Decision Trees

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Agenda 10/28/21

1. Decision Trees
2. Example

`tidymodels` syntax

1. partition the data
2. build a recipe
3. select a model
4. create a workflow
5. fit the model

6. validate the model

Decision trees in action

Figure 1: A visual introduction to machine learning by Yee and Chu.

Yee and Chu created a step-by-step build of a recursive binary tree to model the differences between homes in SF and homes in NYC. http://www.r2d3.us/visual-intro-to-machine-learning-part-1/

Classification and Regression Trees (CART)

Basic Classification and Regression Trees (CART) Algorithm:

1. Start with all observations in one group.
2. Find the variable/split that best separates the response variable (successive binary partitions based on the different predictors / explanatory variables).
    - Evaluation "homogeneity" within each group
    - Divide the data into two groups ("leaves") on that split ("node").
    - Within each split, find the best variable/split that separates the outcomes.
3. Continue until the groups are too small or sufficiently "pure".
4. Prune tree.

Minimize heterogeneity

For every observation that falls into the region R_m,

prediction = the mean of the response values for observations in R_m.

$\Rightarrow$ Minimize Residual Sum of Squares (RSS):

$$RSS = \sum_{m=1}^{|T|} \sum_{i \in R_m} (y_i - \overline{y}_{R_m})^2$$

where $\overline{y}_{R_m}$ is the mean response for observations within the mth region.

Recursive binary splitting

Select the predictor X_j and the cutpoint s such that splitting the predictor space into the regions $\{X|X_j < s\}$ and $\{X|X_j \geq s\}$ lead to the greatest reduction in RSS.

For any j and s, define the pair of half-planes to be

$$R_1(j,s) = \{X|X_j < s\} \text{ and } R_2(j,s) = \{X|X_j \geq s\}$$

Find the value of j and s that minimize the equation:

$$\sum_{i:x_i \in R_1(j,s)} (y_i - \overline{y}_{R_1})^2 + \sum_{i:x_i \in R_2(j,s)} (y_i - \overline{y}_{R_2})^2$$

where $\overline{y}_{R_1}$ is the mean response for observations in $R_1(j,s)$ and $\overline{y}_{R_2}$ is the mean response observations in $R_2(j,s)$.

Trees in action

Measures of impurity

$\hat{p}_{mk}$ = proportion of observations in the mth region from the kth class.

- *classification error rate* = fraction of observations in the node & not in the most common class:

$$E_m = 1 - \max_k(\hat{p}_{mk})$$

- *Gini index*

$$G_m = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$$

- *cross-entropy*

$$D_m = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$

(Gini index & cross-entropy will both take on a value near zero if the $\hat{p}_{mk}$ values are all near zero or all near one.)

Recursive binary splitting

For any j and s, define the pair of half-planes to be

$$R_1(j, s) = \{X | X_j < s\} \text{ and } R_2(j, s) = \{X | X_j \geq s\}$$

Seek the value of j and s that minimize the equation:

$$\sum_{i:x_i \in R_1(j,s)} \sum_{k=1}^{K} \hat{p}_{R_1 k}(1 - \hat{p}_{R_1 k}) + \sum_{i:x_i \in R_2(j,s)} \sum_{k=1}^{K} \hat{p}_{R_2 k}(1 - \hat{p}_{R_2 k}) \tag{1}$$

(2)

equivalently: (3)

$$n_{R_1} \sum_{k=1}^{K} \hat{p}_{R_1 k}(1 - \hat{p}_{R_1 k}) + n_{R_2} \sum_{k=1}^{K} \hat{p}_{R_2 k}(1 - \hat{p}_{R_2 k}) \tag{4}$$

(5)

Stopping

We can always make the tree more "pure" by continuing the split.

Too many splits will overfit the model to the training data!

Ways to control:

- `cost_complexity`
- `tree_depth`
- `min_n`

Overfitting: http://www.r2d3.us/visual-intro-to-machine-learning-part-2/

Cost complexity

There is a cost to having a larger (more complex!) tree.

