16	1.05	-0.18	-0.68
14	GENE1985X	A_06_P3720	DSE2    cell wall organization and biogenesis*    glucan 1,3-beta-glucosidase	1	-0.59	-0.17	1.17	0.85	-0.12	-0.61
15	GENE4728X	A_06_P2774	COX15    cytochrome c oxidase complex assembly*    oxidoreductase activity,	1	-0.28	-0.81	-0.39	0.24	0.01	0.01
16	GENE3153X	A_06_P4597	SPE1    pantothenate biosynthesis*    ornithine decarboxylase activity    YKL18	1	-0.19	0.24	0.03	0.17	0.00	-0.01
17	GENE3704X	A_06_P5667	MTF1    transcription from mitochondrial promoter    S-adenosylmethionine	1	-0.42	-0.43	-0.36	-0.12	0.05	0.24
18	GENE2141X	A_06_P3260	KSS1    invasive growth (sensu Saccharomyces)*    MAP kinase activity    YGR	1	-0.76	-0.32	-0.05	-0.27	-0.31	-0.01
19	GENE2978X	A_06_P3607	biological process unknown    molecular function unknown    YHR036W    1	1	-0.91	-0.43	-0.05	-0.09	-0.27	-0.45
20	GENE1203X	A_06_P5929	biological process unknown    molecular function unknown    YNL158W    1	1	-0.47	-0.43	-0.15	0.08	-0.26	-0.25

