R: A Hitchhikers Guide to Reproducible Research

- Take a parachute and jump (into the tidyverse)

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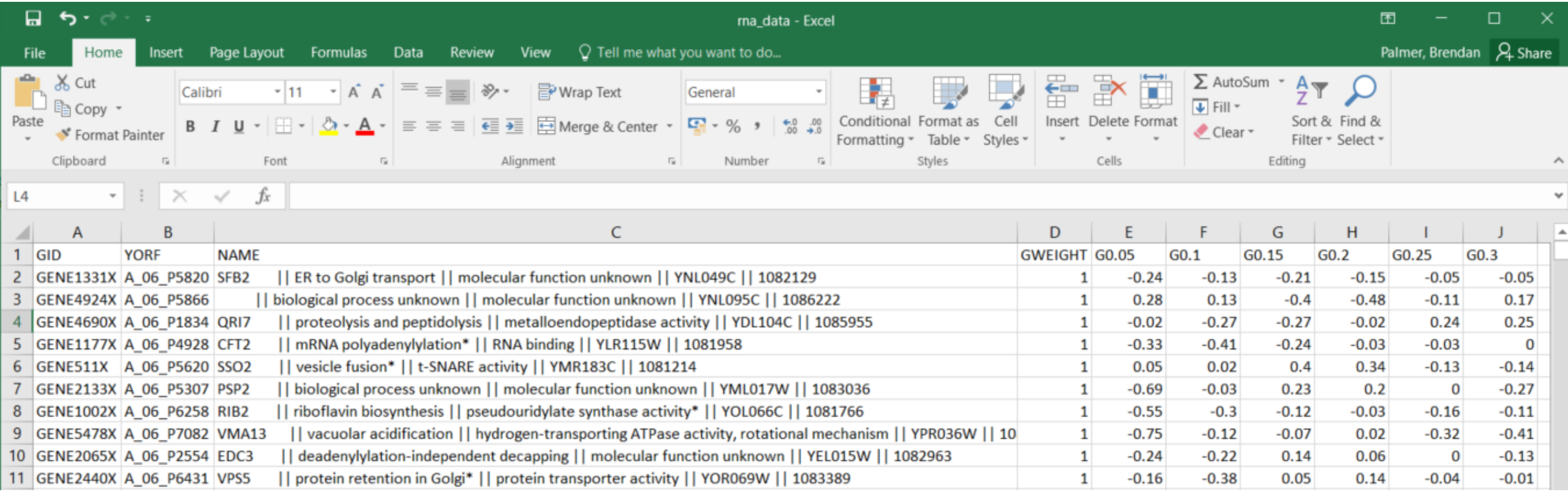
CRF-C
HRB Clinical Research Facility Cork

UCC
University College Cork, Ireland
Coláiste na hOllscoile Corcaigh
School of Public Health

