Data Mining

Thiyanga S. Talagala

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Preface

1 Introduction to Data Mining

1.1 What is Data Mining?

- Process of discovering interesting patterns of knowledge from huge amounts of data.

1.2 What do we mean by interesting patterns?

- Interesting patterns: Valid, Novel, Useful, Understandable

Example

- Retailers collect data about customer purchases at the checkout counters
- Customer purchasing patterns: Identify which items are frequently sold together?
- Products that are likely to be purchased together.

Why it is useful?

- Can make a purchase suggestion to their customers
- Gives an idea that how we can arrange items in a store to as a strategy for boosting sales.

1.3 Characteristics of Big Data: 5 V's of Big Data

1. Volume: size
2. Velocity: how quickly data is generated?
3. Variety: diversity
4. Veracity: quality of data
5. Value: how useful?

1.4 What motivates the development of data mining field?

- Scalability
- High dimensionality
- Heterogeneous and complex data
- Data ownership and distribution

1.5 Data Mining Tasks

1. Predictive tasks: Predict the value of a particular attribute based on the values of other attributes
2. Descriptive tasks: Find human-interpretable patterns that describe data

1.6 Data Quality

1. Range: How narrow or wide of the scope of these data?
2. Relevancy: Is the data relevant to the problem?
3. Recency: How recent the data is generated?
4. Robustness: Signal to noise ratio
5. Reliability: How accurate?

1.7 Applications

1. Web mining: recommendation systems
2. Screening images: Early warning of ecological disasters
3. Marketing and sales
4. Diagnosis
5. Load forecasting
6. Decision involving judgement

Many more...

2 What is Statistical Learing?

In-class explanations

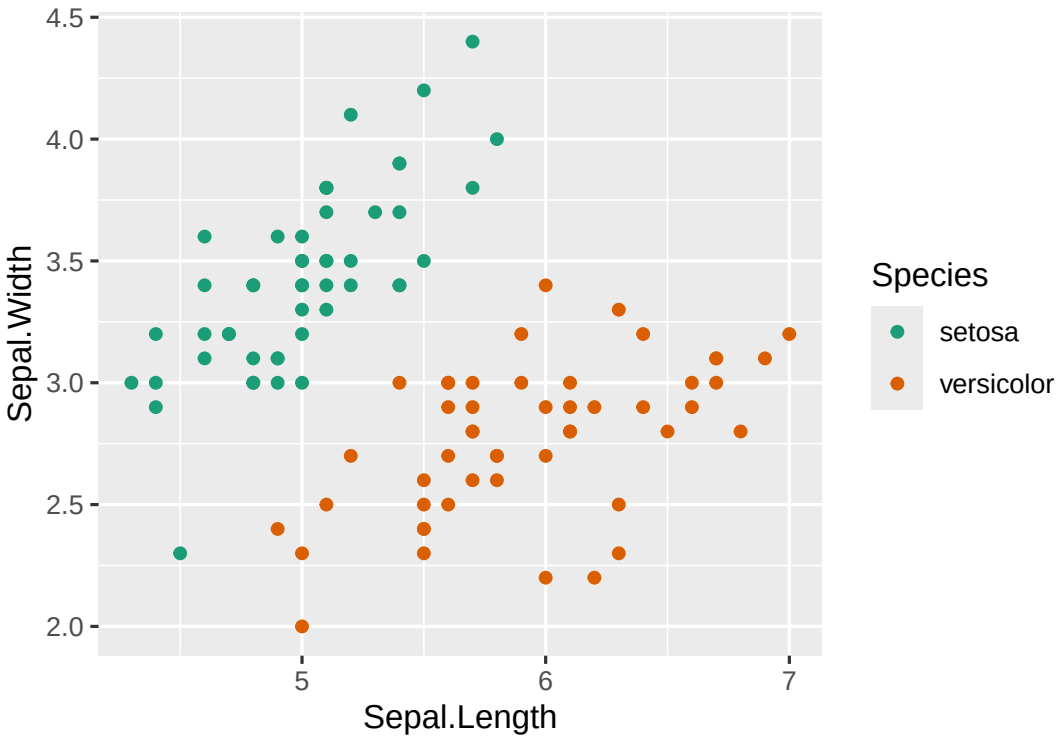
3 Decision Trees

3.1 Motivational Example Dataset

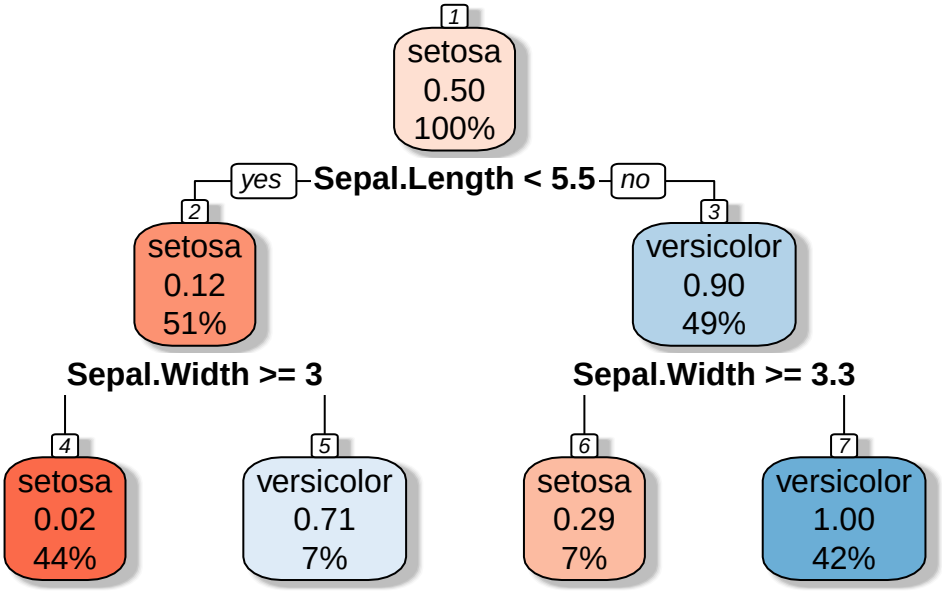
Features: Sepal Length, Sepal Width

Outcome: Species: setosa/versicolor

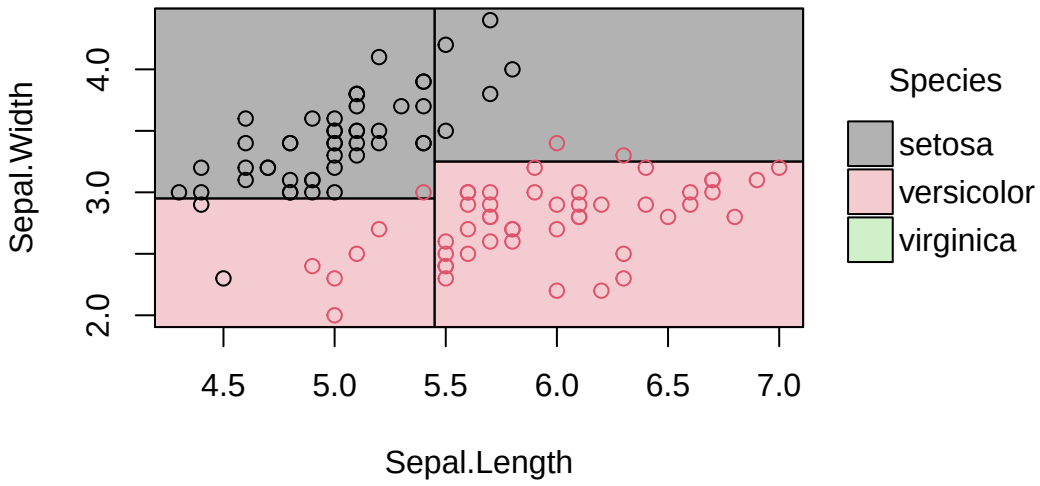
3.1.1 Predictor space

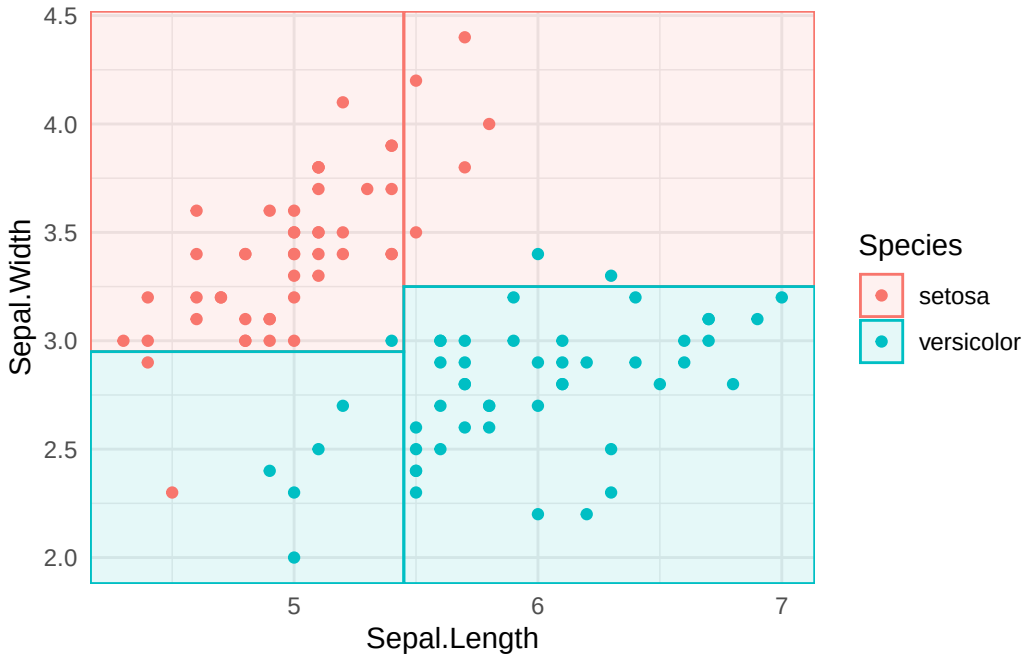


3.1.2 Decision Tree



3.1.3 Partition space





$R1 = \{X | Sepal.Width >= 3, Sepal.Length < 5.5\}$

3.2 Parts of a decision tree

- Root node
- Decision node
- Terminal node/ Leaf node (gives outputs/class assignments)
- Subtree

3.3 Introduction

What happens in the model training phase?

- Stratify or segment the predictor space into a number of non-overlapping regions.
- Set of splitting rules are used to segment the predictor space.
- Decision tree consists of a series of splitting rules.

How to make predictions?

- Mean or mode response value for the training observations in the region which the observation we want to predict belong to.
- We make the same prediction, for the training observations in the j^{th} region R_j.

