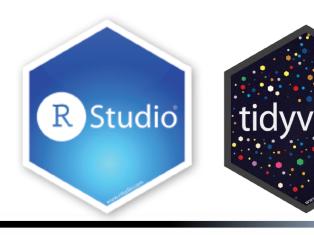
R-eproducible workflows

Half-day workshop Afternoon session



Brendan Palmer,
Statistics & Data Analysis Unit,
Clinical Research Facility - Cork



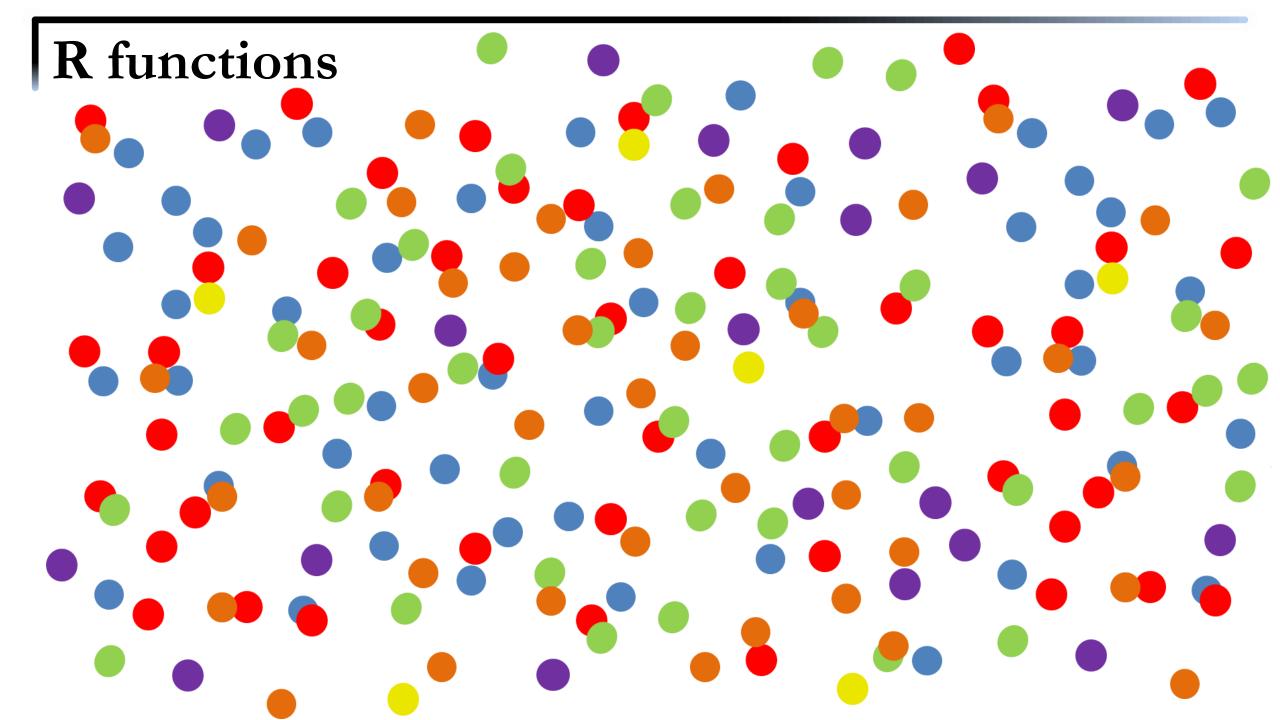




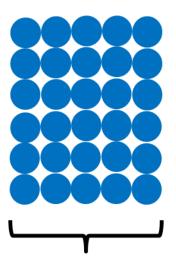
To understand R, remember the following

- Everything that exists is an object

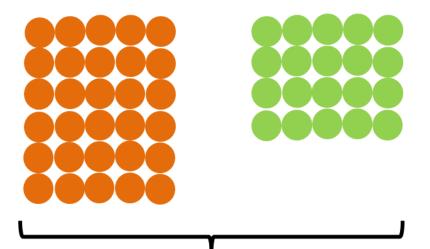
- Everything that happens is a function



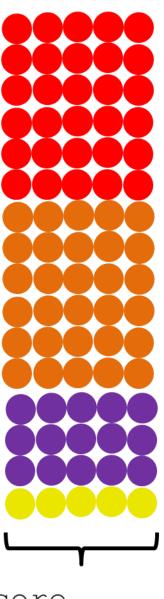
R packages



Base R: Comes preloaded

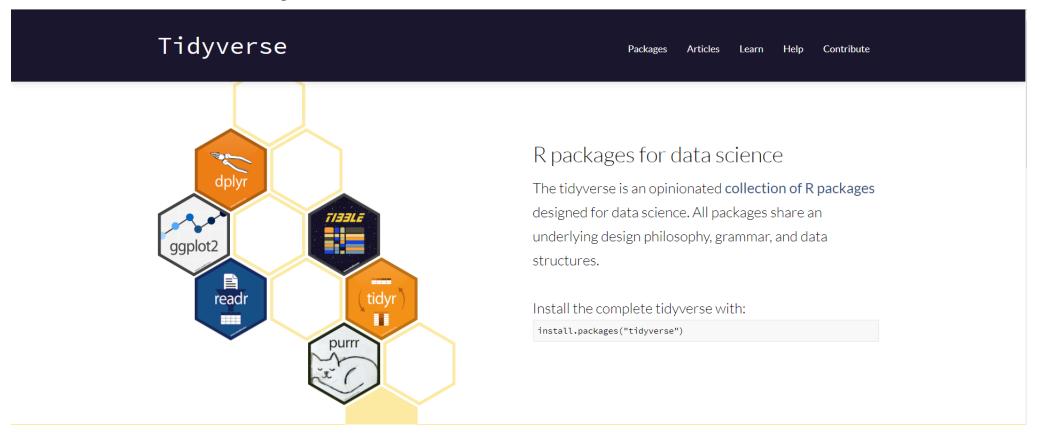


Other packages:
Install once
Update regularly
Load each session



core
tidyverse

What is the tidyverse?



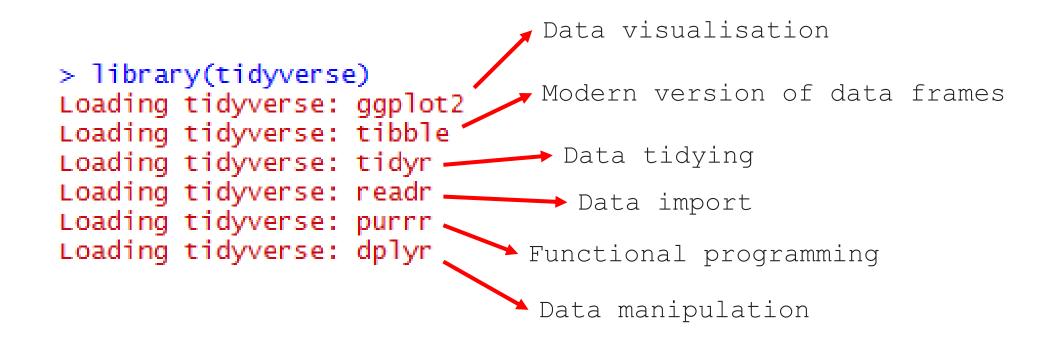
- Joined up collection of packages for data analysis
 - Consistent functions
 - Uses (tidy) data
 - Supports end-to-end workflows

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")