Tidyverse works best with tidy data

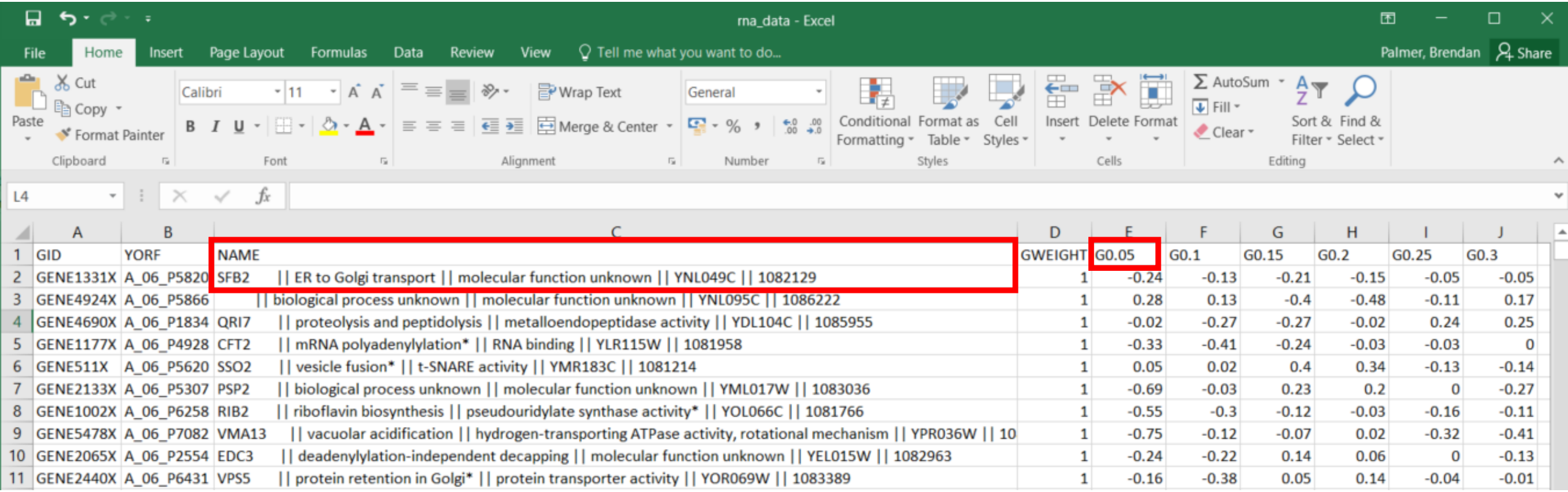
- Each variable forms a column
- Each observation forms a row

Problems with the example RNA data set…



	A	B	C	D	E	F	G	H	I	J
1	GID	YORF	NAME	GWEIGHT	G0.05	G0.1	G0.15	G0.2	G0.25	G0.3
2	GENE1331X	A_06_P5820	SFB2 || ER to Golgi transport || molecular function unknown || YNL049C || 1082129	1	-0.24	-0.13	-0.21	-0.15	-0.05	-0.05
3	GENE4924X	A_06_P5866	|| biological process unknown || molecular function unknown || YNL095C || 1086222	1	0.28	0.13	-0.4	-0.48	-0.11	0.17
4	GENE4690X	A_06_P1834	QRI7 || proteolysis and peptidolysis || metalloendopeptidase activity || YDL104C || 1085955	1	-0.02	-0.27	-0.27	-0.02	0.24	0.25
5	GENE1177X	A_06_P4928	CFT2 || mRNA polyadenylylation* || RNA binding || YLR115W || 1081958	1	-0.33	-0.41	-0.24	-0.03	-0.03	0
6	GENE511X	A_06_P5620	SSO2 || vesicle fusion* || t-SNARE activity || YMR183C || 1081214	1	0.05	0.02	0.4	0.34	-0.13	-0.14
7	GENE2133X	A_06_P5307	PSP2 || biological process unknown || molecular function unknown || YML017W || 1083036	1	-0.69	-0.03	0.23	0.2	0	-0.27
8	GENE1002X	A_06_P6258	RIB2 || riboflavin biosynthesis || pseudouridylate synthase activity* || YOL066C || 1081766	1	-0.55	-0.3	-0.12	-0.03	-0.16	-0.11
9	GENE5478X	A_06_P7082	VMA13 || vacuolar acidification || hydrogen-transporting ATPase activity, rotational mechanism || YPR036W || 10	1	-0.75	-0.12	-0.07	0.02	-0.32	-0.41
10	GENE2065X	A_06_P2554	EDC3 || deadenylylation-independent decapping || molecular function unknown || YEL015W || 1082963	1	-0.24	-0.22	0.14	0.06	0	-0.13
11	GENE2440X	A_06_P6431	VPS5 || protein retention in Golgi* || protein transporter activity || YOR069W || 1083389	1	-0.16	-0.38	0.05	0.14	-0.04	-0.01

Tidyverse works best with tidy data



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5	GENE1177X	A_06_P4928	CFT2 || mRNA polyadenylylation* || RNA binding || YLR115W || 1081958	1	-0.33	-0.41	-0.24	-0.03	-0.03	0
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11	GENE2440X	A_06_P6431	VPS5 || protein retention in Golgi* || protein transporter activity || YOR069W || 1083389	1	-0.16	-0.38	0.05	0.14	-0.04	-0.01