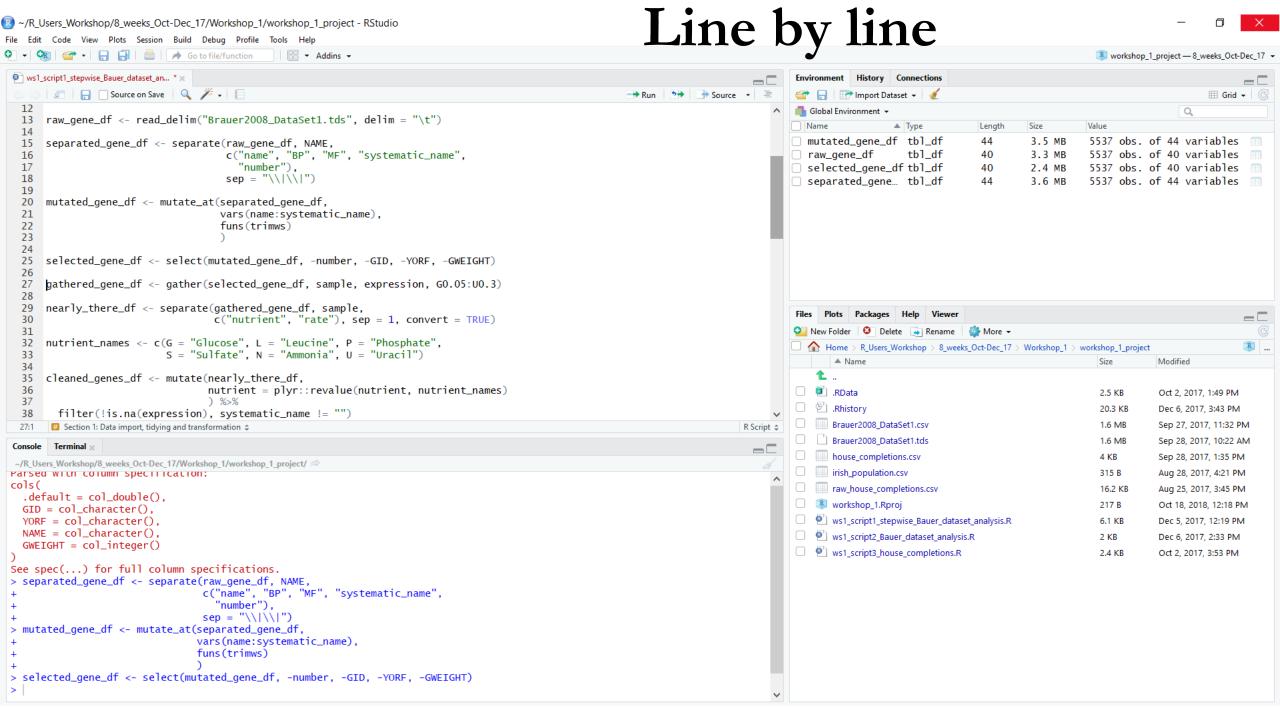
# Try to limit "uninformative" data

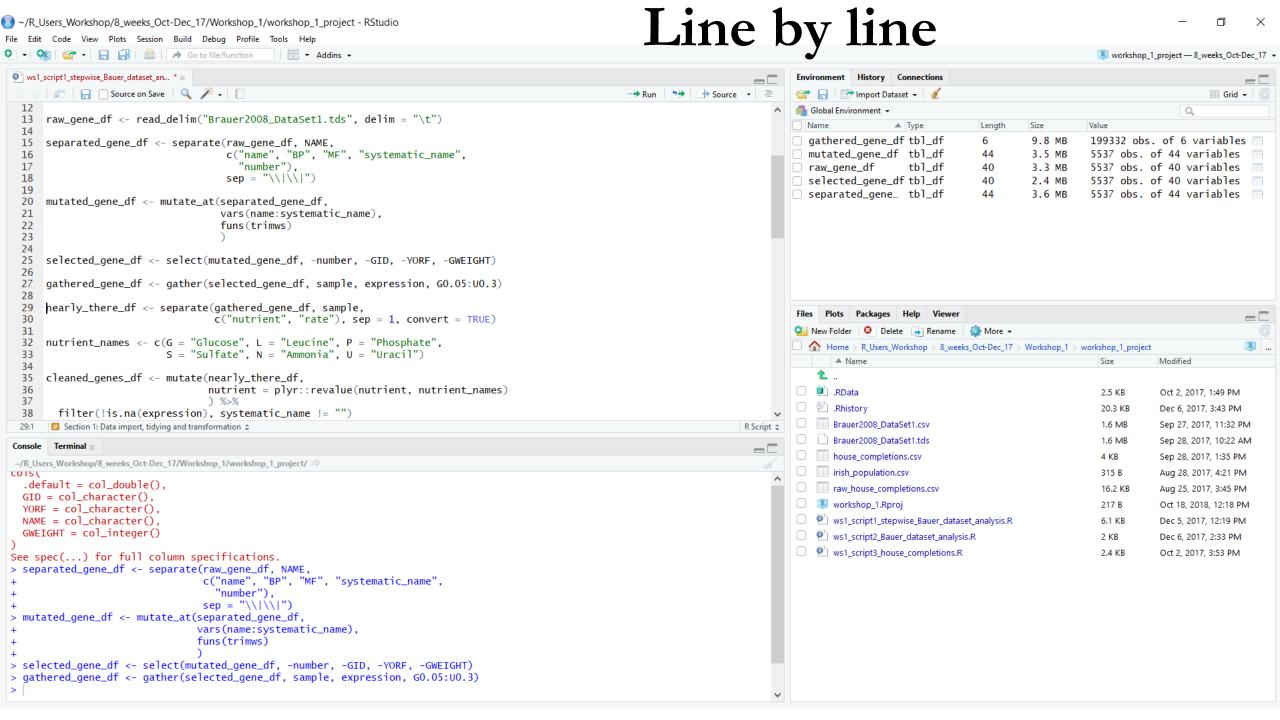
"GWEIGHT" contains the same information in every cell This isn't going to add to our analysis "GID" and "YORF" appear to be study specific IDs "NAME" column contains a lot of information Going back to the previous example; SFB2 || ER to Golgi transport || molecular function unknown || YNL049C || 1082129

