# 11\_decision\_trees

September 20, 2016

### 1 Decision Trees

Adapted from Chapter 8 of An Introduction to Statistical Learning Why are we learning about decision trees?

- Can be applied to both regression and classification problems
- Many useful properties
- Very popular
- Basis for more sophisticated models
- Have a different way of "thinking" than the other models we have studied

## 1.1 Lesson objectives

Students will be able to:

- Explain how a decision tree is created
- Build a decision tree model in scikit-learn
- Tune a decision tree model and explain how tuning impacts the model
- Interpret a tree diagram
- Describe the key differences between regression and classification trees
- Decide whether a decision tree is an appropriate model for a given problem

# 2 Part 1: Regression trees

Major League Baseball player data from 1986-87:

- **Years** (x-axis): number of years playing in the major leagues
- **Hits** (y-axis): number of hits in the previous year
- Salary (color): low salary is blue/green, high salary is red/yellow

#### Group exercise:

- The data above is our **training data**.
- We want to build a model that predicts the Salary of future players based on Years and Hits.
- We are going to "segment" the feature space into regions, and then use the **mean Salary in each region** as the predicted Salary for future players.
- Intuitively, you want to **maximize** the similarity (or "homogeneity") within a given region, and **minimize** the similarity between different regions.



#### Rules for segmenting:

- You can only use **straight lines**, drawn one at a time.
- Your line must either be **vertical or horizontal**.
- Your line **stops** when it hits an existing line.

Above are the regions created by a computer:

- $R_1$ : players with less than 5 years of experience, mean Salary of \$166,000
- $R_2$ : players with **5 or more years** of experience and **less than 118 hits**, mean Salary of **\$403,000**
- $R_3$ : players with 5 or more years of experience and 118 hits or more, mean Salary of \$846,000

**Note:** Years and Hits are both integers, but the convention is to use the **midpoint** between adjacent values to label a split.

These regions are used to make predictions on **out-of-sample data**. Thus, there are only three possible predictions! (Is this different from how **linear regression** makes predictions?)

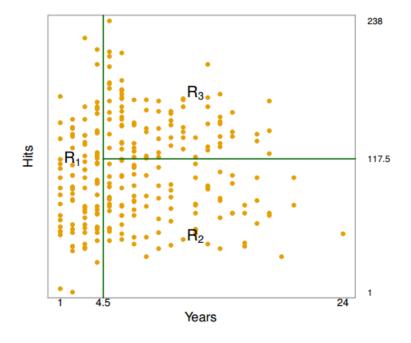
Below is the equivalent regression tree:

The first split is **Years < 4.5**, thus that split goes at the top of the tree. When a splitting rule is **True**, you follow the left branch. When a splitting rule is **False**, you follow the right branch.

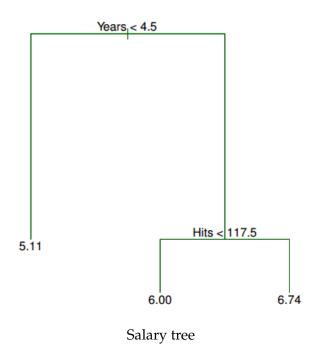
For players in the **left branch**, the mean Salary is \$166,000, thus you label it with that value. (Salary has been divided by 1000 and log-transformed to 5.11.)

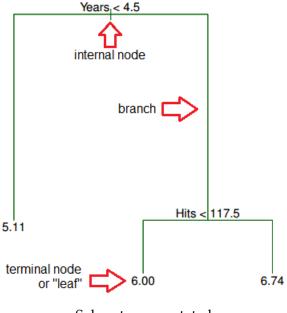
For players in the **right branch**, there is a further split on **Hits < 117.5**, dividing players into two more Salary regions: \$403,000 (transformed to 6.00), and \$846,000 (transformed to 6.74).

What does this tree tell you about your data?



Salary regions





- Salary tree annotated
- Years is the most important factor determining Salary, with a lower number of Years corresponding to a lower Salary.
- For a player with a lower number of Years, Hits is not an important factor determining Salary.
- For a player with a higher number of Years, Hits is an important factor determining Salary, with a greater number of Hits corresponding to a higher Salary.