- Multiple variables are stored in one column
  - e.g. column "NAME" contains values such as;

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

Code structure has two main forms

(1) new_object <- function(input_data,

data_to_b_modified, arguments_to_function)

(2) new_object <- input_data %>% ← magrittr / pipe operator

function(data_to_b_modified, arguments_to_function)

Line by line

ws1_script1_stepwise_Bauer_dataset_an... *

Source on Save | Run | Source

```r
raw_gene_df <- read_delim("Brauer2008_DataSet1.tds", delim = "\t")

separated_gene_df <- separate(raw_gene_df, NAME,
                              c("name", "BP", "MF", "systematic_name",
                                "number"),
                              sep = "\\|\\|")

mutated_gene_df <- mutate_at(separated_gene_df,
                             vars(name:systematic_name),
                             funs(trimws)
                             )

selected_gene_df <- select(mutated_gene_df, -number, -GID, -YORF, -GWEIGHT)

gathered_gene_df <- gather(selected_gene_df, sample, expression, G0.05:U0.3)

nearly_there_df <- separate(gathered_gene_df, sample,
                            c("nutrient", "rate"), sep = 1, convert = TRUE)

nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
                    S = "Sulfate", N = "Ammonia", U = "Uracil")

cleaned_genes_df <- mutate(nearly_there_df,
                           nutrient = plyr::revalue(nutrient, nutrient_names)
                           ) %>%
  filter(!is.na(expression), systematic_name != "")
```

15:1 | Section 1: Data import, tidying and transformation | R Script

Console | Terminal

~/R_Users_Workshop/8_weeks_Oct-Dec_17/Workshop_1/workshop_1_project/

```
> raw_gene_df <- read_delim("Brauer2008_DataSet1.tds", delim = "\t")
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.
>
```

Environment | History | Connections

Import Dataset | Grid

Global Environment

Name	Type	Length	Size	Value
raw_gene_df	tbl_df	40	3.3 MB	5537 obs. of 40 variables

Files | Plots | Packages | Help | Viewer

New Folder | Delete | Rename | More

Home > R_Users_Workshop > 8_weeks_Oct-Dec_17 > Workshop_1 > workshop_1_project

Name	Size	Modified
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Line by line

ws1_script1_stepwise_Bauer_dataset_an... *

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raw_gene_df <- read_delim("Brauer2008_DataSet1.tds", delim = "\t")

separated_gene_df <- separate(raw_gene_df, NAME,
                              c("name", "BP", "MF", "systematic_name",
                                "number"),
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mutated_gene_df <- mutate_at(separated_gene_df,
                             vars(name:systematic_name),
                             funs(trimws)
                             )

selected_gene_df <- select(mutated_gene_df, -number, -GID, -YORF, -GWEIGHT)

gathered_gene_df <- gather(selected_gene_df, sample, expression, G0.05:U0.3)

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nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
                    S = "Sulfate", N = "Ammonia", U = "Uracil")

cleaned_genes_df <- mutate(nearly_there_df,
                           nutrient = plyr::revalue(nutrient, nutrient_names)
                           ) %>%
  filter(!is.na(expression), systematic_name != "")
```

20:1 | Section 1: Data import, tidying and transformation | R Script

Console | Terminal

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```
> raw_gene_df <- read_delim("Brauer2008_DataSet1.tds", delim = "\t")
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  GID = col_character(),
  YORF = col_character(),
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)
See spec(...) for full column specifications.
> separated_gene_df <- separate(raw_gene_df, NAME,
+                               c("name", "BP", "MF", "systematic_name",
+                                 "number"),
+                               sep = "\\|\\|")
> |
```

Environment | History | Connections

Import Dataset | Grid

Global Environment

Name	Type	Length	Size	Value
raw_gene_df	tbl_df	40	3.3 MB	5537 obs. of 40 variables
separated_gene...	tbl_df	44	3.6 MB	5537 obs. of 44 variables

