Summer R

Session 5: Joins, factors, and pivoting

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Agenda

Joins

Factors

Pivoting

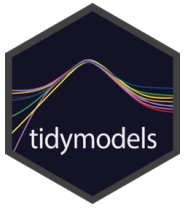
Inference and modeling

Introducing forcats, tidyr, and tidymodels

We've used dplyr for many data frame operations. In our last session, we're trying out three new packages:

- **forcats**: working with factors (categorical variables); tidyverse

- **tidyr**: restructure (pivot) a data frame; tidyverse
- **tidymodels**: inference and modeling



```r
library(tidyverse)
# includes dplyr, forcats, tidyr
library(medicaldata)

# install.packages("tidymodels")
library(tidymodels)
```

Joins

Relational data and table joins

- Much of the world's data lives in *relational database management systems* (RDBMSes), or simply "relational databases"
- Sometimes you might work with one of these directly; other times you might receive CSV files which originated in a RDBMS
- "Relational" == Table A has a relationship to Table B, via column X which appears in both tables ("foreign key relationship")
- Why relational?
  - One big table gets to be unmanageable, but we also don't want to duplicate info in the multiple places that we need it
  - Often-repeated values (e.g., a drug name) can be more efficiently stored/retrieved if they are replaced by a number, which points to the human-readable name.

Joining synthesizes a new a table from two or more parent tables.

Relationship types

- **One-to-one relationships**: one row in Table A corresponds to one row in Table B
- **One-to-many relationships**: “lookup” function; controlled vocabulary; Table B describes categories that are referenced in Table A
- **Many-to-many relationships**: there are many subjects (Table A), and many genetic markers (Table B); a patient may have an unspecified number of markers and vice versa, a relationship described in Table C

It can be helpful to have these relationships in mind when thinking about different ways we might want to join tables together.

Types of joins

Join type asks, “if I have unpaired rows when I join Tables A and B, what do I do with those rows?”

- Full join: keep all rows from both tables, filling NA as needed
- Inner join: keep only rows that appear in *both* tables
- Left join: inner join + keep all of the rows from the *left* table, filling NA as needed
- Right join: inner join + keep all of the rows from the *right* table, filling NA as needed
- Filtering joins: filter rows of Table A based on presence/absence of the row’s ID in Table B

Each of the above joins might produce a different number of rows.

```r
lg_sample <- read_csv("data/lg_sample.csv")
asa_status <- read_csv("data/asa_status.csv")
```

Consider these two tables:

```r
# 6-row sample of licorice_gargle

lg_sample %>%
  select(1:3)
```

```
# A tibble: 6 × 3
  preOp_gender preOp_asa
preOp_calcBMI
         <dbl>     <dbl>
<dbl>
1            0         2
31.3
2            0         1
32.3
3            1         3
30.5
4            0         3
32.2
5            1        NA
36.3
6            0         2
```

```r
# listing of ASA statuses

asa_status
```

```
# A tibble: 4 × 2
  asa_status_id asa_status
          <dbl> <chr>
1             1 a normal healthy
patient
2             2 a patient with mild
systemic disease
3             3 a patient with severe
systemic disease
4             4 UNUSED CATEGORY
```

full_join(): combine all data

```
1  lg_sample %>%
2    select(1:4) %>%
3    full_join(y = asa_status, by = join_by(preOp_asa == asa_status_id))
```

```
# A tibble: 7 × 5
  preOp_gender preOp_asa preOp_calcBMI preOp_age asa_status
         <dbl>     <dbl>          <dbl>     <dbl> <chr>
1            0         2           31.3        80 a patient with mild systemic
d…
2            0         1           32.3        58 a normal healthy patient
3            1         3           30.5        65 a patient with severe
systemic…
4            0         3           32.2        54 a patient with severe
systemic…
5            1        NA           36.3        56 <NA>
6            0         2           28.0        68 a patient with mild systemic
d…
7           NA         4           NA          NA UNUSED CATEGORY
```

Note 7 rows: 5 with matches in both tables; one Table A patient with no pre-op ASA status reported; and one Table B unused

`inner_join()`: keep only rows from both tables

```
lg_sample %>%
  select(1:4) %>%
  inner_join(y = asa_status, by = join_by(preOp_asa == asa_status_id))
```

```
# A tibble: 5 × 5
  preOp_gender preOp_asa preOp_calcBMI preOp_age asa_status
         <dbl>     <dbl>          <dbl>     <dbl> <chr>
1            0         2           31.3        80 a patient with mild systemic
d…
2            0         1           32.3        58 a normal healthy patient
3            1         3           30.5        65 a patient with severe
systemic…
4            0         3           32.2        54 a patient with severe
systemic…
5            0         2           28.0        68 a patient with mild systemic
d…
```

Now we have only the five rows that appear in both tables.

`left_join()`: keep rows from x

```
1  lg_sample %>%
2    select(1:4) %>%
3    left_join(y = asa_status, by = join_by(preOp_asa == asa_status_id))
```

```
# A tibble: 6 × 5
  preOp_gender preOp_asa preOp_calcBMI preOp_age asa_status
         <dbl>     <dbl>          <dbl>     <dbl> <chr>
1            0         2           31.3        80 a patient with mild systemic
d…
2            0         1           32.3        58 a normal healthy patient
3            1         3           30.5        65 a patient with severe
systemic…
4            0         3           32.2        54 a patient with severe
systemic…
5            1        NA           36.3        56 <NA>
6            0         2           28.0        68 a patient with mild systemic
d…
```

Now we have increased to 6 rows, because we kept all of the left table, including the patient with no pre-op ASA status reported.