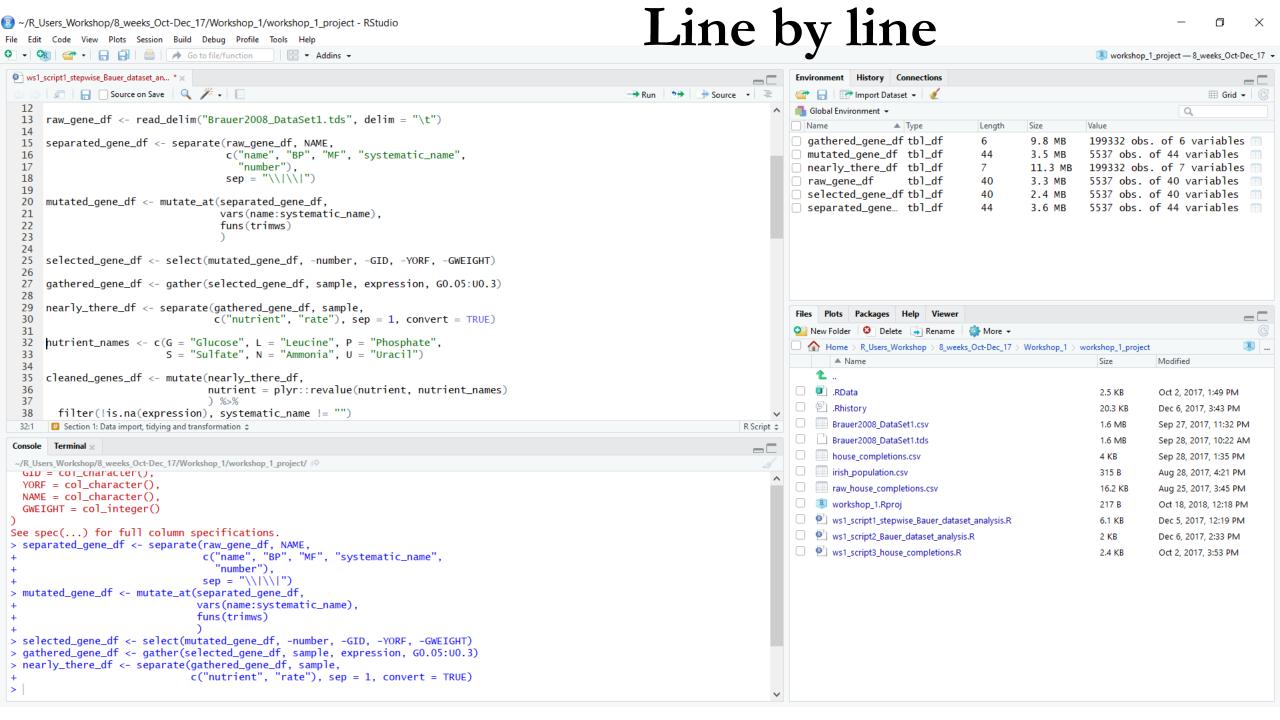
SFB2: Gene names, but not present in all cases ER to Golgi transport: Biological process molecular function unknown: Molecular function YNL049C: Gene ID listed on public repositories 1082129: Another identifier that does not appear to be useful