Files | Plots | Packages | Help | Viewer

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Line by line

ws1_script1_stepwise_Bauer_dataset_an... *

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gathered_gene_df <- gather(selected_gene_df, sample, expression, G0.05:U0.3)

nearly_there_df <- separate(gathered_gene_df, sample,
                            c("nutrient", "rate"), sep = 1, convert = TRUE)

nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
                    S = "Sulfate", N = "Ammonia", U = "Uracil")

cleaned_genes_df <- mutate(nearly_there_df,
                           nutrient = plyr::revalue(nutrient, nutrient_names)
                           ) %>%
  filter(!is.na(expression), systematic_name != "")
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27:1 | Section 1: Data import, tidying and transformation | R Script

Console | Terminal

~/R_Users_Workshop/8_weeks_Oct-Dec_17/Workshop_1/workshop_1_project/

```
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>
```

Environment | History | Connections

Import Dataset | Grid

Global Environment

Name	Type	Length	Size	Value
mutated_gene_df	tbl_df	44	3.5 MB	5537 obs. of 44 variables
raw_gene_df	tbl_df	40	3.3 MB	5537 obs. of 40 variables
selected_gene_df	tbl_df	40	2.4 MB	5537 obs. of 40 variables
separated_gene...	tbl_df	44	3.6 MB	5537 obs. of 44 variables

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29:1 | Section 1: Data import, tidying and transformation | R Script

Console | Terminal

~/R_Users_Workshop/8_weeks_Oct-Dec_17/Workshop_1/workshop_1_project/

```
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>
```

Environment | History | Connections

Import Dataset | Grid

Global Environment

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gathered_gene_df	tbl_df	6	9.8 MB	199332 obs. of 6 variables
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32:1 | Section 1: Data import, tidying and transformation | R Script

Console | Terminal

~/R_Users_Workshop/8_weeks_Oct-Dec_17/Workshop_1/workshop_1_project/

```
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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,
+                              vars(name:systematic_name),
+                              funs(trimws)
+                              )
> selected_gene_df <- select(mutated_gene_df, -number, -GID, -YORF, -GWEIGHT)
> gathered_gene_df <- gather(selected_gene_df, sample, expression, G0.05:U0.3)
> nearly_there_df <- separate(gathered_gene_df, sample,
+                             c("nutrient", "rate"), sep = 1, convert = TRUE)
> nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
+                     S = "Sulfate", N = "Ammonia", U = "Uracil")
>
```

Environment | History | Connections

Import Dataset | Grid

Global Environment

Name	Type	Length	Size	Value
gathered_gene_df	tbl_df	6	9.8 MB	199332 obs. of 6 variables
mutated_gene_df	tbl_df	44	3.5 MB	5537 obs. of 44 variables
nearly_there_df	tbl_df	7	11.3 MB	199332 obs. of 7 variables
nutrient_names	character	6	984 B	Named chr [1:6] "Glucose" "...
raw_gene_df	tbl_df	40	3.3 MB	5537 obs. of 40 variables
selected_gene_df	tbl_df	40	2.4 MB	5537 obs. of 40 variables
separated_gene...	tbl_df	44	3.6 MB	5537 obs. of 44 variables

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Home > R_Users_Workshop > 8_weeks_Oct-Dec_17 > Workshop_1 > workshop_1_project

Name	Size	Modified
..		
.RData	2.5 KB	Oct 2, 2017, 1:49 PM
.Rhistory	20.3 KB	Dec 6, 2017, 3:43 PM
Brauer2008_DataSet1.csv	1.6 MB	Sep 27, 2017, 11:32 PM
Brauer2008_DataSet1.tds	1.6 MB	Sep 28, 2017, 10:22 AM
house_completions.csv	4 KB	Sep 28, 2017, 1:35 PM
irish_population.csv	315 B	Aug 28, 2017, 4:21 PM
raw_house_completions.csv	16.2 KB	Aug 25, 2017, 3:45 PM
workshop_1.Rproj	217 B	Oct 18, 2018, 12:18 PM
ws1_script1_stepwise_Bauer_dataset_analysis.R	6.1 KB	Dec 5, 2017, 12:19 PM
ws1_script2_Bauer_dataset_analysis.R	2 KB	Dec 6, 2017, 2:33 PM
ws1_script3_house_completions.R	2.4 KB	Oct 2, 2017, 3:53 PM