Define the cost complexity criterion, $\alpha > 0$:

$$\text{numerical: } C_\alpha(T) = \sum_{m=1}^{|T|} \sum_{i \in R_m} (y_i - \overline{y}_{R_m})^2 + \alpha \cdot |T| \tag{6}$$

$$\text{categorical: } C_\alpha(T) = \sum_{m=1}^{|T|} \sum_{i \in R_m} I(y_i \neq k(m)) + \alpha \cdot |T| \tag{7}$$

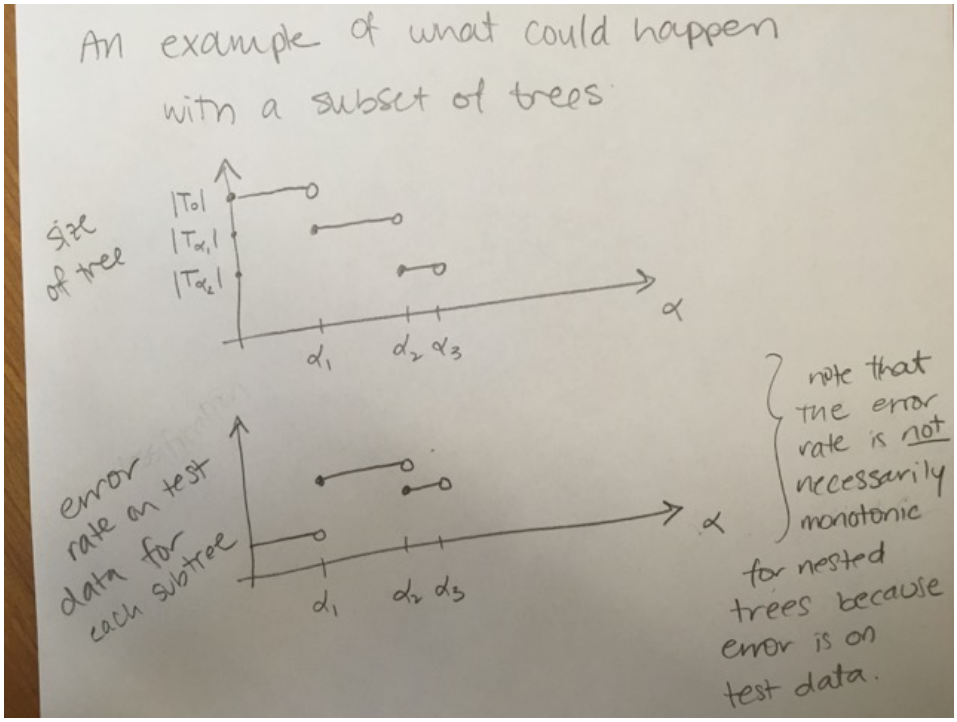
where $k(m)$ is the class with the majority of observations in node m and $|T|$ is the number of terminal nodes in the tree.

- α small: If α is set to be small, we are saying that the risk is more worrisome than the complexity and larger trees are favored because they reduce the risk.
- α large: If α is set to be large, then the complexity of the tree is more worrisome and smaller trees are favored.

In practice

Consider α increasing. As α gets bigger, the "best" tree will be smaller.

The test error will not be monotonically related to the size of the training tree.



A note on α

In the text (*Introduction to Statistical Learning*) and almost everywhere else you might look, the cost complexity is defined as in previous slides.

However, you might notice that in R the `cost_complexity` value is typically less than 1. From what I can tell, the value of the function that is being minimized in R is the **average** of the squared errors and the missclassification **rate**.

$$\text{numerical: } C_\alpha(T) = \frac{1}{n}\sum_{m=1}^{|T|}\sum_{i\in R_m}(y_i - \overline{y}_{R_m})^2 + \alpha\cdot|T| \tag{8}$$

$$\text{categorical: } C_\alpha(T) = \frac{1}{n}\sum_{m=1}^{|T|}\sum_{i\in R_m} I(y_i \neq k(m)) + \alpha\cdot|T| \tag{9}$$

CART algorithm

Algorithm: Building a Regression Tree

1. Use recursive binary splitting to grow a large tree on the training data, stopping only when each terminal node has fewer than some minimum number of observations.
2. Apply cost complexity pruning to the large tree in order to obtain a sequence of best subtrees, as a function of α.
3. Use V-fold cross-validation to choose α. Divide the training observations into V folds, then for each $v = 1, 2, \ldots, V$:
    a. Repeat Steps 1 and 2 on all but the vth fold of the training data.
    b. Evaluate the mean squared prediction error on the data in the left-out kth fold, as a function of α. For each value of α, average the prediction error (either misclassification or RSS), and pick α to minimize the average error.
4. Return the subtree from Step 2 that corresponds to the chosen value of α.