**Question:** What do you like and dislike about decision trees so far?

## 2.1 Building a regression tree by hand

Your training data is a tiny dataset of used vehicle sale prices. Your goal is to predict price for testing data.

- 1. Read the data into a Pandas DataFrame.
- 2. Explore the data by sorting, plotting, or split-apply-combine (aka group\_by).
- 3. Decide which feature is the most important predictor, and use that to create your first splitting rule.
  - Only binary splits are allowed.
- 4. After making your first split, split your DataFrame into two parts, and then explore each part to figure out what other splits to make.
- 5. Stop making splits once you are convinced that it strikes a good balance between underfitting and overfitting.
  - Your goal is to build a model that generalizes well.
  - You are allowed to split on the same variable multiple times!
- 6. Draw your tree, labeling the leaves with the mean price for the observations in that region.

• Make sure nothing is backwards: You follow the **left branch** if the rule is true, and the **right branch** if the rule is false.

## 2.2 How does a computer build a regression tree?

**Ideal approach:** Consider every possible partition of the feature space (computationally infeasible)

"Good enough" approach: recursive binary splitting

- 1. Begin at the top of the tree.
- 2. For **every feature**, examine **every possible cutpoint**, and choose the feature and cutpoint such that the resulting tree has the lowest possible mean squared error (MSE). Make that split.
- 3. Examine the two resulting regions, and again make a **single split** (in one of the regions) to minimize the MSE.
- 4. Keep repeating step 3 until a **stopping criterion** is met:
  - maximum tree depth (maximum number of splits required to arrive at a leaf)
  - minimum number of observations in a leaf

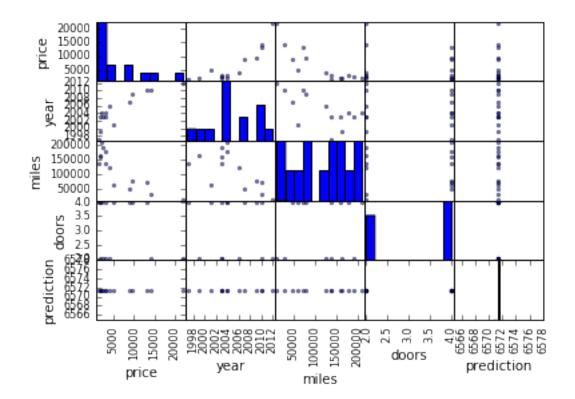
#### 2.2.1 Demo: Choosing the ideal cutpoint for a given feature

%matplotlib inline

```
In [3]: # vehicle data
       import pandas as pd
       url = '../data/vehicles_train.csv'
       train = pd.read_csv(url)
In [4]: # before splitting anything, just predict the mean of the entire dataset
       train['prediction'] = train.price.mean()
       train
Out [4]:
           price year miles doors vtype prediction
           22000 2012
                         13000
                                   2
                                       car 6571.428571
       0
       1
           14000 2010
                                   2
                         30000
                                        car 6571.428571
       2
                                   4 car 6571.428571
           13000 2010
                         73500
       3
            9500 2009
                         78000
                                   4
                                        car 6571.428571
       4
            9000 2007
                       47000
                                   4
                                        car 6571.428571
                                   2
       5
            4000 2006
                       124000
                                        car 6571.428571
       6
            3000 2004
                       177000
                                   4
                                        car 6571.428571
            2000 2004
       7
                        209000
                                   4 truck 6571.428571
       8
            3000 2003
                       138000
                                   2
                                        car 6571.428571
       9
            1900 2003 160000
                                   4
                                        car 6571.428571
       10
            2500 2003 190000
                                   2 truck 6571.428571
       11
            5000 2001
                                   4
                                        car 6571.428571
                       62000
                                   2 truck 6571.428571
       12
            1800 1999
                        163000
       13
            1300 1997
                       138000
                                        car 6571.428571
In [8]: import matplotlib.pyplot as plt
```

