Prediction & Training/Test Set Ideas

In this course we focus on the **predictive modeling** paradigm. In the end, we'll often fit different *families of models* (say some multiple linear regression models, a tree based model, and a random forest model) to a given data set. We'll then judge those models using some model *metric* to determine which model is best at predicting!

Let's break down this process into a few steps.

Predictive Modeling Idea

First we'll choose a form for a model. The types of models to consider often depends on the subject matter at hand. In this course, we'll cover a few general types (or families) of models.

Once we've chosen a model type, we **fit** the model using some algorithm. Usually, we can write this fitting process in terms of minimizing some **loss** function.

We then need to determine the quality of predictions made by the model. We use a model **metric** to do this. Quite often, the loss function and model metric are the same, but this isn't always the case!

For numeric response, the most common model metric is mean squared error (MSE) or root mean squared error (RMSE). For a categorical reponse, the most commmon model metrics are accuracy and log-loss (discussed in detail later).

Training vs Test Sets

Ideally we want our model to predict well for observations **it has yet to see**. We want to avoid *overfitting* to the data we train our model on.

The evaluation of predictions over the observations used to *fit or train the model* is called the **training (set) error**

- Let y_i denote an observed value and $\hat{y}_i$ denote our prediction for that observation. If RMSE was our metric:

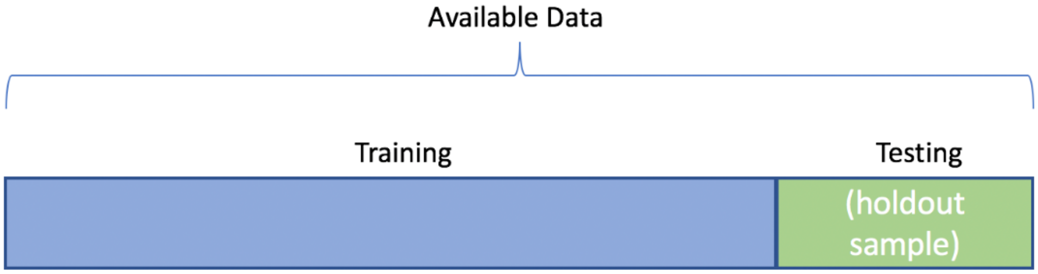
$$\text{Training RMSE} = \sqrt{\frac{1}{\text{\# of obs used to fit model}}\sum_{\text{obs used to fit model}}(y_i - \hat{y}_i)^2}$$

- If we only consider this error, we'll have no idea how the model will fare on data it hasn't seen!

One method to obtain a better idea about model performance is to *randomly* split the data into a **training set** and **test set**.

- On the training set we can fit (or train) our models
- We can then predict for the test set observations and judge effectiveness with

our metric



Example of Fitting and Evaluating Models

Consider our data set on motorcycle sale prices

```
library(tidyverse)
bike_data <- read_csv("https://www4.stat.ncsu.edu/~online/datasets/bikeDetai
bike_data <- bike_data |>
  mutate(log_selling_price = log(selling_price),
         log_km_driven = log(km_driven)) |>
  select(log_km_driven, log_selling_price, everything())
bike_data
```

```
# A tibble: 1,061 × 9
   log_km_driven log_selling_price name    selling_price  year seller_type
owner
           <dbl>             <dbl> <chr>           <dbl> <dbl> <chr>
<chr>
 1          5.86              12.1 Royal …        175000  2019 Individual
1st …
 2          8.64              10.7 Honda …         45000  2017 Individual
1st …
 3          9.39              11.9 Royal …        150000  2018 Individual
1st …
 4         10.0               11.1 Yamaha…         65000  2015 Individual
1st …
 5          9.95               9.90 Yamaha…        20000  2011 Individual
2nd …
 6         11.0                9.80 Honda …        18000  2010 Individual
1st …
 7          9.74              11.3 Honda …         78500  2018 Individual
1st …
 8         10.6               12.1 Royal …        180000  2008 Individual
2nd …
 9         10.4               10.3 Hero H…         30000  2010 Individual
1st …
10         10.6               10.8 Bajaj …         50000  2016 Individual
1st …
# ℹ 1,051 more rows
# ℹ 2 more variables: km_driven <dbl>, ex_showroom_price <dbl>
```

Here our response variable is the `log_selling_price = ln(selling_price)`. We could consider the family of multiple linear regression (MLR) models with differing predictors (x variables).

predictors (x variables).

- The basic MLR model with p predictors models the **average** response variable given the predictors (that's what $E(Y|x_1, x_2, ..., x_p)$ represents, the average or expected Y, given (that's what the vertical bar means) the values of x_1, x_2, ..., x_p) as a linear function (linear in the parameter terms).

$$E(Y|x_1, x_2, ..., x_p) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \beta_p x_p$$

- β_0 is the intercept and each β_j is a slope term associated with a predictor variable.
- As with SLR, we could model the error term with a Normal distribution if we were interested in making inference on the parameters

These basic models find coefficients that minimize the sum of squared residuals (i.e. uses squared error loss to fit the model).