Line by line

ws1_script1_stepwise_Bauer_dataset_an... *

Source on Save | Run | Source

```r
separated_gene_df <- separate(raw_gene_df, NAME,
                              c("name", "BP", "MF", "systematic_name",
                                "number"),
                              sep = "\\|\\|")

mutated_gene_df <- mutate_at(separated_gene_df,
                             vars(name:systematic_name),
                             funs(trimws)
                             )

selected_gene_df <- select(mutated_gene_df, -number, -GID, -YORF, -GWEIGHT)

gathered_gene_df <- gather(selected_gene_df, sample, expression, G0.05:U0.3)

nearly_there_df <- separate(gathered_gene_df, sample,
                            c("nutrient", "rate"), sep = 1, convert = TRUE)

nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
                    S = "Sulfate", N = "Ammonia", U = "Uracil")

cleaned_genes_df <- mutate(nearly_there_df,
                           nutrient = plyr::revalue(nutrient, nutrient_names)
                           ) %>%
  filter(!is.na(expression), systematic_name != "")
```

44:1 | Section 1: Data import, tidying and transformation | R Script

Console | Terminal

~/R_Users_Workshop/8_weeks_Oct-Dec_17/Workshop_1/workshop_1_project/

```
> separated_gene_df <- separate(raw_gene_df, NAME,
+                               c("name", "BP", "MF", "systematic_name",
+                                 "number"),
+                               sep = "\\|\\|")
> mutated_gene_df <- mutate_at(separated_gene_df,
+                              vars(name:systematic_name),
+                              funs(trimws)
+                              )
> selected_gene_df <- select(mutated_gene_df, -number, -GID, -YORF, -GWEIGHT)
> gathered_gene_df <- gather(selected_gene_df, sample, expression, G0.05:U0.3)
> nearly_there_df <- separate(gathered_gene_df, sample,
+                             c("nutrient", "rate"), sep = 1, convert = TRUE)
> nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
+                     S = "Sulfate", N = "Ammonia", U = "Uracil")
> cleaned_genes_df <- mutate(nearly_there_df,
+                            nutrient = plyr::revalue(nutrient, nutrient_names)
+                            ) %>%
+   filter(!is.na(expression), systematic_name != "")
>
```

Environment | History | Connections

Import Dataset | Grid

Global Environment

Name	Type	Length	Size	Value
cleaned_genes_df	tbl_df	7	11.3 MB	198430 obs. of 7 variables
gathered_gene_df	tbl_df	6	9.8 MB	199332 obs. of 6 variables
mutated_gene_df	tbl_df	44	3.5 MB	5537 obs. of 44 variables
nearly_there_df	tbl_df	7	11.3 MB	199332 obs. of 7 variables
nutrient_names	character	6	984 B	Named chr [1:6] "Glucose" "...
raw_gene_df	tbl_df	40	3.3 MB	5537 obs. of 40 variables
selected_gene_df	tbl_df	40	2.4 MB	5537 obs. of 40 variables
separated_gene...	tbl_df	44	3.6 MB	5537 obs. of 44 variables

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Home > R_Users_Workshop > 8_weeks_Oct-Dec_17 > Workshop_1 > workshop_1_project

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ws1_script2_Bauer_dataset_analysis.R	2 KB	Dec 6, 2017, 2:33 PM
ws1_script3_house_completions.R	2.4 KB	Oct 2, 2017, 3:53 PM

Nested

ws1_script1_stepwise_Bauer_dataset_an... *

Source on Save | Run | Source

```r
nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
                    S = "Sulfate", N = "Ammonia", U = "Uracil")

cleaned_genes_df <-
  filter(
    mutate(
      separate(
        gather(
          select(
            mutate_at(
              separate(
                read_delim("Brauer2008_DataSet1.tds", delim = "\t"),
                NAME,
                c("name", "BP", "MF", "systematic_name",  "number"),
                sep = "\\|\\|"), vars(name:systematic_name),
              funs(trimws)),
            -number, -GID, -YORF, -GWEIGHT),
          sample, expression, G0.05:U0.3),
        sample,
        c("nutrient", "rate"),
        sep = 1, convert = TRUE),
      nutrient = plyr::revalue(nutrient, nutrient_names)),
    !is.na(expression), systematic_name != "")
```

24:1 (Top Level) R Script

Console Terminal

~/R_Users_Workshop/8_weeks_Oct-Dec_17/Workshop_1/workshop_1_project/

```
+                 sep = "\\|\\|"), vars(name:systematic_name),
+               funs(trimws)),
+             -number, -GID, -YORF, -GWEIGHT),
+           sample, expression, G0.05:U0.3),
+         sample,
+         c("nutrient", "rate"),
+         sep = 1, convert = TRUE),
+       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.
>
```

Environment | History | Connections

Import Dataset | Grid

Global Environment

Name	Type	Length	Size	Value
cleaned_genes_df	tbl_df	7	11.3 MB	198430 obs. of 7 variables
nutrient_names	character	6	984 B	Named chr [1:6] "Glucose" "Le...

Files | Plots | Packages | Help | Viewer

New Folder | Delete | Rename | More

Home > R_Users_Workshop > 8_weeks_Oct-Dec_17 > Workshop_1 > workshop_1_project

Name	Size	Modified
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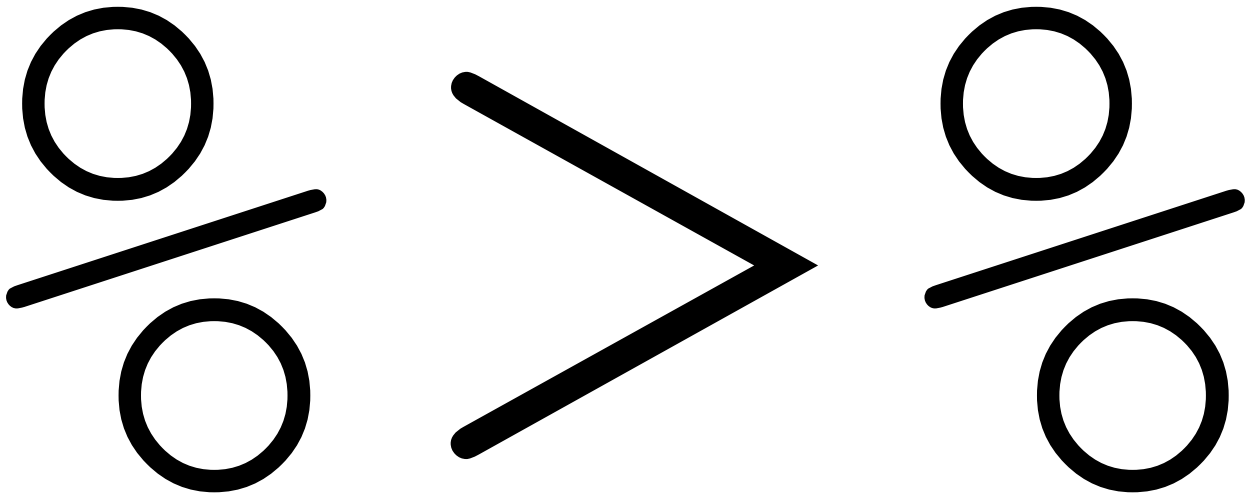
raw_house_completions.csv	16.2 KB	Aug 25, 2017, 3:45 PM
workshop_1.Rproj	217 B	Oct 18, 2018, 12:18 PM
ws1_script1_stepwise_Bauer_dataset_analysis.R	6.1 KB	Dec 5, 2017, 12:19 PM
ws1_script2_Bauer_dataset_analysis.R	2 KB	Dec 6, 2017, 2:33 PM
ws1_script3_house_completions.R	2.4 KB	Oct 2, 2017, 3:53 PM