#### In [9]: pd.scatter\_matrix(train)

```
Out[9]: array([[<matplotlib.axes._subplots.AxesSubplot object at 0x11d593890>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11d71a210>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11d797690>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11d7f5510>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11d874990>],
               [<matplotlib.axes. subplots.AxesSubplot object at 0x11d8db250>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11d95e410>,
                <matplotlib.axes. subplots.AxesSubplot object at 0x11d9e0290>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11da4e250>,
                <matplotlib.axes. subplots.AxesSubplot object at 0x11dad30d0>],
               [<matplotlib.axes._subplots.AxesSubplot object at 0x11dc380d0>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11dcba050>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11dc447d0>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11dd9de90>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11df21d10>],
               [<matplotlib.axes._subplots.AxesSubplot object at 0x11df91610>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11e015490>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11e0794d0>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11e0fd450>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11e135590>],
               [<matplotlib.axes._subplots.AxesSubplot object at 0x11e1ef4d0>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11e373350>,
                <matplotlib.axes. subplots.AxesSubplot object at 0x11d2a2490>,
                <matplotlib.axes._subplots.AxesSubplot object at 0x11e3f0e10>,
                <matplotlib.axes. subplots.AxesSubplot object at 0x11e420690>]], dt
```



```
In [10]: # calculate RMSE for those predictions
         from sklearn import metrics
         import numpy as np
         np.sqrt(metrics.mean_squared_error(train.price, train.prediction))
Out[10]: 5936.9819859959835
In [11]: # define a function that calculates the RMSE for a given split of miles
         def mileage_split(miles):
             lower_mileage_price = train[train.miles < miles].price.mean()</pre>
             higher_mileage_price = train[train.miles >= miles].price.mean()
             train['prediction'] = np.where(train.miles < miles, lower_mileage_price
             return np.sqrt(metrics.mean_squared_error(train.price, train.prediction)
In [12]: # calculate RMSE for tree which splits on miles < 50000
         print 'RMSE:', mileage_split(50000)
         train
RMSE: 3984.09174254
Out [12]:
             price year
                           miles doors
                                                   prediction
                                         vtype
         0
             22000 2012
                           13000
                                      2
                                                 15000.000000
                                            car
             14000 2010
                           30000
                                      2
                                            car 15000.000000
         1
```

```
3
             9500 2009
                        78000
                                     4
                                          car
                                                4272.727273
        4
             9000
                  2007
                         47000
                                     4
                                          car 15000.000000
        5
             4000
                  2006 124000
                                     2
                                                4272.727273
                                          car
             3000 2004 177000
                                     4
        6
                                          car
                                               4272.727273
        7
             2000 2004
                         209000
                                     4
                                      truck
                                               4272.727273
        8
             3000 2003 138000
                                     2
                                          car
                                               4272.727273
        9
             1900 2003 160000
                                     4
                                          car
                                                4272.727273
        10
             2500 2003 190000
                                     2
                                               4272.727273
                                      truck
             5000 2001
                                               4272.727273
        11
                         62000
                                     4
                                          car
             1800 1999 163000
                                     2
                                               4272.727273
        12
                                       truck
        13
             1300 1997 138000
                                     4
                                               4272.727273
                                          car
In [13]: # calculate RMSE for tree which splits on miles < 100000
        print 'RMSE:', mileage_split(100000)
        train
RMSE: 3530.14653008
Out [13]:
            price year
                          miles
                                 doors vtype
                                                prediction
        0
           22000 2012
                          13000
                                     2
                                          car 12083.333333
        1
           14000 2010
                         30000
                                     2
                                          car 12083.333333
        2
            13000 2010
                        73500
                                     4
                                          car 12083.333333
        3
             9500 2009
                        78000
                                     4
                                        car 12083.333333
             9000 2007
                        47000
        4
                                     4
                                         car 12083.333333
                                     2
        5
             4000 2006 124000
                                          car 2437.500000
        6
             3000 2004 177000
                                     4
                                          car
                                               2437.500000
        7
             2000 2004 209000
                                     4 truck
                                               2437.500000
             3000 2003 138000
        8
                                     2
                                               2437.500000
                                          car
                                               2437.500000
        9
             1900 2003 160000
                                     4
                                          car
                                     2 truck
        10
             2500 2003 190000
                                               2437.500000
             5000 2001
                                          car 12083.333333
        11
                         62000
                                     4
        12
             1800 1999 163000
                                     2 truck 2437.500000
        13
             1300 1997 138000
                                               2437.500000
                                          car
In [14]: # check all possible mileage splits
        mileage_range = range(train.miles.min(), train.miles.max(), 1000)
        RMSE = [mileage_split(miles) for miles in mileage_range]
In [15]: # allow plots to appear in the notebook
        %matplotlib inline
        import matplotlib.pyplot as plt
        plt.rcParams['figure.figsize'] = (6, 4)
        plt.rcParams['font.size'] = 14
In [16]: # plot mileage cutpoint (x-axis) versus RMSE (y-axis)
        plt.plot(mileage_range, RMSE)
        plt.xlabel('Mileage cutpoint')
```

