Multiple Linear Regression

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Objectives

This notebook gives an overview of Multiple Linear Regression, where we'll use more than one feature/predictor to predict a numerical response variable. After reviewing this notebook, you should be able to:

- Fit a multiple linear regression model to training data using `tidymodels`
- Assess that model's performance on the training data by looking at global model utility metrics, and by analyzing metrics for the model term.
- Interpret a multiple linear regression model with statistically significant predictors.
- Use a multiple linear regression model to make predictions on new data.
- Evaluate model performance on the test set.

Simple Versus Multiple Linear Regression

In the previous notebook, we learned that a simple linear regression model whose response variable is y and whose sole predictor is x is of the form

$$y = \beta_0 + \beta_1 \cdot x + \varepsilon \quad \text{or} \quad \mathbb{E}\left[y\right] = \beta_0 + \beta_1 \cdot x$$

Multiple linear regression models are quite similar, the difference being that these multiple linear regression models contain multiple predictor variables: $x_1,\ x_2,\ \ldots\ , x_k$. That is, these models take the form

$$y = \beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_2 + \cdots + \beta_k x_k + \varepsilon$$

–or–

$$\mathbb{E}\left[y\right] = \beta_0 + \beta_1 \cdot x_1 + \beta_2 \cdot x_2 + \cdots + \beta_k x_k$$

In a simple linear regression model, we could interpret the coefficient on the term containing the predictor variable as a *slope*. That is, the β coefficient is the expected rate of change in the response variable per unit change in the predictor variable. For example, *a penguin whose bill is* 1*mm longer than average is expected to have about* 88.58*g more mass than the average penguin* or *for each additional millimeter of bill length, we expect a penguin to have about* 88.58*g more mass, on average.*

For multiple linear regression models, we have similar interpretations as long as the model terms are independent of one another (we'll encounter scenarios where they are not when we look at higher-order terms later in our course). That is, the interpretation of β_i, the coefficient on x_i in our model is *the expected change in the response variable associated with a unit change in* x_i*, while all other predictors are held constant.*

Model Coefficients as Slopes

For simple and multiple linear regression models where each model term contains a single numerical predictor, we can interpret the corresponding β-coefficient as a slope, holding all other predictors constant.
That is, for the multiple linear regression model

$$\mathbb{E}\left[y\right] = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k$$

holding all other predictors constant, we expect a unit increase in x_i to be associated with an increase of about β_i in the expected value of y as long as x_1 through x_k are independent, numerical predictors.

Let's move forward and see how to build, assess, and interpret a multiple linear regression model. For simplicity and continuity, we'll continue working with the `palmerpenguins` data and try to predict `body_mass_g` using the other numerical *features* in the data set.

Training and Test Data

We'll start by splitting our data into training and test sets, as usual.

```
set.seed(123)
penguin_splits <- initial_split(penguins)
penguins_train <- training(penguin_splits)
penguins_test <- testing(penguin_splits)
```

As a reminder, here's the first few rows of our training data.

```
penguins_train %>%
  head() %>%
  kable() %>%
  kable_styling()
```

species	island	bill_length_mm	bill_depth_mm	flipper_length_mm	body_mass_g	sex
Gentoo	Biscoe	44.5	14.3	216	4100	NA
Adelie	Torgersen	38.6	21.2	191	3800	male
Gentoo	Biscoe	45.3	13.7	210	4300	female
Chinstrap	Dream	52.8	20.0	205	4550	male
Adelie	Torgersen	37.3	20.5	199	3775	male
Chinstrap	Dream	43.2	16.6	187	2900	female