Nested

```
nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
                    S = "Sulfate", N = "Ammonia", U = "Uracil")

cleaned_genes_df <-
  filter(
    mutate(
      separate(
        gather(
          select(
            mutate_at(
              separate(
                read_delim("Brauer2008_DataSet1.tds", delim = "\t"),
                NAME,
                c("name", "BP", "MF", "systematic_name",  "number"),
                sep = "\\|\\|"), vars(name:systematic_name),
              funs(trimws)),
            -number, -GID, -YORF, -GWEIGHT),
          sample, expression, G0.05:U0.3),
        sample,
        c("nutrient", "rate"),
        sep = 1, convert = TRUE),
      nutrient = plyr::revalue(nutrient, nutrient_names)),
    !is.na(expression), systematic_name != "")
```

Putting the pieces together



Code structure has two main forms

(1) new_object <- function(input_data,

data_to_b_modified, arguments_to_function)

(2) new_object <- input_data

function(data_to_b_modified, arguments_to_function)

Piped

ws1_script1_stepwise_Bauer_dataset_an... | ws1_script2_Bauer_dataset_analysis.R*

Source on Save | Run | Source

```r
nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
                    S = "Sulfate", N = "Ammonia", U = "Uracil"
                    )

cleaned_genes_df <- read_delim("Brauer2008_DataSet1.tds", delim = "\t"
                               ) %>%

  separate(NAME, c("name", "BP", "MF", "systematic_name", "number"), sep = "\\|\\|"
           )  %>%

  mutate_at(vars(name:systematic_name), funs(trimws)
            ) %>%

  select(-number, -GID, -YORF, -GWEIGHT
         ) %>%

  gather(sample, expression, G0.05:U0.3
         ) %>%

  separate(sample, c("nutrient", "rate"), sep = 1, convert = TRUE
           ) %>%

  mutate(nutrient = plyr::revalue(nutrient, nutrient_names)
         ) %>%

  filter(!is.na(expression), systematic_name != ""
         )
```

9:18 (Top Level) R Script

Console | Terminal

~/R_Users_Workshop/8_weeks_Oct-Dec_17/Workshop_1/workshop_1_project/

```
+
+   separate(sample, c("nutrient", "rate"), sep = 1, convert = TRUE
+            ) %>%
+
+   mutate(nutrient = plyr::revalue(nutrient, nutrient_names)
+          ) %>%
+
+   filter(!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.
> |
```

Environment | History | Connections

Import Dataset | Grid

Global Environment

Name	Type	Length	Size	Value
cleaned_genes_df	tbl_df	7	11.3 MB	198430 obs. of 7 variables
nutrient_names	character	6	984 B	Named chr [1:6] "Glucose" "Le...

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ws1_script3_house_completions.R	2.4 KB	Oct 2, 2017, 3:53 PM

Piped

```
nutrient_names <- c(G = "Glucose", L = "Leucine", P = "Phosphate",
                    S = "Sulfate", N = "Ammonia", U = "Uracil"
                    )

cleaned_genes_df <- read_delim("Brauer2008_DataSet1.tds", delim = "\t"
                               ) %>%

  separate(NAME, c("name", "BP", "MF", "systematic_name", "number"), sep = "\\|\\|"
           )  %>%

  mutate_at(vars(name:systematic_name), funs(trimws)
            ) %>%

  select(-number, -GID, -YORF, -GWEIGHT
         ) %>%

  gather(sample, expression, G0.05:U0.3
         ) %>%

  separate(sample, c("nutrient", "rate"), sep = 1, convert = TRUE
           ) %>%

  mutate(nutrient = plyr::revalue(nutrient, nutrient_names)
         ) %>%

  filter(!is.na(expression), systematic_name != ""
         )
```

Moral of the story…

You can go from this

+

tidyverse

=

To this!!

Master Builder!!