Overview of {tidymodels}

August 3, 2024

Table of contents

```r
library(tidyverse)
library(tidymodels)
library(kableExtra)
library(patchwork)
tidymodels_prefer()

penguins <- palmerpenguins::penguins

options(kable_styling_bootstrap_options = c("hover", "striped"))

theme_set(theme_bw(base_size = 14))
```

Objectives

This notebook gives an overview of the `{tidymodels}` modeling framework. After reviewing this notebook, you should be able to:

- Split data into training and testing sets using `initial_split()`
- Identify, construct, and utilize the major components of a modeling `workflow()` in the `{tidymodels}` framework
  - Initialize a model specification for a linear regression model with `linear_reg() %>% set_engine("lm")`

  - Initialize a model recipe with `recipe(response ~ predictors, data)`
  - Package a `model` and `recipe` into a `workflow()`
  - Fit a workflow to training data with `fit()`
  - See global model performance metrics using `glance()`
  - Extract the fitted model summary using `extract_fit_engine() %>% tidy()`
  - Use a fitted workflow to make predictions on new data with `predict()`
  - Use metrics to evaluate the performance of a model

`{tidymodels}` in Action

We'll run through an example to see how the components of a `{tidymodels} workflow()` fit together. We'll use the `palmerpenguins` data set since we've already seen that one before.

```r
penguins %>%
  head()  %>%
  kable() %>%
  kable_styling(bootstrap_options = c("hover", "striped"))
```

species	island	bill_length_mm	bill_depth_mm	flipper_length_mm	body_mass_g	sex	ye
Adelie	Torgersen	39.1	18.7	181	3750	male	20
Adelie	Torgersen	39.5	17.4	186	3800	female	20
Adelie	Torgersen	40.3	18.0	195	3250	female	20
Adelie	Torgersen	NA	NA	NA	NA	NA	20
Adelie	Torgersen	36.7	19.3	193	3450	female	20
Adelie	Torgersen	39.3	20.6	190	3650	male	20

Perhaps a reasonable thing to do might be to try predicting `body_mass_g` of a penguin using their `bill_length_mm`.

Splitting Into Training and Test Sets

We don't want to snoop for relationships, so let's start by splitting our data into training at test sets. We'll use `initial_split()` to do this. **Note:** Please *always* split your data into training and test sets. We will see why later in our course.

```r
set.seed(300)
penguin_splits <- initial_split(penguins, prop = 0.75)
penguins_train <- training(penguin_splits)
penguins_test <- testing(penguin_splits)
```

There are multiple things going on in the code cell above.

- Using `set.seed()` guarantees that every time we run this notebook, we'll get the same training and testing data. This is important so as not to *leak* information from the *test* data into the model *training* process.
- The second line uses `initial_split()` to assign 75% of rows to belong to the training data and the remaining 25% to belong to the testing data. We can change the `prop` argument if we would like different proportions.
    - The `initial_split()` function doesn't actually create the training and test data sets. It just identifies the rows as belonging to belong to one or the other.
- We obtain the *training data* by using the `training()` function on our `split` object.
- Similarly, we obtain the *test data* by using the `testing()` function on our `split` object.

Now we've got our two data sets. Lock up that *test* data and keep it hidden. We don't want to know anything about what is in there. This ensures that `penguins_test` will be an unbiased test for our fitted model.

EDA on Training Data

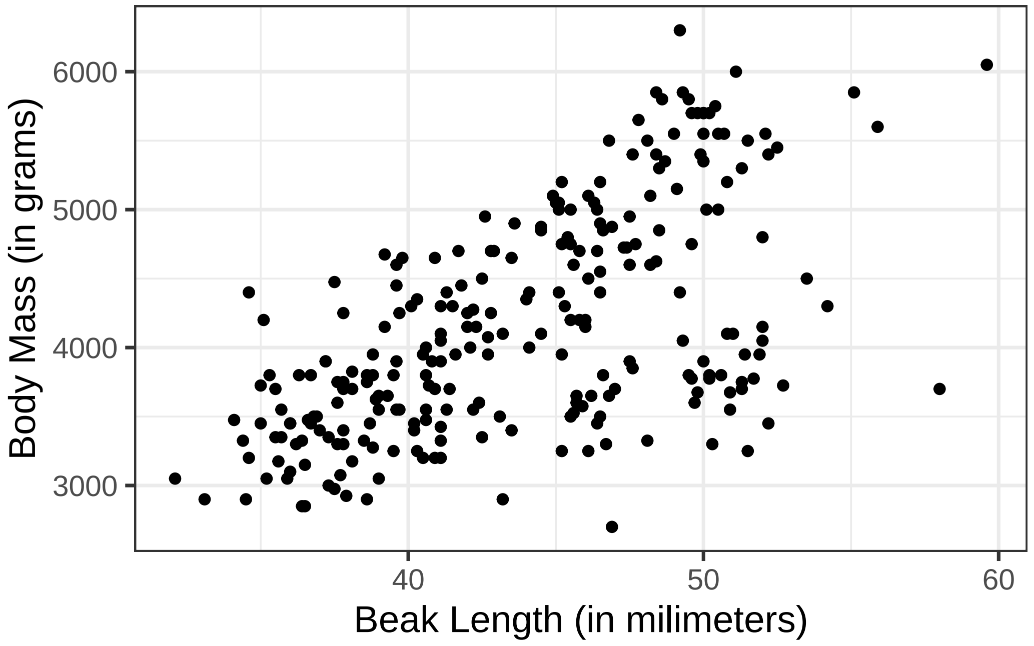
Now that we have our training data, we can look at it. In particular, we may want to know if there is visual evidence of a relationship between `bill_length_mm` and `body_mass_g`.

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

species	island	bill_length_mm	bill_depth_mm	flipper_length_mm	body_mass_g	sex
Adelie	Torgersen	37.2	19.4	184	3900	male
Adelie	Biscoe	41.6	18.0	192	3950	male
Gentoo	Biscoe	50.0	15.2	218	5700	male
Chinstrap	Dream	46.5	17.9	192	3500	female
Adelie	Dream	36.5	18.0	182	3150	female
Chinstrap	Dream	45.7	17.0	195	3650	female

```
penguins_train %>%
  ggplot() +
  geom_point(aes(x = bill_length_mm, y = body_mass_g)) +
  labs(x = "Beak Length (in milimeters)",
       y = "Body Mass (in grams)")
```

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



Okay. It looks like there might be a relationship here!

Specifying a Model Class

For the majority of the semester we'll be working with linear regression models. This means that we'll see the `linear_reg()` model being specified quite often. The great thing about `{tidymodels}` is that everything we do with `linear_reg()` is transferable to other model classes. We'll see that later on in our course.

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

In the code cell above, we created an instance of a linear regression model constructor, and set its fitting engine to `"lm"`. The engine chosen determines how the model will be fit – we'll use `"lm"` almost always. We stored our model constructor in an object called `mass_length_spec`.

Specifying a Recipe

Recipes are very useful aspects of a modeling workflow. We'll use them often. For now, we'll create the simplest recipe possible – a recipe consisting of only a formula. We'll build additional steps into our recipes as we progress through our course.

```r
mass_length_rec <- recipe(body_mass_g ~ bill_length_mm, data = penguins_train)
```

In the code cell above, we specify that our model will predict `body_mass_g`, and it will use only the variable `bill_length_mm` in order to make that prediction. The variables used in this model can be found in `penguins_train`.

Now we're ready to package our model specification and our recipe into a `workflow()`.

Wrapping Everything Into a `workflow()`

We'll see that `workflow()`s are very useful aspects of the `tidymodels` modeling framework. They'll allow us to not only optimize our models, but also optimize decisions that need to be made prior to the models being fit. Additionally, utilizing a `workflow()` will ensure that any new data we ask our model to make predictions for will go through exactly the same transformations as the training data went through.

Let's create a workflow.

```r
mass_length_wf <- workflow() %>%
  add_model(mass_length_spec) %>%
  add_recipe(mass_length_rec)
```

We've created a `workflow()` object and now have added a model and a recipe to it. Now that we've have that simple workflow, let's fit it to our training data!

Fitting our Workflow

What we've essentially done up to this point is we've created a structure which is ready to become a trained model. In terms of a baking analogy, we've taken out all of our ingredients and we know how we want to combine them in order to bake a batch of cookies. We haven't made the cookies (fit the model) yet.

Let's fit the model now.

```r
mass_length_fit <- mass_length_wf %>%
  fit(penguins_train)
```

We just took our workflow object, fit it to the `penguins_train` data, and stored the result in `mass_length_fit`. This is now a fitted model. We can see the structure of that model, use it to make predictions, and more. You may notice that we had to pass the training data as an agument to the `fit()` function again. That's because passing `penguins_train` as a `data` parameter to our `recipe()` earlier only allowed the recipe to learn what kind of variables it was working with. It didn't use that data for anything else.

Extracting the Model Summary

Now that we have a fitted model, let's check out what it looks like! We'll first look at the *global model fit / performance* metrics. We can do this by passing our fitted model object to the `glance()` function.

```
mass_length_fit %>%
  glance() %>%
  kable() %>%
  kable_styling()
```

r.squared	adj.r.squared	sigma	statistic	p.value	df	logLik	AIC	BIC	deviance
0.349806	0.3472461	651.6183	136.6526	0	1	-2020.986	4047.972	4058.607	107850021

We'll talk more about these model metrics in our next class meeting. We can also see information about the individual terms in our model by piping our fitted model object to `extract_fit_engine()` and to `tidy()`, giving us a data frame of metrics for the individual model terms.

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

term	estimate	std.error	statistic	p.value
Intercept	366.84419	326.51140	1.123526	0.2622747
bill_length_mm	86.45721	7.39592	11.689851	0.0000000

Great! We've accessed the model coefficients, and some statistical measures on those estimated values. More on those in our next class meeting as well!

Making Predictions

Since our model is fit, we can also use it to make predictions on new data. Perhaps we have two new penguins whose `bill_length_mm` are 38 and 45 millimeters, respectively.

```
new_data <- tibble(bill_length_mm = c(38, 45))

mass_length_fit %>%
  predict(new_data) %>%
  kable() %>%
  kable_styling(bootstrap_options = c("hover", "striped"))
```

.pred
3652.218
4257.418

We get a predicted body mass for each penguin! We know, almost surely, that these predictions are wrong. We can gain some confidence in our predictions by obtaining an interval of plausible body masses rather than a single point prediction.

```
mass_length_fit %>%
  predict(new_data, type = "conf_int") %>%
  kable() %>%
  kable_styling(bootstrap_options = c("hover", "striped"))
```

.pred_lower	.pred_upper
3535.702	3768.734
4175.341	4339.496

```
mass_length_fit %>%
  predict(new_data, type = "pred_int") %>%
  kable() %>%
  kable_styling(bootstrap_options = c("hover", "striped"))
```

.pred_lower	.pred_upper
2363.676	4940.760
2971.533	5543.304

Perhaps you've noticed that `type = "conf_int"` and `type = "pred_int"` led to different intervals. This is because the *confidence intervals* (`"conf_int"`) attempt to predict the *average* `body_mass_g` for *all* penguins whose `bill_length_mm` is 38 and 45 millimeters, respectively. The *prediction intervals* (`"pred_int"`) are much wider. This is because they attempt to predict the `body_mass_g` for a *single* penguin whose `bill_length_mm` is 38 and 45 millimeters, respectively. It is important to note whether your goal is to predict an *average* response or an *individual* response, and to use the appropriate interval.

Assessing Model Performance

If we are ready to give our model one final test, then we can assess the model's performance on the *test* data using a metric of our choosing.

```r
mass_length_fit %>%
  augment(penguins_test) %>%
  select(bill_length_mm, body_mass_g, .pred) %>%
  head() %>%
  kable() %>%
  kable_styling()
```

bill_length_mm	body_mass_g	.pred
39.1	3750	3747.321
36.6	3700	3531.178
37.7	3600	3626.281
35.9	3800	3470.658
38.2	3950	3669.509
37.9	3150	3643.572

In the code cell above, we used `augment()` rather than `predict()`, which is a special function that appends a `.pred` column (or the corresponding interval columns) to the data frame containing our new data. We then selected only the relevant columns for our small model.

Using this new data frame, we can compare the *truth* (known, actual `body_mass_g`) to our *predictions* (`.pred`) to assess the quality of predictions.

```r
mass_length_fit %>%
  augment(penguins_test) %>%
  select(bill_length_mm, body_mass_g, .pred) %>%
  rmse(body_mass_g, .pred) %>%
  kable() %>%
  kable_styling()
```

.metric	.estimator	.estimate
rmse	standard	631.3512

```r
mass_length_fit %>%
  augment(penguins_test) %>%
  select(bill_length_mm, body_mass_g, .pred) %>%
  rsq(body_mass_g, .pred) %>%
  kable() %>%
  kable_styling()
```

.metric	.estimator	.estimate
rsq	standard	0.3669341

```r
mass_length_fit %>%
  augment(penguins_test) %>%
  select(bill_length_mm, body_mass_g, .pred) %>%
  mae(body_mass_g, .pred) %>%
  kable() %>%
  kable_styling()
```

.metric	.estimator	.estimate
mae	standard	506.5625

There are lots of metrics we could use. If we are interested in multiple metrics, we can collect them all at once by creating a `metric_set()`.

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

mass_length_fit %>%
  augment(penguins_test) %>%
  select(bill_length_mm, body_mass_g, .pred) %>%
  my_metrics(body_mass_g, .pred) %>%
  kable() %>%
  kable_styling()
```

.metric	.estimator	.estimate
rmse	standard	631.3511796
mae	standard	506.5625374
rsq	standard	0.3669341

Summary

The following summary shows the basic steps for using the `{tidymodels}` framework for fitting a statistical model to data.

```r
#create the model specification
lin_reg_spec <- linear_reg() %>%
  set_engine("lm")

#Create a recipe to describe what the model will do
lin_reg_rec <- recipe(response ~ predictors, data)

#package the model and recipe into a workflow
lin_reg_wf <- workflow() %>%
  add_model(lin_reg_spec) %>%
  add_recipe(lin_reg_rec)

#fit the workflow to the training data
lin_reg_fit <- lin_reg_wf %>%
  fit(training_data)
```

Once we have a fitted workflow, there's lots we can do with it. We can see global model-utility and performance metrics.

```r
lin_reg_fit %>%
  glance()
```

We can see the structure of the fitted model.

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

We can also use our fitted workflow to make predictions on new data.

```
lin_reg_fit %>%
  predict(new_data) %>%
  head() %>%
  kable() %>%
  kable_styling()
```

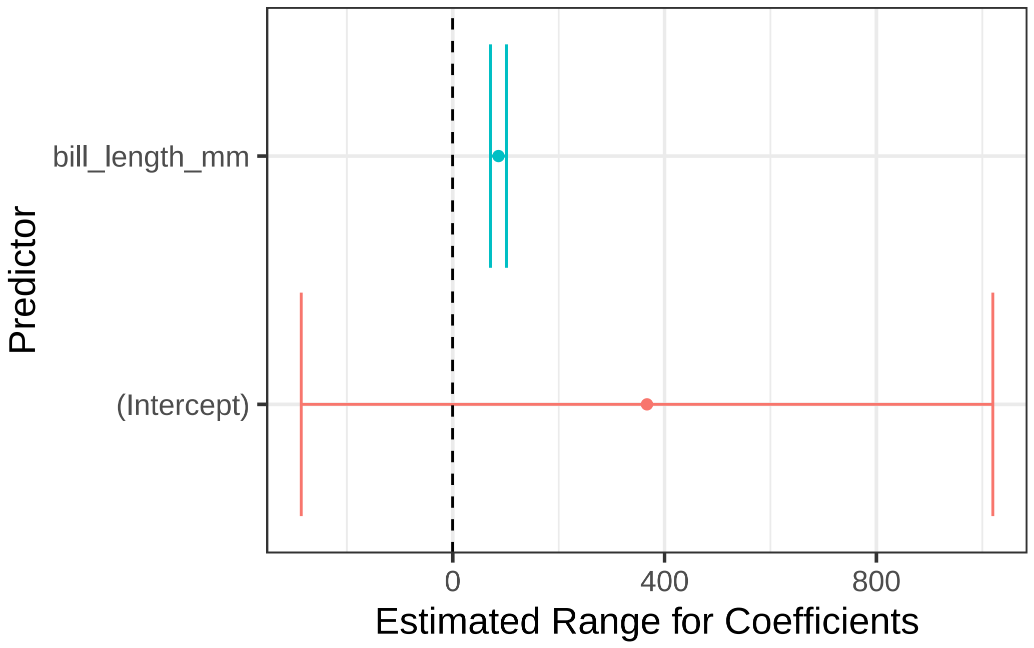
We can append predictions to an existing data frame of new records.