3.4 Decision Trees: Regression - Finding the best split and best splitting variable

The goal is to find $R_1, R_2, R_3 ... R_J$, J distinct and non-overlapping regions that minimize the RSS given by

$$\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2.$$

$\hat{y}_{R_j}$ - mean response for the training observations within the j^{th} region.

In theory, to build the best possible decision tree, we could try every possible way of splitting the data at every step and choose the one that gives the best results. However, this is computationally infeasible, especially when the dataset is large or when there are many predictor variables — the number of possible splits grows exponentially.

Therefore, instead of trying all possible combinations at once, we use a **recursive partitioning approach**. This means:

Start with the entire dataset as one group (the root node).

Find the single best split — the one that most effectively separates the data based on the target variable.

Divide the data into two or more subgroups (child nodes) based on that split.

Repeat the process (recursively) within each subgroup: again find the best split, divide the data, and continue until a stopping rule is met (for example, minimum node size or maximum tree depth).

This recursive process allows the algorithm to build the tree step by step, finding locally optimal splits that approximate the best possible tree without having to evaluate every possible combination.

3.5 Recursive Partitioning for Regression Trees

A regression tree predicts a continuous outcome (for example, house price, temperature, or pH level). The goal is to split the data into smaller and smaller groups (nodes) that are as homogeneous as possible with respect to the response variable.

In-class notation

3.6 Recursive Partitioning for Regression Trees

A **regression tree** is used when the response variable is *continuous* (e.g., house price, temperature, or pH level).

The goal is to split the data into smaller and smaller groups (nodes) that are as **homogeneous as possible** with respect to the response.

3.6.1 Step 1: Start with All Predictors

At the beginning, the algorithm considers **all predictor variables**:

$$X_1, X_2, X_3, \ldots, X_p$$

For each predictor, it looks for the **best split point** that divides the data into two groups such that the prediction error (usually the **sum of squared errors, SSE**) is minimized.

3.6.2 Step 2: Consider All Possible Values

3.6.2.1 Continuous predictors

If a predictor X_j is **continuous**,
then "all possible values" refers to **all unique values** (or **midpoints between consecutive sorted values**) that can be used to split the data.

Example:

Observation	X_j
1	2
2	3
3	5
4	7

Possible split points (midpoints): - $X_j < 2.5$ - $X_j < 4$ - $X_j < 6$

Each of these potential splits is tested to see how well it reduces the SSE of the response variable.

3.6.2.2 Categorical predictors

If X_j is **categorical**,
"all possible values" means all possible **groupings (subsets)** of the categories.

Example:
If the predictor `Species` = {A, B, C}, possible splits are:

- {A} vs {B, C}
- {B} vs {A, C}
- {C} vs {A, B}

Each grouping is evaluated based on how much it reduces the variability in the response.

3.6.3 Step 3: Choose the Best Split

For every predictor and every possible split value, compute:

$$\text{SSE}_{\text{split}} = \text{SSE}_{\text{left node}} + \text{SSE}_{\text{right node}}$$

The **split that minimizes** this total SSE is chosen as the best split for that node.

3.6.4 Step 4: Recursive Partitioning

After splitting the data into two nodes, the same process is applied **recursively** within each node:

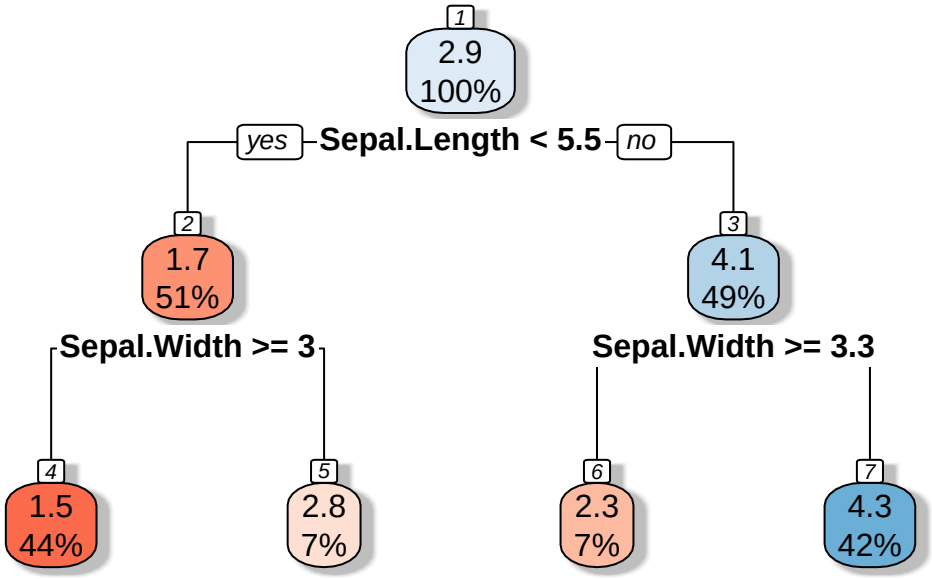
1. Consider all predictors again.
2. For each predictor, test all possible values.
3. Find the best split within that node.
4. Continue until a stopping rule is met (e.g., minimum node size or no significant improvement).

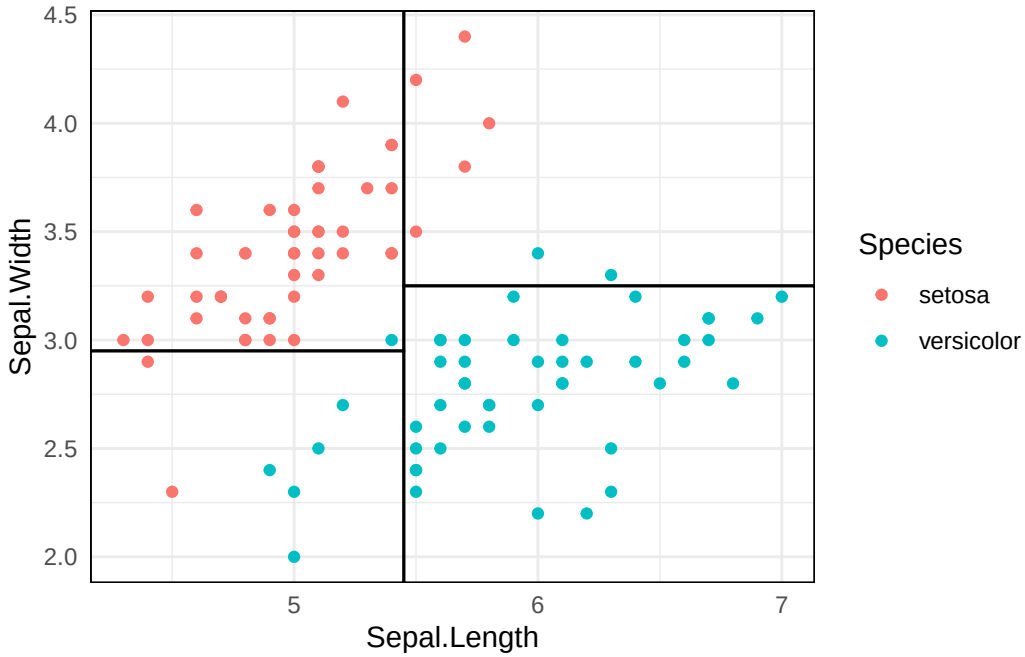
3.6.5 Summary

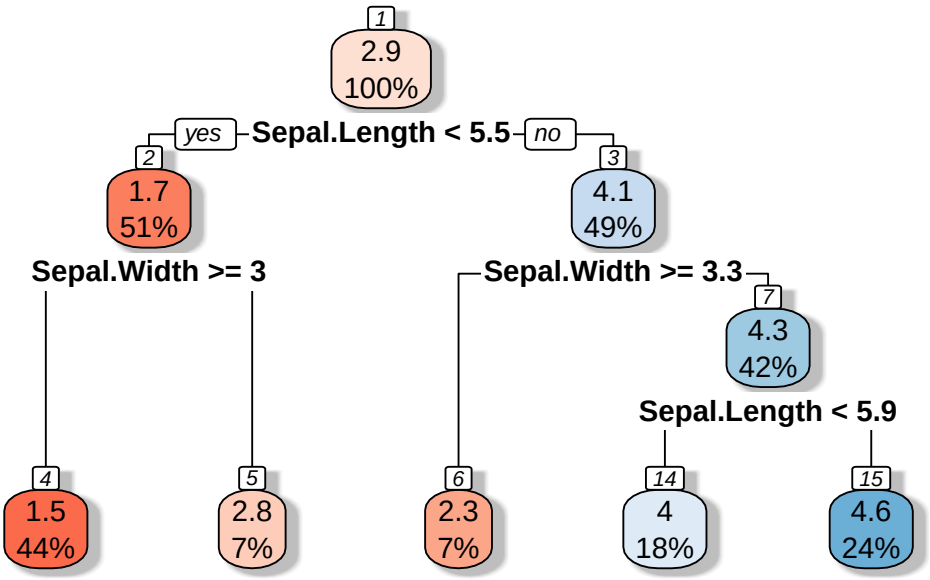
Concept	Explanation
All predictors	Every variable $X_1, X_2, \ldots, X_p$ is considered at each split.
All possible values	Every unique value (or midpoint between values) is tested as a potential split.
Recursive partitioning	The process of repeatedly splitting the data into smaller homogeneous groups until a stopping rule is met.

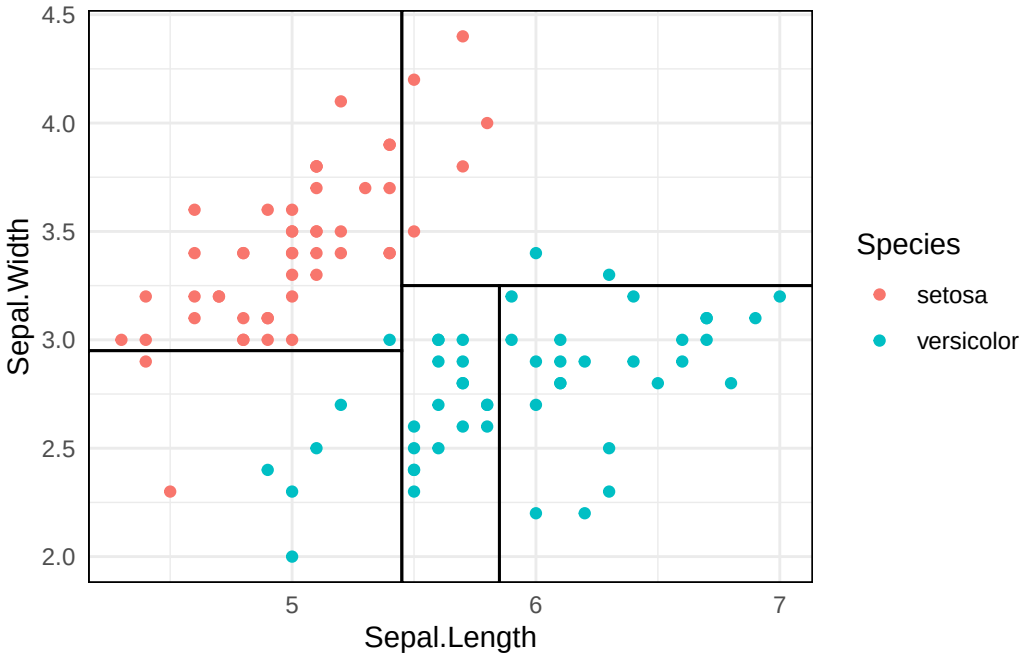
In summary:
Finding every possible combination of splits is computationally infeasible.
Recursive partitioning provides a practical, step-by-step method that finds locally optimal splits efficiently.