EDA with Numerical Features

Let's explore whether the numerical features in our data frame are *visually* associated with penguin body mass.

```
p1 <- penguins_train %>%
  ggplot() +
  geom_point(aes(x = bill_length_mm, y = body_mass_g)) +
  labs(x = "Bill Length (mm)",
       y = "Body Mass (g)")

p2 <- penguins_train %>%
  ggplot() +
  geom_point(aes(x = bill_depth_mm, y = body_mass_g)) +
  labs(x = "Bill Depth (mm)",
       y = "Body Mass (g)")

p3 <- penguins_train %>%
  ggplot() +
  geom_point(aes(x = flipper_length_mm, y = body_mass_g)) +
  labs(x = "Flipper Length (mm)",
       y = "Body Mass (g)")

p4 <- penguins_train %>%
  ggplot() +
  geom_point(aes(x = year, y = body_mass_g)) +
  labs(x = "Year",
       y = "Body Mass (g)")

(p1 + p2 + p3)/p4
```

```
Warning: Removed 2 rows containing missing values or values outside the scale range
(`geom_point()`).
Removed 2 rows containing missing values or values outside the scale range
(`geom_point()`).
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```
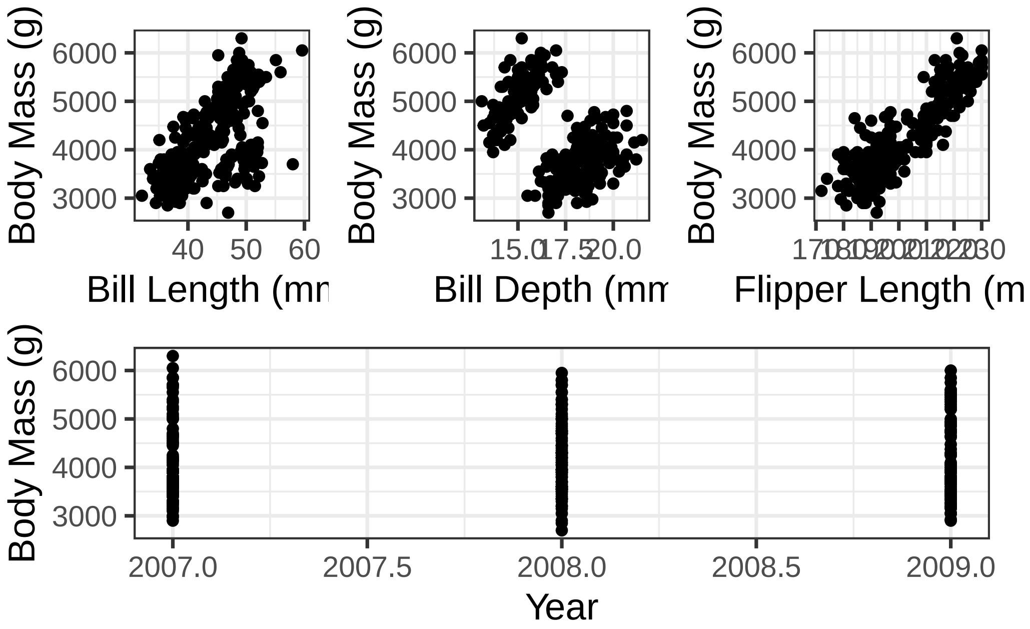



It looks like there are positive associations between penguin body mass and the bill measurements as well as the flipper measurement. The plot with the year variable is difficult to read (which we'll return to later) – for now, we'll include the year variable in our model as another numerical predictor.

Building a Multiple Linear Regression Model

The strategy for building a multiple linear regression model in `{tidymodels}` is exactly the same as the strategy for building a simple linear regression.

- Create a model *specification* using `linear_reg()` and set its fitting engine to `"lm"`.
- Create a model *recipe* by passing the model formula and data to the `recipe()` function.
- Package the model and recipe together into a `workflow()`.
- *Fit* the workflow by passing it to `fit()` with the training data.

Let's see that in action.