```
lin_reg_fit %>%
  augment(new_data) %>%
  head() %>%
  kable() %>%
  kable_styling()
```

Extra Ideas: Visualizing Model Coefficients

Because we can obtain the model coefficients and statistical measures of uncertainty on those estimates, we can plot the confidence intervals on those model coefficients. Plotting the plausible range for the fitted coefficients, and checking to see whether the interval overlaps with 0 is a great way to convey, visually, whether a predictor is significant or not. Furthermore, this provides a convincing description of the direction and magnitude of the estimated effect size, which is understandable even by non-experts!

```
mass_length_fit %>%
  extract_fit_engine() %>%
  tidy() %>%
  ggplot() +
  geom_errorbarh(aes(xmin = estimate - (2*std.error),
                     xmax = estimate + (2*std.error),
                     y = term,
                     color = term),
                 show.legend = FALSE) +
  geom_point(aes(x = estimate, y = term, color = term),
             show.legend = FALSE) +
  geom_vline(xintercept = 0, linetype = "dashed") +
  labs(x = "Estimated Range for Coefficients",
       y = "Predictor")
```



From the plot above, we can see that the range of plausible coefficients on the bill length predictor includes only positive values. That is, penguins with longer bills are expected to be more massive!

Extra Ideas: Residual Analyses

It is important not to treat our models as black boxes or to follow them blindly. The error metrics we compute tell us only part of the story. To understand fully how well our model performs and where/if the model should be trusted, we must understand the types of errors our models make. Building confidence and prediction intervals using our models assumes that the residuals (prediction errors) are distributed randomly, with mean 0 and constant standard deviation. If these assumptions are not satisfied, then our intervals cannot be trusted!

```r
p1 <- mass_length_fit %>%
  augment(penguins_train) %>%
  select(bill_length_mm, body_mass_g, .pred) %>%
  mutate(residual = body_mass_g - .pred) %>%
  ggplot() +
  geom_point(aes(x = bill_length_mm, y = residual)) +
  geom_smooth(aes(x = bill_length_mm, y = residual),
              color = "red") +
  geom_hline(yintercept = 0,
             linetype = "dashed",
             color = "blue") +
  labs(title = "Residuals versus Bill Length",
       x = "Bill Length (in millimeters)",
       y = "Residual Error")

p2 <- mass_length_fit %>%
  augment(penguins_train) %>%
  select(bill_length_mm, body_mass_g, .pred) %>%
  mutate(residual = body_mass_g - .pred) %>%
  ggplot() +
  geom_point(aes(x = body_mass_g, y = residual)) +
  geom_smooth(aes(x = body_mass_g, y = residual),
              color = "red") +
  geom_hline(yintercept = 0,
             linetype = "dashed",
             color = "blue") +
  labs(title = "Residuals versus Body Mass",
       x = "Body Mass (in grams)",
       y = "Residual Error")

p3 <- mass_length_fit %>%
  augment(penguins_train) %>%
  select(bill_length_mm, body_mass_g, .pred) %>%
  mutate(residual = body_mass_g - .pred) %>%
  ggplot() +
  geom_point(aes(x = .pred, y = residual)) +
  geom_smooth(aes(x = .pred, y = residual),
              color = "red") +
  geom_hline(yintercept = 0,
             linetype = "dashed",
             color = "blue") +
  labs(title = "Residuals versus Predicteds",
       x = "Predicted Body Mass (in grams)",
       y = "Residual Error")