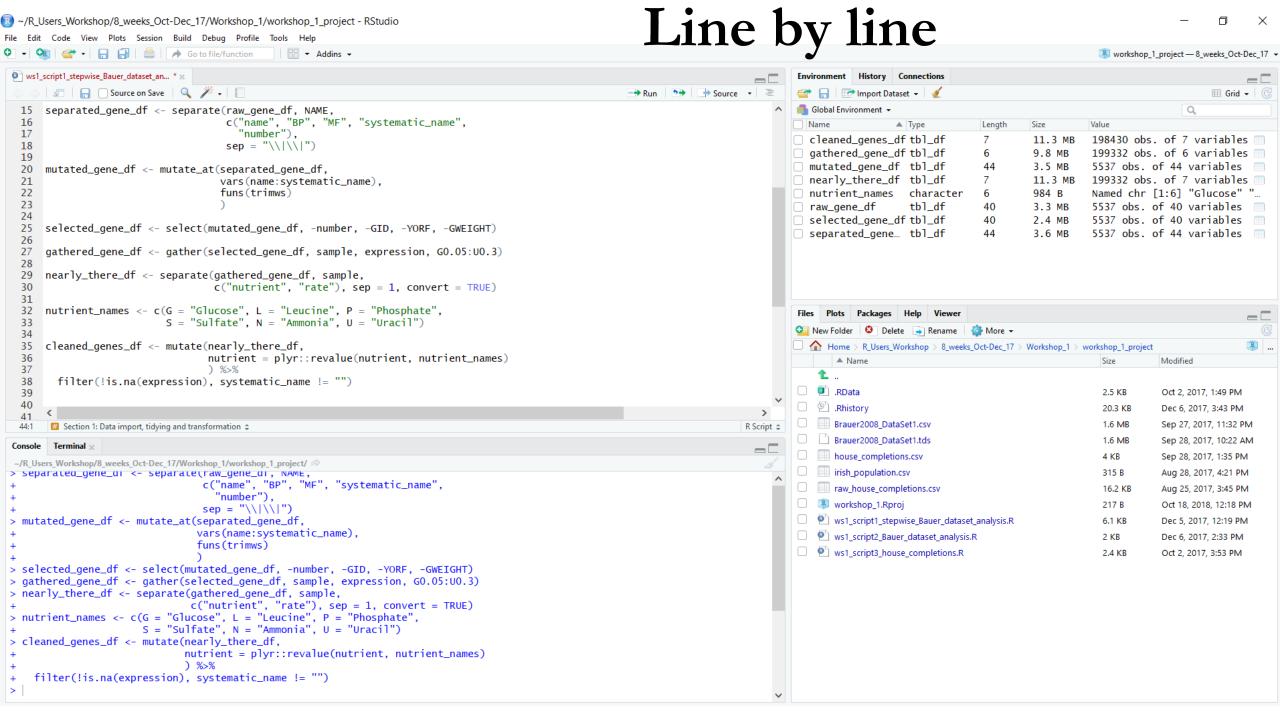


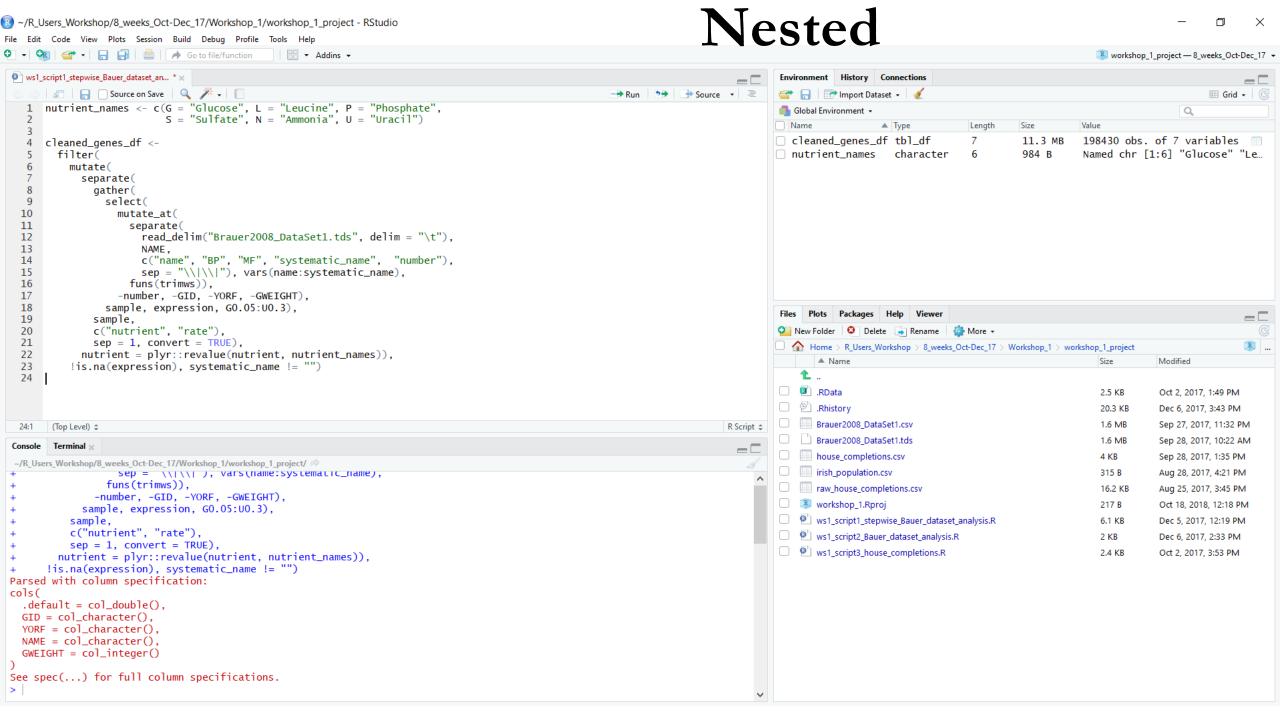






Line by line R\_Users\_Workshop/8\_weeks\_Oct-Dec\_17/Workshop\_1/workshop\_1\_project - RStudio Code View Plots Session Build Debug Profile Tools Help Go to file/function ☐☐☐ ▼ Addins ▼ workshop\_1\_project — 8\_weeks\_Oct-Dec\_17 ws1\_script1\_stepwise\_Bauer\_dataset\_an... \* x Environment History Connections Run 😘 🖶 Source 🔻 🗏 Import Dataset ▼ ⊞ Grid ▼ | © ■ Global Environment ▼ Q. raw\_gene\_df <- read\_delim("Brauer2008\_DataSet1.tds", delim = "\t")</pre> Value Name ■ Type Size Length 14 gathered gene df tbl df 9.8 MB 199332 obs. of 6 variables 15 separated\_gene\_df <- separate(raw\_gene\_df, NAME,</pre> 5537 obs. of 44 variables c("name", "BP", "MF", "systematic\_name", mutated\_gene\_df tbl\_df 3.5 MB 16 17 "number"). nearly\_there\_df tbl\_df 11.3 MB 199332 obs. of 7 variables 18 sep = "\\|\\|") nutrient\_names character Named chr [1:6] "Glucose" ".. 6 984 B 19 5537 obs. of 40 variables raw\_gene\_df tbl df 3.3 MB mutated\_gene\_df <- mutate\_at(separated\_gene\_df, 20 5537 obs. of 40 variables selected\_gene\_df tbl\_df 40 2.4 MB 21 vars(name:systematic\_name), separated\_gene... tbl\_df 5537 obs. of 44 variables 3.6 MB 22 funs(trimws) 23 24 25 selected\_gene\_df <- select(mutated\_gene\_df, -number, -GID, -YORF, -GWEIGHT) 26 gathered\_gene\_df <- gather(selected\_gene\_df, sample, expression, G0.05:U0.3)</pre> 28 nearly\_there\_df <- separate(gathered\_gene\_df, sample,</pre> Files Plots Packages Help Viewer  $=\Box$ c("nutrient", "rate"), sep = 1, convert = TRUE) 30 31 New Folder 🚨 Delete 🗻 Rename 🕍 More 🕶 nutrient\_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",</pre> Home > R Users Workshop > 8 weeks Oct-Dec 17 > Workshop 