2

13000 2010

73500

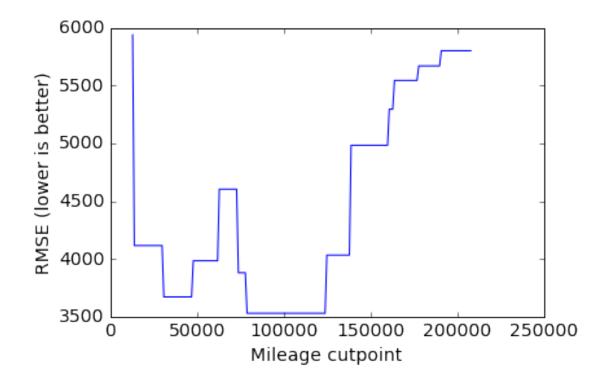
4

car

4272.727273

```
plt.ylabel('RMSE (lower is better)')

# More homogenous groups near 100000. At ends, you are essentially the nu.
Out[16]: <matplotlib.text.Text at 0x121e75e50>
```



**Recap:** Before every split, this process is repeated for every feature, and the feature and cutpoint that produces the lowest MSE is chosen.

# 2.3 Building a regression tree in scikit-learn

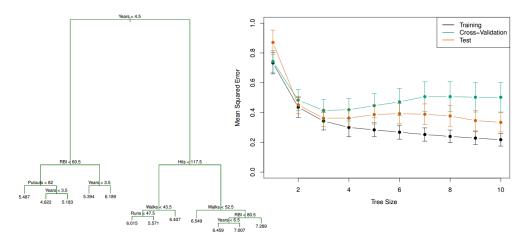
X = train[feature\_cols]

y = train.price

```
In [19]: # instantiate a DecisionTreeRegressor (with random_state=1)
         from sklearn.tree import DecisionTreeRegressor
         treereg = DecisionTreeRegressor(random_state=1)
         treereg
Out[19]: DecisionTreeRegressor(criterion='mse', max_depth=None, max_features=None,
                    max_leaf_nodes=None, min_samples_leaf=1, min_samples_split=2,
                    min_weight_fraction_leaf=0.0, presort=False, random_state=1,
                    splitter='best')
In [20]: # use leave-one-out cross-validation (LOOCV) to estimate the RMSE for this
         from sklearn.cross_validation import cross_val_score
         scores = cross_val_score(treereg, X, y, cv=14, scoring='mean_squared_error
         np.mean(np.sqrt(-scores)) #RMSE. Also, a bug that gives negative number
         # Using LOOCV is because sample size is small.
         # On average how the model will perform in the wild
Out [20]: 3107.1428571428573
In [21]: np.sqrt(-scores)
         # Very different numbers because of variance.
                                 3500., 3500., 4000.,
Out[21]: array([ 8000., 8000.,
                                                         5000.,
                                                                 1000., 1000.,
                               500., 4000., 500., 1700.])
                 1700., 1100.,
```

# 2.4 What happens when we grow a tree too deep?

- Left: Regression tree for Salary **grown deeper**
- Right: Comparison of the training, testing, and cross-validation errors for trees with different numbers of leaves



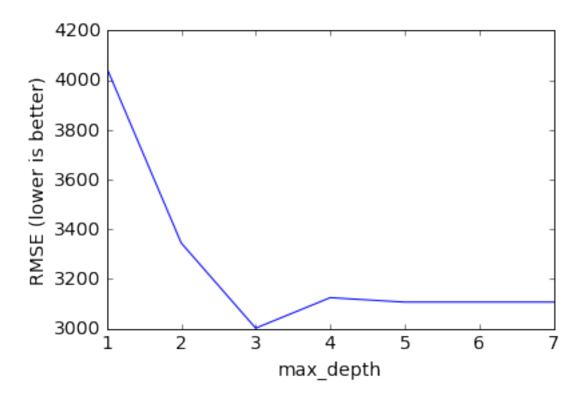
Salary tree grown deep

The **training error** continues to go down as the tree size increases (due to overfitting), but the lowest **cross-validation error** occurs for a tree with 3 leaves.

