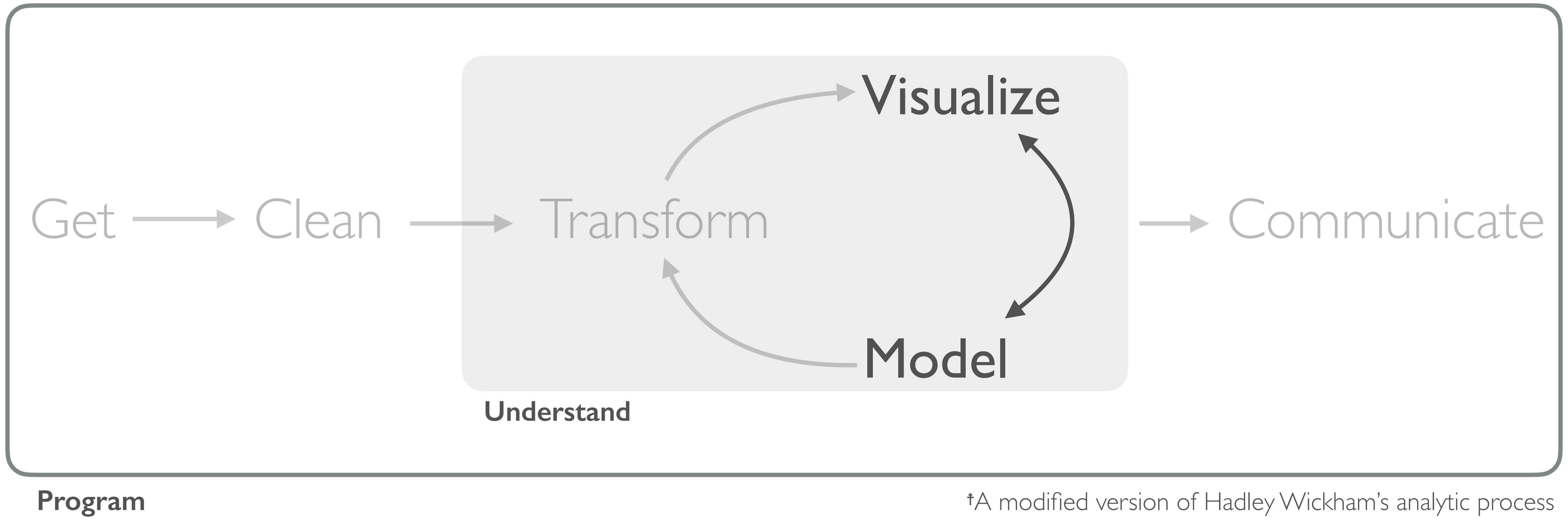
MODELING BASICS



†A modified version of Hadley Wickham's analytic process

"All models are wrong, but some are useful."

– George Box

INTRODUCTION TO APPLIED MODELING

The next three sections are not going to give you a deep understanding of the mathematical theory that underlies models.

They are meant to build your intuition about how modeling works within R, and to give you a family of useful tools that allow you to use models to better understand your data through:

1. modeling basics
2. model building
3. managing many models

INTRODUCTION TO APPLIED MODELING

These sections may feel overwhelming but they are meant to give you a flavor of what you can do in R and to begin preparing you for the Applied Analytics with R course.

We will apply purposeful model specifications

PREREQUISITES

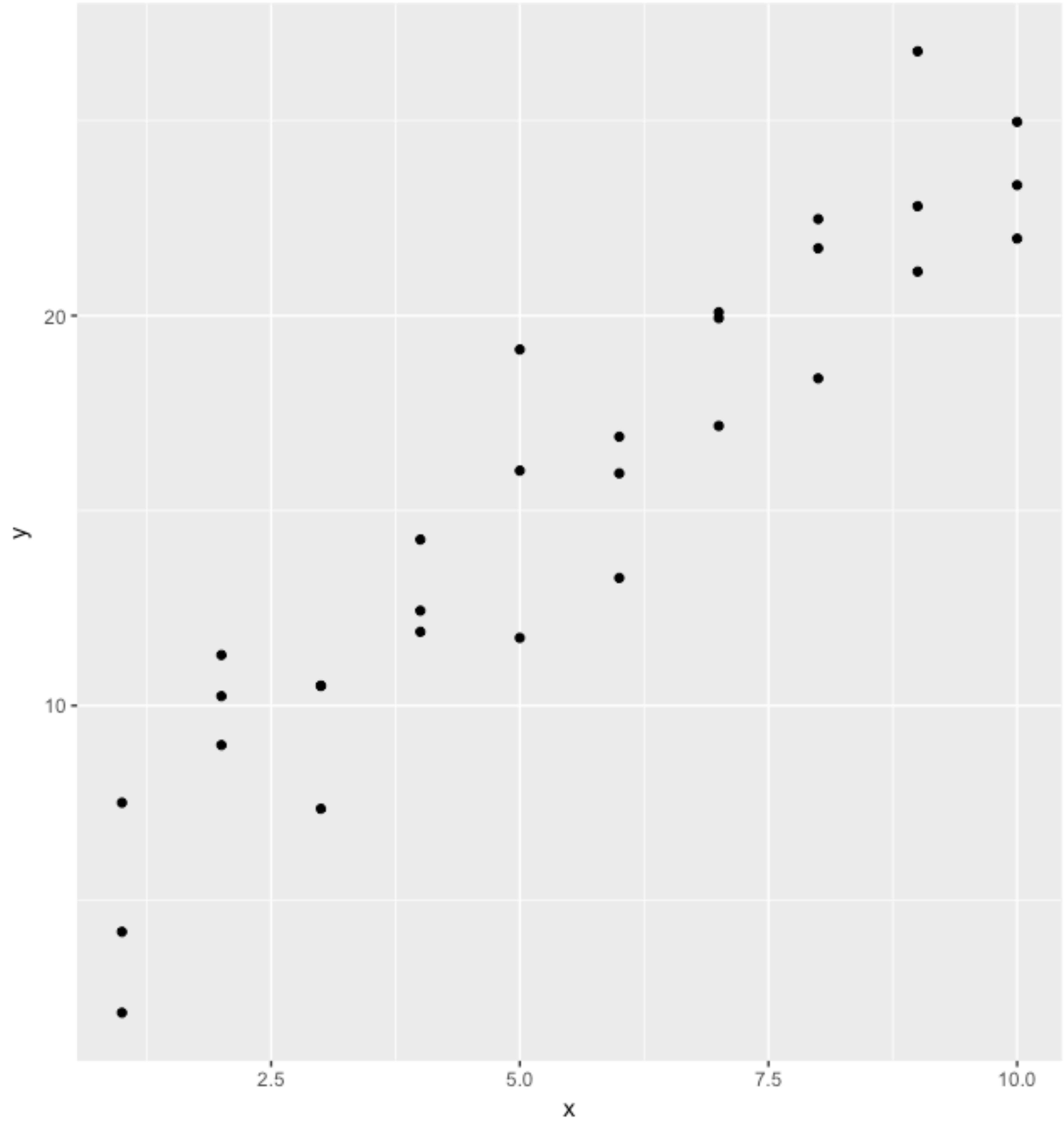
PREREQUISITES

```
library(tidyverse)

library(modelr)

options(na.action = na.warn)
```