3.7 Depth of the decision tree






1
2.9
100%
yes
Sepal.Length < 5.5
no
2
1.7
51%
3
4.1
49%
Sepal.Width >= 3
Sepal.Width >= 3.3
7
4.3
42%
Sepal.Length < 5.9
4
1.5
44%
5
2.8
7%
6
2.3
7%
14
4
18%
15
4.6
24%


4.5
4.0
3.5
3.0
2.5
2.0
Sepal.Width
5
6
7
Sepal.Length
Species
setosa
versicolor

3.8 Pruning Regression Trees

Once a regression tree is grown, it often becomes **too complex** — it may fit the training data very well but perform poorly on new, unseen data.
This problem is known as **overfitting**.

Pruning is the process of **reducing the size** of a fully grown tree to improve its ability to generalize.

3.8.1 Why Prune?

- A large tree captures **noise** as if it were structure.
- It has **low bias** but **high variance**.
- Pruning helps to find a **balance between model complexity and prediction accuracy**.

3.8.2 Types of Pruning

There are two main approaches:

3.8.2.1 (a) Pre-pruning (Early stopping)

Stop the tree growth **before** it becomes too large.

Common stopping rules:

- Minimum number of observations in a node
- Maximum tree depth
- Minimum decrease in SSE required for a split

3.8.2.2 (b) Post-pruning (Cost Complexity Pruning)

Grow a **large tree first**, then prune it **backward** by removing branches that contribute little to predictive accuracy.

3.8.3 Cost Complexity Pruning (a.k.a. Weakest Link Pruning)

The idea is to penalize tree size using a complexity parameter (λ).

For any subtree (T):

$$C(T) = \text{Error}(T) + \lambda L(T)$$

where:

- Error(T): measure of fit (e.g., sum of squared errors)
- $L(T)$: number of leaf nodes in the tree (measure of complexity)
- λ: penalty factor controlling the trade-off between complexity and predictive power

3.8.4 Interpretation of Parameters

Parameter	Meaning
$\lambda = 0$	Fully grown decision tree (no penalty for complexity).
$\lambda = \infty$	Root node only (maximum penalty, no splits).
$0 < \lambda < \infty$	Balances predictive power and complexity.

3.8.5 Total Cost Components

$$\text{Total Cost} = \text{Measure of Fit} + \text{Measure of Complexity}$$

- **Measure of Fit:** Error (e.g., SSE)
- **Measure of Complexity:** Number of leaf nodes $L(T)$

So,

$$C(T) = \text{Error}(T) + \lambda L(T)$$

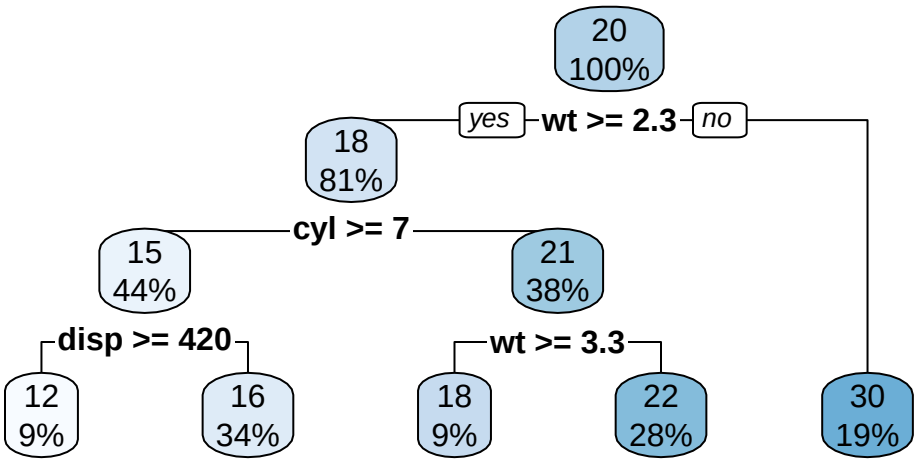
This is sometimes written as:

$$R_\lambda(T) = R(T) + \lambda|T|$$

Both expressions represent the same concept — a **trade-off between model fit and simplicity**.

3.9 Example R code for Pre-pruning and Post-pruning

```r
# Load necessary packages
library(rpart)
library(rpart.plot)

# Use built-in dataset
data(mtcars)

# ----------------------------
#   1. Pre-pruning (Early stopping)
# ----------------------------
# Control parameters limit tree growth
prepruned_tree <- rpart(
  mpg ~ .,
  data = mtcars,
  method = "anova",
  control = rpart.control(
    minsplit = 10,   # minimum observations required to attempt a split
    cp = 0.02,       # minimum improvement in SSE required for a split
    maxdepth = 3     # maximum depth of the tree
  )
)

# Visualize the pre-pruned tree
rpart.plot(prepruned_tree, main = "Pre-pruned Regression Tree")
```




```
# Print summary
print(prepruned_tree)
```

```
n= 32

node), split, n, deviance, yval
      * denotes terminal node

 1) root 32 1126.047000 20.09062
   2) wt>=2.26 26  346.566500 17.78846
     4) cyl>=7 14   85.200000 15.10000
       8) disp>=420 3   12.326670 11.83333 *
       9) disp< 420 11   32.129090 15.99091 *
     5) cyl< 7 12   42.122500 20.92500
      10) wt>=3.3275 3    1.086667 18.36667 *
      11) wt< 3.3275 9   14.855560 21.77778 *
   3) wt< 2.26 6   44.553330 30.06667 *
```

```
summary(prepruned_tree)
```

```
Call:
```

```
rpart(formula = mpg ~ ., data = mtcars, method = "anova", control = rpart.control(minsplit =
    cp = 0.02, maxdepth = 3))
  n= 32

          CP nsplit rel error    xerror       xstd
1 0.65266121      0 1.0000000 1.0455431 0.24712804
2 0.19470235      1 0.3473388 0.6372794 0.17067743
3 0.03618342      2 0.1526364 0.3850991 0.09727425
4 0.02324972      3 0.1164530 0.3849136 0.10418658
5 0.02000000      4 0.0932033 0.3470311 0.10385935

Variable importance
  wt disp   hp drat  cyl qsec   vs
  27   25   19   11    9    5    5

Node number 1: 32 observations,    complexity param=0.6526612
  mean=20.09062, MSE=35.18897
  left son=2 (26 obs) right son=3 (6 obs)
  Primary splits:
      wt   < 2.26   to the right, improve=0.6526612, (0 missing)
      cyl  < 5      to the right, improve=0.6431252, (0 missing)
      disp < 163.8  to the right, improve=0.6130502, (0 missing)
      hp   < 118    to the right, improve=0.6010712, (0 missing)
      vs   < 0.5    to the left,  improve=0.4409477, (0 missing)
  Surrogate splits:
      disp < 101.55 to the right, agree=0.969, adj=0.833, (0 split)
      hp   < 92     to the right, agree=0.938, adj=0.667, (0 split)
      drat < 4      to the left,  agree=0.906, adj=0.500, (0 split)
      cyl  < 5      to the right, agree=0.844, adj=0.167, (0 split)

Node number 2: 26 observations,    complexity param=0.1947024
  mean=17.78846, MSE=13.32948
  left son=4 (14 obs) right son=5 (12 obs)
  Primary splits:
      cyl  < 7      to the right, improve=0.6326174, (0 missing)
      disp < 266.9  to the right, improve=0.6326174, (0 missing)
      hp   < 136.5  to the right, improve=0.5803554, (0 missing)
      wt   < 3.325  to the right, improve=0.5393370, (0 missing)
      qsec < 18.15  to the left,  improve=0.4210605, (0 missing)
  Surrogate splits:
      disp < 266.9  to the right, agree=1.000, adj=1.000, (0 split)
      hp   < 136.5  to the right, agree=0.962, adj=0.917, (0 split)
      wt   < 3.49   to the right, agree=0.885, adj=0.750, (0 split)
```

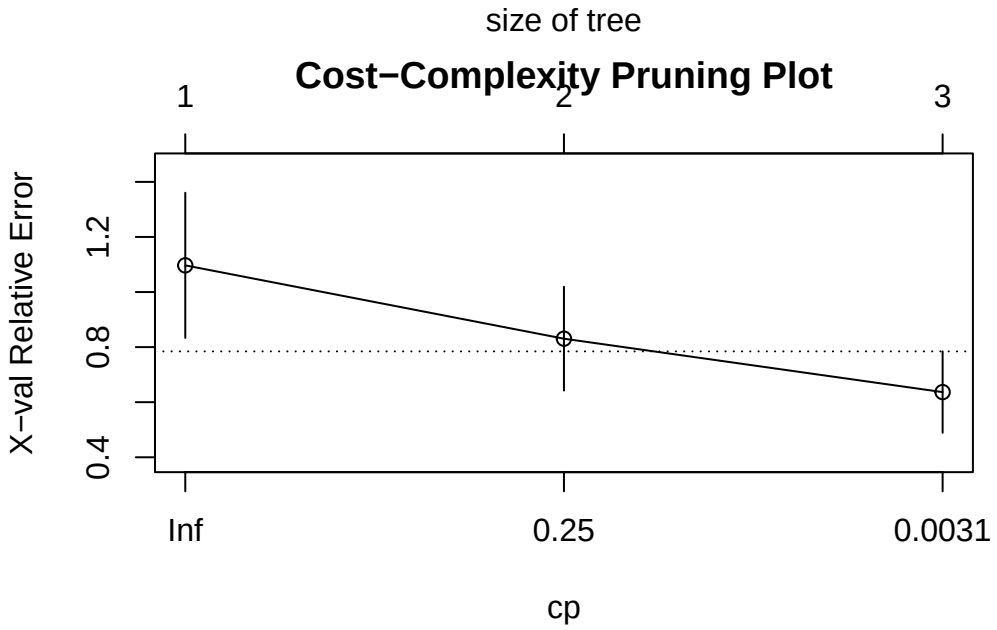
```
      qsec < 18.15  to the left,  agree=0.885, adj=0.750, (0 split)
      vs   < 0.5    to the left,  agree=0.885, adj=0.750, (0 split)

Node number 3: 6 observations
  mean=30.06667, MSE=7.425556

Node number 4: 14 observations,    complexity param=0.03618342
  mean=15.1, MSE=6.085714
  left son=8 (3 obs) right son=9 (11 obs)
  Primary splits:
      disp < 420    to the right, improve=0.4782188, (0 missing)
      wt   < 4.66   to the right, improve=0.4782188, (0 missing)
      hp   < 192.5  to the right, improve=0.4669349, (0 missing)
      carb < 3.5    to the right, improve=0.4669349, (0 missing)
      qsec < 17.71  to the right, improve=0.4306658, (0 missing)
  Surrogate splits:
      wt   < 4.66   to the right, agree=1.000, adj=1.000, (0 split)
      drat < 3.035  to the left,  agree=0.857, adj=0.333, (0 split)
      qsec < 17.41  to the right, agree=0.857, adj=0.333, (0 split)

Node number 5: 12 observations,    complexity param=0.02324972
  mean=20.925, MSE=3.510208
  left son=10 (3 obs) right son=11 (9 obs)
  Primary splits:
      wt   < 3.3275 to the right, improve=0.6215272, (0 missing)
      cyl  < 5      to the right, improve=0.5573591, (0 missing)
      hp   < 96     to the right, improve=0.5507811, (0 missing)
      disp < 163.8  to the right, improve=0.4615111, (0 missing)
      carb < 3      to the right, improve=0.2857431, (0 missing)
  Surrogate splits:
      disp < 163.8  to the right, agree=0.917, adj=0.667, (0 split)
      hp   < 116.5  to the right, agree=0.833, adj=0.333, (0 split)

Node number 8: 3 observations
  mean=11.83333, MSE=4.108889

Node number 9: 11 observations
  mean=15.99091, MSE=2.920826

Node number 10: 3 observations
  mean=18.36667, MSE=0.3622222

Node number 11: 9 observations
```

```
  mean=21.77778, MSE=1.650617
```