- MLR modeling fitting criterion (the 'hats' just imply the parameters are estimates rather than the 'true' underlying values):

$$min_{\hat{\beta}'s} \sum_{i=1}^{n} \left(y_i - \left(\hat{\beta}_0 + \hat{\beta}_1 x_{1i} + ... + \hat{\beta}_p x_{pi}\right)\right)^2$$

This turns out to be equivalent to doing maximum likelihood estimation with the iid error Normal, constant variance, assumption!

- Consider three competing MLR models:
    - Model 1: log_selling_price = intercept + slope*year + Error
    - Model 2: log_selling_price = intercept + slope*log_km_driven + Error
    - Model 3: log_selling_price = intercept + slope*log_km_driven + slope*year + Error

We can split the data randomly into a training set and a testing set. There are a lot of ways to do this. We'll use the `tidymodels::initial_split()` function.

- We commonly use an 80/20 or 70/30 training/test split. The proportion used in this split really depends on the amount of data you have and your subject matter expertise. More data in the test set means a better estimate of the model's performance. However, less data in the training set means a more variable model (bigger changes in predictions from data set to data set).

- Let's split our `bike_data` into a training and test set.
    - Use `initial_split()` to create an initial object
    - Use `training()` and `testing()` on that object to create the two data sets (note the number of observations in each set below!)

```
library(tidymodels)
set.seed(10)
bike_split <- initial_split(bike_data, prop = 0.7)
bike_train <- training(bike_split)
bike_test <- testing(bike_split)
bike_train
```

```
# A tibble: 742 × 9
   log_km_driven log_selling_price name    selling_price  year seller_type
owner
           <dbl>             <dbl> <chr>           <dbl> <dbl> <chr>
<chr>
 1         10.8              10.3  Bajaj …         30000  2012 Individual
1st …
 2          8.95             10.6  Honda …         40000  2015 Individual
1st …
 3          9.99              9.80 Bajaj …         18000  2005 Individual
1st …
 4         10.2              10.5  Hero H…         35000  2017 Individual
1st …
 5         10.8              11.4  Royal …         85000  2013 Individual
1st …
 6          9.88             10.3  Bajaj …         30000  2008 Individual
1st …
 7         10.5              10.5  Hero C…         35000  2014 Individual
1st …
 8          9.68              9.90 Bajaj …         20000  2009 Individual
1st …
 9         11.1              10.1  Hero H…         25000  2008 Individual
3rd …
10          8.94             12.2  Bajaj …        200000  2019 Individual
1st …
# ℹ 732 more rows
# ℹ 2 more variables: km_driven <dbl>, ex_showroom_price <dbl>
```

```
bike_test
```

```
# A tibble: 319 × 9
   log_km_driven log_selling_price name    selling_price  year seller_type
owner
           <dbl>             <dbl> <chr>           <dbl> <dbl> <chr>
<chr>
 1          8.64             10.7  Honda …         45000  2017 Individual
1st …
 2          9.39             11.9  Royal …        150000  2018 Individual
1st …
 3          7.03             12.8  Yamaha…        365000  2019 Individual
1st …
 4          7.44             12.1  Jawa 42        185000  2020 Individual
1st …
 5         10.9              10.1  Suzuki…         25000  2012 Individual
1st …
 6         11.0               9.62 Hero P…         15000  2008 Individual
1st …
 7          7.60             12.1  Jawa S…        180000  2019 Individual
1st …
 8         10.1              10.6  Honda …         42000  2017 Individual
1st …
 9          9.21              9.95 Hero H…         21000  2009 Individual
1st …
```

```
10          9.95              10.7   Hero G…          45000  2018 Individual
1st …
# ℹ 309 more rows
# ℹ 2 more variables: km_driven <dbl>, ex_showroom_price <dbl>
```

We can *fit* or *train* these models on the training set. Recall we use `lm()` to easily fit an MLR model via formula notation. With formula notation we put our response variable on the left and our model for the predictors on the right. The model can include interactions, non-linear terms, etc. If we just want 'main effects' we separate predictors with `+` on the right hand side (we'll cover this in more detail later!)

- Let's fit our three models and save them as objects.

```
reg1 <- lm(log_selling_price ~ year, data = bike_train)
coef(reg1)
```

```
  (Intercept)          year
-186.17235057    0.09777273
```

```
reg2 <- lm(log_selling_price ~ log_km_driven, data = bike_train)
coef(reg2)
```

```
  (Intercept) log_km_driven
   14.6228627    -0.3899342
```

```
reg3 <- lm(log_selling_price ~ year + log_km_driven, data = bike_train)
coef(reg3)
```

```
  (Intercept)          year log_km_driven
-131.66741960    0.07191291   -0.24274055
```

Now we have the fitted models. Want to use them to predict the response

- Model 1: $\widehat{\text{log\_selling\_price}} = -186.1724 + 0.0978 * \text{year}$
- Model 2: $\widehat{\text{log\_selling\_price}} = 14.6229 - 0.3899 * \text{log\_km\_driven}$
- Model 3: $\widehat{\text{log\_selling\_price}} = -131.6674 + 0.0719 * \text{year} - 0.2427 * \text{log\_km\_driven}$

To get predictions from our model, we use the `predict()` function and specify the `newdata` we want to predict for as a data frame with column names matching our predictors in our models. If we don't specify any `newdata`, it returns the predictions made on the training data.

- We can see the first few predictions on the training data from the first model via the code below

```
#year values the predictions are for
bike_train$year |> head()
```

```
[1] 2012 2015 2005 2017 2013 2008
```

```
#predictions made with our first model
predict(reg1) |> head()
```

```
predict(reg1) |> head()
```

```
        1         2         3         4         5         6 
10.546377 10.839696  9.861968 11.035241 10.644150 10.155287 
```

Let's use RMSE as our metric. Although not how we want to compare our models, we can obtain the training RMSE easily with `predict()`. Let's code it up ourselves and also `yardstick::rmse_vec()` to find it (this is the `tidymodels` way).

```
#our own calculation for training RMSE
sqrt(mean((bike_train$log_selling_price - predict(reg1))^2))
```

```
[1] 0.5378694
```

- Now we can supply the actual responses and the model predictions to `yardstick::rmse_vec()`

```
#using yardstick
yardstick::rmse_vec(bike_train$log_selling_price, predict(reg1))
```

```
[1] 0.5378694
```

```
#second and third models
#using yardstick
rmse_vec(bike_train$log_selling_price, predict(reg2))
```

```
[1] 0.5669127
```

```
#using yardstick
rmse_vec(bike_train$log_selling_price, predict(reg3))
```

```
[1] 0.4924924
```

- These values represent a measure of quality of prediction by these models (as judged by our metric RMSE).
- This estimate of RMSE for the predictions is too **optimistic** compared to how the model would perform with new data!
- Really, what we want to compare is how the models do on data they weren't trained on.
- We want to find this type of metric on the test set. That means we want to use the **truth** from the test set (y_i for the test set) and compare that to predictions made for that test set observation ($\hat{y}_i$).

$$\text{Test Set RMSE} = \sqrt{\frac{1}{n_{test}}\sum_{i=1}^{n_{test}}(y_i - \hat{y}_i)^2}$$

To do this in R we need to tell `predict()` about the `newdata` being the test set (`bike_test`). As this is a data frame with columns for our predictors, we can just (bike_test). As this is a data frame with columns for our predictors, we can just pass the entire data frame for ease and `predict()` uses appropriate/needed columns to find our predictions.

```
#look at a few observations and predictions
bike_test |>
  select(log_km_driven, log_selling_price) |>
  mutate(model_1_preds = predict(reg1, newdata = bike_test))
```

```
# A tibble: 319 × 3
   log_km_driven log_selling_price model_1_preds
           <dbl>             <dbl>         <dbl>
 1          8.64             10.7           11.0
 2          9.39             11.9           11.1
 3          7.03             12.8           11.2
 4          7.44             12.1           11.3
 5         10.9              10.1           10.5
 6         11.0               9.62          10.2
 7          7.60             12.1           11.2
 8         10.1              10.6           11.0
 9          9.21              9.95          10.3
10          9.95             10.7           11.1
# ℹ 309 more rows
```

- Now let's find the **test set error** for each model

```
#obtain the test set RMSE for each model
rmse_vec(bike_test$log_selling_price, predict(reg1, newdata = bike_test))
```

```
[1] 0.5746992
```

```
rmse_vec(bike_test$log_selling_price, predict(reg2, newdata = bike_test))
```

```
[1] 0.6548019
```

```
rmse_vec(bike_test$log_selling_price, predict(reg3, newdata = bike_test))
```

```
[1] 0.554596
```

We see that our third model with both `year` and `log_km_driven` gives a better (by our metric) set of predictions!

When choosing a model, if the RMSE values were 'close', we'd want to consider the interpretability of the model (and perhaps the assumptions required by each model if we wanted to do inference too!)

- Note: we can do this with `yardstick::rmse()` if our predictions are in the data frame. `rmse()` takes in the `data` as the first argument, the `truth` column as the second, and the `estimate` (or predictions) as the third.

```
#look at a few observations and predictions
bike_test |>
  select(log_selling_price, log_km_driven) |>
```

```
  select(log_selling_price, log_km_driven) |>
  mutate(model_1_preds = predict(reg1, newdata = bike_test)) |>
  rmse(truth = log_selling_price, estimate = model_1_preds)
```

```
# A tibble: 1 × 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 rmse    standard       0.575
```

Recap

We generally need to go through a few steps when training and testing our model(s):

- Choose form of model
- Fit model to data using some algorithm
  - Usually can be written as a problem where we minimize some loss function
- Evaluate the model using a metric
  - RMSE very common for a numeric response
- Ideally we want our model to predict well for observations **it has yet to see**!