`right_join()`: keep rows from y

```
1  lg_sample %>%
2    select(1:4) %>%
3    right_join(y = asa_status, by = join_by(preOp_asa == asa_status_id))
```

```
# A tibble: 6 × 5
  preOp_gender preOp_asa preOp_calcBMI preOp_age asa_status
         <dbl>     <dbl>          <dbl>     <dbl> <chr>
1            0         2           31.3        80 a patient with mild systemic
d…
2            0         1           32.3        58 a normal healthy patient
3            1         3           30.5        65 a patient with severe
systemic…
4            0         3           32.2        54 a patient with severe
systemic…
5            0         2           28.0        68 a patient with mild systemic
d…
6           NA         4           NA          NA UNUSED CATEGORY
```

6 rows again, but this time we have dropped the nonreporting patient, and we see instead the unused category.

`semi_join()`, `anti_join()`: filter x vs. y

Filtering joins decide which rows to keep from x, based on the presence (or absence) of the value in y

Example: you applied inclusion criteria to get a list of patient ID's to include in analysis, and now you would like to filter just those patients' records into a data frame.

```
inclusion_ids <- tibble(subject_id = c(9134, 663, 5408))

covid_testing %>%
  semi_join(y = inclusion_ids, by = join_by(subject_id))
```

```
# A tibble: 3 × 17
  subject_id fake_…¹ fake_…² gender pan_day test_id clini…³ result demo_…⁴   age
       <dbl> <chr>   <chr>   <chr>    <dbl> <chr>   <chr>   <chr>  <chr>   <dbl>
1       9134 grunt   rivers  male         7 covid   clinic… negat… patient   0.8
2        663 ithoke  targar… male         9 covid   clinic… negat… patient   0.8
3       5408 alia    ryswell female      10 covid   clinic… negat… patient   0.9
# … with 7 more variables: drive_thru_ind <dbl>, ct_result <dbl>,
#   orderset <dbl>, payor_group <chr>, patient_class <chr>, col_rec_tat <dbl>,
#   rec_ver_tat <dbl>, and abbreviated variable names ¹fake_first_name,
#   ²fake_last_name, ³clinic_name, ⁴demo_group
```

Factors

Factors

- Factors are special vectors for categorical variables
- A factor has one or more **levels** of accepted values
- Values are integers with a human-readable label
- Levels may be ordered or unordered

```
1 c("A", "B", "C", "B", "A", "B") %>% summary()
```

```
   Length     Class      Mode 
        6 character character 
```

```
1 as_factor(c("A", "B", "C", "B", "A", "B")) %>% summary()
```

```
A B C 
2 3 1 
```

Jobs involving factors

Typical things you'll need to do with factors:

- Convert character vector into factor: `as_factor()`
- Change the label associated with a level: `fct_recode()`
- Collapse two or more levels into one level (e.g., "Other"): `fct_collapse()`
- Change factor's order of levels: several functions

```
1 my_fct <- as_factor(c("A", "B", "C", "B", "A", "B"))
2
3 my_fct
```

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

```
1 my_fct %>% fct_recode(beta = "B")
```

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

```
1 my_fct %>% fct_collapse(Other = c("A", "B"))
```

```
[1] Other Other C     Other Other Other
Levels: Other C
```

```
1 my_fct %>% fct_infreq()
```

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

forcats::fct_infreq()

reorder FACTOR LEVELS by # of observations in each level

(default: largest n = 1st level)

(df)

animal	mass
alligator	281.5
cat	9.4
cat	11.6
whale	52300
alligator	427.9
cat	7.3
cat	10.8

LEVELS REORDERED BASED on COUNTS

see also:

fct_inorder: reorder by order of appearance

fct_reorder: reorder by another variable

fct_relevel: reorder manually

+ more!

forcats.tidyverse.org

Artwork by @allison_horst

ICA 5.1: Joins and factors

Pivoting

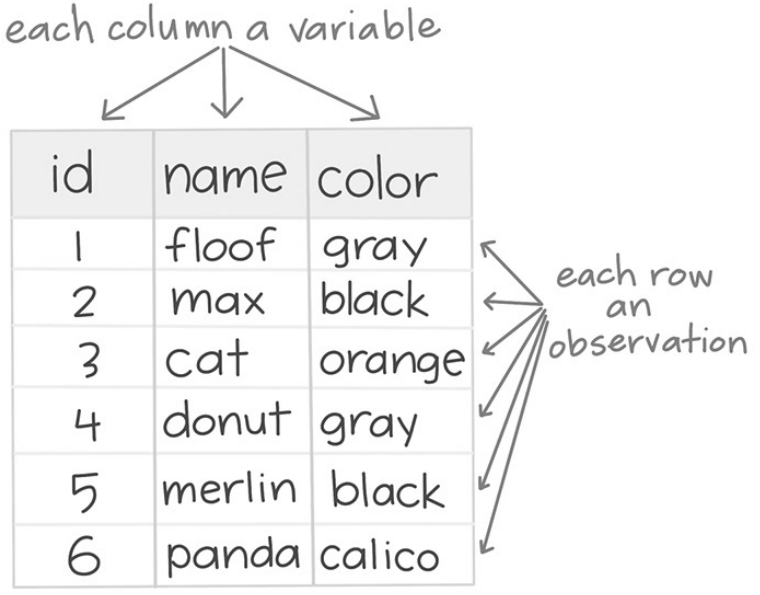
Pivoting: what and why

- To “pivot” tabular data means to restructure part of it in terms of column and row definition
- Example: a variable described by *one column per year* of interest
  - But ggplot expects all values to be in the same column
  - Solution: all values into a new `value` column, and each year into a new `year` column
  - n columns $\rightarrow$ 2 columns
- The goal is often “tidy data”: one observation per row, one variable per column

> TIDY DATA is a standard way of mapping the meaning of a dataset to its structure.
>
> –HADLEY WICKHAM

In tidy data:

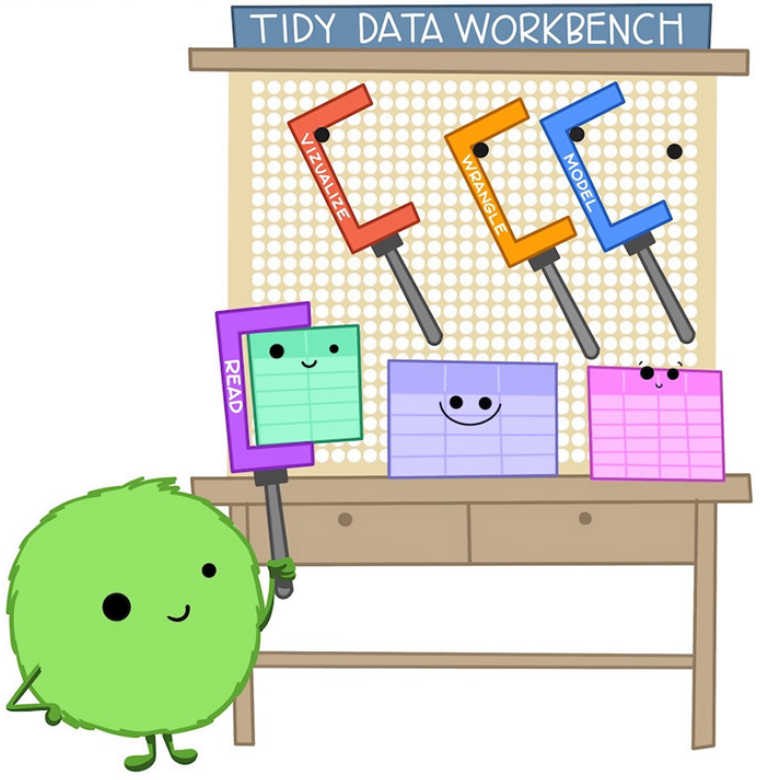
- each variable forms a column
- each observation forms a row
- each cell is a single measurement



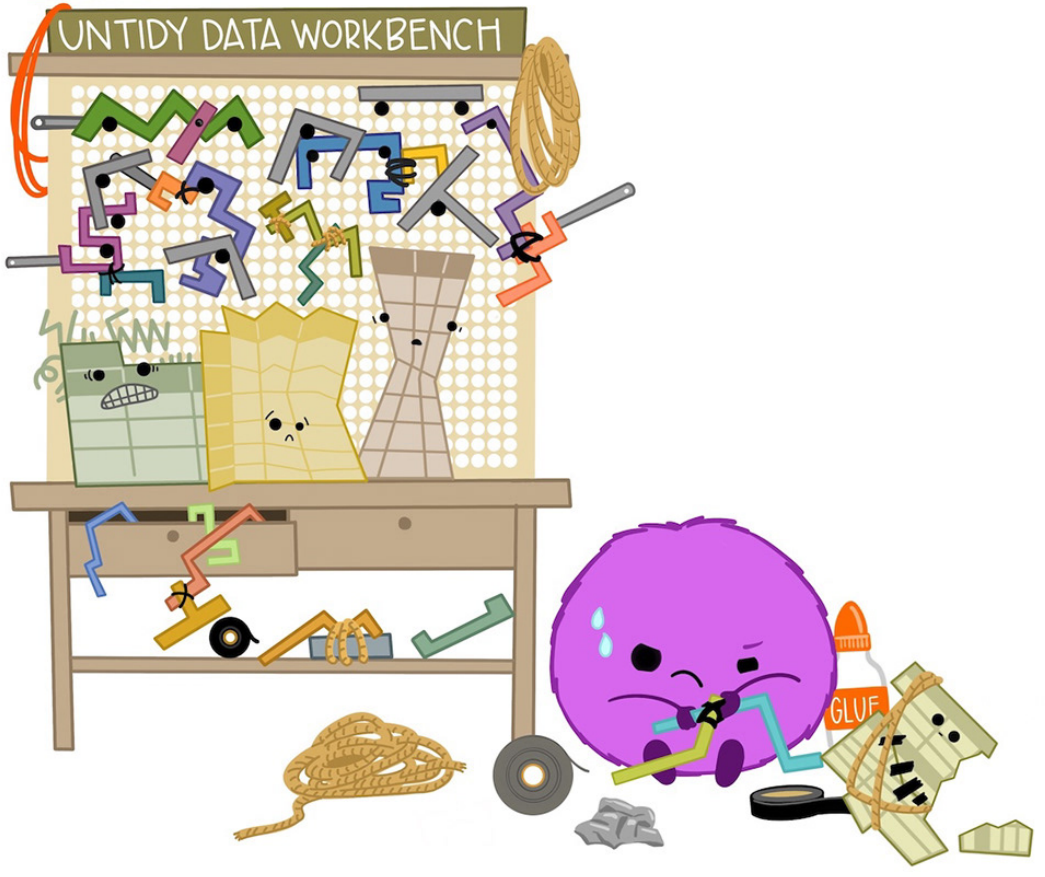
Wickham, H. (2014). Tidy Data. Journal of Statistical Software *59* (10). DOI: 10.18637/jss.v059.i10

Artwork by @allison_horst

When working with tidy data, we can use the same tools in similar ways for different datasets...



...but working with untidy data often means reinventing the wheel with one-time approaches that are hard to iterate or reuse.



Artwork by @allison_horst

`pivot_longer()`

- For when you need reduce the number of columns, making the table *longer* with more rows
- Or: when multiple *observations* are compressed into a single row
- Note required arguments (given in example below)
- Example: annual teen birth counts by state, one column for each year (2013-19); source: CDC
  - `cols =` the year columns (`` `2013`:`2019` ``)
  - `names_to =` new column where you want the years recorded (`year`)
  - `values_to =` new column where you want the values recorded (`births`)

Before pivoting

```
1  teen_births %>% print(width=58)
```

```
# A tibble: 52 × 8
# Groups:   State [52]
   State  `2013` `2014` `2015` `2016` `2017` `2018`
`2019`
   <chr>   <dbl>  <dbl>  <dbl>  <dbl>  <dbl>  <dbl>
<dbl>
 1 Alaba…  10784  10018   9478   8960   8482   7848
7910
 2 Alaska   1416   1290   1324   1166    972    846
786
 3 Arizo…  14464  13244  11820  10714  10050   9300
8636
 4 Arkan…   8310   7564   7354   6744   6356   5856
5764
 5 Calif…  61010  54050  48350  42824  37870  33858
30712
 6 Color…   7668   6754   6540   6136   5580   5044
4942
 7 Conne…   3212   2840   2482   2272   2106   1976
1804
 8 Delaw…   1456   1232   1080   1166   1104    994
888
```

After pivoting longer

```
1  teen_births %>%
2    pivot_longer(cols = `2013`:`2019`,
3                 names_to = "year",
4                 values_to = "births")
```

```
# A tibble: 364 × 3
# Groups:   State [52]
   State    year  births
   <chr>    <chr>  <dbl>
 1 Alabama  2013   10784
 2 Alabama  2014   10018
 3 Alabama  2015    9478
 4 Alabama  2016    8960
 5 Alabama  2017    8482
 6 Alabama  2018    7848
 7 Alabama  2019    7910
 8 Alaska   2013    1416
 9 Alaska   2014    1290
10 Alaska   2015    1324
# … with 354 more rows
```

Data source: CDC

`pivot_wider()`

- For when you need to increase the number of columns, making the table *wider* with fewer rows
- Rare that you will need to use this for tidying; usually for generating a summary/comparison table, or for transforming to the format expected by another tool
- Note required arguments `names_from`, `values_from`

ICA 5.2: Pivoting

Inference and modeling

Checking for normality: histogram + theoretical

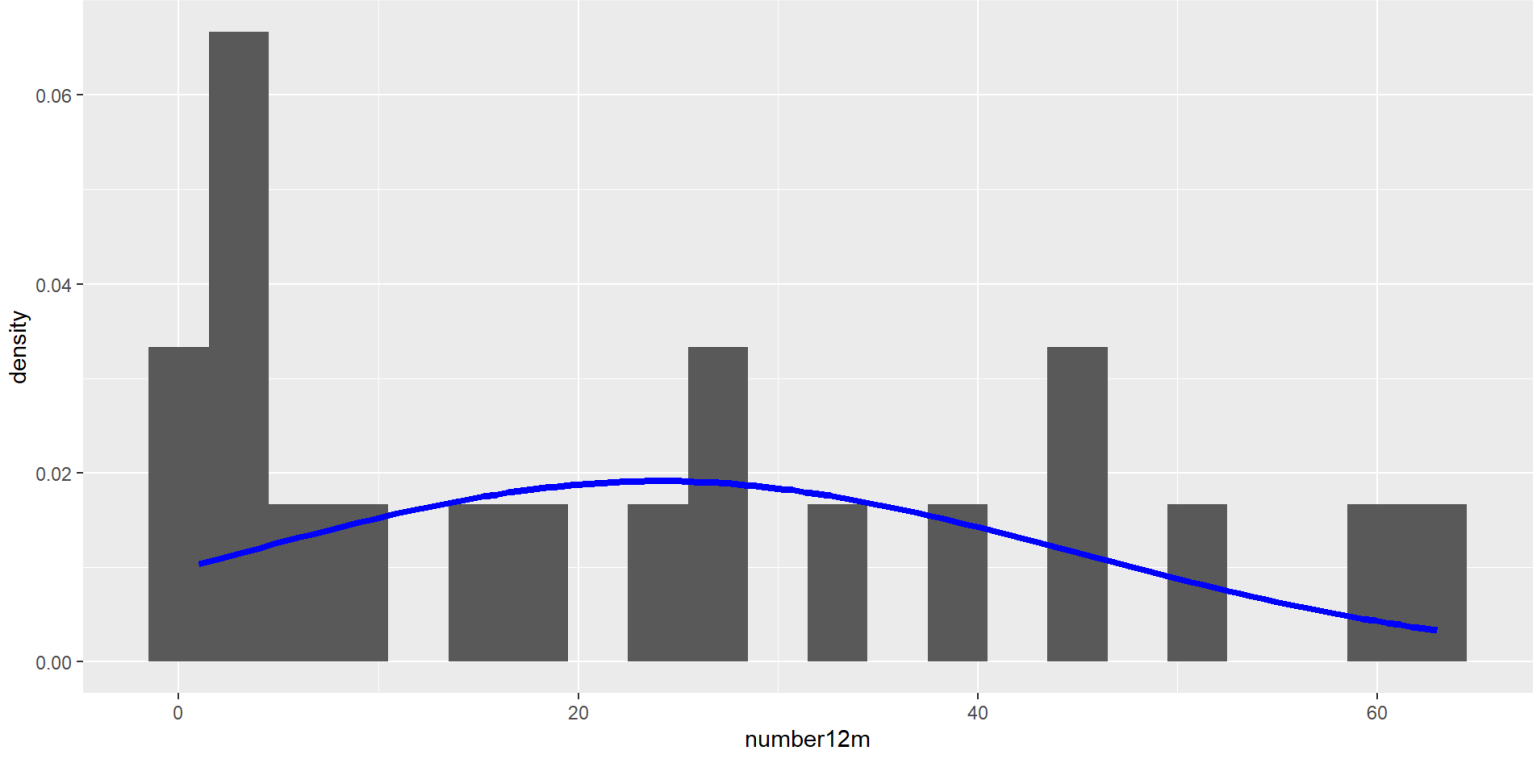
The ggplot2 `stat_function()` layer allows you to plot various statistical functions (such as a theoretical distribution). Note that for the two layers to be compatible, we transform the histogram's `y` to density. `dnorm()` is the base R function for the Normal distribution.

```
mu <- mean(polyps$number12m, na.rm=TRUE)
sigma <- sd(polyps$number12m, na.rm=TRUE)

polyps %>%
  drop_na(number12m) %>%
  ggplot() +
  geom_histogram(aes(x=number12m, y=after_stat(density)), binwidth = 3) +
  stat_function(fun=dnorm, geom="line", color="blue", linewidth=1.5,
                args=list(mean=mu, sd=sigma))
```

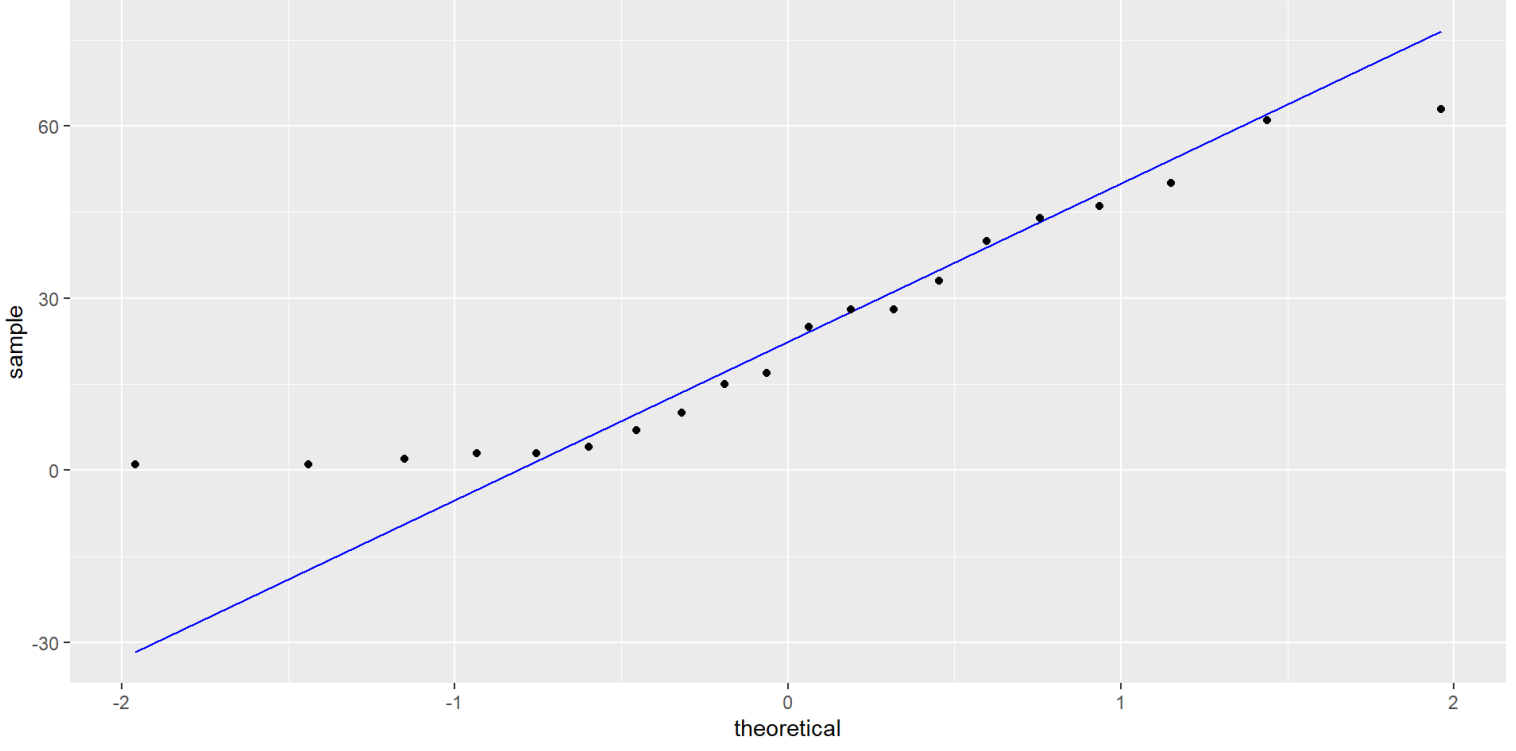
```r
mu <- mean(polyps$number12m, na.rm=TRUE)
sigma <- sd(polyps$number12m, na.rm=TRUE)

polyps %>%
  drop_na(number12m) %>%
  ggplot() +
  geom_histogram(aes(x=number12m, y=after_stat(density)), binwidth = 3) +
  stat_function(fun=dnorm, geom="line", color="blue", linewidth=1.5,
                args=list(mean=mu, sd=sigma))
```



Checking for normality: Q-Q plot

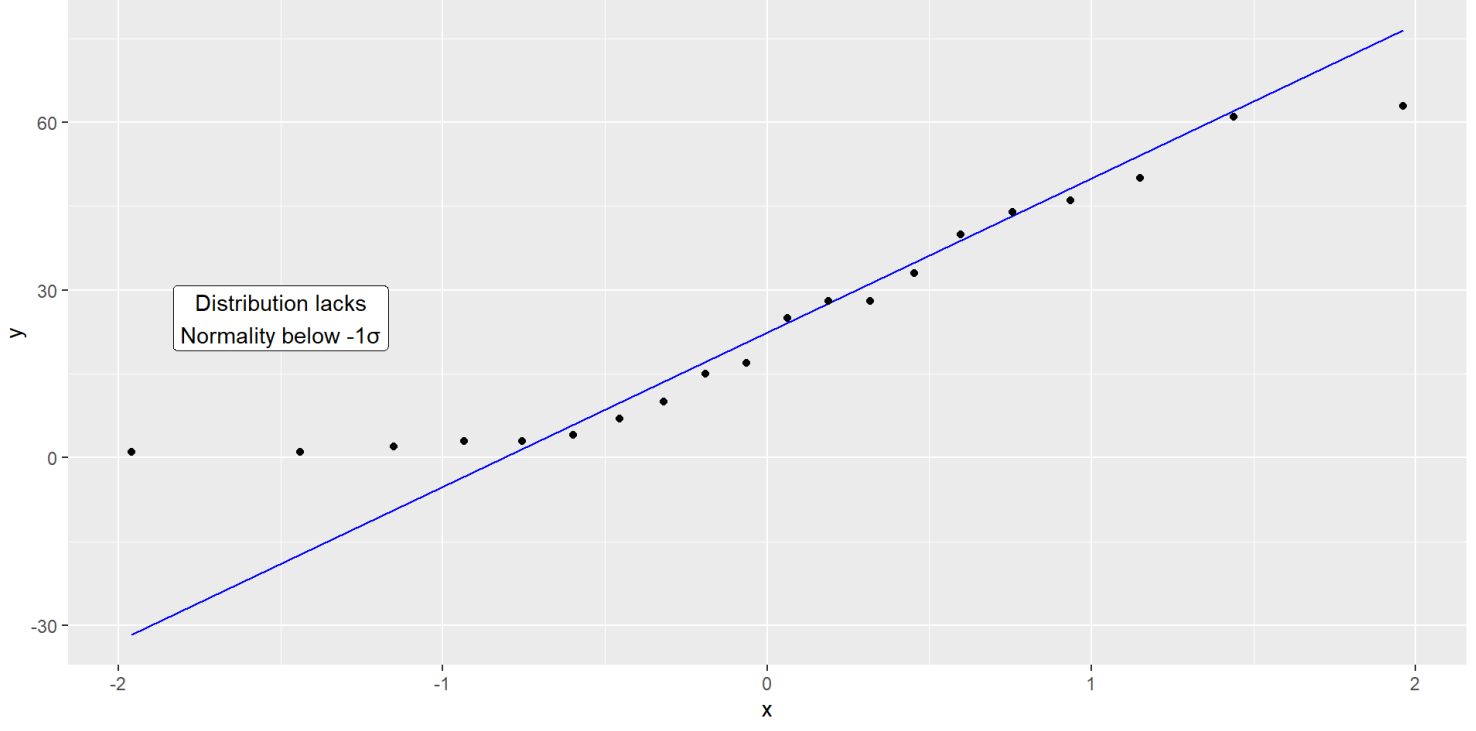
```
num12m_qqp <- polyps %>%
  drop_na(number12m) %>%
  ggplot(aes(sample=number12m)) +
  geom_qq_line(color="blue") +
  geom_qq()
num12m_qqp
```