1 > workshop 1 project S = "Sulfate", N = "Ammonia", U = "Uracil") 33 ▲ Name Modified 34 **1**... cleaned\_genes\_df <- mutate(nearly\_there\_df,</pre> 36 nutrient = plyr::revalue(nutrient, nutrient\_names) □ ■ .RData 2.5 KB Oct 2, 2017, 1:49 PM 37 ) %>% ☐ <a>♠</a> .Rhistory 20.3 KB Dec 6, 2017, 3:43 PM 38 filter(!is.na(expression), systematic\_name != "") Brauer2008\_DataSet1.csv 1.6 MB Sep 27, 2017, 11:32 PM Section 1: Data import, tidying and transformation \$ ☐ Brauer2008 DataSet1.tds 1.6 MB Sep 28, 2017, 10:22 AM Console Terminal house\_completions.csv 4 KB Sep 28, 2017, 1:35 PM ~/R\_Users\_Workshop/8\_weeks\_Oct-Dec\_17/Workshop\_1/workshop\_1\_project/ A irish\_population.csv 315 B Aug 28, 2017, 4:21 PM NAME = COI\_CHARACTER(), GWEIGHT = col\_integer() raw\_house\_completions.csv 16.2 KB Aug 25, 2017, 3:45 PM workshop\_1.Rproj 217 B Oct 18, 2018, 12:18 PM See spec(...) for full column specifications. ws1\_script1\_stepwise\_Bauer\_dataset\_analysis.R > separated\_gene\_df <- separate(raw\_gene\_df, NAME, 6.1 KB Dec 5, 2017, 12:19 PM c("name", "BP", "MF", "systematic\_name", ws1\_script2\_Bauer\_dataset\_analysis.R 2 KB Dec 6, 2017, 2:33 PM "number"), ws1\_script3\_house\_completions.R 2.4 KB Oct 2, 2017, 3:53 PM sep = "\\|\\|") mutated\_gene\_df <- mutate\_at(separated\_gene\_df,</pre> vars(name:systematic\_name), funs(trimws) > selected\_gene\_df <- select(mutated\_gene\_df, -number, -GID, -YORF, -GWEIGHT)</pre> gathered\_gene\_df <- gather(selected\_gene\_df, sample, expression, G0.05:U0.3)</pre> > nearly\_there\_df <- separate(gathered\_gene\_df, sample,</pre> c("nutrient", "rate"), sep = 1, convert = TRUE) > nutrient\_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",</pre> S = "Sulfate", N = "Ammonia", U = "Uracil")