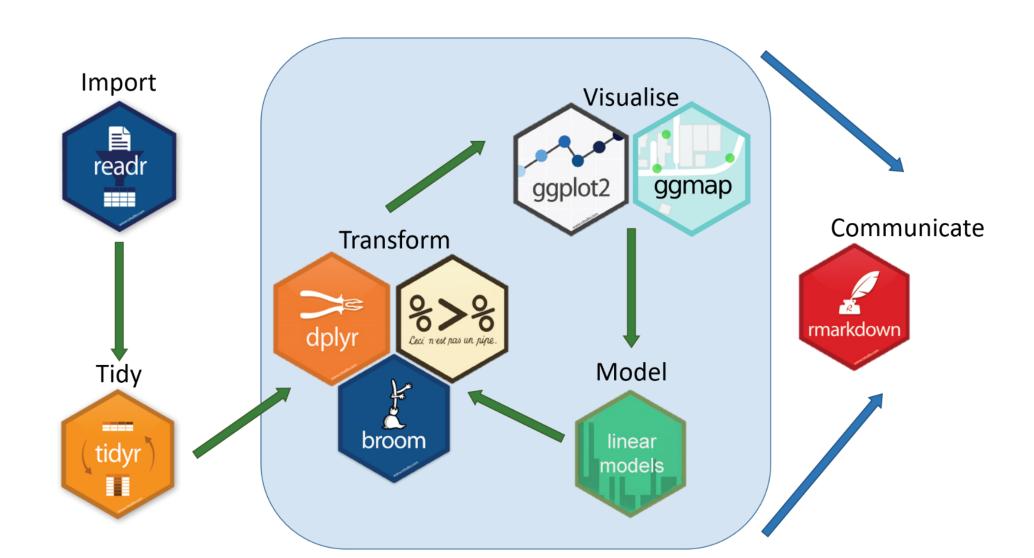
The tidyverse Oct 2017



The tidyverse Feb 2019

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
```

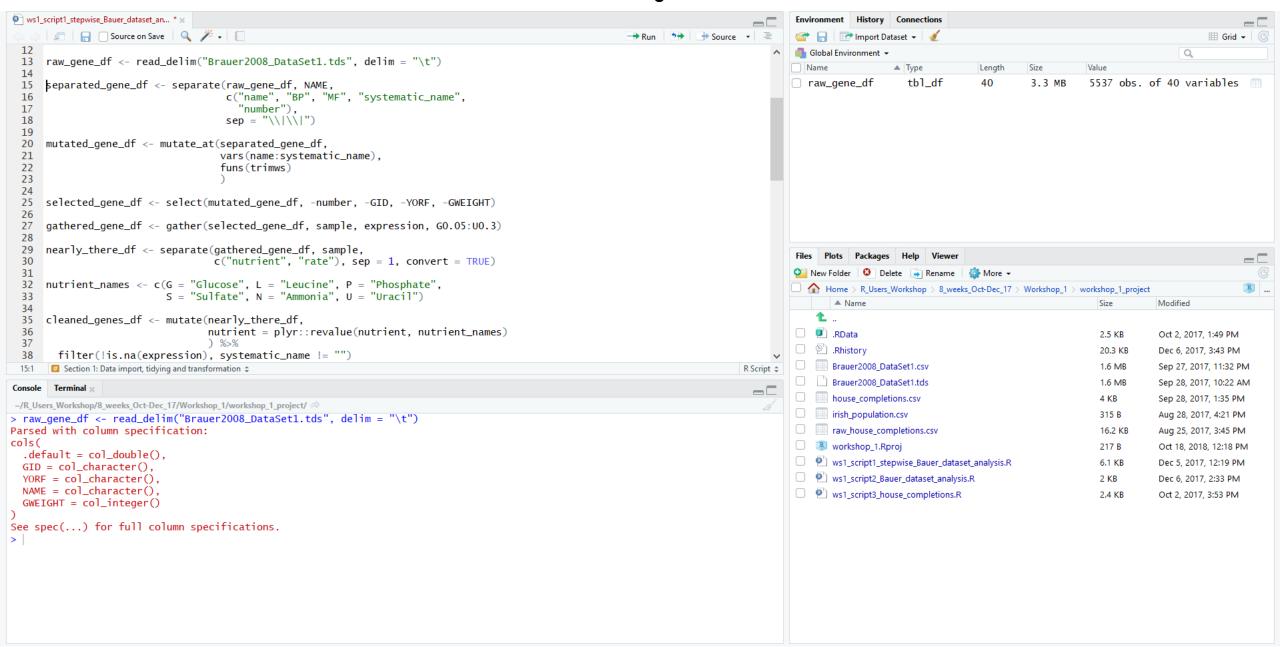
sep = "\\|\\|") - identify the separator to be used

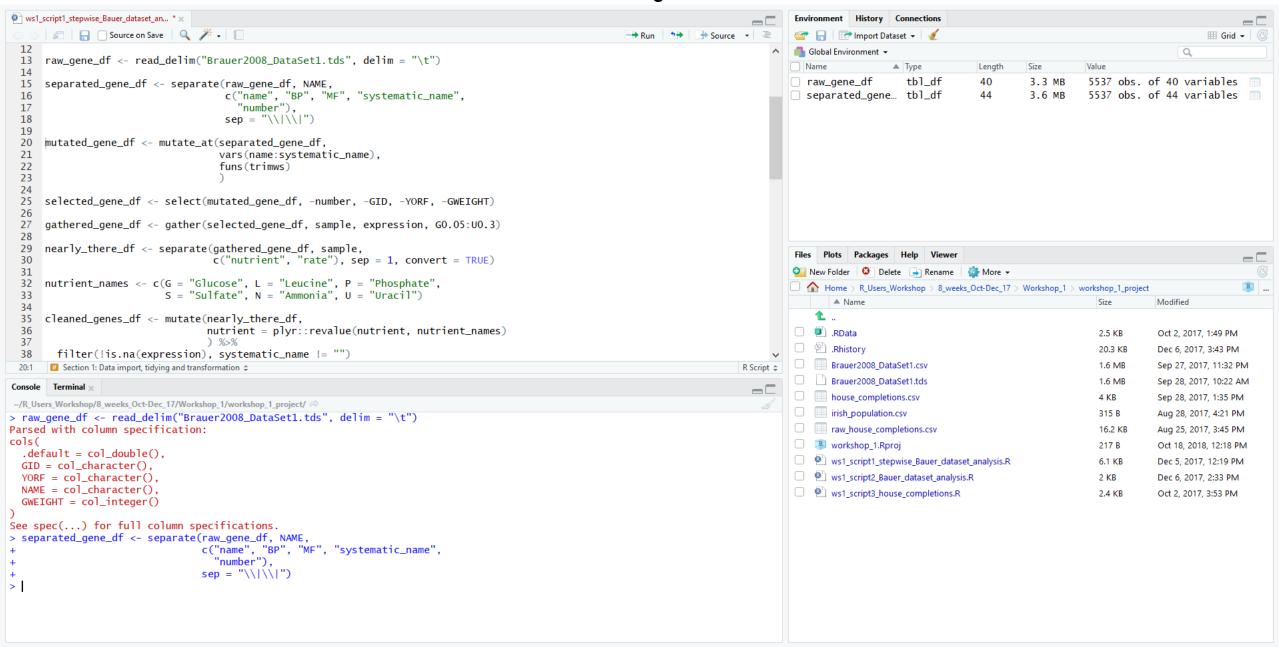
(▽ Filter							(C,
•	GID [‡]	YORF [‡]	NAME ÷	GWEIGHT [‡]	G0.05 [‡]	G0.1 [‡]	G0.15 [‡]	G0.2 [‡]	G0.25 [‡]	G0.3 [‡] I
1	GENE1331X	A_06_P5820	SFB2 ER to Golgi transport molecular function unknown YNL049C 108	1	-0.24	-0.13	-0.21	-0.15	-0.05	-0.05
2	GENE4924X	A_06_P5866	biological process unknown molecular 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

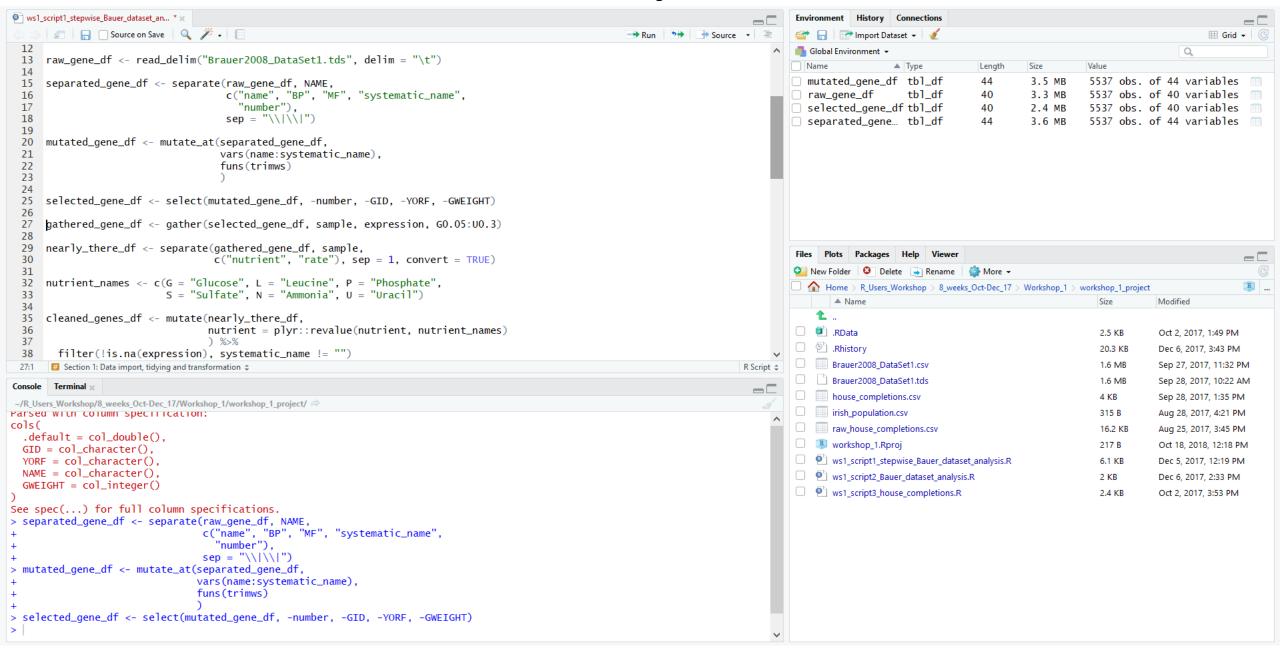
Try to limit "uninformative" data

"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



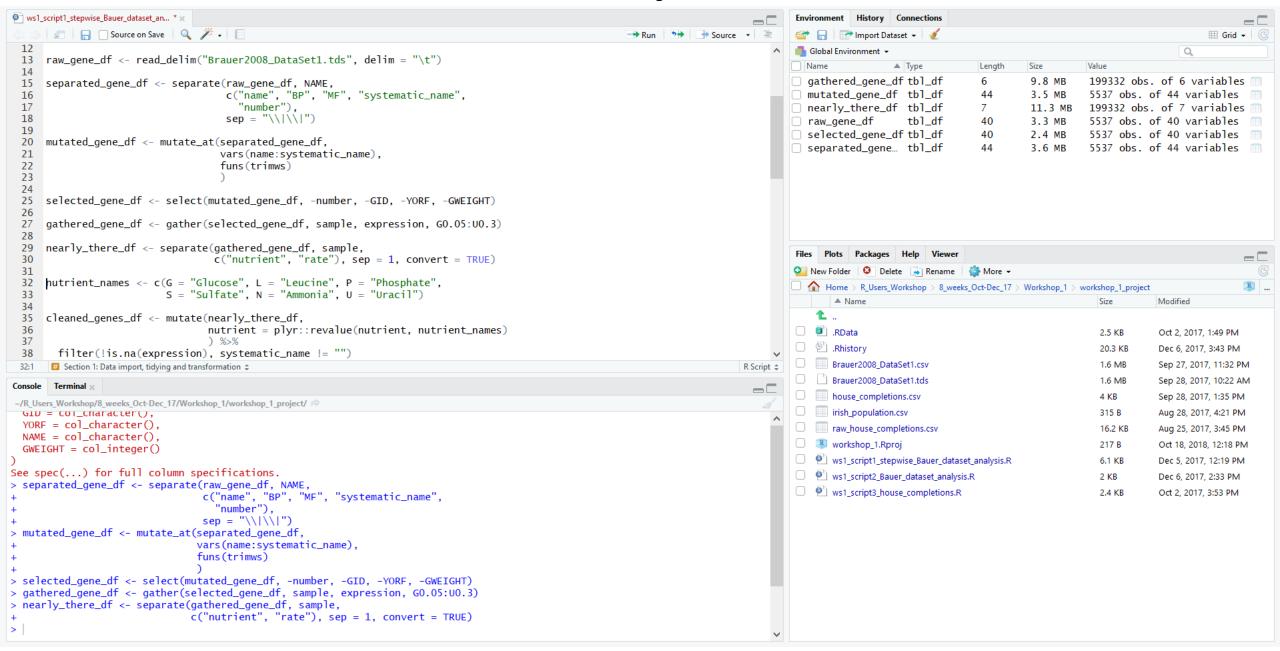


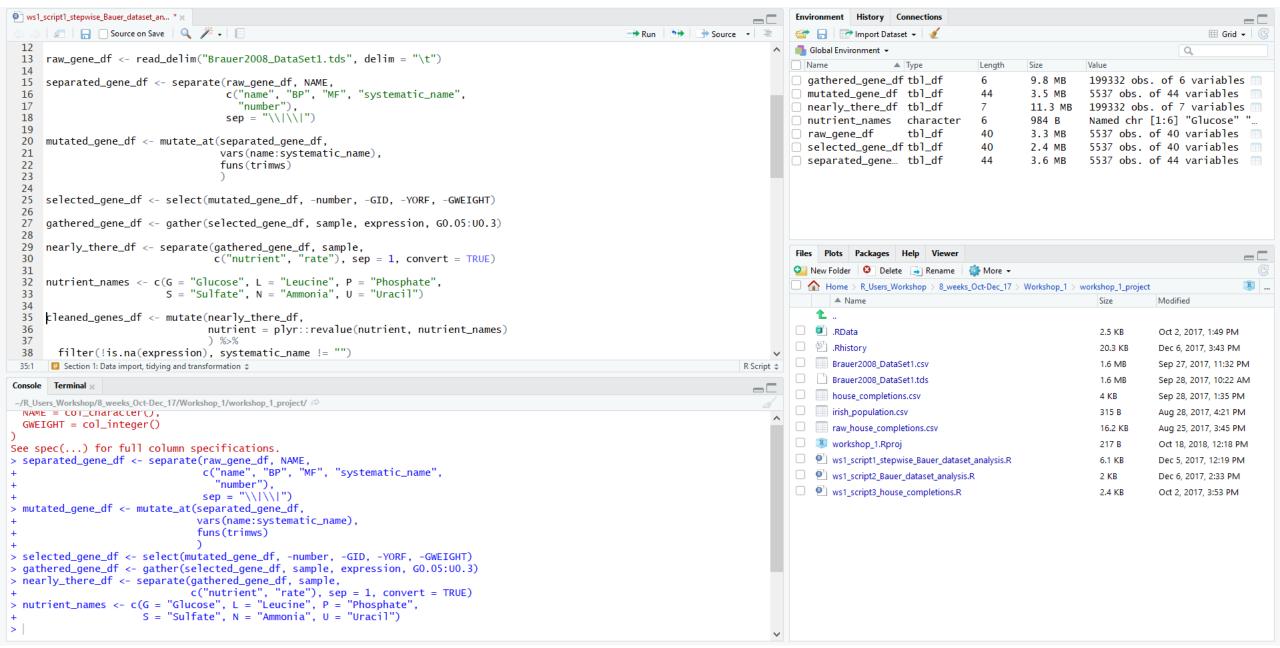


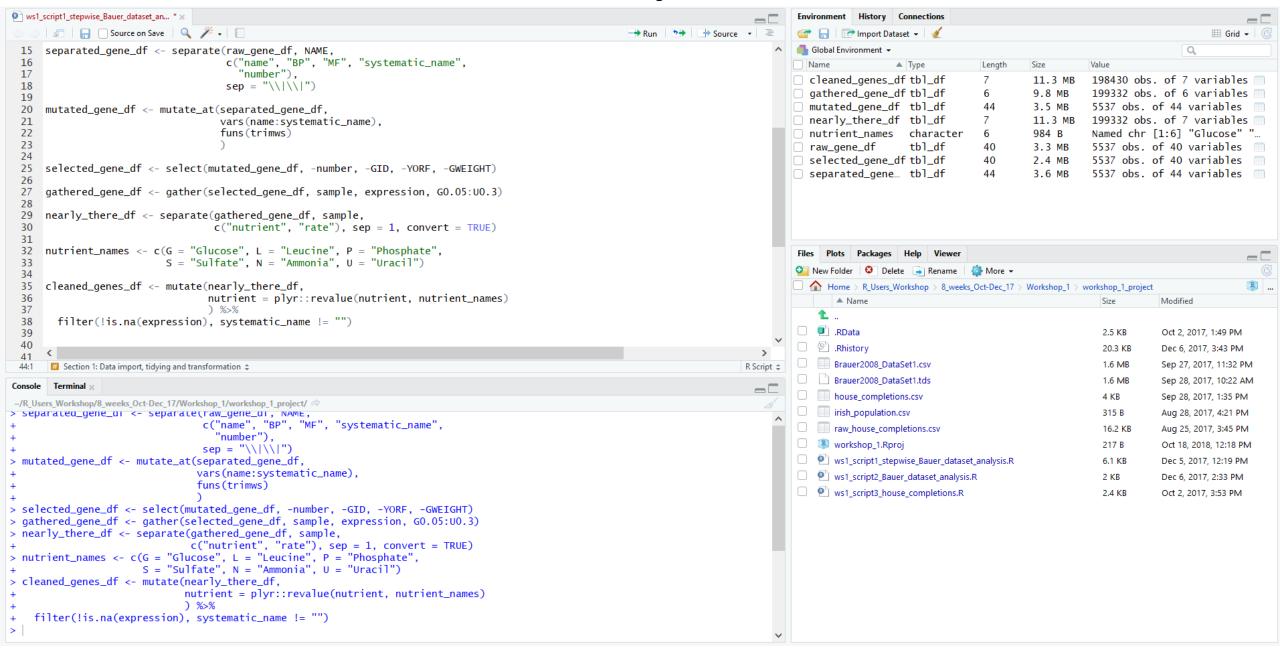
```
ws1_script1_stepwise_Bauer_dataset_an... * x
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       ⊞ Grid → G
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                                                                                                                                                ■ Global Environment ▼
  13
      raw_gene_df <- read_delim("Brauer2008_DataSet1.tds", delim = "\t")</pre>
                                                                                                                                                  Name
                                                                                                                                                                  ■ Type