PRE-MODELING

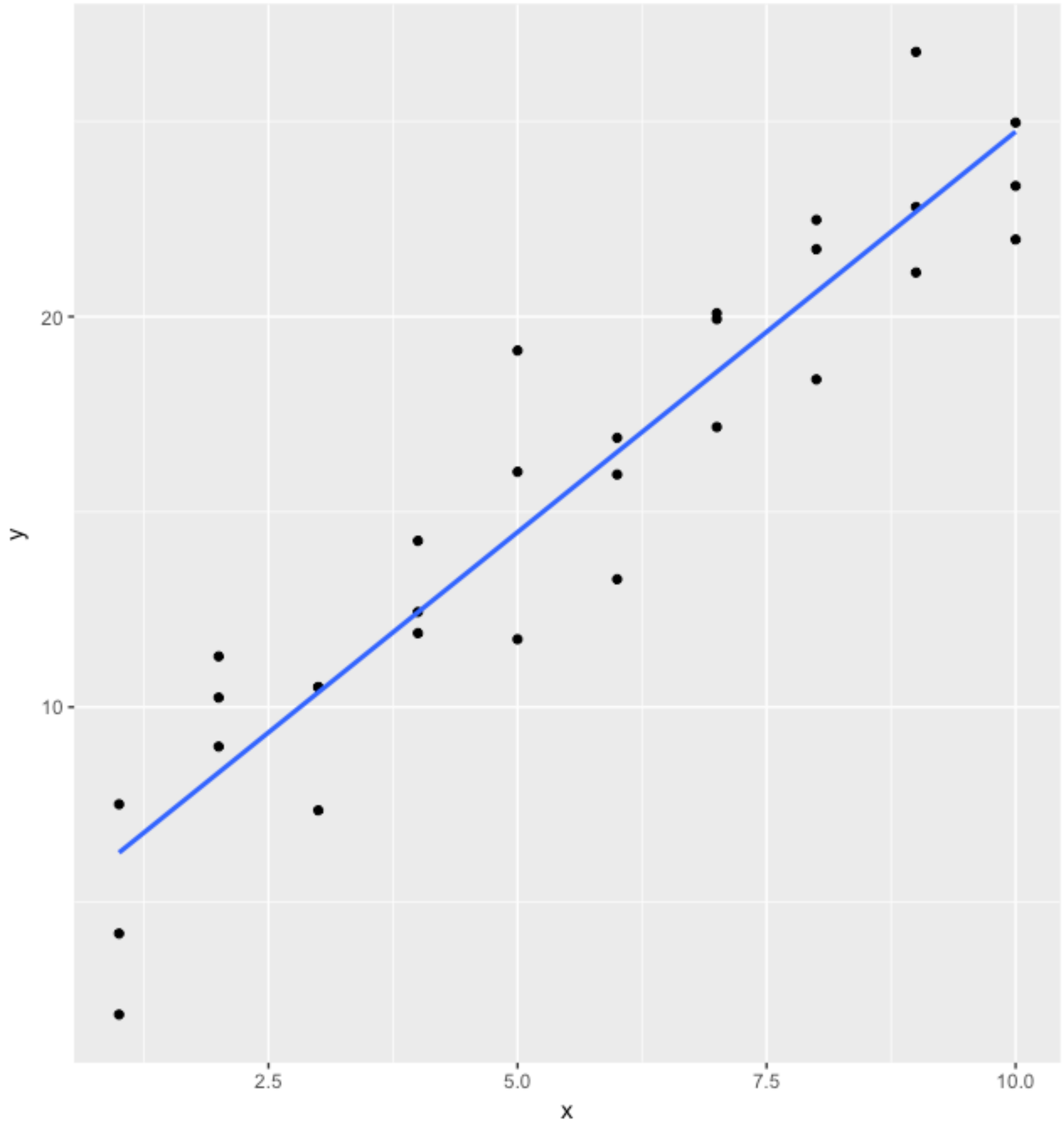
IDENTIFYING (LINEAR) RELATIONSHIPS

```
ggplot(sim1, aes(x, y)) +
  geom_point()
```



IDENTIFYING (LINEAR) RELATIONSHIPS

```
ggplot(sim1, aes(x, y)) +
  geom_point() +
  geom_smooth(method = "lm", se = FALSE)
```



MEASURING (LINEAR) RELATIONSHIPS

```
cor(sim1$x, sim1$y)
[1] 0.9405384
```

Correlation measures the linear relationship between two variables

Can be an indicator of a predictive relationship to be exploited but does not mean it should be…

nor does it imply a causal relationship

MEASURING (LINEAR) RELATIONSHIPS

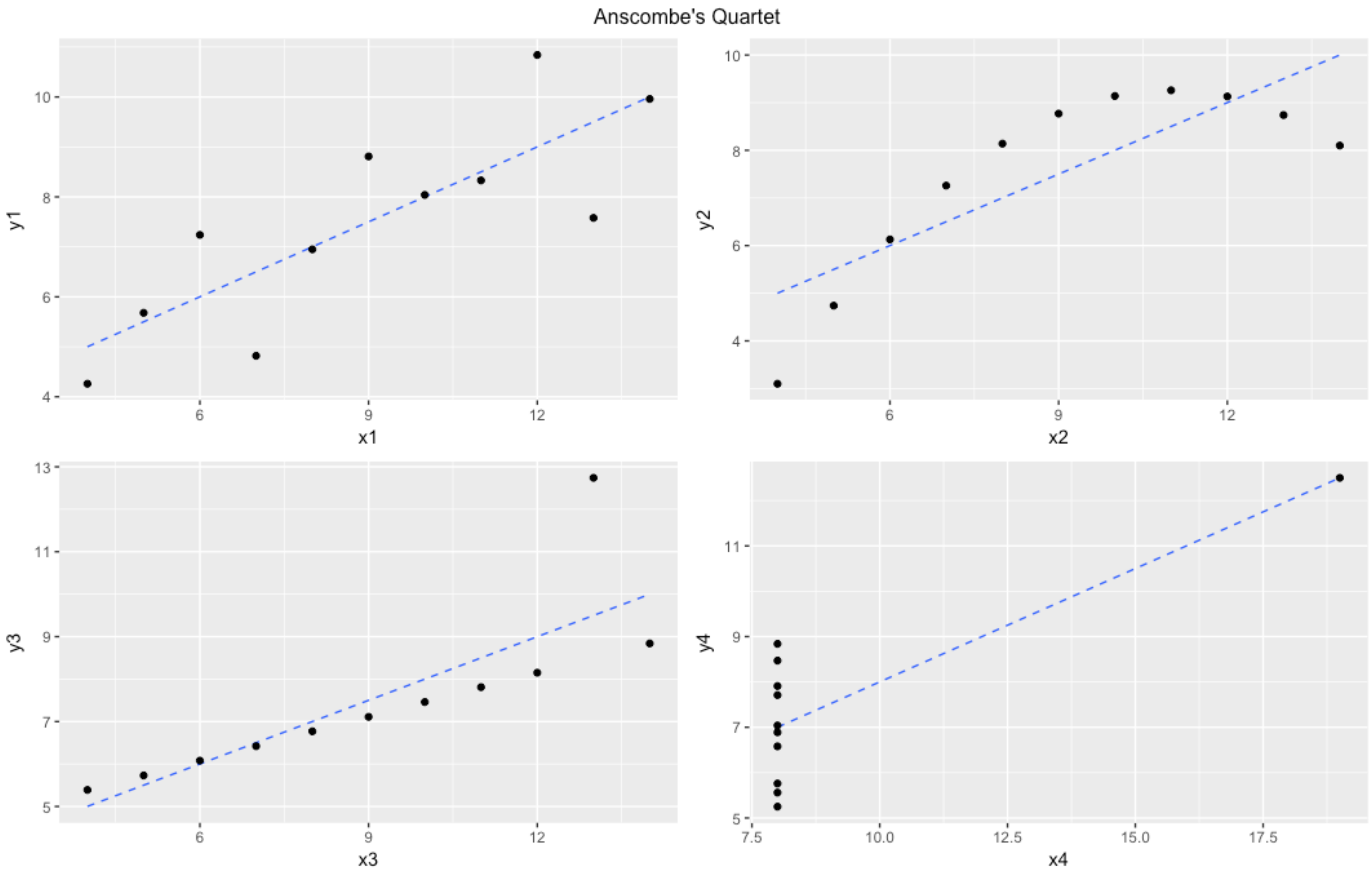
```
cor.test(sim1$x, sim1$y)
 Pearson's product-moment correlation

data:  sim1$x and sim1$y
t = 14.651, df = 28, p-value = 1.173e-14
alternative hypothesis: true correlation is not
equal to 0
95 percent confidence interval:
 0.8776625 0.9715879
sample estimates:
      cor
0.9405384
```

The `cor()` function provides the correlation coefficient…

but `cor.test()` provides additional insights

WHY IS VISUALIZING RELATIONSHIPS IMPORTANT?

WHY IS VISUALIZING RELATIONSHIPS IMPORTANT?



4 different data sets

4 different relationships

All have `cor(x, y) = .816`

Don’t interpret numbers blindly!

YOUR TURN!

- *Assess the linear relationship between* `mpg` *and* `wt` *in the* `mtcars` *data set*
- *How could you do this using* `dplyr` *(hint:* `summarise()`*)?*
- *How could you visually compare a linear vs. non-linear relationship (hint:* `geom_smooth()`*)?*

MULTIPLE RELATIONSHIPS

```
sim4
# A tibble: 300 × 4
      x1         x2   rep           y
   <dbl>      <dbl> <int>       <dbl>
1     -1 -1.0000000     1  4.24767769
2     -1 -1.0000000     2  1.20599701
3     -1 -1.0000000     3  0.35347770
4     -1 -0.7777778     1 -0.04665814
5     -1 -0.7777778     2  4.63868987
6     -1 -0.7777778     3  1.37709540
7     -1 -0.5555556     1  0.97522088
8     -1 -0.5555556     2  2.49963753
9     -1 -0.5555556     3  2.70474837
10    -1 -0.3333333     1  0.55751522
# ... with 290 more rows
```

What if we want to look for multiple relationships?