```
mass_multi_spec <- linear_reg() %>%
  set_engine("lm")

mass_multi_rec <- recipe(body_mass_g ~ bill_length_mm + bill_depth_mm + flipper_length_mm + y

mass_multi_wf <- workflow() %>%
  add_model(mass_multi_spec) %>%
  add_recipe(mass_multi_rec)

mass_multi_fit <- mass_multi_wf %>%
  fit(penguins_train)
```

There it is – we have our model. Let's check it out.

Assessing our Fitted Model

As a reminder, we'll run several levels of assessment.

- A global model assessment (using `glance()`), including
  - the *global test for model utility* (looking at the `p.value`)
  - an assessment of the proportion of variation in the response variable explained by our model (looking at the `adj.r.squared`)

    - understanding the expected “accuracy” of our model (looking at the `sigma` value, which measures the *residual standard error*, and constructing a naive confidence interval)

- Individual model-term analysis (using `fitted_model %>% extract_fit_engine() %>% tidy()`), including

    - assessing the statistical significance of individual model terms (looking at the `p.values`)
    - identifying and interpreting estimated model coefficients (looking at the `estimate`)
    - identifying and interpreting the uncertainty in these coefficient estimates (looking at the `std.error` to construct confidence intervals)

- An unbiased assessment of model performance

    - Since the model knew the true body masses of the penguins that it is attempting to predict, it had an unfair advantage in predicting those values. Think of it this way, if you have a practice exam with an answer key (which you get to look at), then just because you do well on the practice exam doesn’t mean you are well-prepared for the real exam – the same holds true for the model.

    - We’ll use our model to make predictions for the body mass of penguins in our test data.

    - Once we have those questions, we’ll compute global model performance metrics like RMSE and R-Squared.

        * Because the model didn’t know that these penguins existed, the model has no advantage in predicting their body mass. Assessing the model performance on these *test* penguins leaves the assessment unbiased.

Global Model Assessment

Let’s use `glance()` to get some very high-level metrics about our overall model’s estimated performance.

```
mass_multi_fit %>%
  glance() %>%
  kable() %>%
  kable_styling(bootstrap_options = c("hover", "striped"))
```

r.squared	adj.r.squared	sigma	statistic	p.value	df	logLik	AIC	BIC	deviance
0.7808404	0.7773478	387.1782	223.571	0	4	-1886.198	3784.396	3805.667	37626655

First, we can conduct the *global test for model utility.* Since this is the first time we've really done such a test, a reminder of the hypotheses appears below.

$$\begin{array}{rcl} H_0 & : & \beta_1 = \beta_2 = \beta_3 = \beta_4 = 0 \\ H_a & : & \text{At least one of the coefficients is non-zero} \end{array}$$

The `p.value` for this test is extremely small, so we have evidence to suggest that at least one of the model's predictor terms has a non-zero coefficient. That's good news – there is *atleast some* value to our model!

We can see from the `adj.r.squared` value that *approximately 77.73% of the variation in penguin body mass is explained by this model.*

Finally, we can assess the *residual standard error* (`sigma`) for the model. This value helps us estimate how accurate we should expect our predictions to be. At approximately 95% confidence, we can expect our predictions to be accurate to within about ± 774.36 grams. As a reminder, however, this estimate is biased and may be *too optimistic* about the errors our model will make in the future. We should recalculate this metric (and the adjusted R squared metric) using unseen data, such as the *test* data.

Assessment of Individual Model Terms

We'll pipe our fitted model to `extract_fit_engine()` and `tidy()` to obtain the data frame of model terms and corresponding metrics.

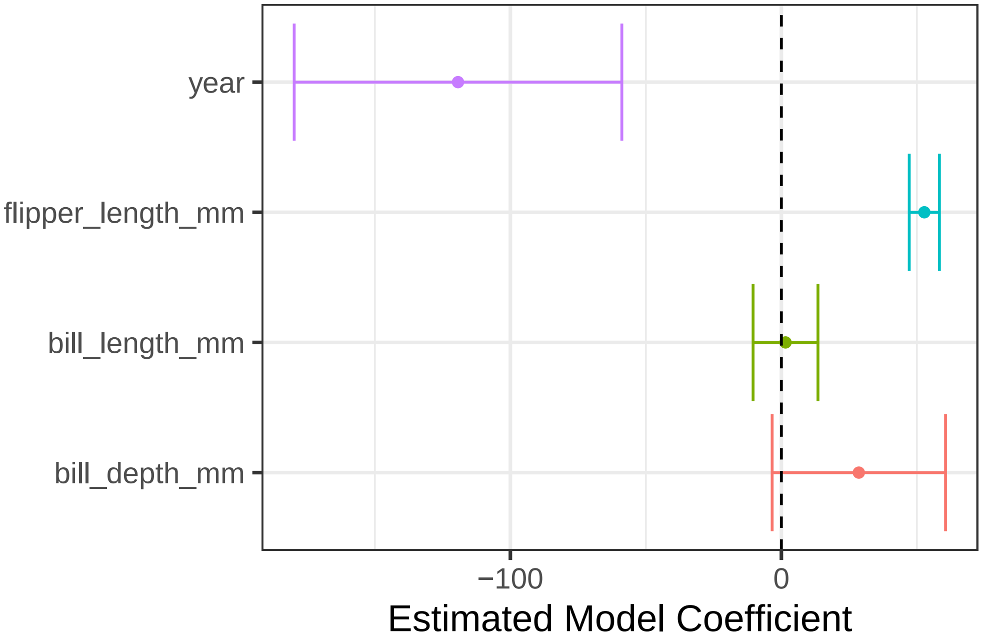
```r
mass_multi_fit %>%
  extract_fit_engine() %>%
  tidy() %>%
  kable() %>%
  kable_styling()
```

term	estimate	std.error	statistic	p.value
Intercept	232658.774875	60591.365347	3.8398008	0.0001560
bill_length_mm	1.530334	5.984567	0.2557134	0.7983815
bill_depth_mm	28.587515	15.997312	1.7870199	0.0751409
flipper_length_mm	52.753150	2.783871	18.9495697	0.0000000
year	-119.323909	30.224297	-3.9479466	0.0001024

The first thing we should do is look at the `p.value`s associated with the individual model terms. At this stage, if any model terms are not statistically significant we should remove them one-by-one. We'll do so by removing the predictor with the highest `p.value` first.

Before we begin removing predictors from the model, perhaps this process seems a bit mysterious. It is worth looking at a visual of the estimated model coefficients and their plausible ranges.