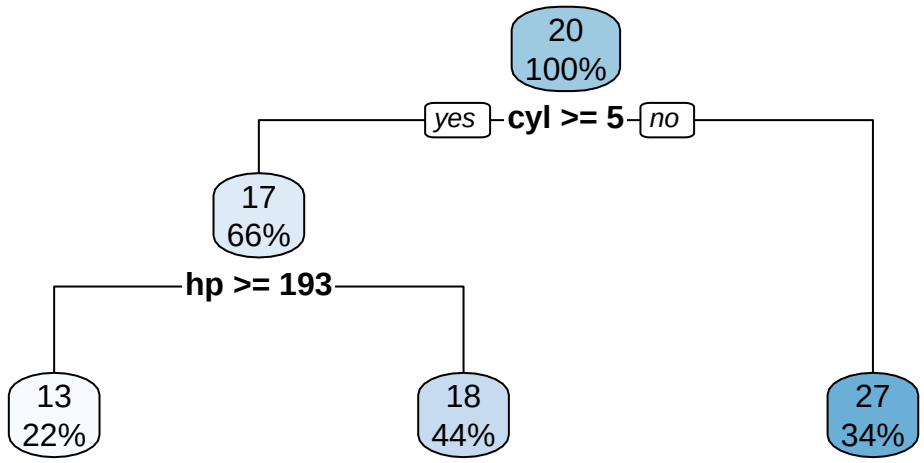
```r
# -----------------------------
#   2. Post-pruning (Cost-complexity pruning)
# -----------------------------
# Step 1: Grow a large tree first
full_tree <- rpart(
  mpg ~ .,
  data = mtcars,
  method = "anova",
  control = rpart.control(cp = 0.0001)  # allow the tree to grow large
)

# Step 2: Display complexity parameter (CP) table
printcp(full_tree)
```

```
Regression tree:
rpart(formula = mpg ~ ., data = mtcars, method = "anova", control = rpart.control(cp = 1e-04)

Variables actually used in tree construction:
[1] cyl hp

Root node error: 1126/32 = 35.189

n= 32

        CP nsplit rel error  xerror    xstd
1 0.643125      0   1.00000 1.09687 0.26357
2 0.097484      1   0.35687 0.83062 0.18855
3 0.000100      2   0.25939 0.63665 0.14784
```

```r
# Step 3: Plot cross-validation results
plotcp(full_tree, main = "Cost-Complexity Pruning Plot")
```




```r
# Step 4: Select the cp value that minimizes cross-validation error
optimal_cp <- full_tree$cptable[which.min(full_tree$cptable[,"xerror"]), "CP"]

# Step 5: Prune the tree at the optimal cp value
pruned_tree <- prune(full_tree, cp = optimal_cp)

# Step 6: Visualize the pruned tree
rpart.plot(pruned_tree, main = "Post-pruned Regression Tree")
```




```
# Step 7: Summarize pruned model
summary(pruned_tree)
```

```
Call:
rpart(formula = mpg ~ ., data = mtcars, method = "anova", control = rpart.control(cp = 1e-04)
  n= 32

          CP nsplit rel error    xerror      xstd
1 0.64312523      0 1.0000000 1.0968692 0.2635747
2 0.09748407      1 0.3568748 0.8306178 0.1885469
3 0.00010000      2 0.2593907 0.6366477 0.1478392

Variable importance
 cyl disp   hp   wt qsec   vs carb
  20   20   19   16   12   11    1

Node number 1: 32 observations,    complexity param=0.6431252
  mean=20.09062, MSE=35.18897
  left son=2 (21 obs) right son=3 (11 obs)
  Primary splits:
      cyl  < 5      to the right, improve=0.6431252, (0 missing)
      wt   < 2.3925 to the right, improve=0.6356630, (0 missing)
```

```
      disp < 163.8  to the right, improve=0.6130502, (0 missing)
      hp   < 118    to the right, improve=0.6010712, (0 missing)
      vs   < 0.5    to the left,  improve=0.4409477, (0 missing)
  Surrogate splits:
      disp < 142.9  to the right, agree=0.969, adj=0.909, (0 split)
      hp   < 101    to the right, agree=0.938, adj=0.818, (0 split)
      wt   < 2.5425 to the right, agree=0.906, adj=0.727, (0 split)
      qsec < 18.41  to the left,  agree=0.844, adj=0.545, (0 split)
      vs   < 0.5    to the left,  agree=0.844, adj=0.545, (0 split)

Node number 2: 21 observations,    complexity param=0.09748407
  mean=16.64762, MSE=9.451066
  left son=4 (7 obs) right son=5 (14 obs)
  Primary splits:
      hp   < 192.5  to the right, improve=0.5530828, (0 missing)
      cyl  < 7      to the right, improve=0.5068475, (0 missing)
      disp < 266.9  to the right, improve=0.5068475, (0 missing)
      wt   < 3.49   to the right, improve=0.4414890, (0 missing)
      drat < 3.075  to the left,  improve=0.1890739, (0 missing)
  Surrogate splits:
      disp < 334    to the right, agree=0.857, adj=0.571, (0 split)
      wt   < 4.66   to the right, agree=0.810, adj=0.429, (0 split)
      qsec < 15.455 to the left,  agree=0.810, adj=0.429, (0 split)
      carb < 3.5    to the right, agree=0.762, adj=0.286, (0 split)
      gear < 4.5    to the right, agree=0.714, adj=0.143, (0 split)

Node number 3: 11 observations
  mean=26.66364, MSE=18.48959

Node number 4: 7 observations
  mean=13.41429, MSE=4.118367

Node number 5: 14 observations
  mean=18.26429, MSE=4.276582
```

3.10 Classification Trees: Best Split, Entropy, and Gini Coefficients

Classification trees are used when the response variable is **categorical**.
At each node, the algorithm tries to find the **best split** — the one that produces the most **homogeneous** (pure) child nodes.

3.10.1 The Idea of "Best Split"

At any node in the tree:

- The data are divided into two (or more) groups based on a predictor.
- The **best split** is the one that makes each resulting group as **pure** as possible with respect to the class labels.

To measure **purity**, we use **impurity measures** such as:

- **Entropy**
- **Gini index**
- (Sometimes) **Misclassification error**

3.10.2 Entropy

Entropy measures the **disorder** or **uncertainty** in a node.

If there are (K) classes and (p_k) is the proportion of observations belonging to class (k), then:

$$\text{Entropy} = -\sum_{k=1}^{K} p_k \log_2(p_k)$$

3.10.2.1 Properties:

- Entropy $= 0 \rightarrow$ Node is perfectly pure (all observations belong to one class).
- Entropy is maximum when all classes are equally likely.

3.10.2.2 Example:

Class	Count	p_k	$-p_k \log_2(p_k)$
A	8	0.8	0.257
B	2	0.2	0.464

$$\text{Entropy} = 0.257 + 0.464 = 0.721$$

3.10.3 Gini Index

The **Gini coefficient** (or **Gini impurity**) is another measure of node impurity.

$$\text{Gini} = 1 - \sum_{k=1}^{K} p_k^2$$

3.10.3.1 Properties:

- Gini $= 0 \rightarrow$ Perfectly pure node
- Gini is smaller when the node is more homogeneous

3.10.3.2 Example:

Using the same proportions as above ($p_1 = 0.8, p_2 = 0.2$):

$$\text{Gini} = 1 - (0.8^2 + 0.2^2) = 1 - (0.64 + 0.04) = 0.32$$

3.10.4 Misclassification Error (less common)

A simpler impurity measure sometimes used:

$$\text{Error} = 1 - \max(p_k)$$

For the same node ($\max(p_k) = 0.8$):

$$\text{Error} = 1 - 0.8 = 0.2$$

3.10.5 Choosing the Best Split

For each possible split:

1. Compute the impurity (Entropy or Gini) **before** splitting — call this I_{parent}.
2. Compute the impurity of the **child nodes** (weighted by their sizes):

$$I_{\text{split}} = \frac{n_L}{n} I_L + \frac{n_R}{n} I_R$$

3. Compute the **information gain** (reduction in impurity):

$$\text{Gain} = I_{\text{parent}} - I_{\text{split}}$$

4. The **best split** is the one that maximizes this gain (i.e., gives the largest reduction in impurity).

3.10.6 Comparing Entropy and Gini

Property	Entropy	Gini
Range	0 to 1	0 to 0.5
Shape	Logarithmic	Quadratic
Interpretation	Information theory measure	Probability of misclassification
Behavior	Slightly more sensitive to rare classes	Computationally simpler
Commonly used in	C4.5, ID3 algorithms	CART algorithm

Both criteria often lead to **similar splits** in practice.