# 2.5 Tuning a regression tree

Let's try to reduce the RMSE by tuning the **max\_depth** parameter:

```
In [20]: # try different values one-by-one
         treereg = DecisionTreeRegressor(max_depth=1, random_state=1)
         scores = cross_val_score(treereg, X, y, cv=14, scoring='mean_squared_error
         np.mean(np.sqrt(-scores))
Out [20]: 4050.1443001442999
  Or, we could write a loop to try a range of values:
In [21]: # list of values to try
         max_depth_range = range(1, 8)
                                                             # At most 8 questions in
         # list to store the average RMSE for each value of max_depth
         RMSE_scores = []
         # use LOOCV with each value of max_depth
         for depth in max_depth_range:
             treereg = DecisionTreeRegressor(max_depth=depth, random_state=1)
             MSE_scores = cross_val_score(treereg, X, y, cv=14, scoring='mean_square
             RMSE_scores.append(np.mean(np.sqrt(-MSE_scores)))
In [22]: # plot max_depth (x-axis) versus RMSE (y-axis)
         plt.plot(max_depth_range, RMSE_scores)
         plt.xlabel('max_depth')
         plt.ylabel('RMSE (lower is better)')
Out[22]: <matplotlib.text.Text at 0x11774ee10>
```



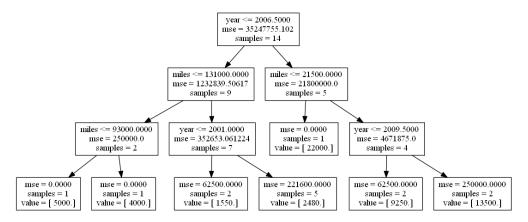
```
In [23]: # max_depth=3 was best, so fit a tree using that parameter
         treereg = DecisionTreeRegressor(max_depth=3, random_state=1)
         treereg.fit(X, y)
Out[23]: DecisionTreeRegressor(criterion='mse', max_depth=3, max_features=None,
                    max_leaf_nodes=None, min_samples_leaf=1, min_samples_split=2,
                    min_weight_fraction_leaf=0.0, presort=False, random_state=1,
                    splitter='best')
In [24]: # "Gini importance" of each feature: the (normalized) total reduction of each
         pd.DataFrame({'feature':feature_cols, 'importance':treereg.feature_importa
         # Each tree might be different. One may say miles is more important.
Out [24]:
           feature
                    importance
         0
              year
                      0.798744
             miles
         1
                      0.201256
                      0.000000
             doors
             vtype
                      0.000000
```

# 2.6 Creating a tree diagram

```
In [25]: # create a Graphviz file
     from sklearn.tree import export_graphviz
```

export\_graphviz(treereg, out\_file='tree\_vehicles.dot', feature\_names=feature

```
# At the command line, run this to convert to PNG:
# dot -Tpng tree_vehicles.dot -o tree_vehicles.png
```



Tree for vehicle data

Reading the internal nodes:

- samples: number of observations in that node before splitting
- mse: MSE calculated by comparing the actual response values in that node against the mean response value in that node
- rule: rule used to split that node (go left if true, go right if false)

Reading the leaves:

- samples: number of observations in that node
- value: mean response value in that node
- mse: MSE calculated by comparing the actual response values in that node against "value"

# 2.7 Making predictions for the testing data

```
In [26]: # read the testing data
         url = '../data/vehicles_test.csv'
         test = pd.read csv(url)
         test['vtype'] = test.vtype.map({'car':0, 'truck':1})
         test
Out [26]:
            price year
                          miles
                                 doors
                                        vtype
             3000 2003
                        130000
                                             1
             6000
                   2005
                          82500
         1
                                             0
           12000 2010
                          60000
                                      2
                                             0
```

**Question:** Using the tree diagram above, what predictions will the model make for each observation?

### 3 Part 2: Classification trees

**Example:** Predict whether Barack Obama or Hillary Clinton will win the Democratic primary in a particular county in 2008:

### **Questions:**

- What are the observations? How many observations are there?
- What is the response variable?
- What are the features?
- What is the most predictive feature?
- Why does the tree split on high school graduation rate twice in a row?
- What is the class prediction for the following county: 15% African-American, 90% high school graduation rate, located in the South, high poverty, high population density?
- What is the predicted probability for that same county?