                                                                                                                                                                                  Length
                                                                                                                                                                                           Size
                                                                                                                                                                                                      Value
  14
                                                                                                                                                  gathered_gene_df tb1_df
                                                                                                                                                                                                      199332 obs. of 6 variables
                                                                                                                                                                                   6
                                                                                                                                                                                           9.8 MB
  15
      separated_gene_df <- separate(raw_gene_df, NAME,</pre>
                                       c("name", "BP", "MF", "systematic_name",
                                                                                                                                                  mutated_gene_df tbl_df
                                                                                                                                                                                           3.5 MB
                                                                                                                                                                                                      5537 obs. of 44 variables
  16
  17
                                         "number"),
                                                                                                                                                  raw_gene_df
                                                                                                                                                                     tbl_df
                                                                                                                                                                                   40
                                                                                                                                                                                           3.3 MB
                                                                                                                                                                                                      5537 obs. of 40 variables
  18
                                       sep = "\\|\\|")
                                                                                                                                                  selected_gene_df tbl_df
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                                                                                                                                                                                   40
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  19
                                                                                                                                                  separated_gene... tbl_df
                                                                                                                                                                                   44
                                                                                                                                                                                            3.6 MB
                                                                                                                                                                                                      5537 obs. of 44 variables
      mutated_gene_df <- mutate_at(separated_gene_df,</pre>
  20
  21
                                      vars(name:svstematic_name).
  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
      hearly_there_df <- separate(gathered_gene_df, sample,
                                                                                                                                                Files Plots Packages Help Viewer
  30
                                     c("nutrient", "rate"), sep = 1, convert = TRUE)
  31
                                                                                                                                                New Folder 

Delete 
Rename 

More ▼
      nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
                                                                                                                                                  Home > R Users Workshop > 8 weeks Oct-Dec 17 > Workshop 1 > workshop 1 project
  33
                            S = "Sulfate". N = "Ammonia". U = "Uracil")
                                                                                                                                                        ■ Name
                                                                                                                                                                                                        Size
                                                                                                                                                                                                                   Modified
  34
                                                                                                                                                    1...
  35
      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
                                                                                                                                                ☐ ❷ .Rhistory
                                                                                                                                                                                                        20.3 KB
                                                                                                                                                                                                                   Dec 6, 2017, 3:43 PM
  38
        filter(!is.na(expression), systematic_name != "")
                                                                                                                                                ☐ Brauer2008 DataSet1.csv
                                                                                                                                                                                                                   Sep 27, 2017, 11:32 PM
       # Section 1: Data import, tidying and transformation $
                                                                                                                                       R Script $
                                                                                                                                                                                                        1.6 MB
                                                                                                                                                ☐ Brauer2008_DataSet1.tds
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       Terminal
                                                                                                                                                house_completions.csv
                                                                                                                                                                                                        4 KB
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~/R_Users_Workshop/8_weeks_Oct-Dec_17/Workshop_1/workshop_1_project/ A
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  .default = col_double(),
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  GID = col character().
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                                                                                                                                                                                                        217 B
  YORF = col_character(),
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  NAME = col_character(),
                                                                                                                                                                                                        6.1 KB
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  GWEIGHT = col_integer()
                                                                                                                                                       ws1_script2_Bauer_dataset_analysis.R
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                                                                                                                                                ws1 script3_house_completions.R
                                                                                                                                                                                                                   Oct 2, 2017, 3:53 PM
See spec(...) for full column specifications.
> separated_gene_df <- separate(raw_gene_df, NAME,
                                   c("name", "BP", "MF", "systematic_name",
                                      "number"),
                                   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>
```







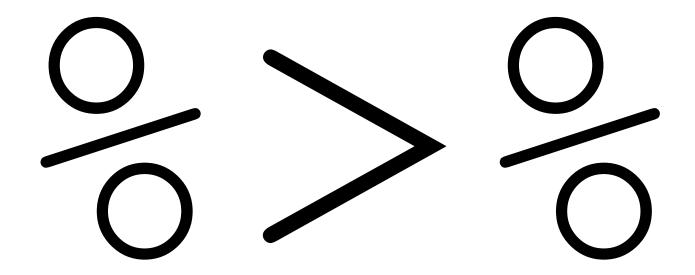
Nested

```
ws1_script1_stepwise_Bauer_dataset_an... * x
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                                                                                                                                          ⊞ Grid ▼ G
     nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate".</pre>
                                                                                                                                          Global Environment •
                                                                                                                                                                                                                  Q.
                           S = "Sulfate", N = "Ammonia", U = "Uracil")
                                                                                                                                          Name
                                                                                                                                                            ■ Type
                                                                                                                                                                            Length
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                                                                                                                                            cleaned_genes_df tbl_df
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                                                                                                                                                                                                198430 obs. of 7 variables
      cleaned_genes_df <-
                                                                                                                                            nutrient_names character
                                                                                                                                                                                     984 B
                                                                                                                                                                                                Named chr [1:6] "Glucose" "Le...
        filter(
                                                                                                                                                                            6
          mutate(
            separate(
              gather(
                select(
  10
                   mutate_at(
  11
                     separate(
                       read_delim("Brauer2008_DataSet1.tds", delim = "\t"),
  12
  13
                       c("name", "BP", "MF", "systematic_name", "number"),
  14
  15
                       sep = "\\|\\|"), vars(name:systematic_name),
  16
                     funs(trimws)).
  17
                   -number, -GID, -YORF, -GWEIGHT),
 18
                sample, expression, G0.05:U0.3).
                                                                                                                                          Files Plots Packages Help Viewer
  19
               sample,
  20
              c("nutrient", "rate"),
                                                                                                                                          New Folder Delete 🗐 Rename 🤹 More 🕶
  21
               sep = 1, convert = TRUE),
                                                                                                                                                                                                                             R ...
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 22
            nutrient = plyr::revalue(nutrient, nutrient_names)),
                                                                                                                                                 ▲ Name
                                                                                                                                                                                                              Modified
 23
          !is.na(expression), systematic_name != "")
                                                                                                                                              £.
 24
                                                                                                                                         RData
                                                                                                                                                                                                   2.5 KB
                                                                                                                                                                                                              Oct 2, 2017, 1:49 PM
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                   sep = \\\\\\ ), vars(name:systematic_name),
                 funs(trimws)).
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               -number, -GID, -YORF, -GWEIGHT),
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                                                                                                                                                                                                              Oct 18, 2018, 12:18 PM
            sample, expression, G0.05:U0.3),
          sample.
                                                                                                                                             ws1 script1 stepwise Bauer dataset analysis.R
                                                                                                                                                                                                    6.1 KB
                                                                                                                                                                                                              Dec 5, 2017, 12:19 PM
          c("nutrient", "rate"),
                                                                                                                                             ws1_script2_Bauer_dataset_analysis.R
                                                                                                                                                                                                    2 KB
                                                                                                                                                                                                              Dec 6, 2017, 2:33 PM
          sep = 1, convert = TRUE),
                                                                                                                                          ws1 script3 house completions.R
                                                                                                                                                                                                    2.4 KB
                                                                                                                                                                                                              Oct 2, 2017, 3:53 PM
        nutrient = plyr::revalue(nutrient, nutrient_names)),
      !is.na(expression), systematic_name != "")
Parsed with column specification:
cols(
  .default = col_double(),
  GID = col_character(),
  YORF = col_character(),
  NAME = col_character(),
  GWEIGHT = col_integer()
See spec(...) for full column specifications.
```

Nested

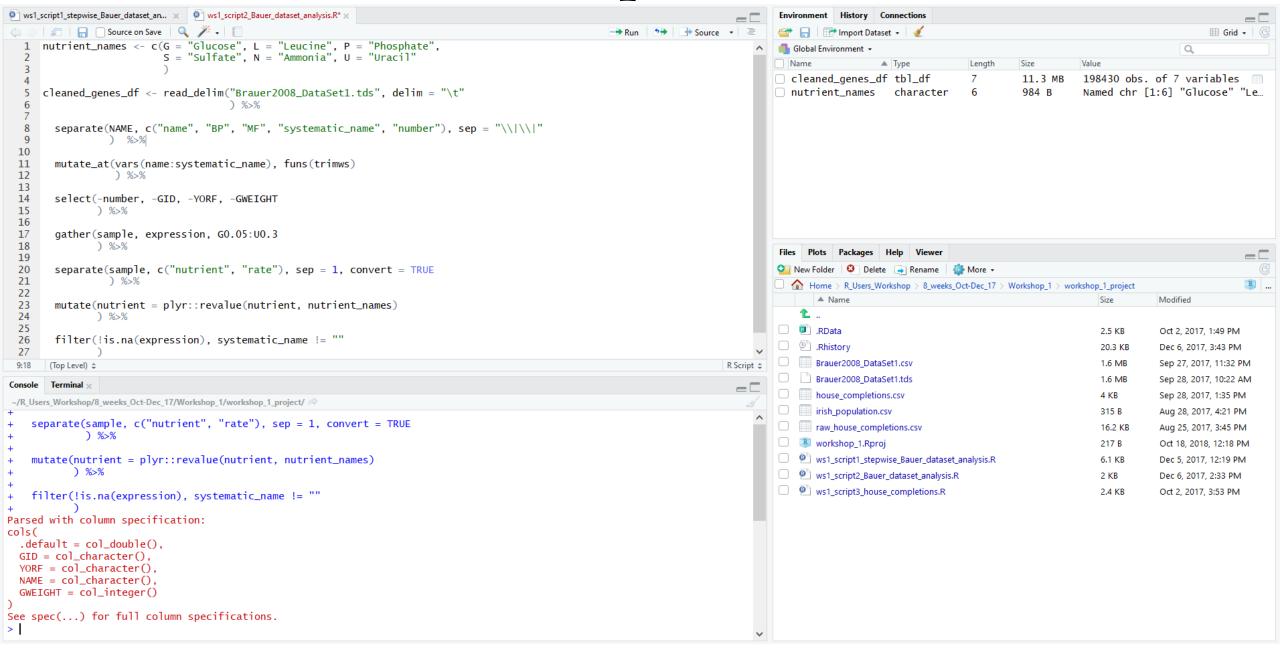
```
nutrient\_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
                        S = "Sulfate", N = "Ammonia", U = "Uracil")
 2
 3
    cleaned_genes_df <-
      filter(
 5
        mutate(
 6
          separate(
 8
            gather(
 9
              select(
10
                mutate_at(
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