4 Random Forests

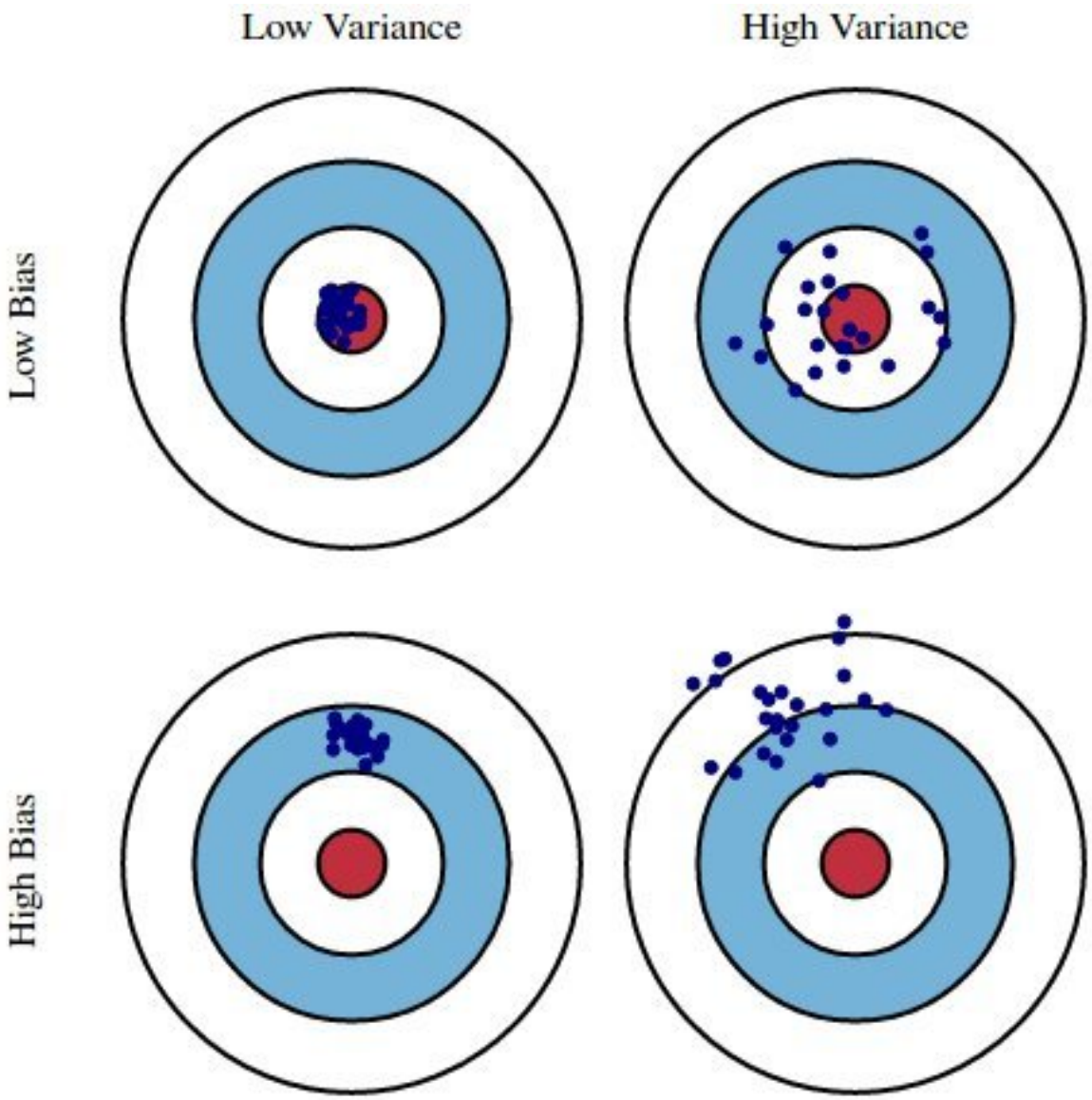
4.1 Decision trees - Limitation

To capture a complex decision boundary we need to use a deep tree

In-class explanation

4.2 Bias-Variance Trade off

- A deep decision tree has low bias and high variance.



4.3 Bagging (Bootstrap Aggregation)

- Technique for reducing the variance of an estimated predicted function
- Works well for high-variance, low-bias procedures, such as trees

4.4 Ensemble Methods

- Combines several base models
- **Bagg**ing (**B**ootstrap **Agg**regation) is an ensemble method

4.5 Ensemble Methods

"Ensemble learning gives credence to the idea of the "wisdom of crowds," which suggests that the decision-making of a larger group of people is typically better than that of an individual expert."

Source: https://www.ibm.com/cloud/learn/boosting

4.6 Bootstrap

- Generate multiple samples of training data, via bootstrapping

Example

Training data: $\{(y_1, x_1), (y_2, x_2), (y_3, x_3), (y_4, x_4)\}$

Three samples generated from bootstrapping

Sample 1 = $\{(y_1, x_1), (y_2, x_2), (y_3, x_3), (y_4, x_4)\}$

Sample 2 = $\{(y_1, x_1), (y_1, x_1), (y_1, x_1), (y_4, x_4)\}$

Sample 3 = $\{(y_1, x_1), (y_2, x_2), (y_1, x_1), (y_4, x_4)\}$

4.7 Aggregation

- Train a decision tree on each bootstrap sample of data without pruning.
- Aggregate prediction using either voting or averaging

4.8 Bagging - in class diagram

4.9 Bagging

Pros

- Ease of implementation
- Reduction of variance

Cons

- Loss of interpretability
- Computationally expensive

4.10 Bagging

- Bootstrapped subsamples are created
- A Decision Tree is formed on each bootstrapped sample.
- The results of each tree are aggregated

4.11 Random Forests: Improving on Bagging

- The ensembles of trees in Bagging tend to be highly correlated.
- All of the bagged trees will look quite similar to each other. Hence, the predictions from the bagged trees will be highly correlated.

4.12 Random Forests

1. Bootstrap samples
2. At each split, randomly select a set of predictors from the full set of predictors
3. From the selected predictors we select the optimal predictor and the optimal corresponding threshold for the split.
4. Grow multiple trees and aggregate

4.13 Random Forests - Hyper parameters

1. Number of variables randomly sampled as candidates at each split
2. Number of trees to grow
3. Minimum size of terminal nodes. Setting this number larger causes smaller trees to be grown (and thus take less time).

Note: In theory, each tree in the random forest is full (not pruned), but in practice this can be computationally expensive,thus, imposing a minimum node size is not unusual.

4.14 Random Forests

- Bagging ensemble method
- Gives final prediction by aggregating the predictions of bootstrapped decision tree samples.
- Trees in a random forest are independent of each other.

4.15 Random Forests

Pros

- Accuracy

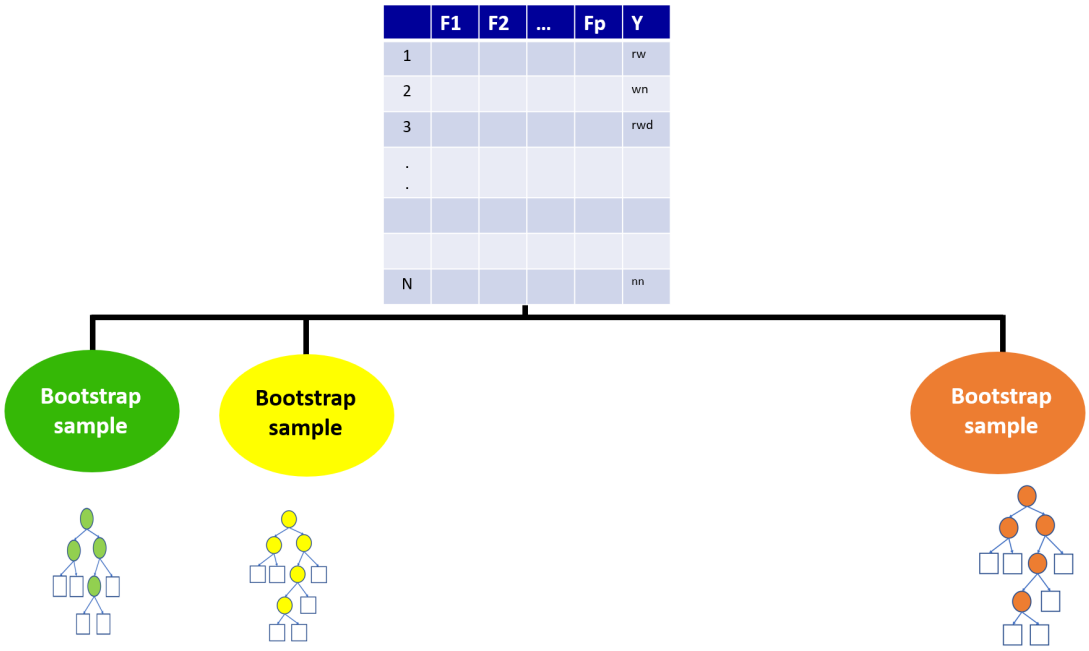
Cons

- Speed
- Interpretability
- Overfitting

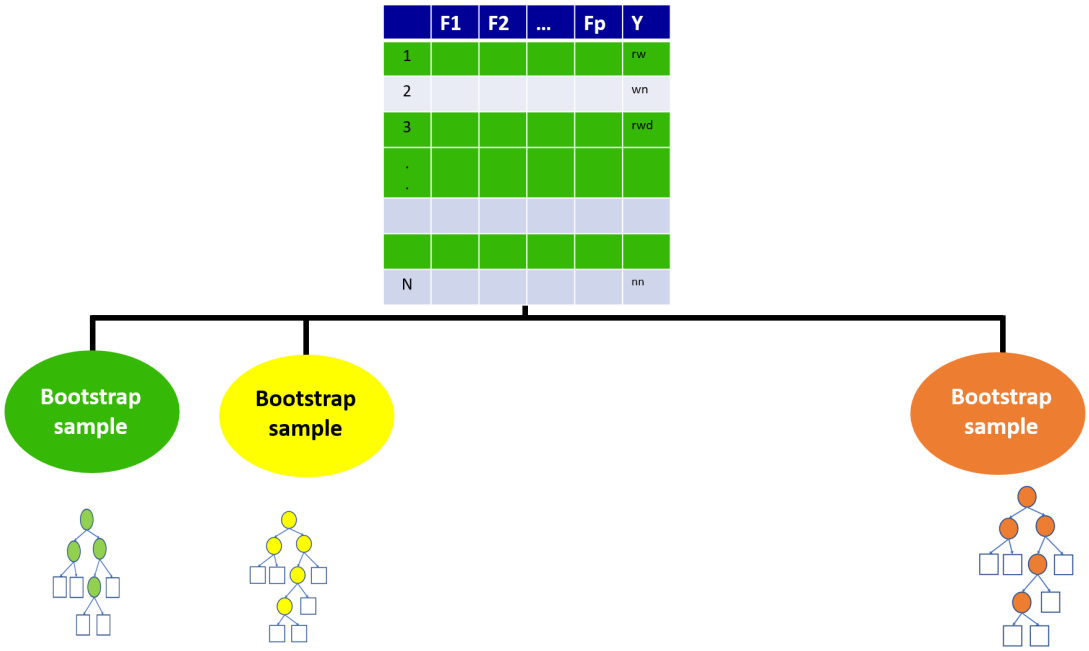
4.16 Out-of-bag error

With ensemble methods, we get a new metric for assessing the predictive performance of the model, the out-of-bag error

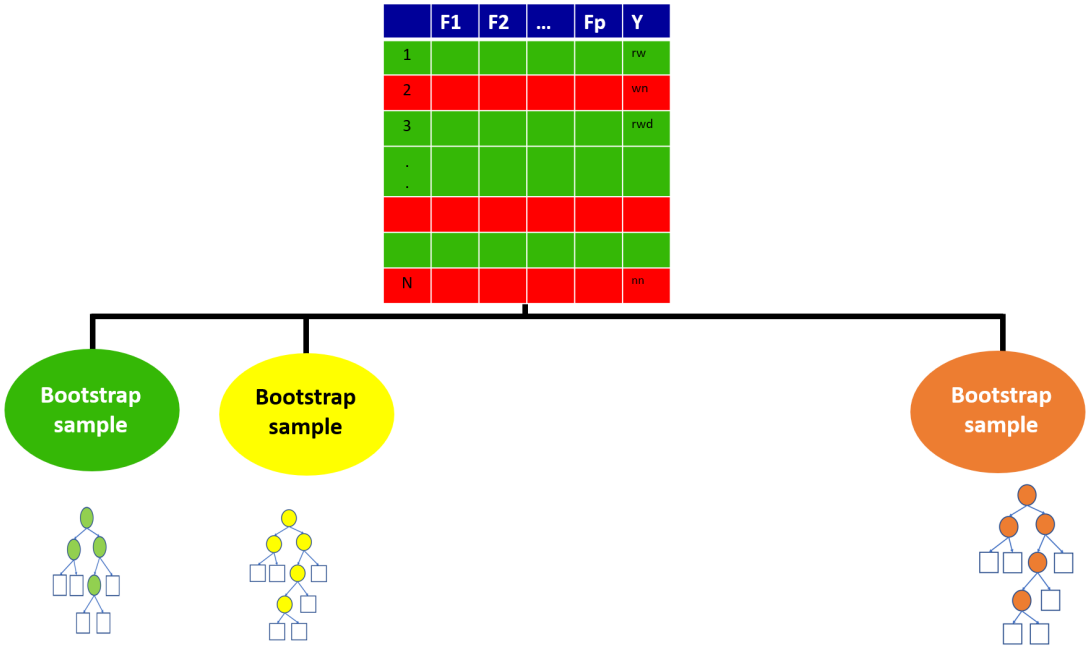
4.17 Random Forests



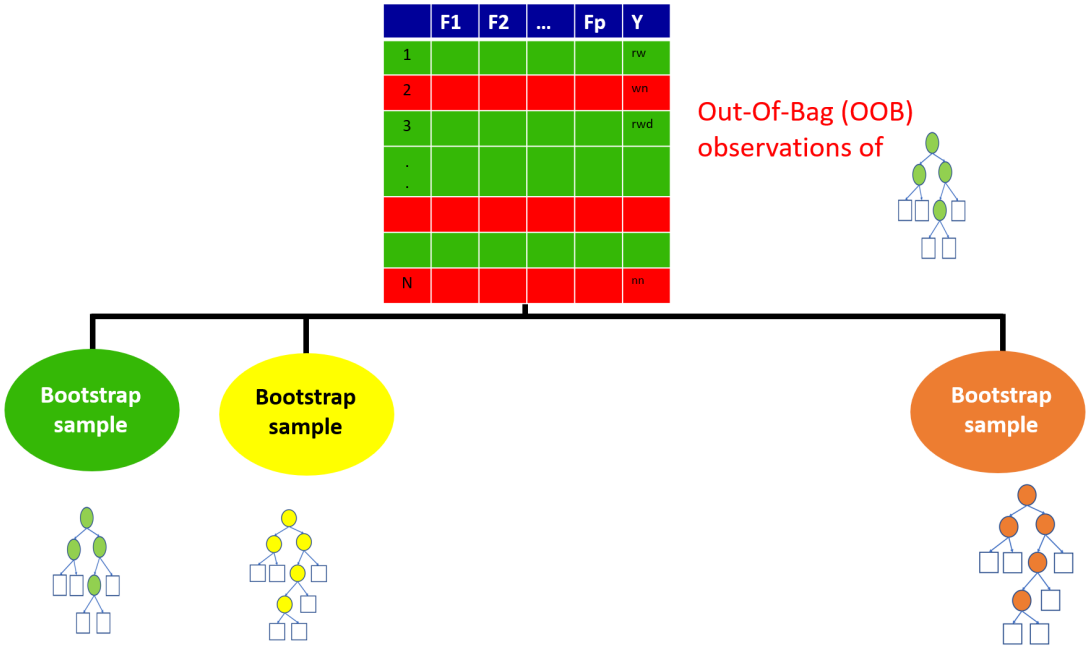
4.18 Random Forests



4.19 Out-of-Bag (OOB) Samples

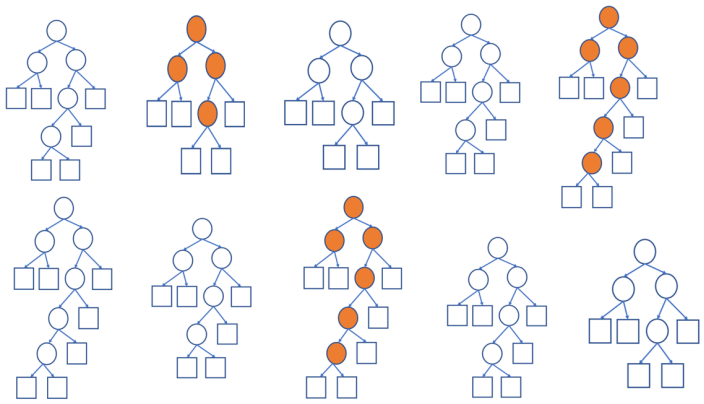


4.20 Out-of-Bag (OOB) Samples



4.21 Predictions based on OOB observations

	F1	F2	...	Fp	Y
1					rw
2					wn
3					rwd
. .					
N					nn



4.22 Predictions based on OOB observations

Figure 1

	F1	F2	...	Fp	Y
1					rw
2					wn
3					rwd
. .					
N					nn

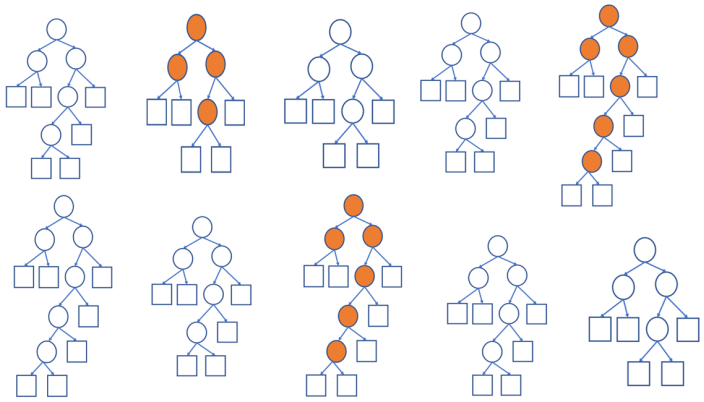


Figure 2

	F1	F2	...	Fp	Y
1					rw
2					wn
3					rwd
. .					
N					nn

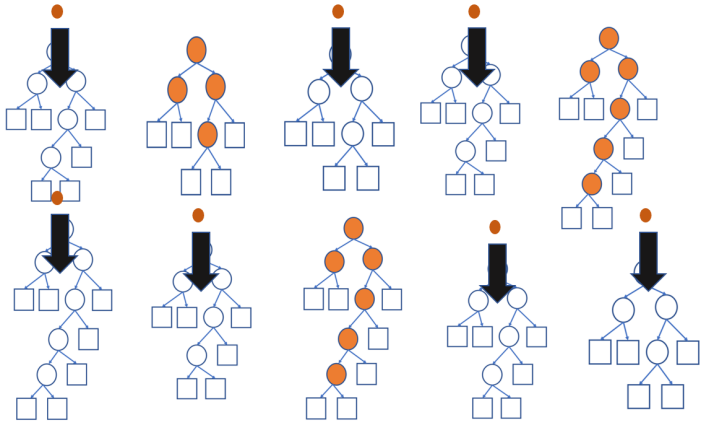


Figure 3

	F1	F2	...	Fp	Y	rw	rwd	wn	...	ARIMA	nn
1					rw						
2					wn	0	0	5	0	0	2
3					rwd						
. .						. .					
N					nn						

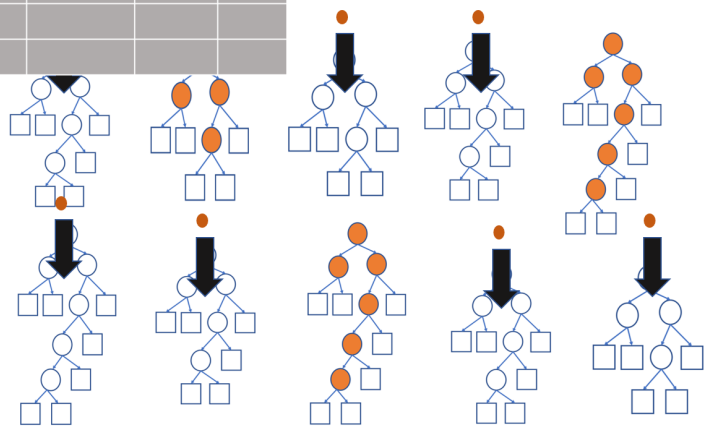


Figure 4

	F1	F2	...	Fp	Y	rw	rwd	wn	...	ARIMA	nn
1					rw						
2					wn	0	0	0.7	0	0	0.3
3					rwd						
. .						. .					
N					nn						

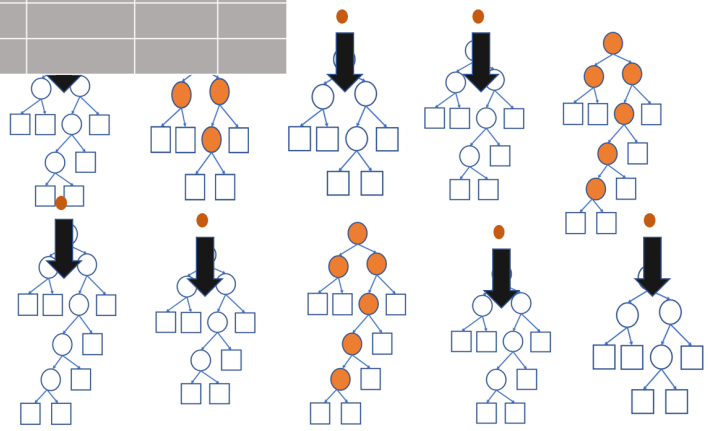


Figure 5

	F1	F2	...	Fp	Y	rw	rwd	wn	...	ARIMA	nn
1					rw	1	0	0	0	0	0
2					wn	0	0	0.7	0	0	0.3
3					rwd						
. .						. .					
N					nn						