CART example w defaults

recipe

```
penguin_cart_recipe <-
  recipe(species ~ . ,
         data = penguin_train) |>
  step_unknown(sex, new_level = "unknown") |>
  step_mutate(year = as.factor(year))

summary(penguin_cart_recipe)
```

```
# A tibble: 8 x 4
  variable          type      role      source
  <chr>             <list>    <chr>     <chr>
1 island            <chr [3]> predictor original
2 bill_length_mm    <chr [2]> predictor original
3 bill_depth_mm     <chr [2]> predictor original
4 flipper_length_mm <chr [2]> predictor original
5 body_mass_g       <chr [2]> predictor original
6 sex               <chr [3]> predictor original
7 year              <chr [2]> predictor original
8 species           <chr [3]> outcome   original
```

model

```
penguin_cart <- decision_tree() |>
  set_engine("rpart") |>
  set_mode("classification")

penguin_cart
```

```
Decision Tree Model Specification (classification)

Computational engine: rpart
```

workflow

```
penguin_cart_wflow <- workflow() |>
  add_model(penguin_cart) |>
  add_recipe(penguin_cart_recipe)

penguin_cart_wflow
```

```
== Workflow ====================================================================
Preprocessor: Recipe
Model: decision_tree()

-- Preprocessor ----------------------------------------------------------------
2 Recipe Steps

* step_unknown()
* step_mutate()

-- Model -----------------------------------------------------------------------
Decision Tree Model Specification (classification)

Computational engine: rpart
```

fit

```
penguin_cart_fit <- penguin_cart_wflow |>
  fit(data = penguin_train)

penguin_cart_fit
```

```
== Workflow [trained] ==========================================================
Preprocessor: Recipe
Model: decision_tree()

-- Preprocessor ----------------------------------------------------------------
2 Recipe Steps

* step_unknown()
* step_mutate()

-- Model -----------------------------------------------------------------------
n= 258

node), split, n, loss, yval, (yprob)
      * denotes terminal node

1) root 258 139 Adelie (0.461240310 0.189922481 0.348837209)
  2) flipper_length_mm< 206.5 164  46 Adelie (0.719512195 0.274390244 0.006097561)
    4) bill_length_mm< 43.15 118   3 Adelie (0.974576271 0.025423729 0.000000000) *
    5) bill_length_mm>=43.15 46   4 Chinstrap (0.065217391 0.913043478 0.021739130) *
  3) flipper_length_mm>=206.5 94   5 Gentoo (0.010638298 0.042553191 0.946808511)
    6) bill_depth_mm>=17.15 7   3 Chinstrap (0.142857143 0.571428571 0.285714286) *
    7) bill_depth_mm< 17.15 87   0 Gentoo (0.000000000 0.000000000 1.000000000) *
```

pred

```
penguin_cart_fit |>
  predict(new_data = penguin_train) |>
  cbind(penguin_train) |>
  select(.pred_class, species) |>
  table()
```