# 3.1 Comparing regression trees and classification trees

regressiclassification
trees trees

predict predict
a a con- catetinu- gorious cal
responsæsponse

```
regressidassification
trees
       trees
predictpredict
us-
       us-
ing
       ing
mean most
       com-
sponse monly
of
       oc-
each
       cur-
leaf
       ing
       class
       of
       each
       leaf
splits splits
are
       are
cho-
       cho-
       sen
sen
       to
to
min-
       min-
       i-
mize
       mize
MSE
       Gini
       in-
       dex
       (dis-
       cussed
       below)
```

#### 3.1.1 Comparing classification error rate and Gini index

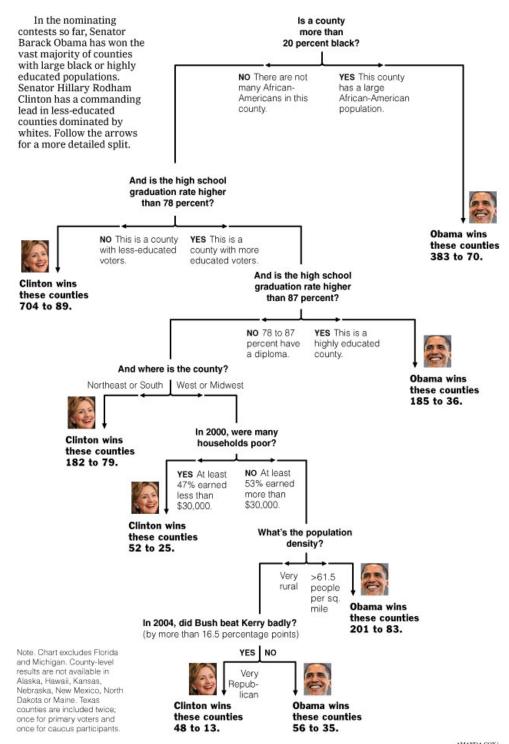
- Gini index is generally preferred because it will make splits that **increase node purity**, even if that split does not change the classification error rate.
- Node purity is important because we're interested in the **class proportions** in each region, since that's how we calculate the **predicted probability** of each class.
- scikit-learn's default splitting criteria for classification trees is Gini index.

Note: There is another common splitting criteria called **cross-entropy**. It's numerically similar to Gini index, but slower to compute, thus it's not as popular as Gini index.

# 3.2 Building a classification tree in scikit-learn

We'll build a classification tree using the Titanic data:

# Decision Tree: The Obama-Clinton Divide



Sources: Election results via The Associated Press; Census Bureau; Dave Leip's Atlas of U.S. Presidential Elections