```r
mass_multi_fit %>%
  extract_fit_engine() %>%
  tidy() %>%
  filter(term != "Intercept") %>%
  ggplot() +
  geom_errorbarh(aes(y = term,
                     xmin = estimate - (2*std.error),
                     xmax = estimate + (2*std.error),
                     color = term),
                 show.legend = FALSE) +
  geom_point(mapping = aes(x = estimate, y = term, color = term),
             show.legend = FALSE) +
  geom_vline(xintercept = 0, linetype = "dashed") +
  labs(x = "Estimated Model Coefficient",
       y = "")
```



We can see that the plausible ranges for coefficients on `bill_length_mm` and `bill_depth_mm` overlap with 0. If these coefficients were 0, then the corresponding model terms would drop out of the model. This is what *statistical insignificance* means.

Let's refit the model without the `bill_length_mm` predictor and see whether `bill_length_mm` should still be removed.

```r
mass_multi_spec <- linear_reg() %>%
  set_engine("lm")

mass_multi_rec <- recipe(body_mass_g ~ bill_length_mm + flipper_length_mm + year, data = peng

mass_multi_wf <- workflow() %>%
  add_model(mass_multi_spec) %>%
  add_recipe(mass_multi_rec)

mass_multi_fit <- mass_multi_wf %>%
  fit(penguins_train)

mass_multi_fit %>%
  extract_fit_engine() %>%
  tidy() %>%
  kable() %>%
  kable_styling()
```

term	estimate	std.error	statistic	p.value
Intercept	225991.977989	60739.032170	3.7207043	0.0002450
bill_length_mm	3.794827	5.874269	0.6460083	0.5188618
flipper_length_mm	49.895057	2.288486	21.8026532	0.0000000
year	-115.523634	30.280317	-3.8151395	0.0001713

Bill length in millimeters is still just above the threshold for statistical significance. We'll drop it from our model and refit.