Sidebar: plot annotations

`annotate()` is an additional ggplot layer you can add to plots:

```
num12m_qqp <- num12m_qqp +
  annotate(geom="label", x=-1.5, y=25,
           label="Distribution lacks\nNormality below -1σ")
num12m_qqp
```



Sidebar: saving plots

`ggplot2::ggsave()` allows us to save plot objects in a variety of formats and parameters. Here are example calls:

```
# scalable vector graphics (SVG) format:
ggsave(filename="num12m-qq.svg", plot=num12m_qqp)

# 500 x 400 px PNG file, 100dpi:
ggsave(filename="num12m-qq.png", plot=num12m_qqp,
       width=500, height=400, units="px", dpi=100)

# 4 in. x 6 in. PDF, 300dpi:
ggsave(filename="num12m-qq.pdf", plot=num12m_qqp,
       width=4, height=6, units="in")
# note that this plot will be in a portrait format
```

Inference and modeling - the base R way

- A variety of functions are available depending on the test / probability distribution / regression you need
- These functions usually expect vectors as input; usually produce some printable object (`summary()` also usable)
- Student's t-test: `t.test()`
- Chi-squared test: `chisq.test()` (note: expects a matrix for 2-way)
- Linear model: `lm()` with `predict()`

These functions can be compatible with tidyverse work (but not `%>%`)

Are mean 12-month counts significantly different between sulindac (treatment) and placebo groups?

```r
sulindac12m <- polyps %>%
  filter(treatment == "sulindac") %>%
  pull(number12m)
sulindac12m
```

```
[1] NA  2 17  1 25  3 33 NA  3  1  4
```

```r
placebo12m <- polyps %>%
  filter(treatment == "placebo") %>%
  pull(number12m)
placebo12m
```

```
[1] 63 28 61  7 15 44 28 10 40 46 50
```

```r
t.test(sulindac12m, placebo12m)
```

```
    Welch Two Sample t-test

data:  sulindac12m and placebo12m
t = -3.6114, df = 16.901, p-value = 0.002172
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 -40.79597 -10.69898
sample estimates:
mean of x mean of y
 9.888889 35.636364
```

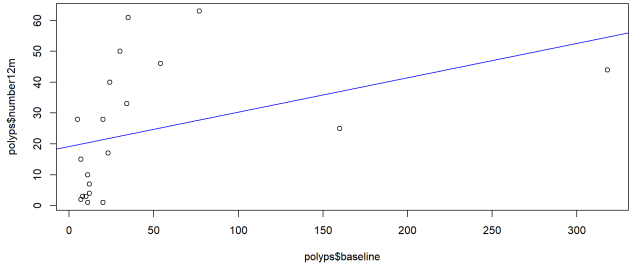
Is there a relationship between baseline and 12-month counts?

```r
polyps_model <- lm(number12m ~ baseline, data=polyps)
polyps_model
```

```
Call:
lm(formula = number12m ~ baseline, data = polyps)

Coefficients:
(Intercept)     baseline
    19.1647       0.1113
```

```r
plot(polyps$baseline, polyps$number12m)
abline(polyps_model, col="blue")
```



What 12-month count does this model predict for a baseline of 50? of 100?

```r
new_baseline <- tibble(
  baseline = c(50, 100)
)
predict(polyps_model, newdata=new_baseline)
```

```
       1        2
24.72882 30.29290
```

Inference and modeling - the tidymodels way

- Specifically, the {infer} and {parsnip} packages
- New verbs for the tidyverse pipeline: (or you can use wrappers like `t_test()`)
  - `specify()` variable/relationship of interest
  - `hypothesize()` the null hypothesis
  - `generate()` (or simulate if theoretical) the null distribution
  - `calculate()` a test statistic like `Chisq, F, t,` or `z`
- Good vignettes for getting started: Getting to Know infer, Introduction to parsnip

Are mean 12-month counts significantly different between sulindac (treatment) and placebo groups?

```r
# infer::t_test()

polyps %>%
  t_test(response = number12m,
         explanatory = treatment)
```

```
# A tibble: 1 × 7
  statistic  t_df p_value alternative estimate lower_ci upper_ci
      <dbl> <dbl>   <dbl> <chr>          <dbl>    <dbl>    <dbl>
1      3.61  16.9 0.00217 two.sided       25.7     10.7     40.8
```

Is there a relationship between baseline and 12-month counts?

```r
# parsnip::linear_reg()

polyps_model <- linear_reg() %>%
  set_engine("lm") %>%
  fit(number12m ~ baseline, data = polyps)
polyps_model
```

```
parsnip model object


Call:
stats::lm(formula = number12m ~ baseline, data = data)

Coefficients:
(Intercept)     baseline
    19.1647       0.1113
```

What 12-month count does this model predict for a baseline of 50? of 100?

```r
new_baseline <- tibble(
  baseline = c(50, 100)
)
predict(polyps_model, new_baseline)
```

```
# A tibble: 2 × 1
  .pred
  <dbl>
1  24.7
2  30.3
```

Plotting a model (without `geom_smooth`)