(p1 / p2 / p3)
```

```
`geom_smooth()` using method = 'loess' and formula = 'y ~ x'

Warning: Removed 2 rows containing non-finite outside the scale range
(`stat_smooth()`).

Warning: Removed 2 rows containing missing values or values outside the scale range
```

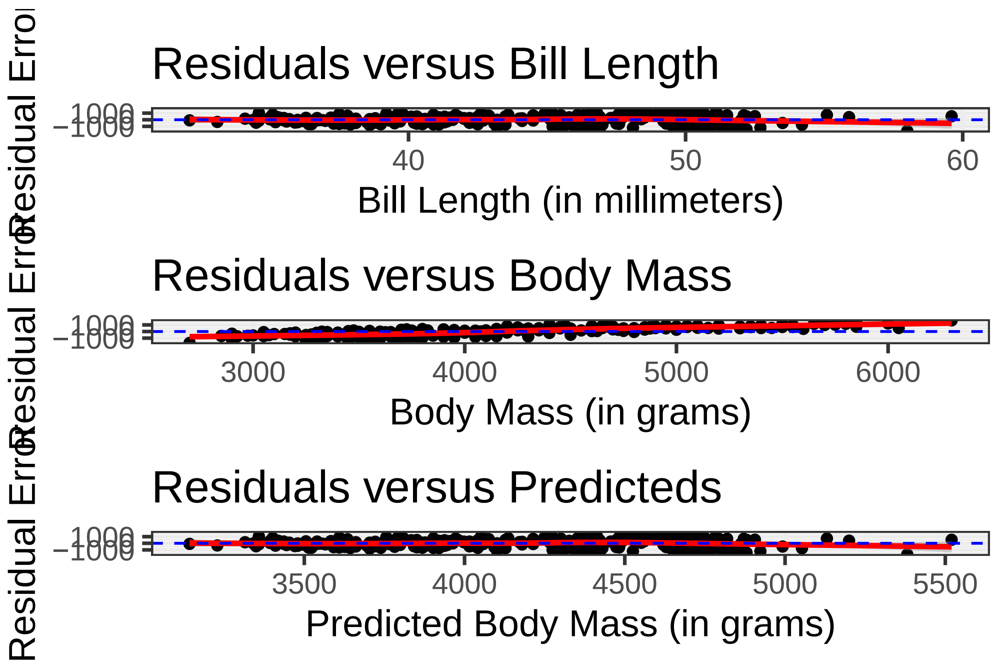
```
(`geom_point()`).

`geom_smooth()` using method = 'loess' and formula = 'y ~ x'

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

`geom_smooth()` using method = 'loess' and formula = 'y ~ x'

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



Note: There are several concerning take-aways of the previous three plots.

- In the first and third plots, we see evidence that the spread of the residuals widens for lengthier bills and for heavier body masses.
    - This means that any confidence or prediction intervals we build using our models will be unreliable!

  - The intervals we construct will be *too optimistic* for penguins with above average bill lengths or body mass. Those confidence and prediction intervals smaller penguins will also not be narrow enough.

- In the second plot, we see a clear linear trend in the relationship between our prediction errors and the true penguin body mass.

  - This indicates that the our model is *over-predicting* (predicting body masses that are too high) for penguins whose actual body mass is below average, and *underpredicting* (predicting body masses that are too low) for penguins whose actual body mass is above average.
  - This means that our model's prediction's are not to be trusted – if we obtain a prediction of low body mass then we know it is likely not low enough, while we know that obtaining a prediction of high body mass is not likely a high enough prediction. Hopefully we can improve the model.