AMANDA COX/ THE NEW YORK TIMES

#### Obama-Clinton decision tree

```
# encode female as 0 and male as 1
         titanic['Sex'] = titanic.Sex.map({'female':0, 'male':1})
         # fill in the missing values for age with the median age
         titanic.Age.fillna(titanic.Age.median(), inplace=True)
         # create a DataFrame of dummy variables for Embarked
         embarked_dummies = pd.get_dummies(titanic.Embarked, prefix='Embarked')
         embarked_dummies.drop(embarked_dummies.columns[0], axis=1, inplace=True)
         # concatenate the original DataFrame and the dummy DataFrame
         titanic = pd.concat([titanic, embarked_dummies], axis=1)
         # print the updated DataFrame
         titanic.head()
Out [29]:
            PassengerId Survived
                                   Pclass
         0
                      1
                                 0
                      2
         1
                                 1
                                         1
         2
                      3
                                 1
                                         3
         3
                      4
                                 1
                                         1
         4
                      5
                                         3
                                                                             SibSp
                                                           Name
                                                                 Sex
                                                                        Age
         0
                                       Braund, Mr. Owen Harris
                                                                       22.0
                                                                                 1
         1
            Cumings, Mrs. John Bradley (Florence Briggs Th...
                                                                       38.0
                                                                                 1
         2
                                        Heikkinen, Miss. Laina
                                                                      26.0
                                                                                 0
         3
                 Futrelle, Mrs. Jacques Heath (Lily May Peel)
                                                                   0
                                                                      35.0
                                                                                 1
         4
                                      Allen, Mr. William Henry
                                                                       35.0
                                                                                 \cap
                      Ticket
                                  Fare Cabin Embarked
                                                        Embarked_Q Embarked_S
         0
                   A/5 21171
                                7.2500
                                                               0.0
                                         NaN
                                                     S
                                                                            1.0
                    PC 17599
                              71.2833
                                         C85
                                                     С
                                                               0.0
                                                                            0.0
         1
                                                     S
            STON/02. 3101282
                               7.9250
                                         NaN
                                                               0.0
                                                                            1.0
         3
                      113803
                               53.1000 C123
                                                     S
                                                               0.0
                                                                            1.0
                      373450
                                8.0500
                                         NaN
                                                     S
                                                               0.0
                                                                            1.0
```

- **Survived:** 0=died, 1=survived (response variable)
- Pclass: 1=first class, 2=second class, 3=third class
  - What will happen if the tree splits on this feature?
- **Sex:** 0=female, 1=male
- Age: numeric value
- Embarked: C or Q or S

```
y = titanic.Survived
In [31]: # fit a classification tree with max_depth=3 on all data
          from sklearn.tree import DecisionTreeClassifier
          treeclf = DecisionTreeClassifier(max_depth=3, random_state=1)
          treeclf.fit(X, y)
Out[31]: DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=3,
                        max_features=None, max_leaf_nodes=None, min_samples_leaf=1,
                        min_samples_split=2, min_weight_fraction_leaf=0.0,
                        presort=False, random_state=1, splitter='best')
In [32]: # create a Graphviz file
          export_graphviz(treeclf, out_file='tree_titanic.dot', feature_names=feature
          # At the command line, run this to convert to PNG:
               dot -Tpng tree_titanic.dot -o tree_titanic.png
                                     Sex <= 0.5000
gini = 0.473012957861
                               Pclass <= 2.5000
gini = 0.382835003448
                                           Age <= 6.5000
gini = 0.306443716228
```

Pclass <= 2.5000 gini = 0.444444444444

> gini = 0.4898 samples = 14 value = [ 8. 6.]

gini = 0.0000 samples = 10 value = [ 0. 10.] Pclass <= 1.5000 ini = 0.279782478606 samples = 553

gini = 0.4599

gini = 0.2043

samples = 433 value = [ 383. 50

X = titanic[feature\_cols]

Age <= 2.5000 gini = 0.100276816609 samples = 170

gini = 0.0907 samples = 168 value = [ 8. 160.]

gini = 0.5000 samples = 2 value = [1. 1.]

Tree for Titanic data

Embarked\_S <= 0.5000 gini = 0.5 samples = 144

> gini = 0.4688 samples = 88 value = [ 55. 33.]

gini = 0.4228 samples = 56 value = [ 17. 39.]

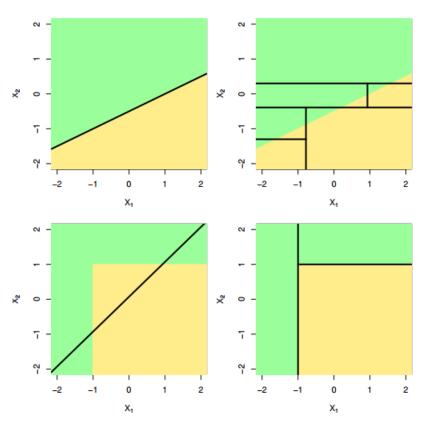
Notice the split in the bottom right: the **same class** is predicted in both of its leaves. That split didn't affect the **classification error rate**, though it did increase the **node purity**, which is important because it increases the accuracy of our predicted probabilities.

```
In [33]: # compute the feature importances
         pd.DataFrame({ 'feature':feature_cols, 'importance':treeclf.feature_importance'
         # Importance for purity
Out [33]:
                feature
                          importance
         0
                 Pclass
                            0.242664
         1
                            0.655584
                    Sex
         2
                    Age
                            0.064494
         3
            Embarked Q
                            0.000000
             Embarked S
                            0.037258
```