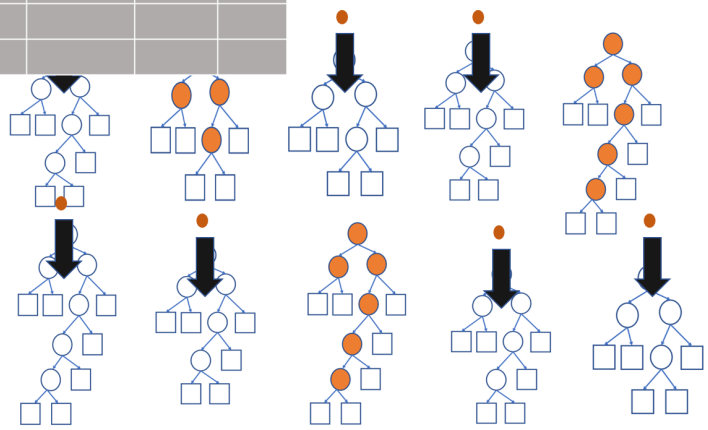


Figure 6

	F1	F2	...	Fp	Y	rw	rwd	wn	...	ARIMA	nn
1					rw	1	0	0	0	0	0
2					wn	0	0	0.7	0	0	0.3
3					rwd	0	0.5	0	0	0.5	0
. .						. .					
N					nn	0.2	0.25	0.1		0.2	0.25

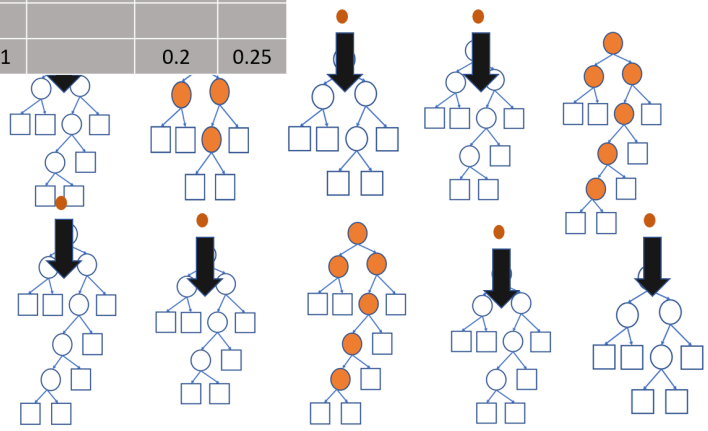


Figure 7

	F1	F2	...	Fp	Y	rw	rwd	wn	...	ARIMA	nn
1					rw	1	0	0	0	0	0
2					wn	0	0	0.7	0	0	0.3
3					rwd	0	0.5	0	0	0.5	0
. .						. .					
N					nn	0.2	0.25	0.1		0.2	0.25

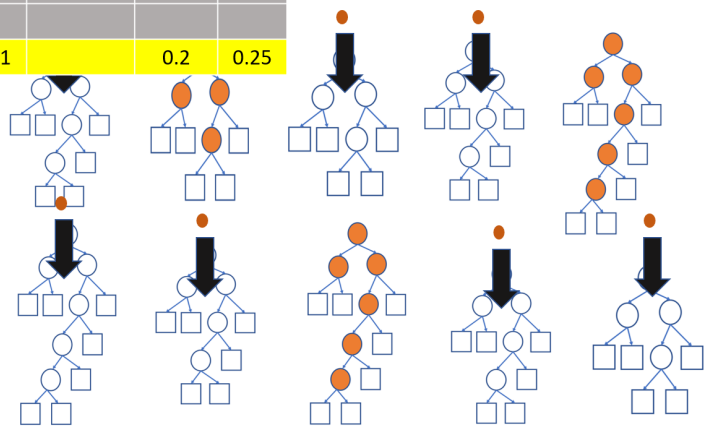
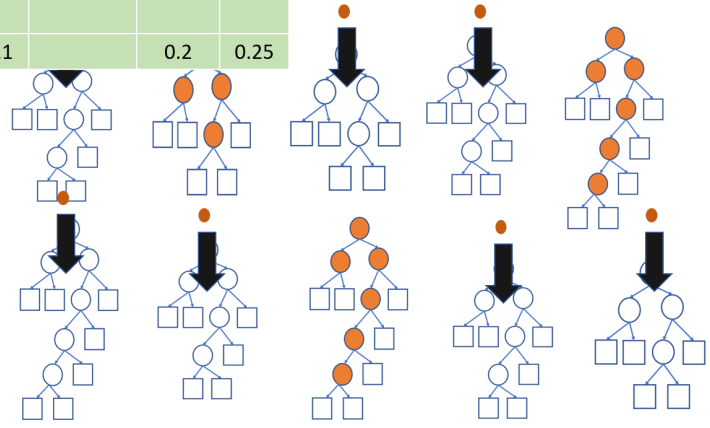


Figure 8

	F1	F2	...	Fp	Y	rw	rwd	wn	...	ARIMA	nn
1					rw	1	0	0	0	0	0
2					wn	0	0	0.7	0	0	0.3
3					rwd	0	0.5	0	0	0.5	0
. .						. .					
N					nn	0.2	0.25	0.1		0.2	0.25



4.23 Variable Importance in Random Forest

contribution to predictive accuracy

- Permutation-based variable importance
- Mean decrease in Gini coefficient

4.24 Permutation-based variable importance

- the OOB samples are passed down the tree, and the prediction accuracy is recorded
- the values for the j^{th} variable are randomly permuted in the OOB samples, and the accuracy is again computed.
- the decrease in accuracy as a result of this permuting is averaged over all trees, and is used as a measure of the importance of variable j in the random forests

4.25 Mean decrease in Gini coefficient

- Measure of how each variable contributes to the homogeneity of the nodes and leaves in the resulting random forest
- The higher the value of mean decrease accuracy or mean decrease Gini score, the higher the importance of the variable in the model

4.26 Boosting

- Bagging and boosting are two main types of ensemble learning methods.
- The main difference between bagging and boosting is the way in which they are trained.
- In bagging, weak learners (decision trees) are trained in parallel, but in boosting, they learn sequentially.

4.27 Boosting

1. Fit a single tree
2. Draw a sample that gives higher selection probabilities to misclassified records
3. Fit a tree to the new sample
4. Repeat Steps 2 and 3 multiple times
5. Use weighted voting to classify records, with heavier weights for later trees

4.28 Boosting

- Iterative process.
- Each tree is dependent on the previous one. Hence, it is hard to parallelize the training process of boosting algorithms.
- The training time will be higher. This is the main drawback of boosting algorithms.

4.29 Boosting Algorithms

- Adaptive boosting or AdaBoost
- Gradient boosting
- Extreme gradient boosting or XGBoost

5 Measures of Performance

Task: Build a tree-based model to predict species

5.1 Load libraries

```
library(palmerpenguins)
library(rsample)       # for initial_split
library(dplyr)
library(caret)
library(randomForest)
library(ada)
library(gbm)
library(tidyverse)
library(yardstick) #roc_curve
```

5.2 Clean data

```
penguins_clean <- na.omit(penguins)
penguins_clean$species <- as.factor(penguins_clean$species)
```

5.3 Stratified train-test split

```
set.seed(123)
split <- initial_split(penguins_clean, prop = 0.7, strata = "species")
train_data <- training(split)
table(train_data$species)
```

```
   Adelie Chinstrap    Gentoo
      102        47        83
```

```
test_data  <- testing(split)
table(test_data$species)
```

```
   Adelie Chinstrap    Gentoo
       44        21        36
```

5.4 Variables

```
predictors <- c("bill_length_mm", "bill_depth_mm", "flipper_length_mm", "body_mass_g", "sex"
response <- "species"
```

5.5 Random Forest Model

```
set.seed(123)
rf_model <- randomForest(
  as.formula(paste(response, "~", paste(predictors, collapse = "+"))),
  data = train_data,
  importance = TRUE
)
rf_model
```

```
Call:
 randomForest(formula = as.formula(paste(response, "~", paste(predictors,      collapse = "+
               Type of random forest: classification
                     Number of trees: 500
No. of variables tried at each split: 2

        OOB estimate of  error rate: 3.45%
Confusion matrix:
          Adelie Chinstrap Gentoo class.error
```

```
Adelie       100         1      1  0.01960784
Chinstrap      4        42      1  0.10638298
Gentoo         0         1     82  0.01204819
```

```
rf_pred <- predict(rf_model, newdata = test_data)
rf_pred
```

```
       1         2         3         4         5         6         7         8
  Adelie    Adelie    Adelie    Adelie    Adelie    Adelie    Adelie    Adelie
       9        10        11        12        13        14        15        16
  Adelie    Adelie    Adelie    Adelie    Adelie    Adelie    Adelie    Adelie
      17        18        19        20        21        22        23        24
  Adelie    Adelie    Adelie    Adelie    Adelie    Adelie    Adelie    Adelie
      25        26        27        28        29        30        31        32
  Adelie Chinstrap    Adelie    Adelie    Adelie    Adelie    Adelie    Adelie
      33        34        35        36        37        38        39        40
  Adelie    Adelie    Adelie    Adelie    Adelie    Adelie    Adelie    Adelie
      41        42        43        44        45        46        47        48
  Adelie    Adelie    Adelie    Adelie    Gentoo    Gentoo    Gentoo    Gentoo
      49        50        51        52        53        54        55        56
  Gentoo    Gentoo    Gentoo    Gentoo    Gentoo    Gentoo    Gentoo    Gentoo
      57        58        59        60        61        62        63        64
  Gentoo    Gentoo    Gentoo    Gentoo    Gentoo    Gentoo    Gentoo    Gentoo
      65        66        67        68        69        70        71        72
  Gentoo    Gentoo    Gentoo    Gentoo    Gentoo    Gentoo    Gentoo    Gentoo
      73        74        75        76        77        78        79        80
  Gentoo    Gentoo    Gentoo    Gentoo    Gentoo    Gentoo    Gentoo    Gentoo
      81        82        83        84        85        86        87        88
Chinstrap Chinstrap Chinstrap Chinstrap Chinstrap Chinstrap Chinstrap Chinstrap
      89        90        91        92        93        94        95        96
Chinstrap Chinstrap Chinstrap Chinstrap Chinstrap Chinstrap Chinstrap Chinstrap
      97        98        99       100       101
Chinstrap Chinstrap Chinstrap Chinstrap Chinstrap
Levels: Adelie Chinstrap Gentoo
```

```
rf_cm <- confusionMatrix(rf_pred, test_data$species)
print(rf_cm)
```

```
Confusion Matrix and Statistics

          Reference
```

```
Prediction  Adelie Chinstrap Gentoo
  Adelie        43         0      0
  Chinstrap      1        21      0
  Gentoo         0         0     36

Overall Statistics

               Accuracy : 0.9901
                 95% CI : (0.9461, 0.9997)
    No Information Rate : 0.4356
    P-Value [Acc > NIR] : < 2.2e-16

                  Kappa : 0.9846

 Mcnemar's Test P-Value : NA

Statistics by Class:

                     Class: Adelie Class: Chinstrap Class: Gentoo
Sensitivity                 0.9773           1.0000        1.0000
Specificity                 1.0000           0.9875        1.0000
Pos Pred Value              1.0000           0.9545        1.0000
Neg Pred Value              0.9828           1.0000        1.0000
Prevalence                  0.4356           0.2079        0.3564
Detection Rate              0.4257           0.2079        0.3564
Detection Prevalence        0.4257           0.2178        0.3564
Balanced Accuracy           0.9886           0.9938        1.0000
```

5.6 Exercise

Compute the following measures manually and interpret them.