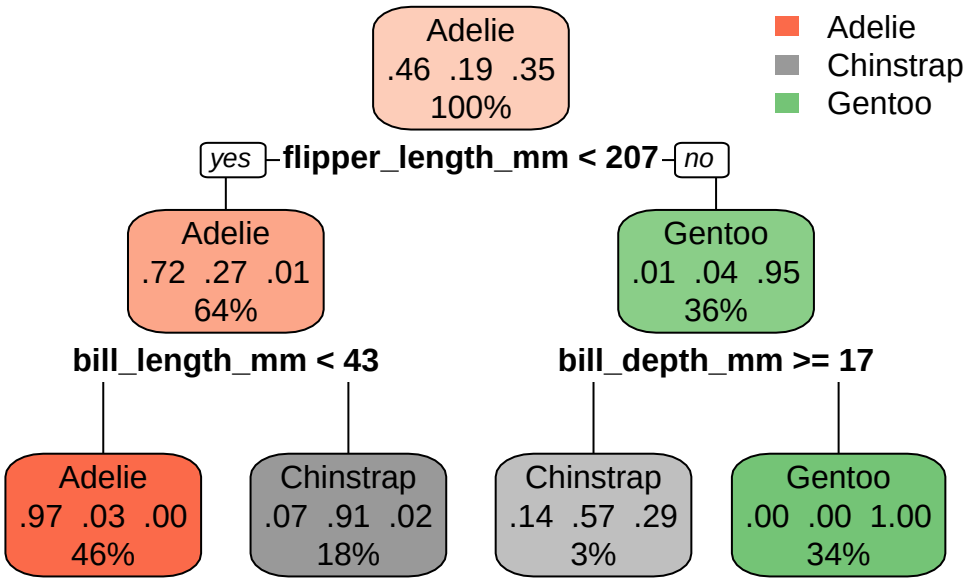
```
           species
.pred_class Adelie Chinstrap Gentoo
```

```
  Adelie        115          3       0
  Chinstrap       4         46       3
  Gentoo          0          0      87
```

Plotting the tree (not tidy)

plot 1

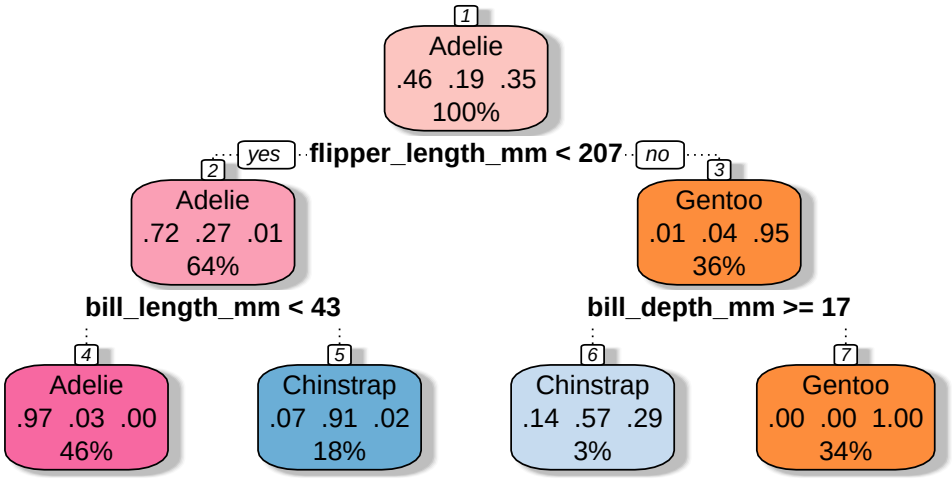
```
library(rpart.plot)
penguins_cart_plot <-
  penguin_cart_fit |>
  extract_fit_parsnip()

rpart.plot(
  penguins_cart_plot$fit,
  roundint = FALSE)
```



plot 2

```
library(rattle)
penguins_cart_plot <-
  penguin_cart_fit |>
  extract_fit_parsnip()
```

```
fancyRpartPlot(
  penguins_cart_plot$fit,
  sub = NULL,
  palettes = "RdPu")
```