MULTIPLE RELATIONSHIPS

```
cor(sim4)
               x1            x2        rep           y
x1   1.000000e+00 -8.870745e-21 0.00000000  0.38941683
x2  -8.870745e-21  1.000000e+00 0.00000000 -0.59481723
rep  0.000000e+00  0.000000e+00 1.00000000  0.02629568
y    3.894168e-01 -5.948172e-01 0.02629568  1.00000000

pairs(sim4)
```

What if we want to look for multiple relationships?

`cor()` will work on a full data frame (assuming all variables are numeric)

`pairs()` will provide x-y scatter plot pairs

MULTIPLE RELATIONSHIPS

```
sim4 %>%
  gather(var, value, -y) %>%
  group_by(var) %>%
  summarise(corr = cor(y, value),
            p_value = cor.test(y, value)$p.value) %>%
  filter(p_value < 0.05)
# A tibble: 2 × 3
    var       corr      p_value
  <chr>      <dbl>        <dbl>
1    x1  0.3894168 2.656616e-12
2    x2 -0.5948172 4.279573e-30
```

…but this can still be difficult to see the strongest patterns

nor do we get the p-values to tell which linear relationships are insignificant

we can get this info by leveraging **`tidyr`** and **`dplyr`** functions

Work through this code line by line to see how it works

YOUR TURN!

- *Visualize relationships across all* **`mtcars`** *variables; which ones appear to have the strongest relationship to* **`mpg`?**
- *Quantify the correlations and find the ones that are statistically significant at $p <= 0.05$*

MANY QUESTIONS REMAIN

Many questions remain such as:

- What can we infer from these relationships (other than just strength)
- How should we treat categorical variables
- Are there interactions between variables
- How well do these variables predict an output
- and a host of others

We can <u>start</u> to answer some of these questions with regression modeling

MODELING BASICS

MODELS AS AN EDA TOOL

Here we are going to use models as a tool for exploratory analysis, not confirmatory analysis

In Applied Analytics with R you will learn how to use regression models for confirmatory analysis which includes:

- Partitioning your data for training, querying, and testing your model
- A more in-depth assessment of model performance
- Correct hypothesis inference

MODEL FORMULAE IN R

```
response variable ~ explanatory variable(s)
```

Read ~ as "is modeled as a function of"

MODEL FORMULAE IN R

`response variable ~ explanatory variable(s)`

`Read ~ as "is modeled as a function of"`

Thus, a simple linear regression of `y` on `x` would be written as:

```
y ~ x
```

MODEL FORMULAE IN R

`response variable ~ explanatory variable(s)`

`Read ~ as "is modeled as a function of"`

`Thus, a simple linear regression of y on x would be written as:`

```
y ~ x
```

And a one-way ANOVA where sex is a two-level factor would be written as:

```
y ~ sex
```

MODEL FORMULAE IN R

```
sim1$y ~ sim1$x
str(sim1$y ~ sim1$x)
```

Execute these in R, what do they do?

MODEL FORMULAE IN R

```
sim1$y ~ sim1$x
str(sim1$y ~ sim1$x)
Class 'formula'  language sim1$y ~ sim1$x
  ..- attr(*, ".Environment")=<environment:
R_GlobalEnv>
```

Execute these in R, what do they do?

They simply create a formula object but we need a function to model this formula

LINEAR MODEL FUNCTION

```
sim1_mod <- lm(y ~ x, data = sim1)
```

In R, `lm()` is the function to perform a linear model.

LINEAR MODEL FUNCTION

```
sim1_mod <- lm(y ~ x, data = sim1)
sim1_mod
Call:
lm(formula = y ~ x, data = sim1)

Coefficients:
(Intercept)            x
      4.221        2.052
```

In R, `lm()` is the function to perform a linear model.

This creates an object that contains a lot of results from the `lm()` model

LINEAR MODEL FUNCTION

```
sim1_mod <- lm(y ~ x, data = sim1)
sim1_mod
summary(sim1_mod)
Call:
lm(formula = y ~ x, data = sim1)

Residuals:
    Min      1Q  Median      3Q     Max
-4.1469 -1.5197  0.1331  1.4670  4.6516

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   4.2208     0.8688   4.858 4.09e-05 ***
x             2.0515     0.1400  14.651 1.17e-14 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.203 on 28 degrees of freedom
```

In R, `lm()` is the function to perform a linear model.

This creates an object that contains a lot of results from the `lm()` model

`summary()` prints off many useful results

LINEAR MODEL FUNCTION

```
sim1_mod <- lm(y ~ x, data = sim1)
sim1_mod
summary(sim1_mod)
str(sim1_mod)
coef(sim1_mod)
residuals(sim1_mod)
fitted.values(sim1_mod)
```

The `lm()` object is just a list so we can access many results just by knowing their names

Try these functions

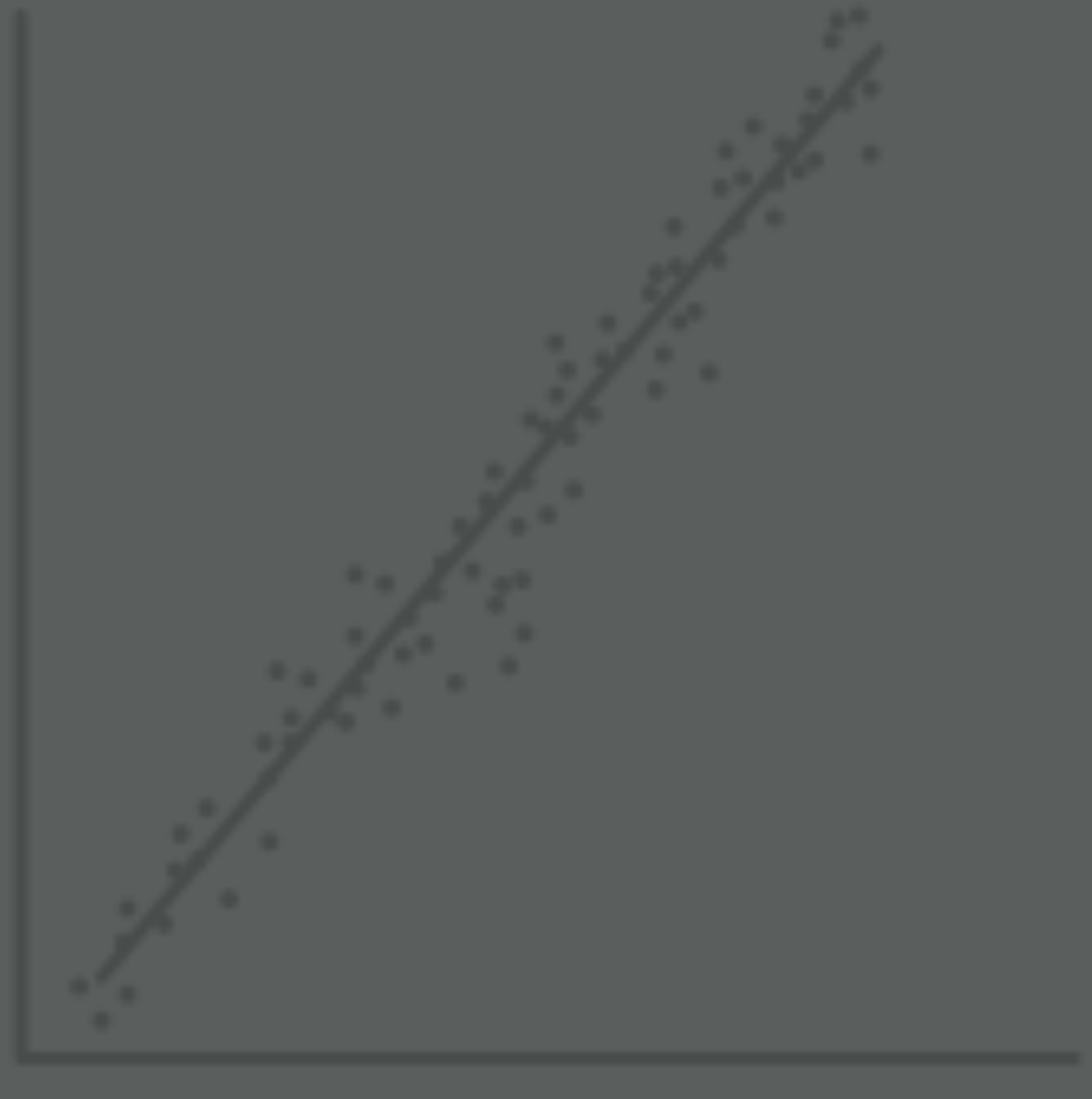
YOUR TURN!