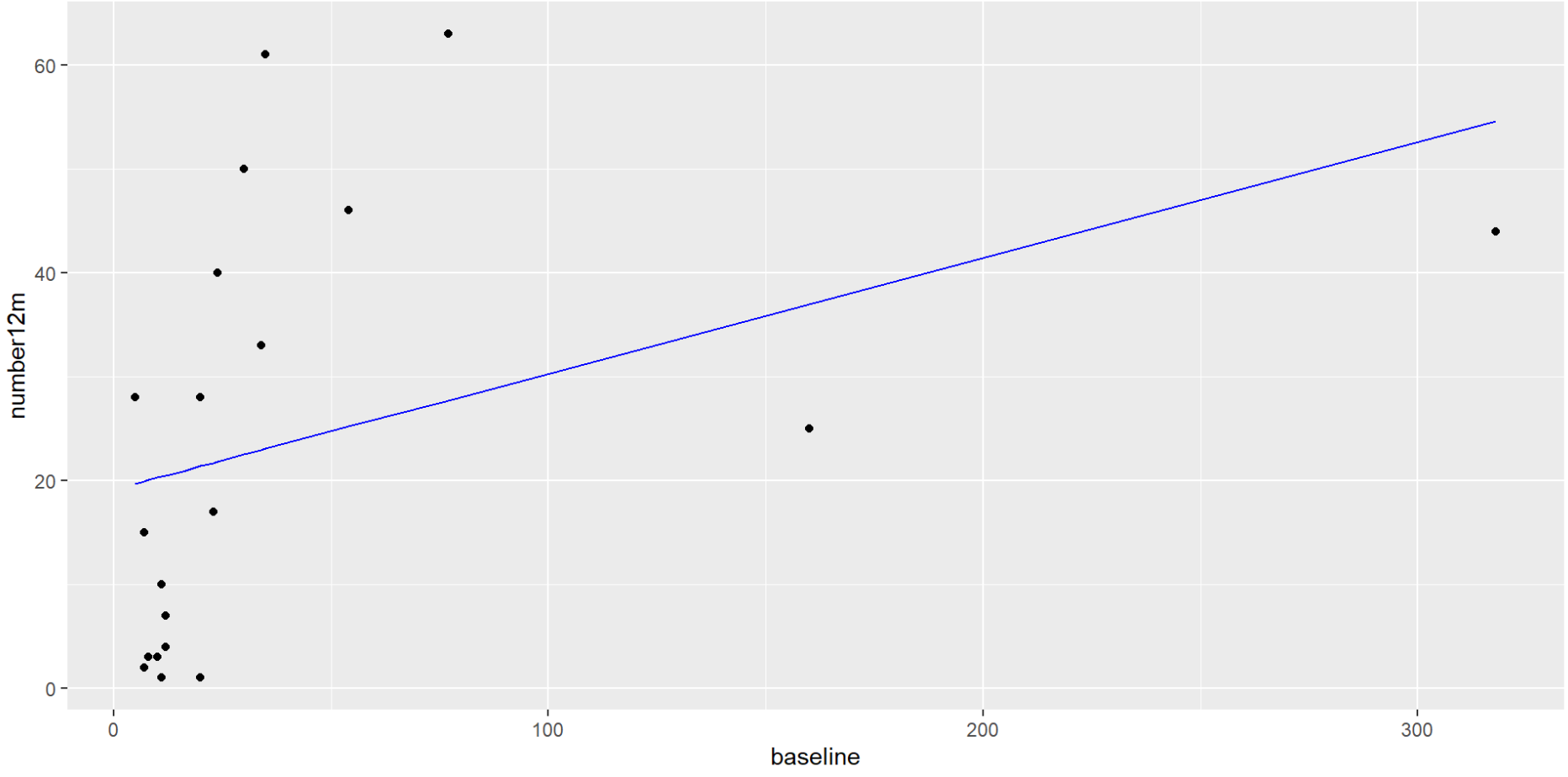
Run `predict()` on a data frame of your explanatory values. Then bind the predicted column back with the original data frame and plot the predictions with their own `geom_line()`.

```
baseline_df <- polyps %>%
  select(baseline)

predicted_df <- predict(polyps_model, new_data = baseline_df) %>%
  rename(predicted_12m = ".pred") %>%
  mutate(predicted_12m = round(predicted_12m, 1))
predicted_df
```

```
# A tibble: 22 × 1
   predicted_12m
           <dbl>
 1          19.9
 2          27.7
 3          19.9
 4          19.7
 5          21.7
 6          23.1
 7          20.4
 8          20.5
 9          19.9
10          54.6
# … with 12 more rows
```

```r
polyps %>%
  bind_cols(predicted_df) %>%
  ggplot() +
  geom_point(aes(x=baseline, y=number12m)) +
  geom_line(aes(x=baseline, y=predicted_12m),
            color="blue")
```



ICA 5.3: Inference and modeling

Wrap up

Conclusion

We learned about:

- joining tables to combine data
- working with factors for categorical variables
- pivoting a data frame to restructure it
- what inference and modeling look like in R

Potential next directions

- Exploring more of tidymodels
- Computational Genomics with R (free ebook)
- …or one of many other topics in the Big Book of R directory

Always feel free to reach out! dbordelon@pitt.edu