CART example w CV

new recipe

```
penguin_cart_tune_recipe <-
  recipe(sex ~ body_mass_g + bill_length_mm + species,
         data = penguin_train)
```

creating folds

```
set.seed(470)
penguin_vfold <- vfold_cv(penguin_train,
                          v = 5, strata = sex)
```

alpha

```r
cart_grid <- expand.grid(
  cost_complexity = c(0, 10^(seq(-5,-1,1))),
  tree_depth = seq(1,6, by = 1))

cart_grid
```

```
   cost_complexity tree_depth
1            0e+00          1
2            1e-05          1
3            1e-04          1
4            1e-03          1
5            1e-02          1
6            1e-01          1
7            0e+00          2
8            1e-05          2
9            1e-04          2
10           1e-03          2
11           1e-02          2
12           1e-01          2
13           0e+00          3
14           1e-05          3
15           1e-04          3
16           1e-03          3
17           1e-02          3
18           1e-01          3
19           0e+00          4
20           1e-05          4
21           1e-04          4
22           1e-03          4
23           1e-02          4
24           1e-01          4
25           0e+00          5
26           1e-05          5
27           1e-04          5
28           1e-03          5
29           1e-02          5
30           1e-01          5
31           0e+00          6
32           1e-05          6
33           1e-04          6
34           1e-03          6
35           1e-02          6
```

```
36           1e-01          6
```

tune wkflow

```
penguin_cart_tune <-
  decision_tree(cost_complexity = tune(),
                tree_depth = tune()) |>
  set_engine("rpart") |>
  set_mode("classification")

penguin_cart_wflow_tune <- workflow() |>
  add_model(penguin_cart_tune) |>
  add_recipe(penguin_cart_tune_recipe)
```

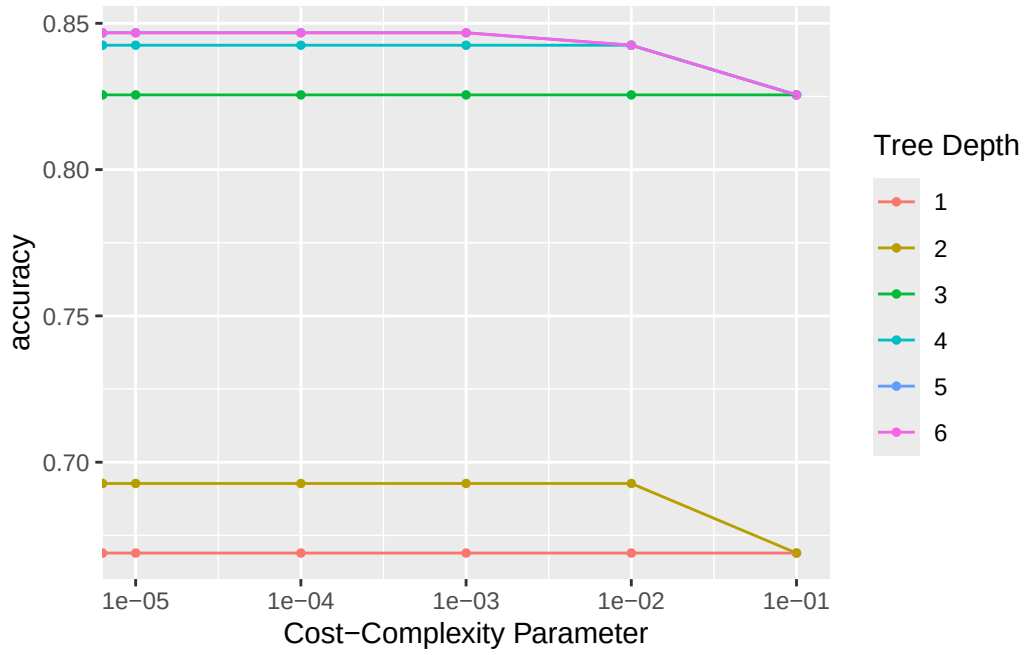
tuning

```
penguin_tuned <- penguin_cart_wflow_tune |>
  tune_grid(resamples = penguin_vfold,
            grid = cart_grid)

penguin_tuned |> collect_metrics() |>
  filter(.metric == "accuracy")
```

```
# A tibble: 36 x 8
   cost_complexity tree_depth .metric  .estimator  mean     n std_err .config
             <dbl>      <dbl> <chr>    <chr>      <dbl> <int>   <dbl> <chr>
 1         0               1 accuracy binary     0.669     5  0.0152 Preproces~
 2         0.00001         1 accuracy binary     0.669     5  0.0152 Preproces~
 3         0.0001          1 accuracy binary     0.669     5  0.0152 Preproces~
 4         0.001           1 accuracy binary     0.669     5  0.0152 Preproces~
 5         0.01            1 accuracy binary     0.669     5  0.0152 Preproces~
 6         0.1             1 accuracy binary     0.669     5  0.0152 Preproces~
 7         0               2 accuracy binary     0.693     5  0.0226 Preproces~
 8         0.00001         2 accuracy binary     0.693     5  0.0226 Preproces~
 9         0.0001          2 accuracy binary     0.693     5  0.0226 Preproces~
10         0.001           2 accuracy binary     0.693     5  0.0226 Preproces~
# i 26 more rows
```

Parameter choice

```
penguin_tuned |>
  autoplot(metric = "accuracy")
```




```
penguin_tuned |>
  select_best(metric = "accuracy")
```

```
# A tibble: 1 x 3
  cost_complexity tree_depth .config
            <dbl>      <dbl> <chr>
1            0           5 Preprocessor1_Model25
```

Best model

```
penguin_best <- finalize_model(
  penguin_cart_tune,
  select_best(penguin_tuned, metric = "accuracy"))
```

```r
workflow() |>
  add_model(penguin_best) |>
  add_recipe(penguin_cart_tune_recipe) |>
  fit(data = penguin_train)
```

```
== Workflow [trained] ==========================================================
Preprocessor: Recipe
Model: decision_tree()

-- Preprocessor ----------------------------------------------------------------
0 Recipe Steps

-- Model ---------------------------------------------------------------------
n=248 (10 observations deleted due to missingness)

node), split, n, loss, yval, (yprob)
      * denotes terminal node

 1) root 248 116 female (0.53225806 0.46774194)
   2) body_mass_g< 3712.5 90  15 female (0.83333333 0.16666667)
     4) bill_length_mm< 38.95 44   1 female (0.97727273 0.02272727) *
     5) bill_length_mm>=38.95 46  14 female (0.69565217 0.30434783)
      10) body_mass_g< 3312.5 11   0 female (1.00000000 0.00000000) *
      11) body_mass_g>=3312.5 35  14 female (0.60000000 0.40000000)
        22) species=Chinstrap 20   5 female (0.75000000 0.25000000)
          44) bill_length_mm< 48.3 11   0 female (1.00000000 0.00000000) *
          45) bill_length_mm>=48.3 9   4 male (0.44444444 0.55555556) *
        23) species=Adelie 15   6 male (0.40000000 0.60000000) *
   3) body_mass_g>=3712.5 158  57 male (0.36075949 0.63924051)
     6) species=Gentoo 86  39 female (0.54651163 0.45348837)
      12) body_mass_g< 4987.5 41   1 female (0.97560976 0.02439024) *
      13) body_mass_g>=4987.5 45   7 male (0.15555556 0.84444444) *
     7) species=Adelie,Chinstrap 72  10 male (0.13888889 0.86111111)
      14) body_mass_g< 3962.5 35   9 male (0.25714286 0.74285714)
        28) bill_length_mm< 48.3 25   9 male (0.36000000 0.64000000)
          56) bill_length_mm>=40.85 7   3 female (0.57142857 0.42857143) *
          57) bill_length_mm< 40.85 18   5 male (0.27777778 0.72222222) *
        29) bill_length_mm>=48.3 10   0 male (0.00000000 1.00000000) *
      15) body_mass_g>=3962.5 37   1 male (0.02702703 0.97297297) *
```

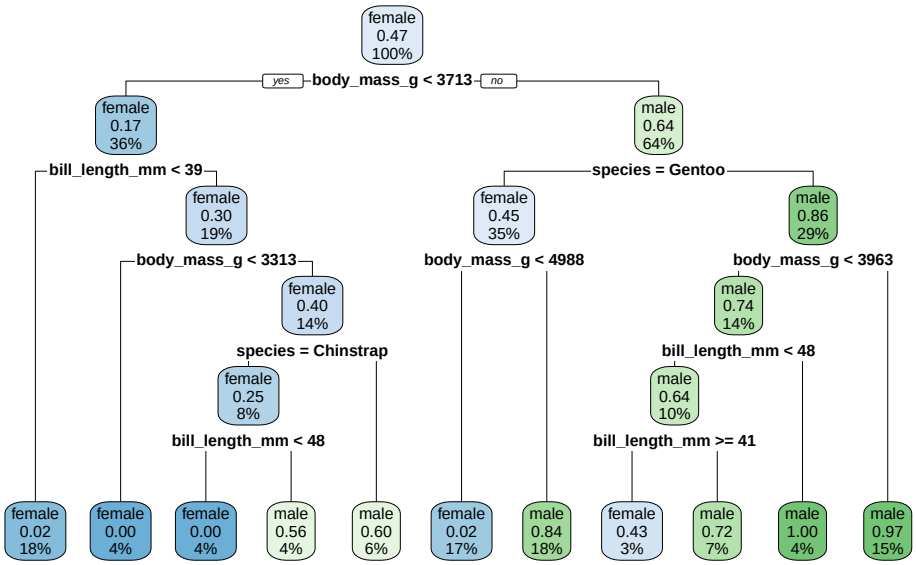
Best Model Predictions

```
workflow() |>
  add_model(penguin_best) |>
  add_recipe(penguin_cart_tune_recipe) |>
  fit(data = penguin_train) |>
  predict(new_data = penguin_test) |>
  cbind(penguin_test) |>
  select(.pred_class, sex) |>
  table()
```

```
           sex
.pred_class female male
     female     26    5
     male        7   47
```

Best Model Predictions

```
library(rpart.plot)
penguins_cart_plot <-
workflow() |>
  add_model(penguin_best) |>
  add_recipe(penguin_cart_tune_recipe) |>
  fit(data = penguin_train) |>
  extract_fit_parsnip()

rpart.plot(
  penguins_cart_plot$fit,
  roundint = FALSE)
```



Bias-Variance Tradeoff

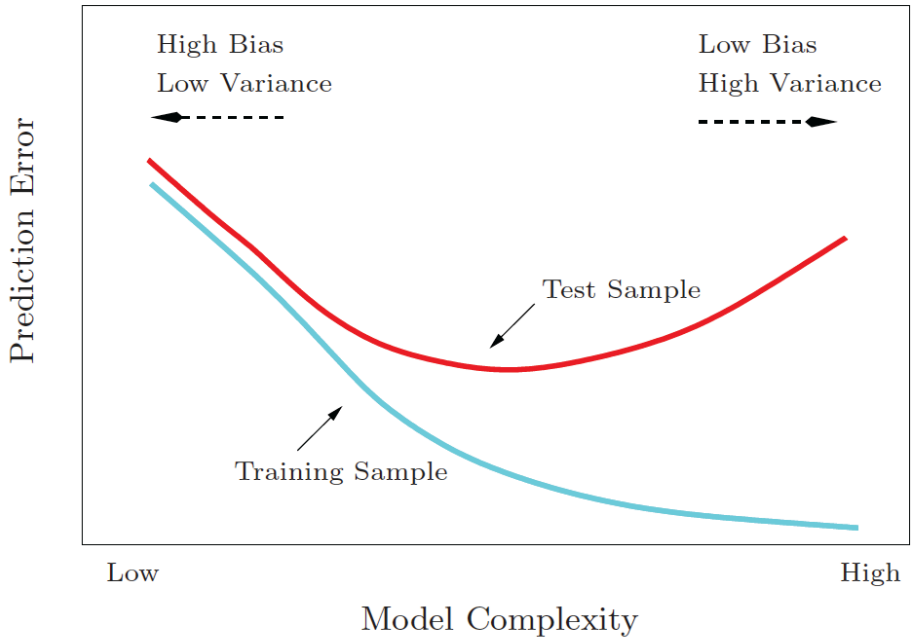


Figure 2: Test and training error as a function of model complexity. Note that the error goes down monotonically only for the training data. Be careful not to overfit!! image credit: ISLR

Reflecting on Model Building

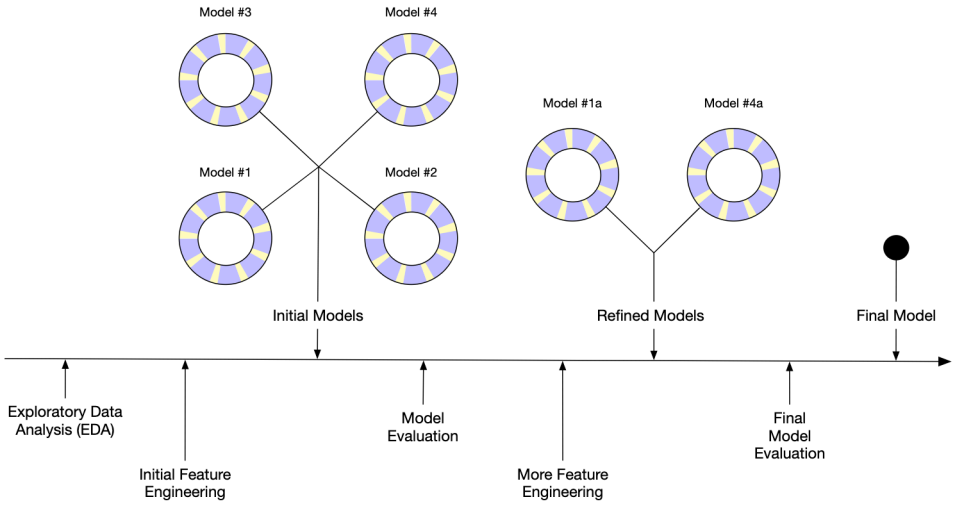


Figure 1.3: A schematic for the typical modeling process.

Figure 3: Image credit: https://www.tmwr.org/

Reflecting on Model Building

- **Exploratory data analysis (EDA):** Initially there is a back and forth between numerical analysis and visualization of the data (represented in Figure 1.2) where different discoveries lead to more questions and data analysis "side-quests" to gain more understanding.
- **Feature engineering:** The understanding gained from EDA results in the creation of specific model terms that make it easier to accurately model the observed data. This can include complex methodologies (e.g., PCA) or simpler features (using the ratio of two predictors). Chapter 8 focuses entirely on this important step.
- **Model tuning and selection (circles with blue and yellow segments):** A variety of models are generated and their performance is compared. Some models require *parameter tuning* where some structural parameters are required to be specified or optimized. The colored segments within the circles signify the repeated data splitting used during resampling (see Chapter 10).
- **Model evaluation:** During this phase of model development, we assess the model's performance metrics, examine residual plots, and conduct other EDA-like analyses to understand how well the models work. In some cases, formal between-model comparisons (Chapter 11) help you to understand whether any differences in models are within the experimental noise.

Figure 4: Image credit: https://www.tmwr.org/

Reflecting on Model Building

Thoughts	Activity
The daily ridership values between stations are extremely correlated.	EDA
Weekday and weekend ridership look very different.	EDA
One day in the summer of 2010 has an abnormally large number of riders.	EDA
Which stations had the lowest daily ridership values?	EDA
Dates should at least be encoded as day-of-the-week, and year.	Feature Engineering
Maybe PCA could be used on the correlated predictors to make it easier for the models to use them.	Feature Engineering
Hourly weather records should probably be summarized into daily measurements.	Feature Engineering
Let's start with simple linear regression, K-nearest neighbors, and a boosted decision tree.	Model Fitting
How many neighbors should be used?	Model Tuning
Should we run a lot of boosting iterations or just a few?	Model Tuning
How many neighbors seemed to be optimal for these data?	Model Tuning
Which models have the lowest root mean squared errors?	Model Evaluation
Which days were poorly predicted?	EDA
Variable importance scores indicate that the weather information is not predictive. We'll drop them from the next set of models.	Model Evaluation
It seems like we should focus on a lot of boosting iterations for that model.	Model Evaluation
We need to encode holiday features to improve predictions on (and around) those dates.	Feature Engineering
Let's drop K-NN from the model list.	Model Evaluation

Figure 5: Image credit: https://www.tmwr.org/