```r
mass_multi_spec <- linear_reg() %>%
  set_engine("lm")

mass_multi_rec <- recipe(body_mass_g ~ flipper_length_mm + year, data = penguins_train)

mass_multi_wf <- workflow() %>%
  add_model(mass_multi_spec) %>%
  add_recipe(mass_multi_rec)

mass_multi_fit <- mass_multi_wf %>%
  fit(penguins_train)

coef_df <- mass_multi_fit %>%
  extract_fit_engine() %>%
  tidy()

coef_df %>%
  kable() %>%
  kable_styling()
```

term	estimate	std.error	statistic	p.value
Intercept	227916.26652	60596.048460	3.76124	0.0002101
flipper_length_mm	50.87429	1.712514	29.70736	0.0000000
year	-116.49701	30.207960	-3.85650	0.0001460

Okay, both of the remaining predictors, `flipper_length_mm` and `year` are statistically significant. This gives us our "*final*" model form of $\mathbb{E}\left[\text{body\_mass\_g}\right] = \beta_0 + \beta_1 \cdot \text{flipper\_length\_mm} + \beta_2 \cdot \text{year}$, where the estimated model has $\beta_0 \approx 227916.3$, $\beta_1 \approx 50.87$, and $\beta_2 \approx$ -116.5.

At this point, we have a model that we can make predictions and interpretations with. In terms of the model coefficients,

- We expect penguins with longer flippers to have greater mass. On average, with year being held constant, we expect a unit increase in flipper length to be associated with approximately 50.87g additional mass.
- We expect penguins to have lower body mass with each passing year. On average, holding the flipper length constant, similar penguins from one year to the next are expected to have approximately 116.5g less body mass.

Interpreting Marginal Effects with `{marginaleffects}`

So far, we have been able to interpret each model coefficient as a slope. This is relatively straight forward. However, as we explore more complex models – particularly those with mixed effects and higher order terms – the interpretation of the impact of a predictor on the response is more difficult to extract. This is particularly true for those without a calculus background.

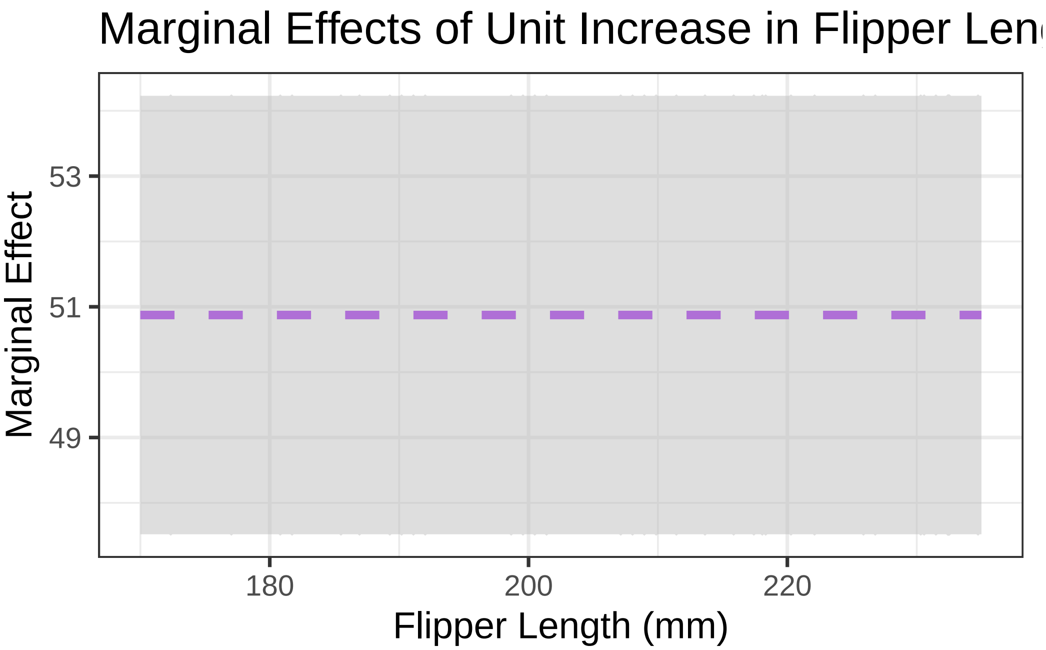
Fortunately, the `{marginaleffects}` package can help us. We'll introduce it now because this is a simple case and this early exposure will make it easier for us to use the functionality later.