1. Sensitivity
2. Specificity
3. Prevalence
4. Positive Prediction Value (PPV)
5. Negative Prediction Value (NPV)
6. Detection rate

7. Detection prevalence
8. Balanced accuracy
9. Precision
10. Recall
11. F1 score

5.7 Receiver Operating Characteristic (ROC) curves

ROC curves are normally for binary classification, but penguins$species has three classes. For multiclass ROC, we compute one-vs-all ROC curves.

It's a plot of:

- True Positive Rate (TPR / Sensitivity) on the y-axis
- False Positive Rate (FPR = 1 - Specificity) on the x-axis
- It shows the trade-off between sensitivity and specificity for different decision thresholds of a classifier.

5.7.1 Metric Formula

True Positive Rate (Sensitivity)

$$TPR = TP/(TP + FN)$$

False Positive Rate

$$FPR = FP/(FP + TN)$$

Specificity

$$TN/(TN + FP) = 1 - FPR$$

Where:

TP = True Positives

FP = False Positives

TN = True Negatives

FN = False Negatives

```
# Predict class probabilities
rf_prob <- predict(rf_model, newdata = test_data, type = "prob")
rf_prob
```

```
    Adelie Chinstrap Gentoo
1    0.978     0.022  0.000
2    0.924     0.076  0.000
3    0.990     0.010  0.000
4    0.976     0.024  0.000
5    0.972     0.028  0.000
6    0.994     0.006  0.000
7    0.994     0.006  0.000
8    0.964     0.036  0.000
9    0.994     0.006  0.000
10   0.984     0.016  0.000
11   0.718     0.280  0.002
12   0.998     0.002  0.000
13   0.998     0.002  0.000
14   0.994     0.006  0.000
15   0.952     0.048  0.000
16   0.966     0.034  0.000
17   1.000     0.000  0.000
18   0.996     0.004  0.000
19   0.966     0.034  0.000
20   0.992     0.008  0.000
21   0.894     0.068  0.038
22   0.984     0.016  0.000
23   0.990     0.010  0.000
24   1.000     0.000  0.000
25   0.974     0.026  0.000
26   0.262     0.734  0.004
27   0.802     0.196  0.002
28   0.864     0.088  0.048
29   0.978     0.022  0.000
30   0.934     0.060  0.006
31   0.980     0.020  0.000
32   0.750     0.250  0.000
33   0.986     0.014  0.000
34   0.998     0.002  0.000
```

35	0.982	0.018	0.000
36	0.968	0.032	0.000
37	0.988	0.012	0.000
38	0.998	0.002	0.000
39	1.000	0.000	0.000
40	0.980	0.020	0.000
41	0.986	0.014	0.000
42	0.990	0.010	0.000
43	0.958	0.042	0.000
44	0.898	0.060	0.042
45	0.000	0.000	1.000
46	0.000	0.004	0.996
47	0.000	0.000	1.000
48	0.000	0.000	1.000
49	0.002	0.006	0.992
50	0.006	0.014	0.980
51	0.000	0.000	1.000
52	0.000	0.012	0.988
53	0.000	0.000	1.000
54	0.000	0.004	0.996
55	0.016	0.008	0.976
56	0.000	0.000	1.000
57	0.000	0.000	1.000
58	0.014	0.004	0.982
59	0.016	0.026	0.958
60	0.000	0.000	1.000
61	0.002	0.008	0.990
62	0.004	0.026	0.970
63	0.002	0.000	0.998
64	0.000	0.000	1.000
65	0.000	0.000	1.000
66	0.000	0.000	1.000
67	0.000	0.004	0.996
68	0.000	0.000	1.000
69	0.000	0.000	1.000
70	0.000	0.000	1.000
71	0.000	0.000	1.000
72	0.000	0.002	0.998
73	0.000	0.000	1.000
74	0.000	0.000	1.000
75	0.002	0.006	0.992
76	0.012	0.020	0.968
77	0.000	0.000	1.000

```
78   0.000     0.000  1.000
79   0.000     0.000  1.000
80   0.000     0.000  1.000
81   0.018     0.982  0.000
82   0.032     0.968  0.000
83   0.040     0.960  0.000
84   0.022     0.978  0.000
85   0.162     0.838  0.000
86   0.052     0.944  0.004
87   0.038     0.958  0.004
88   0.070     0.920  0.010
89   0.030     0.966  0.004
90   0.204     0.794  0.002
91   0.030     0.966  0.004
92   0.036     0.940  0.024
93   0.026     0.968  0.006
94   0.334     0.506  0.160
95   0.022     0.976  0.002
96   0.250     0.456  0.294
97   0.004     0.990  0.006
98   0.030     0.966  0.004
99   0.034     0.960  0.006
100  0.202     0.722  0.076
101  0.328     0.474  0.198
attr(,"class")
[1] "matrix" "array"  "votes"
```

```r
# Combine predicted probabilities with true labels for tidymodels
rf_results <- test_data %>%
  select(species) %>%
  bind_cols(as.data.frame(rf_prob))
rf_results
```

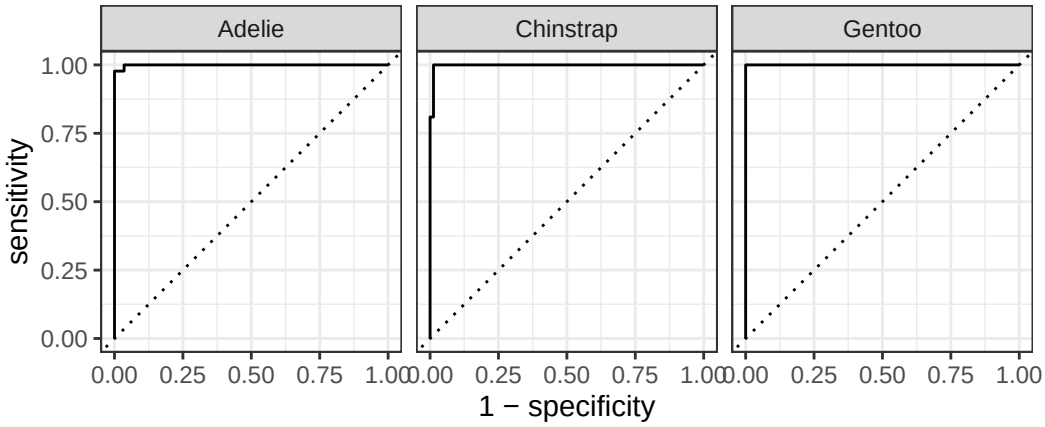
```
# A tibble: 101 x 4
   species Adelie Chinstrap Gentoo
 * <fct>    <dbl>     <dbl>  <dbl>
 1 Adelie   0.978     0.022      0
 2 Adelie   0.924     0.076      0
 3 Adelie   0.99      0.01       0
 4 Adelie   0.976     0.024      0
 5 Adelie   0.972     0.028      0
 6 Adelie   0.994     0.006      0
```

```
 7 Adelie   0.994     0.006      0
 8 Adelie   0.964     0.036      0
 9 Adelie   0.994     0.006      0
10 Adelie   0.984     0.016      0
# i 91 more rows
```

```r
# Compute ROC curves
# roc_curve() for multiclass expects:
# truth column and all class probability columns
roc_data <- rf_results %>%
  roc_curve(truth = species, Adelie, Chinstrap, Gentoo)
roc_data
```

```
# A tibble: 129 x 4
   .level .threshold specificity sensitivity
   <chr>       <dbl>       <dbl>       <dbl>
 1 Adelie   -Inf           0               1
 2 Adelie      0           0               1
 3 Adelie      0.002       0.456           1
 4 Adelie      0.004       0.526           1
 5 Adelie      0.006       0.561           1
 6 Adelie      0.012       0.579           1
 7 Adelie      0.014       0.596           1
 8 Adelie      0.016       0.614           1
 9 Adelie      0.018       0.649           1
10 Adelie      0.022       0.667           1
# i 119 more rows
```

```r
# Plot ROC curves
roc_data |> autoplot()
```




```
# Compute AUC for each class
auc_data <- rf_results |>
  roc_auc(truth = species, Adelie, Chinstrap, Gentoo)
auc_data
```

```
# A tibble: 1 x 3
  .metric .estimator .estimate
  <chr>   <chr>          <dbl>
1 roc_auc hand_till      0.999
```

5.8 Illustration of How ROC Curves Are Plotted

Let's do that for one species (Adelie) vs others, using predicted probabilities from a Random Forest.

```
test_data_adelie <- test_data |>
  mutate(actual = ifelse(species == "Adélie", 1, 0))
test_data_adelie
```

```
# A tibble: 101 x 9
```

```
   species island    bill_length_mm bill_depth_mm flipper_length_mm body_mass_g
   <fct>   <fct>              <dbl>         <dbl>             <int>       <int>
 1 Adelie  Torgersen           39.1          18.7               181        3750
 2 Adelie  Torgersen           39.5          17.4               186        3800
 3 Adelie  Torgersen           39.3          20.6               190        3650
 4 Adelie  Torgersen           36.6          17.8               185        3700
 5 Adelie  Biscoe              37.7          18.7               180        3600
 6 Adelie  Biscoe              35.9          19.2               189        3800
 7 Adelie  Biscoe              38.2          18.1               185        3950
 8 Adelie  Biscoe              38.8          17.2               180        3800
 9 Adelie  Biscoe              37.9          18.6               172        3150
10 Adelie  Dream               39.5          17.8               188        3300
# i 91 more rows
# i 3 more variables: sex <fct>, year <int>, actual <dbl>
```