1. *Fit a linear model that regresses* **`mpg`** *onto* **`wt`** *with the* **`mtcars`** *data*

2. *How does this model appear to fit (hint: summary)?*

3. *Can you access the fitted (aka predicted) values and residuals?*

VISUALIZING MODELS



DO OUR RELATIONSHIPS HOLD VISUALLY?

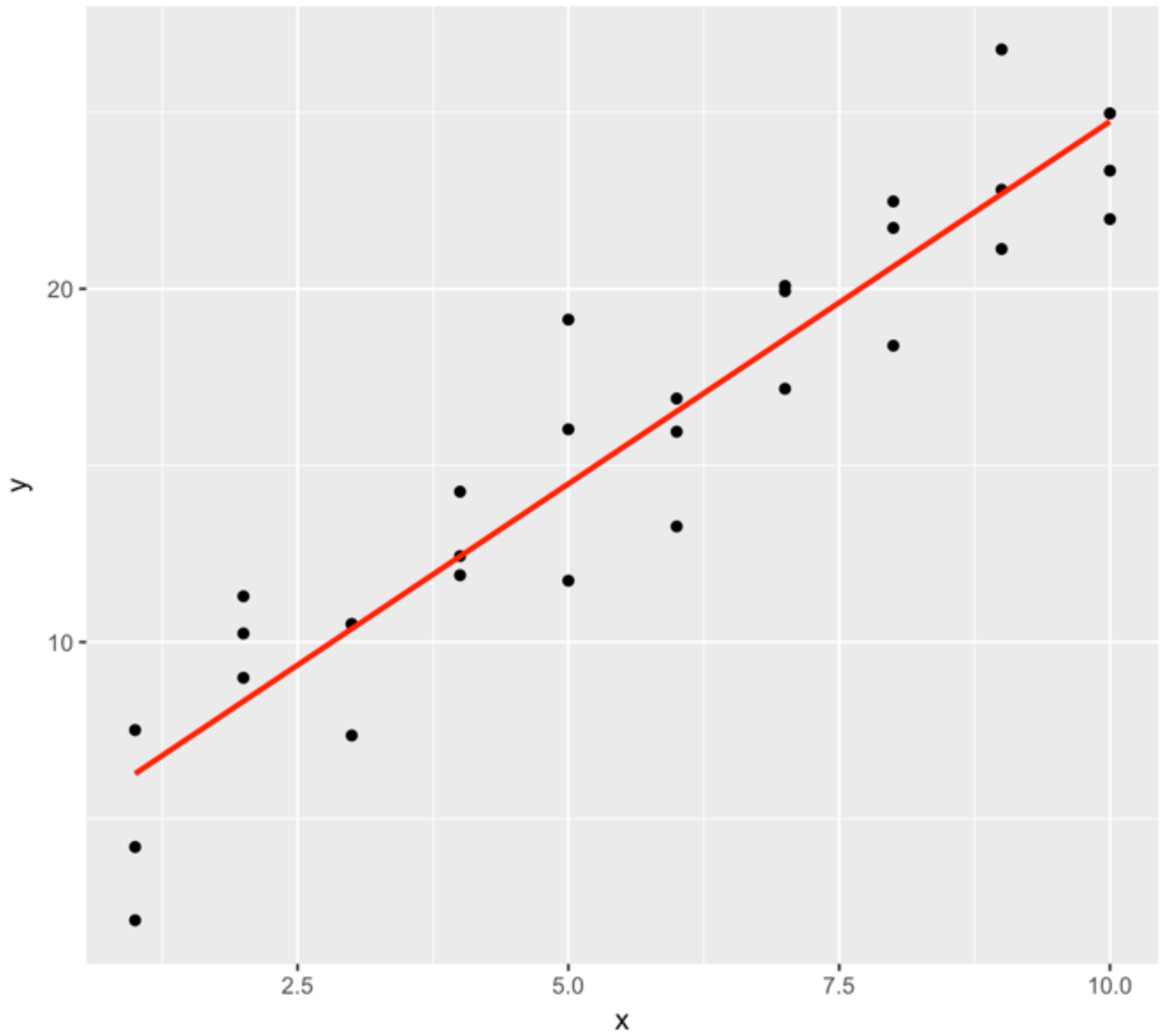
```
sim1_mod <- lm(y ~ x, data = sim1)
sim1 %>%
  add_predictions(sim1_mod) %>%
  add_residuals(sim1_mod)
# A tibble: 30 x 4
       x         y      pred        resid
   <int>     <dbl>     <dbl>        <dbl>
1      1  4.199913  6.272355 -2.072442018
2      1  7.510634  6.272355  1.238279125
3      1  2.125473  6.272355 -4.146882207
4      2  8.988857  8.323888  0.664969362
5      2 10.243105  8.323888  1.919217378
6      2 11.296823  8.323888  2.972935148
7      3  7.356365 10.375421 -3.019056466
8      3 10.505240 10.375421  0.129938253
```

We can add the fitted values and residuals to our original `sim1` data frame with `add_predictions()` and `add_residuals()`...

DO OUR RELATIONSHIPS HOLD VISUALLY?

```
sim1_mod <- lm(y ~ x, data = sim1)
sim1 %>%
  add_predictions(sim1_mod) %>%
  add_residuals(sim1_mod) %>%
  ggplot(aes(x, y)) +
  geom_point() +
  geom_line(aes(y = pred),
            color = "red", size = 1)
```

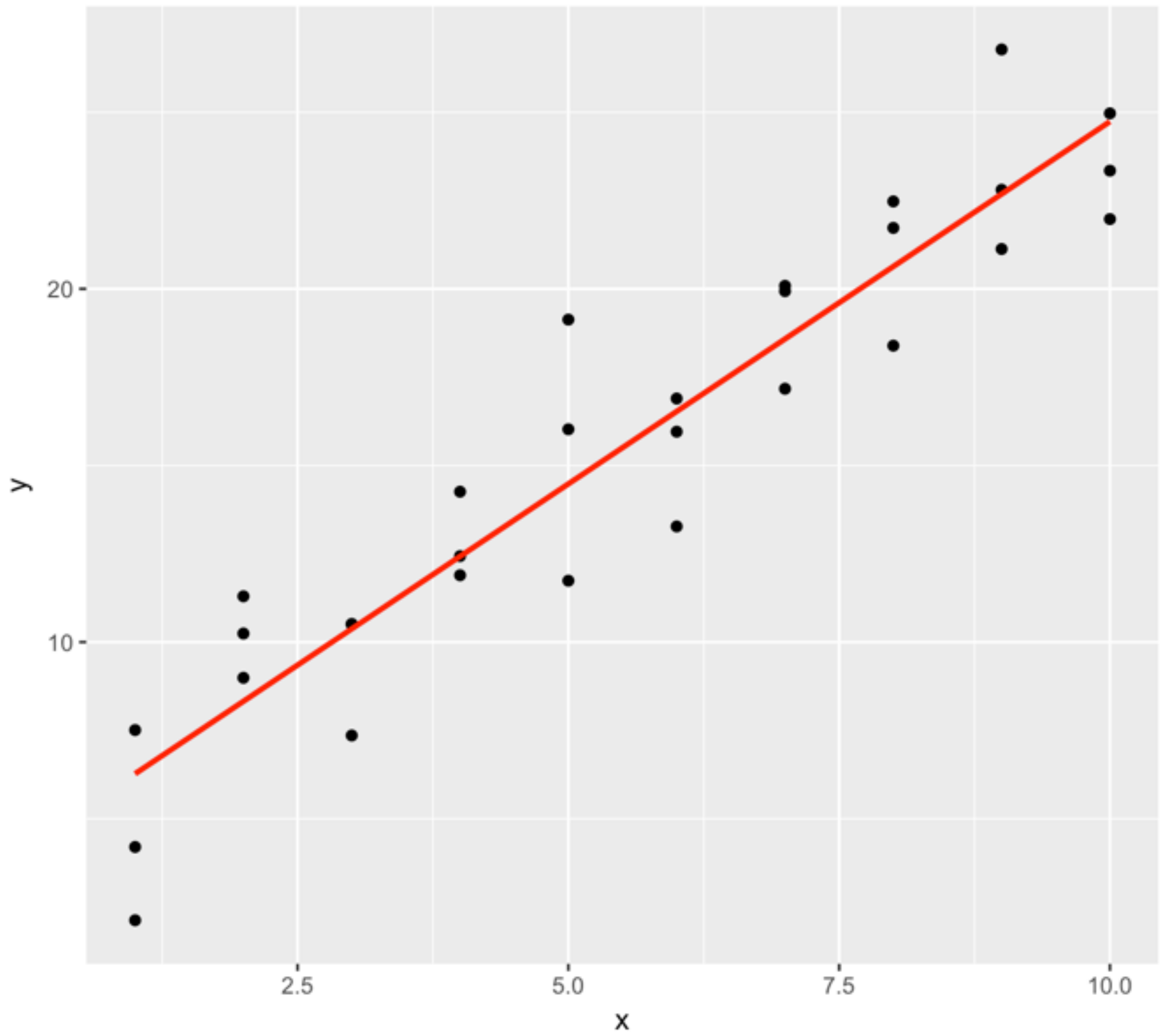
…which makes it easy to pipe right into a visualization of the fitted values



DO OUR RELATIONSHIPS HOLD VISUALLY?

```
sim1_mod <- lm(y ~ x, data = sim1)
sim1 %>%
  add_predictions(sim1_mod) %>%
  add_residuals(sim1_mod) %>%
  ggplot(aes(x, y)) +
  geom_point() +
  geom_line(aes(y = pred),
            color = "red", size = 1)

# do you see how these relate????
ggplot(sim1, aes(x, y)) +
  geom_point() +
  geom_smooth(method = "lm")
```

…which makes it easy to pipe right into a visualization of the fitted values



DO OUR RELATIONSHIPS HOLD VISUALLY?

```
sim1_mod <- lm(y ~ x, data = sim1)
sim1 %>%
  add_residuals(sim1_mod) %>%
  ggplot(aes(resid)) +
  geom_histogram(binwidth = .5)

sim1 %>%
  add_residuals(sim1_mod) %>%
  ggplot(aes(x, resid)) +
  geom_ref_line(h = 0) +
  geom_point()
```

…we also want to plot the residuals

Try these - what do they tell you?

DO OUR RELATIONSHIPS HOLD VISUALLY?

```
sim1_mod <- lm(y ~ x, data = sim1)
sim1 %>%
  add_residuals(sim1_mod) %>%
  ggplot(aes(resid)) +
  geom_histogram(binwidth = .5)

sim1 %>%
  add_residuals(sim1_mod) %>%
  ggplot(aes(x, resid)) +
  geom_ref_line(h = 0) +
  geom_point()
```

…we also want to plot the residuals

The residuals look like random noise, suggesting the model has done a good job capturing the pattern

YOUR TURN!

1. *Fit a linear model that regresses* **`mpg`** *onto* **`wt`** *with the* **`mtcars`** *data*

2. *How does this model appear to fit numerically (hint: summary)?*

3. *Add the predicted and residual values to the* **`mtcars`** *data set and plot them? How do they visually fit?*

MODELING CATEGORICAL VARIABLES

CATEGORICAL PREDICTORS

Regression is straight forward when the predictor is continuous, but things get a bit more complicated when the predictor is categorical.

```
sim2
# A tibble: 40 × 2
        x          y
    <chr>      <dbl>
1       a  1.9353632
2       a  1.1764886
3       a  1.2436855
4       a  2.6235489
5       a  1.1120381
6       a  0.8660030
7       a -0.9100875
8       a  0.7207628
```

CATEGORICAL PREDICTORS

Regression is straight forward when the predictor is continuous, but things get a bit more complicated when the predictor is categorical.

```
sim2_mod <- lm(y ~ x, data = sim2)
```

Luckily, the syntax for categorical variables does not change as R takes care of the dirty work…

CATEGORICAL PREDICTORS

Regression is straight forward when the predictor is continuous, but things get a bit more complicated when the predictor is categorical.

```
sim2_mod <- lm(y ~ x, data = sim2)
summary(sim2_mod)
Call:
lm(formula = y ~ x, data = sim2)

Residuals:
     Min       1Q   Median       3Q      Max 
-2.40131 -0.43996 -0.05776  0.49066  2.63938 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)   1.1522     0.3475   3.316  0.00209 ** 
xb            6.9639     0.4914  14.171 2.68e-16 ***
xc            4.9750     0.4914  10.124 4.47e-12 ***
xd            0.7588     0.4914   1.544  0.13131
```

Luckily, the syntax for categorical variables does not change as R takes care of the dirty work…

but how we interpret the results changes slightly

Who can interpret these results?

CATEGORICAL PREDICTORS

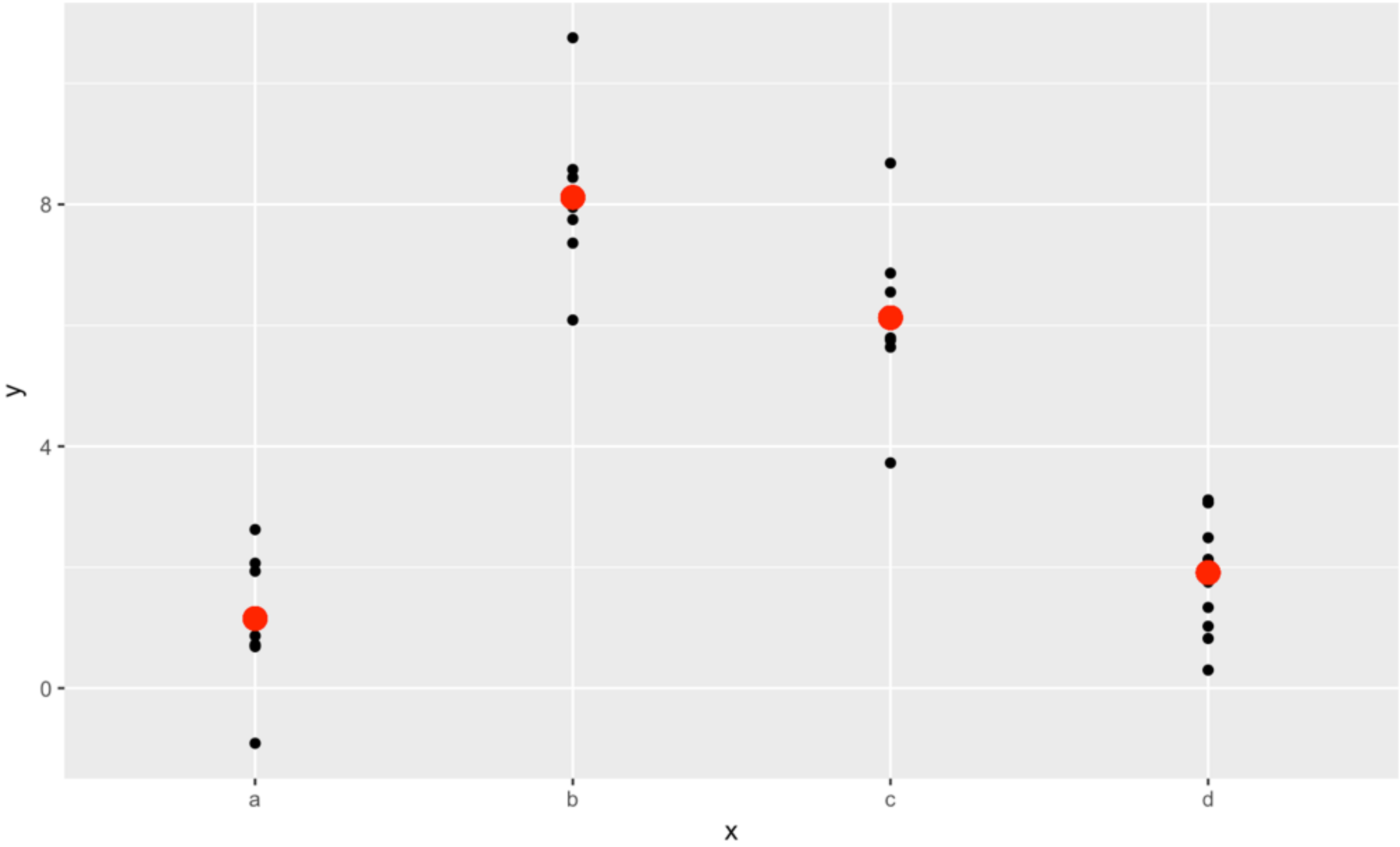
Regression is straight forward when the predictor is continuous, but things get a bit more complicated when the predictor is categorical.

```
sim2_mod <- lm(y ~ x, data = sim2)
summary(sim2_mod)
Call:
lm(formula = y ~ x, data = sim2)

Residuals:
     Min       1Q   Median       3Q      Max
-2.40131 -0.43996 -0.05776  0.49066  2.63938

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   1.1522     0.3475   3.316  0.00209 **
xb            6.9639     0.4914  14.171 2.68e-16 ***
xc            4.9750     0.4914  10.124 4.47e-12 ***
xd            0.7588     0.4914   1.544  0.13131
```

```
sim2_mod <- lm(y ~ x, data = sim2)
sim2 %>%
  data_grid(x) %>%
  add_predictions(sim2_mod)
# A tibble: 4 × 2
      x     pred
  <chr>    <dbl>
1     a 1.152166
2     b 8.116039
3     c 6.127191
4     d 1.910981
```

CATEGORICAL PREDICTORS

Regression is straight forward when the predictor is continuous, but things get a bit more complicated when the predictor is categorical.




```
sim2_mod <- lm(y ~ x, data = sim2)
sim2 %>%
  data_grid(x) %>%
  add_predictions(sim2_mod)
# A tibble: 4 x 2
      x     pred
  <chr>    <dbl>
1     a 1.152166
2     b 8.116039
3     c 6.127191
4     d 1.910981
```

CATEGORICAL PREDICTORS

Regression is straight forward when the predictor is continuous, but things get a bit more complicated when the predictor is categorical.

What if we want to change the order of the categorical variables?

CATEGORICAL PREDICTORS

Regression is straight forward when the predictor is continuous, but things get a bit more complicated when the predictor is categorical.

```
sim2b <- sim2 %>%
  mutate(x = as.factor(x),
         x = relevel(x, ref = "b"))

sim2b_mod <- lm(y ~ x, data = sim2b)
summary(sim2b_mod)
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)   8.1160     0.3475  23.356  < 2e-16 ***
xa           -6.9639     0.4914 -14.171 2.68e-16 ***
xc           -1.9888     0.4914  -4.047 0.000263 ***
xd           -6.2051     0.4914 -12.627 8.67e-15 ***
```

What if we want to change the order of the categorical variables?

This is where understanding factors is handy.

Use `relevel()` to establish a new reference level.

YOUR TURN!

1. *Fit a model that regresses* **`mpg`** *onto* **`cyl`** *with the* **`mtcars`** *data. Make sure* **`cyl`** *is being used as a categorical variable and not a continuous.*

2. *Can you plot the predictions?*

3. *How about plotting the residuals?*

INTERACTIONS BETWEEN CONTINUOUS AND CATEGORICAL

INTERACTIONS

What happens when you combine a continuous and a categorical variable? `sim3` contains a categorical predictor and a continuous predictor.

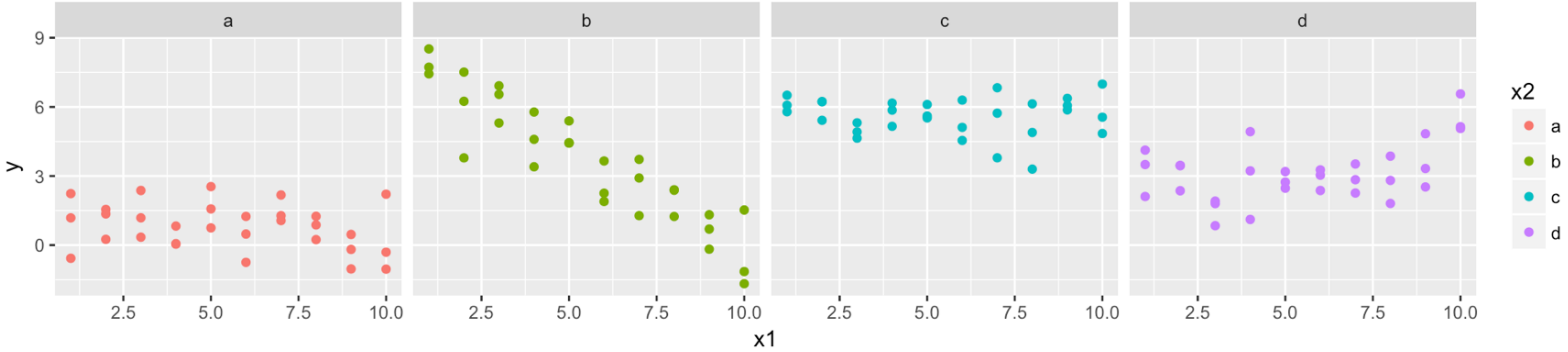
```
sim3
# A tibble: 120 × 5
     x1     x2   rep          y    sd
  <int> <fctr> <int>      <dbl> <dbl>
1     1      a     1 -0.5707363     2
2     1      a     2  1.1841503     2
3     1      a     3  2.2373204     2
4     1      b     1  7.4366963     2
5     1      b     2  8.5182934     2
6     1      b     3  7.7239098     2
7     1      c     1  6.5067480     2
8     1      c     2  5.7900643     2
```

INTERACTIONS

What happens when you combine a continuous and a categorical variable? **`sim3`** contains a categorical predictor and a continuous predictor.

```
ggplot(sim3, aes(x1, y, color = x2)) +
  geom_point() +
  facet_wrap(~ x2)
```

There clearly appears to be different relationships across the categorical variable levels



INTERACTIONS

```
mod1 <- lm(y ~ x1 + x2, data = sim3)
mod2 <- lm(y ~ x1 * x2, data = sim3)
```

We can model this two different ways:

- + will model the variables independent of one another

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

INTERACTIONS

```
mod1 <- lm(y ~ x1 + x2, data = sim3)
mod2 <- lm(y ~ x1 * x2, data = sim3)
```

We can model this two different ways:

- + will model the variables independent of one another

- * will model the variables with interactions

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2$$

INTERACTIONS

```r
mod1 <- lm(y ~ x1 + x2, data = sim3)
mod2 <- lm(y ~ x1 * x2, data = sim3)

# run summaries to compare the difference
summary(mod1)
summary(mod2)
```

We can model this two different ways:

- + will model the variables independent of one another
- * will model the variables with interactions

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2$$

INTERACTIONS

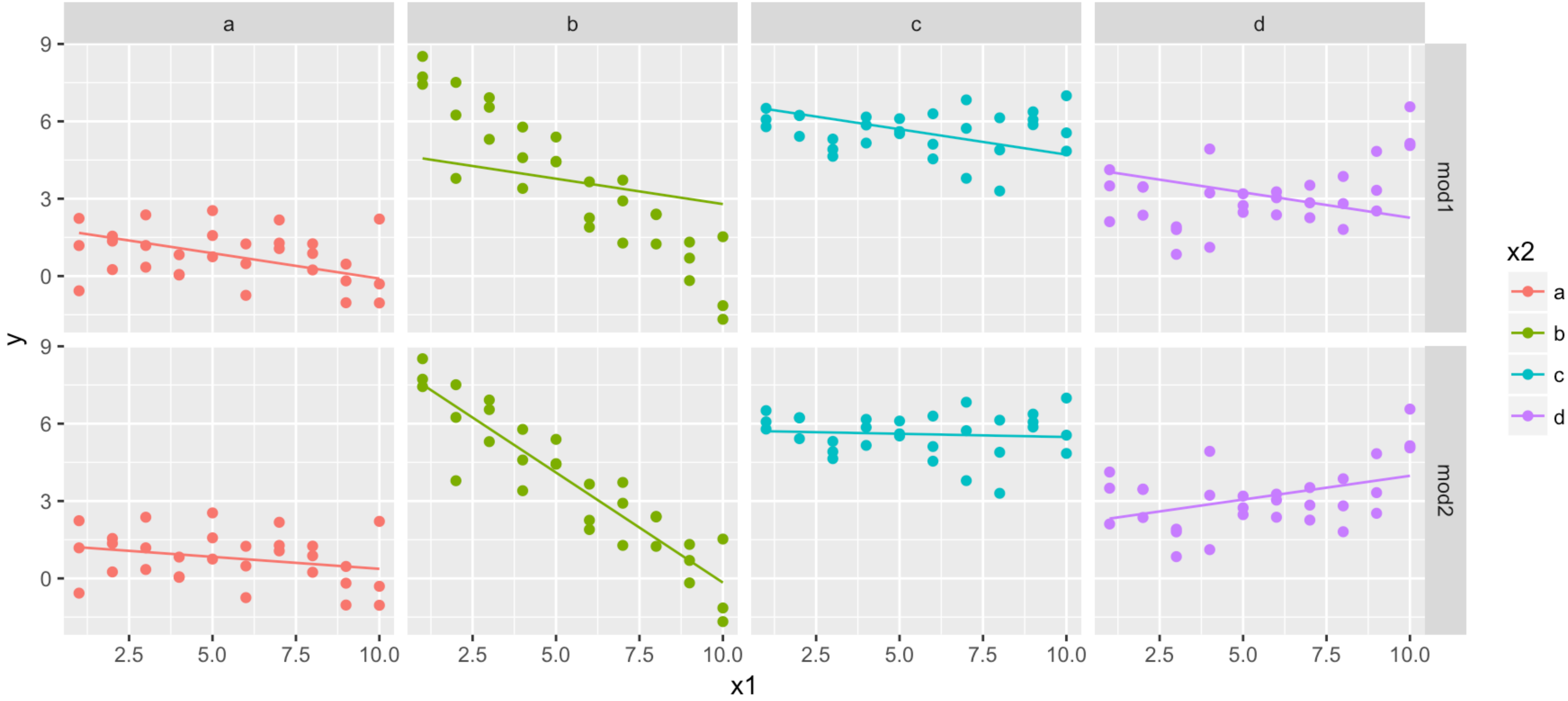
```
sim3 %>%
  gather_predictions(mod1, mod2) %>%
  ggplot(aes(x1, y, color = x2)) +
  geom_point() +
  geom_line(aes(y = pred)) +
  facet_grid(model ~ x2)
```

We can compare the difference in these models using a similar process as before…

Except here we use `gather_predictions` to incorporate results from both models

Run this code line-by-line to see what is happening? What do the results suggest?

INTERACTIONS



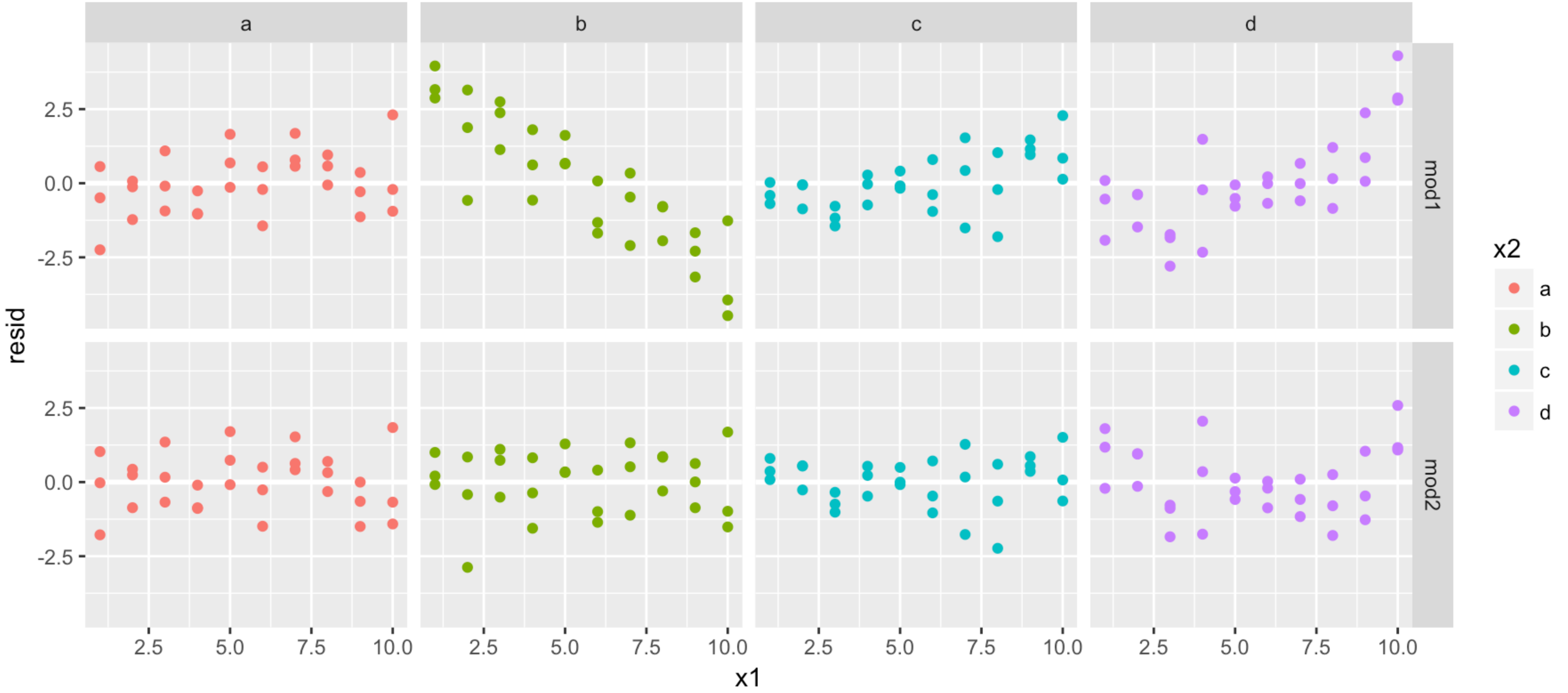
INTERACTIONS

```
sim3 %>%
  gather_residuals(mod1, mod2) %>%
  ggplot(aes(x1, resid, color = x2)) +
  geom_ref_line(h = 0, size = 1) +
  geom_point() +
  facet_grid(model ~ x2)
```

Using a similar process with `gather_residuals` will allow you to compare residuals in a similar manner

Run this code line-by-line to see what is happening? What do the results suggest?

INTERACTIONS



YOUR TURN!

1. *compute the following two models for the mtcars data*

```
mtcars_mod3 <- lm(mpg ~ wt + as.factor(cyl), data = mtcars)
mtcars_mod4 <- lm(mpg ~ wt * as.factor(cyl), data = mtcars)
```

2. *Compare the summaries*
3. *Compare the predicted values*
4. *Compare the residuals*
5. *What are your thoughts?*

$$\hat{Y} = \alpha + \beta X$$

MODEL SPECIFICATION

MODEL SPECIFICATION

```
model_matrix(sim1, y ~ x)
model_matrix(sim2, y ~ x)
model_matrix(sim3, y ~ x1 + x2)
model_matrix(sim3, y ~ x1 * x2)
```

As you are learning to specify models in R you may get confused, or forget, just how to interpret the model your specifying.

You can easily assess your model using **`model_matrix`**

`Run these functions and observe the difference`

MODEL SPECIFICATION

```
model_matrix(sim1, y ~ x)
model_matrix(sim2, y ~ x)
model_matrix(sim3, y ~ x1 + x2)
model_matrix(sim3, y ~ x1 * x2)
# A tibble: 120 × 5
   `(Intercept)`    x1   x2b   x2c   x2d
           <dbl> <dbl> <dbl> <dbl> <dbl>
1              1     1     0     0     0
2              1     1     0     0     0
3              1     1     0     0     0
4              1     1     1     0     0
5              1     1     1     0     0
6              1     1     1     0     0
7              1     1     0     1     0
8              1     1     0     1     0
```

As you are learning to specify models in R you may get confused, or forget, just how to interpret the model your specifying.