```r
library(marginaleffects)

counterfactual_flipper_df <- tibble(flipper_length_mm = seq(170, 235, length.out = 500),
                                    year = 2019)
```

```
mfx <- mass_multi_fit %>%
  extract_fit_engine() %>%
  slopes(newdata = counterfactual_flipper_df,
         variables = "flipper_length_mm",
         conf_level = 0.95) %>%
  tibble()

mfx %>%
  select(term, flipper_length_mm, estimate, conf.low, conf.high, std.error) %>%
  head(n = 10) %>%
  kable() %>%
  kable_styling()
```

term	flipper_length_mm	estimate	conf.low	conf.high	std.error
flipper_length_mm	170.0000	50.87429	47.51951	54.22906	1.71165
flipper_length_mm	170.1303	50.87429	47.51951	54.22906	1.71165
flipper_length_mm	170.2605	50.87429	47.51951	54.22906	1.71165
flipper_length_mm	170.3908	50.87429	47.51951	54.22906	1.71165
flipper_length_mm	170.5210	50.87429	47.51951	54.22906	1.71165
flipper_length_mm	170.6513	50.87429	47.51951	54.22906	1.71165
flipper_length_mm	170.7816	50.87429	47.51951	54.22906	1.71165
flipper_length_mm	170.9118	50.87429	47.51951	54.22906	1.71165
flipper_length_mm	171.0421	50.87429	47.51951	54.22906	1.71165
flipper_length_mm	171.1723	50.87429	47.51951	54.22906	1.71165

```
mfx %>%
  select(flipper_length_mm, estimate, conf.low, conf.high) %>%
  ggplot() +
  geom_line(aes(x = flipper_length_mm, y = estimate), color = "purple", lty = "dashed", lwd =
  geom_ribbon(aes(x = flipper_length_mm, ymin = conf.low, ymax = conf.high),
              fill = "grey", alpha = 0.5) +
  labs(x = "Flipper Length (mm)",
       y = "Marginal Effect",
       title = "Marginal Effects of Unit Increase in Flipper Length")
```



Reading off of the graph, we can see that the estimated marginal effect of an increase of 1mm in flipper length is associated with an estimated increase of just under 50g, and that this expected increase is independent of the current flipper length. Furthermore, we can see that we are 95% confident that the marginal effect of a unit increase in flipper length on expected body mass is somewhere between 47.5g/mm and 54.25g/mm. These estimates agree with the values we calculated from the tabular output of the regression model above.

Returning to Global Performance Metrics

Since our model form has changed, we need to reassess our global model metrics. They will have all shifted.

```
mass_multi_fit %>%
  glance() %>%
  kable() %>%
  kable_styling(bootstrap_options = c("hover", "striped"))
```

r.squared	adj.r.squared	sigma	statistic	p.value	df	logLik	AIC	BIC	deviance
0.7776845	0.775927	388.4116	442.5111	0	2	-1888.028	3784.056	3798.237	38168479

It is no surprise that our model as a whole still has a significant `p.value`. We removed those predictors which we we were not confident had non-zero coefficients.

Our `adj.r.squared` value has changed slightly, and our final model explains approximately 77.59% of the variability in penguin body mass.

Finally, our *residual standard error* has also changed slightly. We now expect our predictions to be accurate to within about ± 776.82g.

Assessing Model Performance on Unseen (Test) Observations

We recognize that the `adj.r.squared` and *residual standard error* estimates from the global model metrics may be too optimistic. Again, this is because these measures are associated with how well our model predicts the *training* observations, where the model knew the answers. We can reconstruct these metrics using the *test* data to obtain unbiased estimates of model performance. We'll do the following:

- Create a set of metrics (using `metric_set()`) that we wish to use to evaluate our model.
- Augment our test data set with a column of predictions of body mass coming from our model.
- Evaluate our metrics by comparing the true responses (`body_mass_g`) to the predicted responses (`.pred`)

```
my_metrics <- metric_set(rmse, rsq)

mass_multi_fit %>%
  augment(penguins_test) %>%
  select(body_mass_g, .pred) %>%
  my_metrics(body_mass_g, .pred) %>%
  kable() %>%
  kable_styling(bootstrap_options = c("hover", "striped"))
```

.metric	.estimator	.estimate
rmse	standard	376.6980462
rsq	standard	0.7450228

We see that the R Squared value is slightly lower on the test data than it was on the training data. As a reminder, a lower R Squared value indicates that a lower proportion of the variation in the response is explained by our model – that is, the model performs slightly worse on the test data according to the R Squared metric.

Note that *root mean squared error* is comparable to the *residual standard error* (`sigma`), as it measures the average prediction error. Similarly, we see a slightly lower `rmse` on the test data than we saw on the training data. As a reminder, lower `rmse` indicates better predictive performance, so this model performs slightly *better* on the test data according to the `rmse` metric. More on this later in our course as well.

A Note on Comparing Model Metrics: The *residual standard error* (`sigma`) from the `glance()` function and the `rmse` metric we've computed just now utilize slightly different formulas, so they aren't directly comparable (particularly in cases with very small data). One thing we can do is to use `glance()` for the *global test of model utility* only (interpreting that `p.value`), and then we can compute `rsq` and `rmse` for both the training and test sets and compare those to one another.

```r
(mass_multi_fit %>%
  augment(penguins_test) %>%
  select(body_mass_g, .pred) %>%
  my_metrics(body_mass_g, .pred) %>%
   mutate(type = "test")) %>%
  bind_rows(
    (mass_multi_fit %>%
       augment(penguins_train) %>%
       select(body_mass_g, .pred) %>%
       my_metrics(body_mass_g, .pred) %>%
       mutate(type = "train"))
  ) %>%
  pivot_wider(id_cols = type,
              names_from = .metric,
              values_from = .estimate) %>%
  kable() %>%
  kable_styling(bootstrap_options = c("hover", "striped"))
```

type	rmse	rsq
test	376.698	0.7450228
train	386.129	0.7776845

Summary

Okay, we've covered quite a bit in this notebook! Here's a recap of the most important ideas.

- Multiple linear regressions are extensions of simple linear regression models, in which we have *multiple* model terms containing predictor variables.

- A multiple linear regression model takes the form $\mathbb{E}\left[y\right] = \beta_0 + \beta_1\cdot x_1 + \beta_2\cdot x_2 + \cdots + \beta_k x_k$, where y is the response variable and $x_1,~x_2,~\cdots,~x_k$ are predictors.
- The β_0 "coefficient" is the intercept for the model – the expected response if all predictor variables take on the value 0.
- Each β_i for $i > 0$ can be interpreted as a *slope* coefficient for the corresponding model term, when all other predictors are held constant.
- We run multiple levels of assessment on our models.
  - We use `fitted_model %>% glance()` to obtain the `p.value` associated with a *global test for model utility*. That is, we test the hypotheses

    $$\begin{array}{rcl} H_0 & : & \beta_1 = \beta_2 = \cdots = \beta_k = 0\\ H_a & : & \text{At least one of the model coefficients is non-zero}\end{array}$$

  - We use `fitted_model %>% extract_fit_engine() %>% tidy()` to obtain estimated model coefficients and diagnostics.
    - In general, we look to the `p.value` column to determine whether model terms are statistically significant or not.
    - In the case where model terms are not statistically significant, we remove one predictor at a time (according to the highest `p.value`), and refit the model. We continue in this fashion until all remaining terms are statistically significant.
    - At this point, we have an estimated model and we can construct it using the estimated β coefficients found in the `estimate` column.
    - The corresponding values in the `std.error` column help us build confidence intervals for the β coefficients, giving us greater understanding of the uncertainty in our model.
  - Finally, we can compute performance metrics for our model on both the *training* and *test* data sets.
    - In general, we should expect our models to perform better on *training* data (since the model has access to the true responses during the fitting process), however this is not always the case.
    - Comparing these *training* and *test* metrics is a great way to gain insight into the current *fit* of our model and how we might be able to improve it. (More on this idea later in our course)