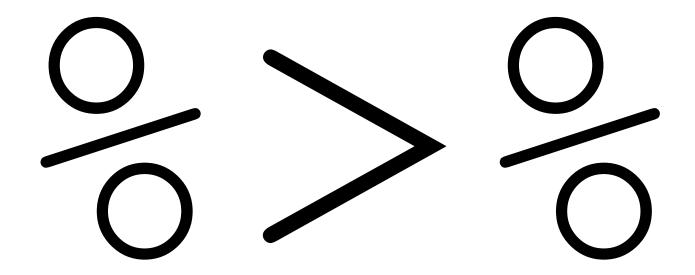




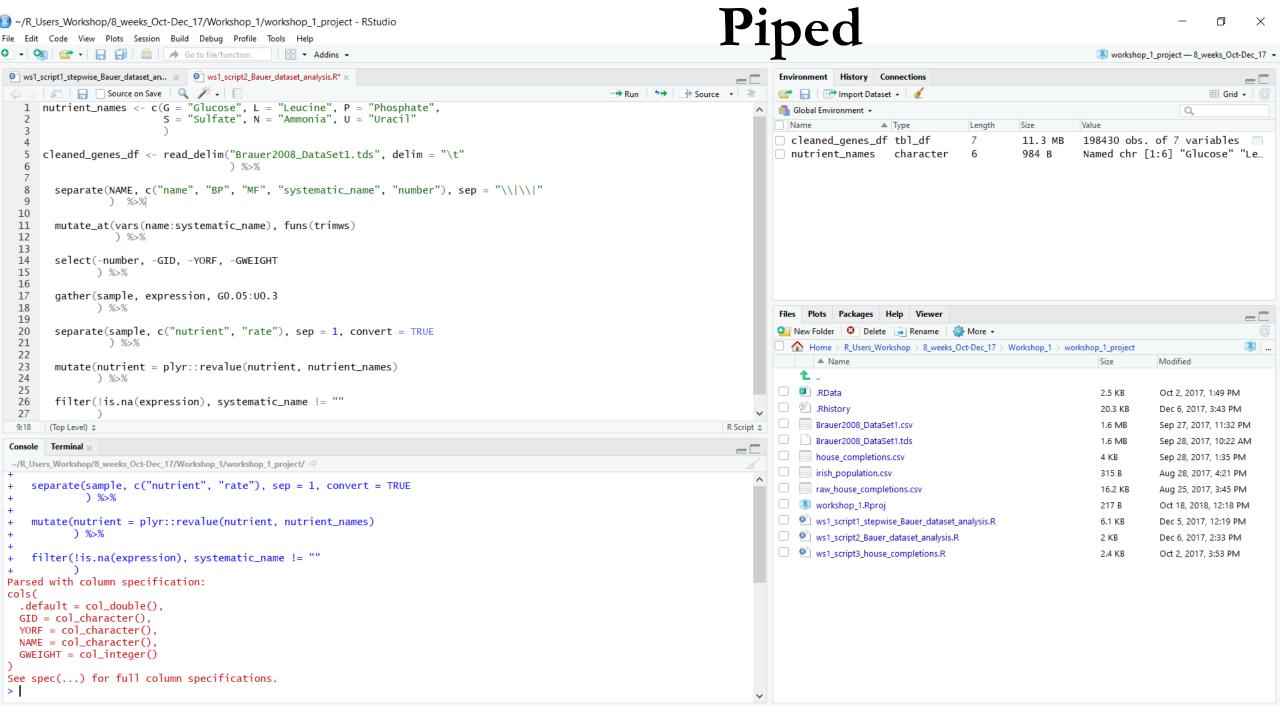
#### Nested

```
nutrient\_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
 2
                        S = "Sulfate", N = "Ammonia", U = "Uracil")
 3
    cleaned_genes_df <-
      filter(
 5
        mutate(
 6
          separate(
 8
            gather(
 9
              select(
10
                mutate_at(
11
                  separate(
                    read_delim("Brauer2008_DataSet1.tds", delim = "\t"),
12
13
                    NAME.
14
                    c("name", "BP", "MF", "systematic_name", "number"),
15
                    sep = "\\|\\|"), vars(name:systematic_name),
                  funs(trimws)),
16
17
                -number, -GID, -YORF, -GWEIGHT),
18
              sample, expression, G0.05:U0.3),
19
            sample.
20
            c("nutrient", "rate"),
21
            sep = 1, convert = TRUE),
          nutrient = plyr::revalue(nutrient, nutrient_names)),
22
        !is.na(expression), systematic_name != "")
23
24
```

# Putting the pieces together



#### Code structure v2

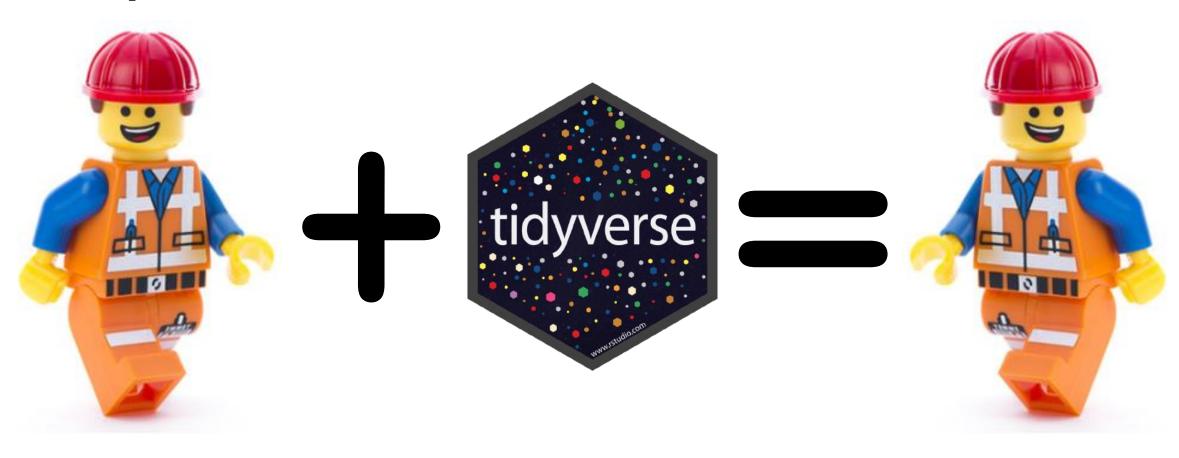


### Piped

```
nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",</pre>
 2
                         S = "Sulfate", N = "Ammonia", U = "Uracil"
 3
 4
    cleaned_genes_df <- read_delim("Brauer2008_DataSet1.tds", delim = "\t"</pre>
 6
                                    ) %>%
 8
      separate(NAME, c("name", "BP", "MF", "systematic_name", "number"), sep = "\\|\\|"
 9
               ) %>%
10
11
      mutate_at(vars(name:systematic_name), funs(trimws)
12
                ) %>%
13
      select(-number, -GID, -YORF, -GWEIGHT
14
15
             ) %>%
16
17
      gather(sample, expression, G0.05:U0.3
18
             ) %>%
19
20
      separate(sample, c("nutrient", "rate"), sep = 1, convert = TRUE
21
               ) %>%
22
23
      mutate(nutrient = plyr::revalue(nutrient, nutrient_names)
24
             ) %>%
25
26
      filter(!is.na(expression), systematic_name !=
27
```

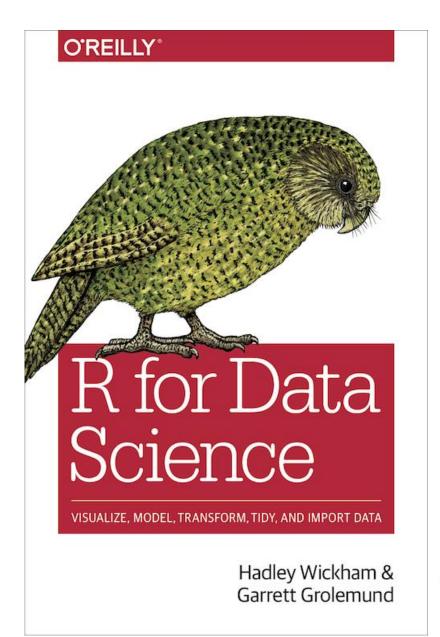
# The moral of the story......

You can go from this



To this!!

#### You could write a book on that!!



## And on this!!

Use R! Hadley Wickham ggplot2 **Elegant Graphics for Data Analysis** Second Edition 2 Springer