You can easily assess your model using **`model_matrix`**

Run these functions and observe the difference

TRANSFORMATIONS

You can also perform transformations inside the model formula

TRANSFORMATIONS

You can also perform transformations inside the model formula

```
lm(log(y) ~ sqrt(x1) + x2)
```

log and square root transformations

TRANSFORMATIONS

You can also perform transformations inside the model formula

```
lm(log(y) ~ sqrt(x1) + x2)

lm(y ~ x + I(x ^ 2))
```

log and square root transformations

transformations involving +, *, ^, or -, will need to be wrapped in `I()`

TRANSFORMATIONS

You can also perform transformations inside the model formula

```
lm(log(y) ~ sqrt(x1) + x2)

lm(y ~ x + I(x ^ 2))

model_matrix(sim1, y ~ x + x^2)
model_matrix(sim1, y ~ x + I(x^2))
```

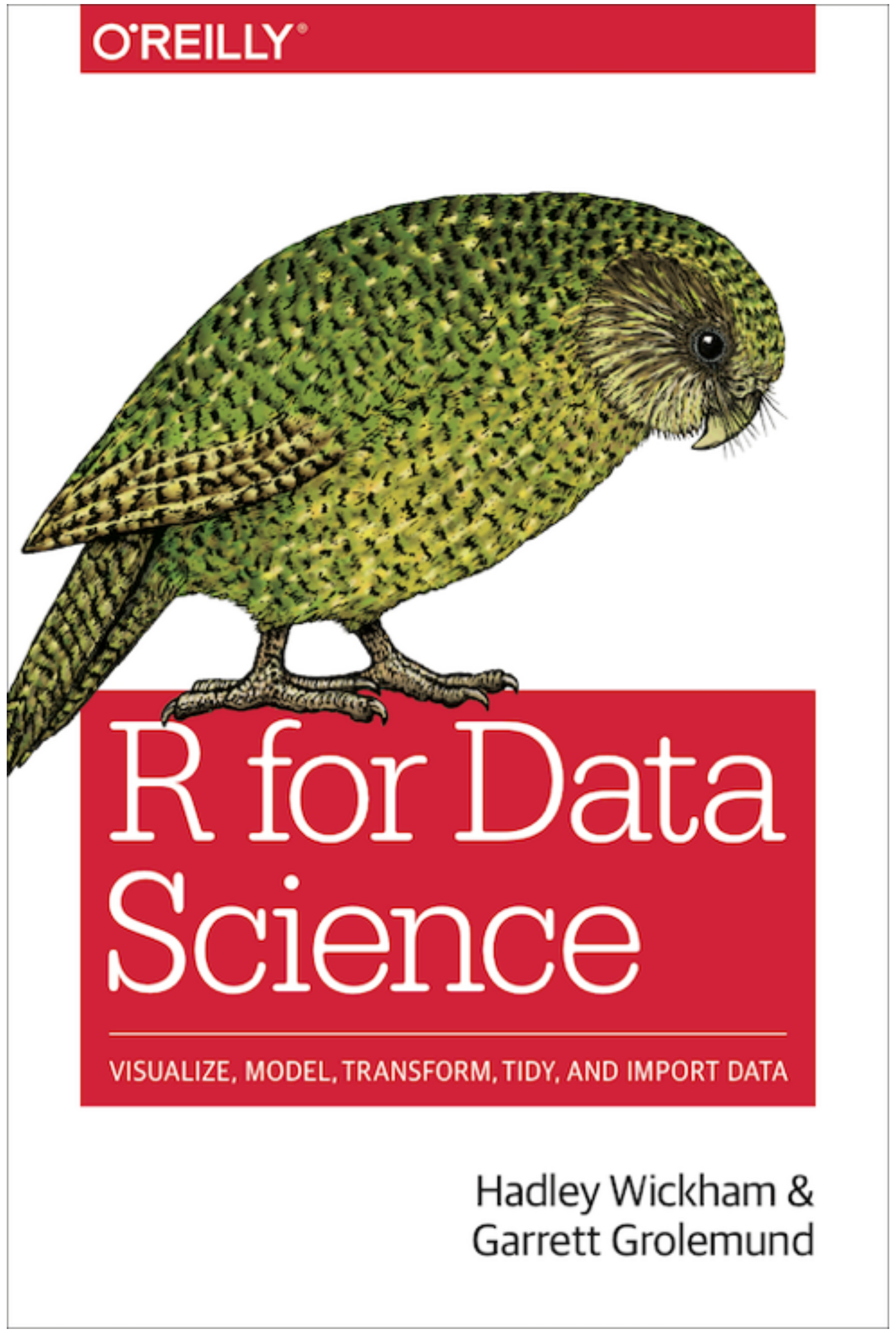
log and square root transformations

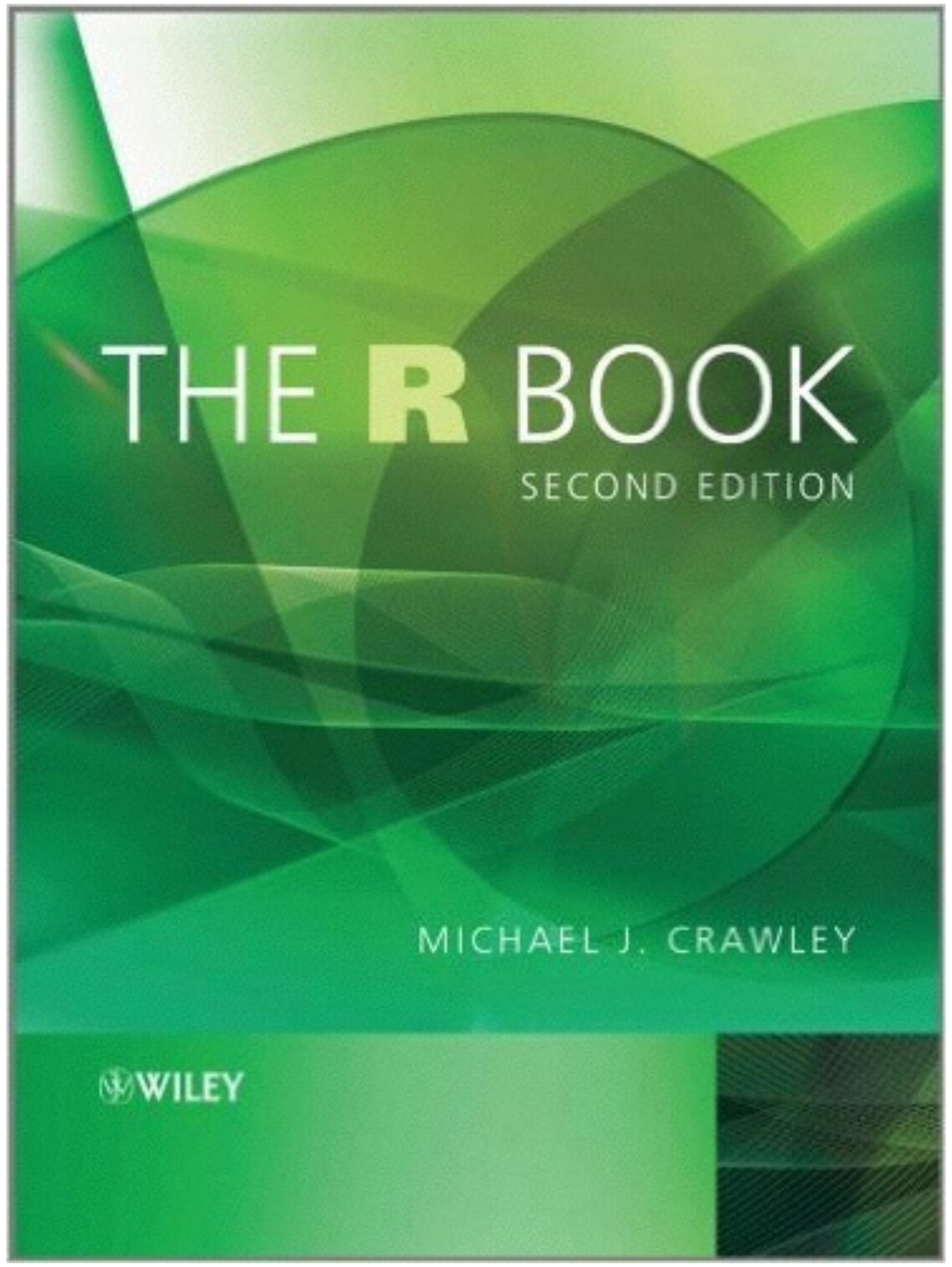
transformations involving +, *, ^, or -, will need to be wrapped in I()

If you get confused, just use `model_matrix`

SO LITTLE TIME!

LEARN MORE


O'REILLY
R for Data Science
VISUALIZE, MODEL, TRANSFORM, TIDY, AND IMPORT DATA
Hadley Wickham &
Garrett Grolemund


THE R BOOK
SECOND EDITION
MICHAEL J. CRAWLEY
WILEY

WHAT TO REMEMBER

FUNCTIONS TO REMEMBER

Operator/Function	Description
`cor, cor.test`	Compute correlation
`pairs, geom_ref_line`	Plot pairwise x-y scatterplots, add reference line to ggplot (great for assessing residual)
`lm(y ~ x, data = df)`	Linear model specification
`summary, residuals, fitted.values, coef`	Summarize and extract components out of the `lm()` object
`add_predictions, add_residuals, gather_predictions, gather_residuals`	Shortcut functions to add predicted values and residuals from an `lm()` object to a new or existing data frame
`model_matrix`	assess model specification