Piped

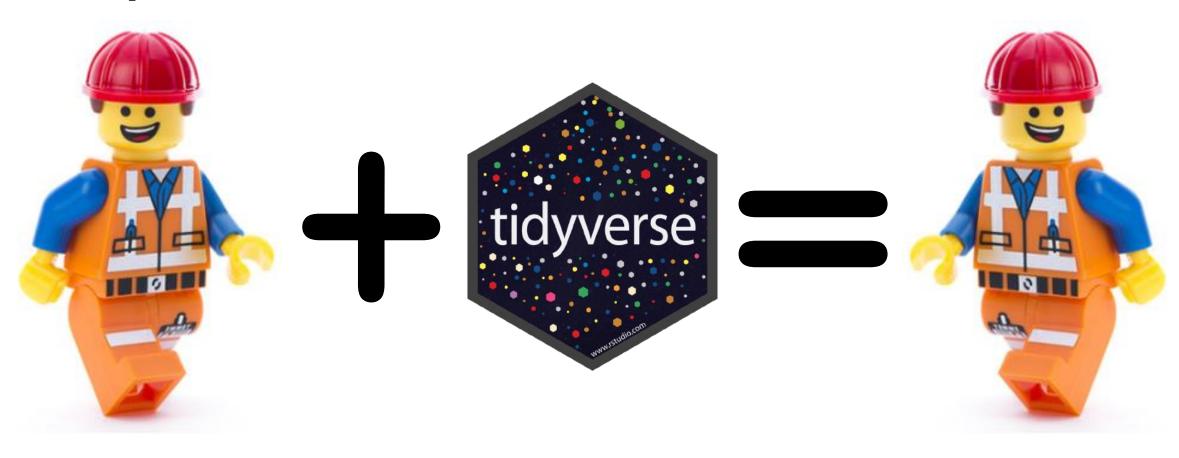
```
nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",</pre>
 2
                         S = "Sulfate", N = "Ammonia", U = "Uracil"
 3
 4
    cleaned_genes_df <- read_delim("Brauer2008_DataSet1.tds", delim = "\t"</pre>
 6
                                    ) %>%
 8
      separate(NAME, 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
```

Magrittr package

- Tidyverse packages automatically make %>% available
- Magrittr has other tools that you might find useful

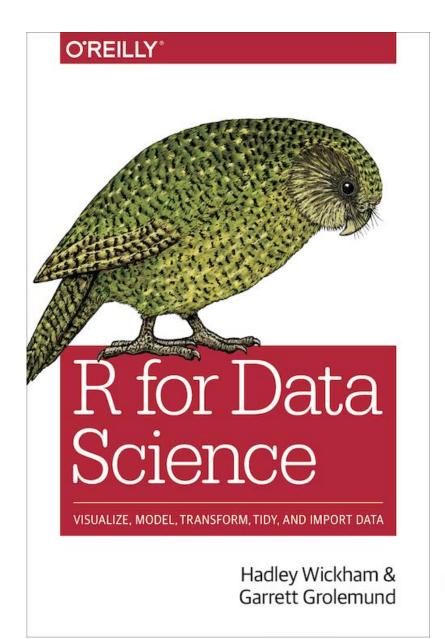
The moral of the story......

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