# 4 Part 3: Comparing decision trees with other models

## Advantages of decision trees:

- Can be used for regression or classification
- Can be displayed graphically
- Highly interpretable
- Can be specified as a series of rules, and more closely approximate human decision-making than other models
- Prediction is fast
- Features don't need scaling
- Automatically learns feature interactions
- Tends to ignore irrelevant features
- Non-parametric (will outperform linear models if relationship between features and response is highly non-linear)



Trees versus linear models

### Disadvantages of decision trees:

- Performance is (generally) not competitive with the best supervised learning methods (low bias)
- Can easily overfit the training data (tuning is required)
- Small variations in the data can result in a completely different tree (high variance)

- Recursive binary splitting makes "locally optimal" decisions that may not result in a globally optimal tree
- Doesn't tend to work well if the classes are highly unbalanced
- Doesn't tend to work well with very small datasets

## 5 BONUS Dive into Gini

## 5.1 Splitting criteria for classification trees

Common options for the splitting criteria:

- **classification error rate:** fraction of training observations in a region that don't belong to the most common class
- Gini index: measure of total variance across classes in a region

#### 5.1.1 Example of classification error rate

Pretend we are predicting whether someone buys an iPhone or an Android:

- At a particular node, there are **25 observations** (phone buyers), of whom **10 bought iPhones** and **15 bought Androids**.
- Since the majority class is **Android**, that's our prediction for all 25 observations, and thus the classification error rate is 10/25 = 40%.

Our goal in making splits is to reduce the classification error rate. Let's try splitting on gender:

- Males: 2 iPhones and 12 Androids, thus the predicted class is Android
- Females: 8 iPhones and 3 Androids, thus the predicted class is iPhone
- Classification error rate after this split would be 5/25 = 20%

Compare that with a split on age:

- 30 or younger: 4 iPhones and 8 Androids, thus the predicted class is Android
- 31 or older: 6 iPhones and 7 Androids, thus the predicted class is Android
- Classification error rate after this split would be 10/25 = 40%

The decision tree algorithm will try **every possible split across all features**, and choose the split that **reduces the error rate the most.** 

#### 5.1.2 Example of Gini index

Calculate the Gini index before making a split:

$$1 - \left(\frac{iPhone}{Total}\right)^2 - \left(\frac{Android}{Total}\right)^2 = 1 - \left(\frac{10}{25}\right)^2 - \left(\frac{15}{25}\right)^2 = 0.48$$

- The **maximum value** of the Gini index is 0.5, and occurs when the classes are perfectly balanced in a node.
- The **minimum value** of the Gini index is 0, and occurs when there is only one class represented in a node.

• A node with a lower Gini index is said to be more "pure".

Evaluating the split on **gender** using Gini index:

Males: 
$$1 - \left(\frac{2}{14}\right)^2 - \left(\frac{12}{14}\right)^2 = 0.24$$

Females: 
$$1 - \left(\frac{8}{11}\right)^2 - \left(\frac{3}{11}\right)^2 = 0.40$$

Weighted Average: 
$$0.24\left(\frac{14}{25}\right) + 0.40\left(\frac{11}{25}\right) = 0.31$$

Evaluating the split on age using Gini index:

30 or younger: 
$$1 - \left(\frac{4}{12}\right)^2 - \left(\frac{8}{12}\right)^2 = 0.44$$

31 or older: 
$$1 - \left(\frac{6}{13}\right)^2 - \left(\frac{7}{13}\right)^2 = 0.50$$

Weighted Average: 
$$0.44\left(\frac{12}{25}\right) + 0.50\left(\frac{13}{25}\right) = 0.47$$

Again, the decision tree algorithm will try **every possible split**, and will choose the split that **reduces the Gini index (and thus increases the "node purity") the most.** 

- In [ ]:
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- In [ ]: