Day 10: Classification, Entropy and Decision Trees

Classifying - Histograms

Let's imagine that we want to classify observations based on a binary dependent variable, y.

- Two possible outcomes
- We classify each observation based on which outcome is most likely

$$p(y|x) \geq .5 \Rightarrow \hat{y} = 1$$

$$p(y|x) < .5 \Rightarrow \hat{y} = 0$$

Classifying - Histograms

Let's draw some classifiers on the white board.

- Divide the data in half for each of two x variables
- Each separate bin can then be classified separately
- We can increase the granularity of our classifier by adding more breaks to each x variable

Classifying - Histograms

Is there a more efficient way?

- Imagine we only divide variables in half
- How many discrete bins of data would exist if we looked at each of 16 variables in this way?

Classifying - Histograms

Is there a more efficient way?

- Imagine we only divide variables in half
- How many discrete bins of data would exist if we looked at each of 16 variables in this way?
  - $2^{16} = 65,536$ possible bins
  - We would then need 65,536 observations at the **minimum** to obtain **any** information about each cell
- This is **not** efficient

Classification - A Better Algorithm

If we don't want to use histograms, what tools are available?

- Logistic Regression
- Naïve Bayes Classifier
- Nearest Neighbor Algorithms
- Decision Trees
- Support Vector Machines
- Neural Networks

What is Entropy?

Entropy is a measure of uncertainty (or information) about the world, or, more specifically, uncertainty about the true value of an outcome in a given model.

Lower entropy: less uncertainty

Higher entropy: greater uncertainty

Measuring Entropy

Entropy can be calculated using the following equation

$$H(x) = -\sum_{i=0}^{n} p(x_i)\ ln\ p(x_i)$$

This is *Nat* Entropy (Shannon entropy is calculated using log_2, and Hartley entropy uses log_{10})

Measuring Entropy

1. More options leads to higher entropy
2. Equal probabilities of outcomes lead to higher entropy

The goal of all of our predictive measures will be to reduce entropy (or maximize information gain) at each step in our model

Remember: information gain should be relative to the universe, not our sample

Exercise

Write a function to estimate the Shannon Entropy of a set of outcomes, given the observed probability for each outcome in an arbitrary set. Use your function to answer:

1. If the probability of 5 outcomes are .2, .3, .1, .1, and .3, then what is the entropy of the system?
2. If the probabilty of each of 5 outcomes is .2, then what is the entropy of the system?
3. If the probability of each of 10 outcomes is .1, then what is the entropy of the system?

Exercise Answer

```
import numpy as np

def sEnt(listP):
    entropy = 0
    n = len(listP)
    for i in range(n):
        entropy += listP[i] * np.log2(listP[i])
    entropy *= -1
    return entropy

print(natEnt([.2,.3,.1,.1,.3]))
print(natEnt([.2]*5))
print(natEnt([.1]*10))
```

Using Entropy

We need to determine how we can reduce the entropy of our system by dividing data.

1. Choose the most informative Variable
2. Choose how to best divide the selected variable in order to gain information
3. Repeat until we reach a stopping point
    - We need to predetermine a stopping rule

Using Entropy

In order to choose the most informative variable, we need to first determine how informative each variable is

- Search across each variable for the optimal decision point
- Determine the information gain from that variable and decision point
- Compare the information gain across the available variables

Information Gain

We can define information gain from a binary split of our data as follows:

$$IG = H_0(x) - H_1(x)$$

Where H_0 is the original entropy, and H_1 is the entropy after the split.

Information Gain

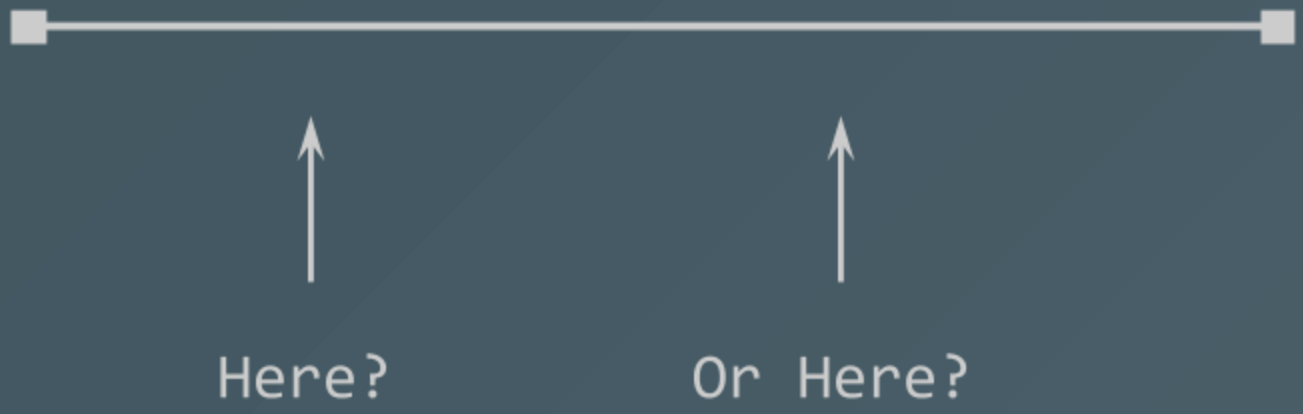
We can calculate H_1 as

$$H_1(x) = \omega_1 \cdot H_{11}(x) + \omega_2 \cdot H_{12}(x)$$

- ω_1 and ω_2: the ratio of elements in each respective child node relative to the parent node (should add up to 1)
- H_{11} and H_{12}: the entropy of each child node

Where is the Cutoff?

Where do we draw the line when dividing observations based on a given variable?



Where is the Cutoff?

We need an algorithm that will **search** across possible cutoffs for our variable, and return the most advantageous split.

- Gradient Descent is frequently used on continuous variables
- For binary variables, we can simply separate the groups/classes
- For count variables, determine which cutoff will generate the greatest gain

Concept Code

```
# Determine the number of classes in dep. var,
#       and calculate the probability of each
# NOTE: this is NOT efficient code

def prob(depVar):
    vals = np.unique(depVar)
    k = len(vals)
    n = len(depVar)
    probs = [0]*k
    for i in range(n):
        for j in range(k):
            if (depVar[i]==vals[j]):
                probs[j]+=(1/n)
    return probs
```

Concept Code

```
def searchFn(y, x):
    minx = np.min(x)
    maxx = np.max(x)
    base = sEnt(prob(y))
    ent = [0]*len(y)
    bestx = minx
    gain = 0
    for i in np.linspace(minx, maxx,
                num=len(np.unique(y))):
        a = y[(x>=i)]
        b = y[(x<i)]
        if ((sEnt(prob(a)*len(a)) +
        sEnt(prob(b))*len(b)) / len(y) < base):
            bestx = i
            gain = base - (sEnt(prob(a)*len(a)) +
                sEnt(prob(b))*len(b)) / len(y)
    return gain, bestx
```

Concept Code

```
# Determine the x variable that will most reduce entropy

def bestGain(y, x):
    base = sEnt(prob(y))
    best = [0,0,0,None]
    for i in range(np.shape(x)[1]):
        if (searchFn(y,x[:,i])[0] > best[0]):
            best = [searchFn(y,x[:,i])[0],
                searchFn(y,x[:,i])[1], i, None]
    return best
```

Repeating these functions recursively until we reach our stopping rule would create a decision tree using our most informative variables.

Implementing a Decision Tree

We will start using the `sklearn` library today. It is the most robust machine learning library available, and allows us to implement many kinds of tests and algorithms. sci-kit learn documentation

```
from sklearn.tree import DecisionTreeClassifier
from sklearn.metrics import accuracy_score
from sklearn.model_selection import train_test_split
```

This is all the extra code that we will need to start using our new Decision Tree Classifiers.

Fitting Data with Sci-kit Learn

```
# Our import statements for this problem
import pandas as pd
import numpy as np
import patsy as pt

from sklearn.tree import DecisionTreeClassifier
from sklearn.metrics import accuracy_score
from sklearn.model_selection import train_test_split
```

Fitting Data with Sci-kit Learn

```
# The code to implement a decision tree
data = pd.read_csv(
        "/home/dusty/DatasetsDA/Titanic/train.csv")


model = DecisionTreeClassifier()

y, x = pt.dmatrices("Survived ~ -1 + Sex + Age
                + SibSp + Pclass", data=data)

x, xt, y, yt = train_test_split(x, y,
                test_size=0.33, random_state=42)

res = model.fit(x,y)

print("\n\nIn-sample accuracy: %s%%\n\n"
 % str(round(100*accuracy_score(y, model.predict(x)), 2)))
```

How does it do?

Using the Titanic dataset, and predicting survival with sex, age, siblings, and class (how fancy the passenger was traveling) results in the following printout:

In-sample accuracy: 94.35%

For being easy to implement, that is a pretty good prediction!

Today's Lab Exercise

With your teammates, find your best decision tree with the student performance data provided.

Once you have a tree that you are satisfied with, compare it to the models made by other groups. It's time to start comparing the performance of the preferred model from each team on new student data.

The winning team will get some bonus points!

Day 11 - Decision Trees and Overfitting

Fitting Data with Sci-kit Learn

Recall the model that we used last week to predict survival of Titanic passengers

```
# Our import statements for this problem
import pandas as pd
import numpy as np
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from sklearn.tree import DecisionTreeClassifier
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```

Fitting Data with Sci-kit Learn

```
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x, xt, y, yt = train_test_split(x, y,
                test_size=0.33, random_state=42)

res = model.fit(x,y)

print("\n\nIn-sample accuracy: %s%%\n\n"
 % str(round(100*accuracy_score(y, model.predict(x)), 2)))
```
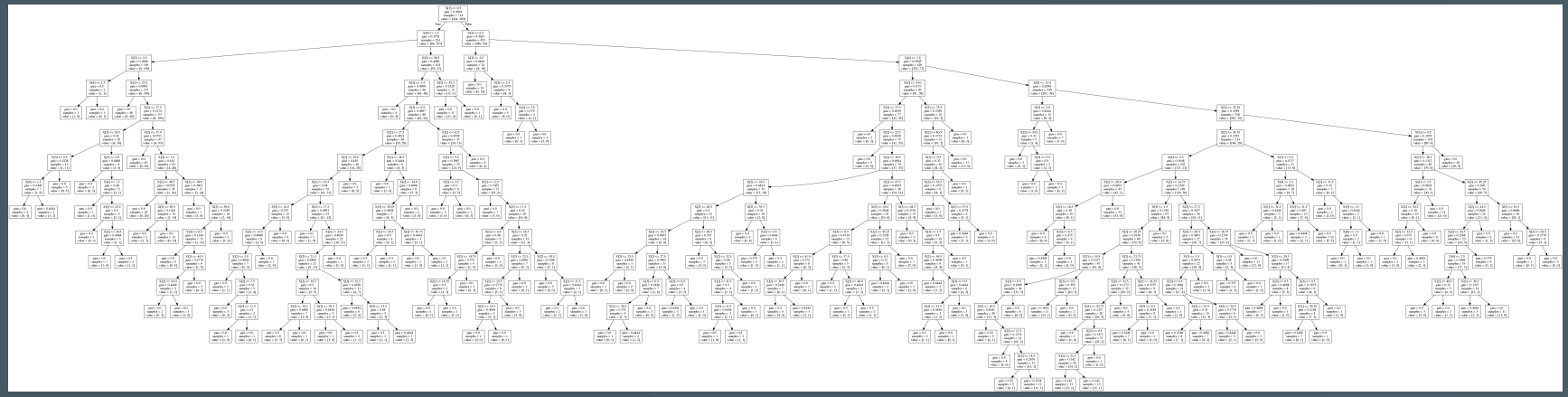

Visualizing the Model

- A decision tree is just one (possibly long) logical statement
- We can quickly present a diagram of it to non-experts
- Even better, they will be able to read and **understand** that model

Visualizing the Model



Didn't you say that this would be **human** readable?

Overfitting in Decision Trees

If we want a model to be readable for a human, we should probably try to keep the model simpler. This will also aid in out-of-sample prediction accuracy.

```
print("\n\nIn-sample accuracy: %s%%\n\n"
 % str(round(100*accuracy_score(y, model.predict(x)), 2)))
print("\n\nOut-of-sample accuracy: %s%%\n\n"
%str(round(100*accuracy_score(yt, model.predict(xt)), 2)))
```

In-sample accuracy: 94.35%
Out-of-sample accuracy: 75.85%

So we are doing much worse on our out-of-sample observations than we do in-sample

Overfitting Decision Trees

Let's restrict our tree to only 5 levels, and see what happens. We only need to modify one line of our code:

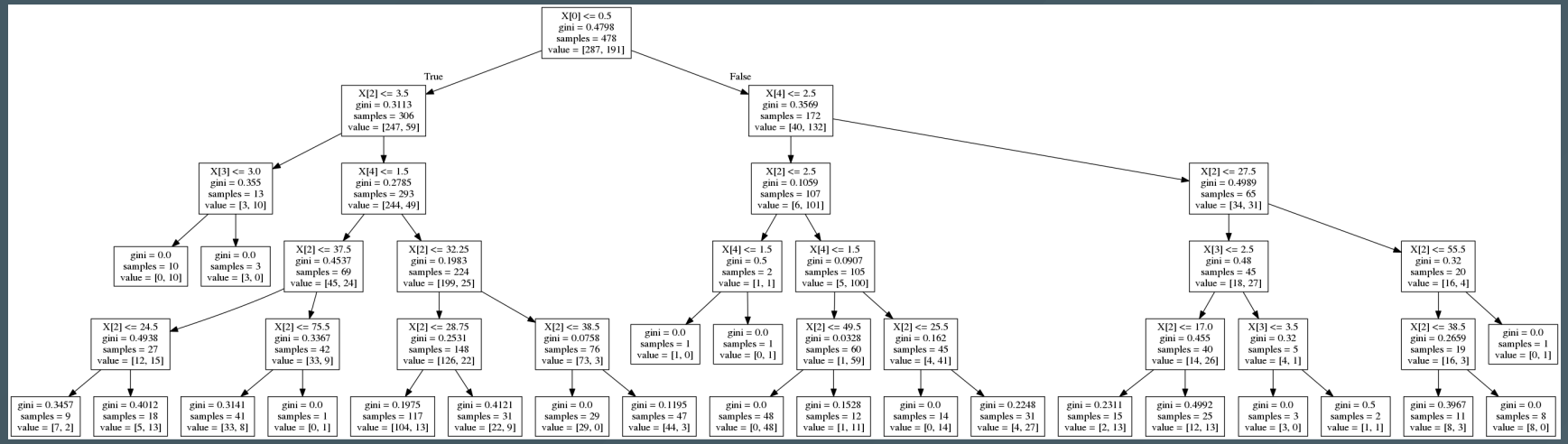
```
model = DecisionTreeClassifier(max_depth=5)
```

In-sample accuracy: 86.82%

Out-of-sample accuracy: 77.12%

By simplifying, we actually do **better** out of sample

The Tree


X[0] <= 0.5
gini = 0.4798
samples = 478
value = [287, 191]
True
False
X[2] <= 3.5
gini = 0.3113
samples = 306
value = [247, 59]
X[4] <= 2.5
gini = 0.3569
samples = 172
value = [40, 132]
X[3] <= 3.0
gini = 0.355
samples = 13
value = [3, 10]
X[4] <= 1.5
gini = 0.2785
samples = 293
value = [244, 49]
X[2] <= 2.5
gini = 0.1059
samples = 107
value = [6, 101]
X[2] <= 27.5
gini = 0.4989
samples = 65
value = [34, 31]
gini = 0.0
samples = 10
value = [0, 10]
gini = 0.0
samples = 3
value = [3, 0]
X[2] <= 37.5
gini = 0.4537
samples = 69
value = [45, 24]
X[2] <= 32.25
gini = 0.1983
samples = 224
value = [199, 25]
X[4] <= 1.5
gini = 0.5
samples = 2
value = [1, 1]
X[4] <= 1.5
gini = 0.0907
samples = 105
value = [5, 100]
X[3] <= 2.5
gini = 0.48
samples = 45
value = [18, 27]
X[2] <= 55.5
gini = 0.32
samples = 20
value = [16, 4]
X[2] <= 24.5
gini = 0.4938
samples = 27
value = [12, 15]
X[2] <= 75.5
gini = 0.3367
samples = 42
value = [33, 9]
X[2] <= 28.75
gini = 0.2531
samples = 148
value = [126, 22]
X[2] <= 38.5
gini = 0.0758
samples = 76
value = [73, 3]
gini = 0.0
samples = 1
value = [1, 0]
gini = 0.0
samples = 1
value = [0, 1]
X[2] <= 49.5
gini = 0.0328
samples = 60
value = [1, 59]
X[2] <= 25.5
gini = 0.162
samples = 45
value = [4, 41]
X[2] <= 17.0
gini = 0.455
samples = 40
value = [14, 26]
X[3] <= 3.5
gini = 0.32
samples = 5
value = [4, 1]
X[2] <= 38.5
gini = 0.2659
samples = 19
value = [16, 3]
gini = 0.0
samples = 1
value = [0, 1]
gini = 0.3457
samples = 9
value = [7, 2]
gini = 0.4012
samples = 18
value = [5, 13]
gini = 0.3141
samples = 41
value = [33, 8]
gini = 0.0
samples = 1
value = [0, 1]
gini = 0.1975
samples = 117
value = [104, 13]
gini = 0.4121
samples = 31
value = [22, 9]
gini = 0.0
samples = 29
value = [29, 0]
gini = 0.1195
samples = 47
value = [44, 3]
gini = 0.0
samples = 48
value = [0, 48]
gini = 0.1528
samples = 12
value = [1, 11]
gini = 0.0
samples = 14
value = [0, 14]
gini = 0.2248
samples = 31
value = [4, 27]
gini = 0.2311
samples = 15
value = [2, 13]
gini = 0.4992
samples = 25
value = [12, 13]
gini = 0.0
samples = 3
value = [3, 0]
gini = 0.5
samples = 2
value = [1, 1]
gini = 0.3967
samples = 11
value = [8, 3]
gini = 0.0
samples = 8
value = [8, 0]

Overfitting Decision Trees

Let's make one more change, and restrict our tree to leaves with 10 or more observations:

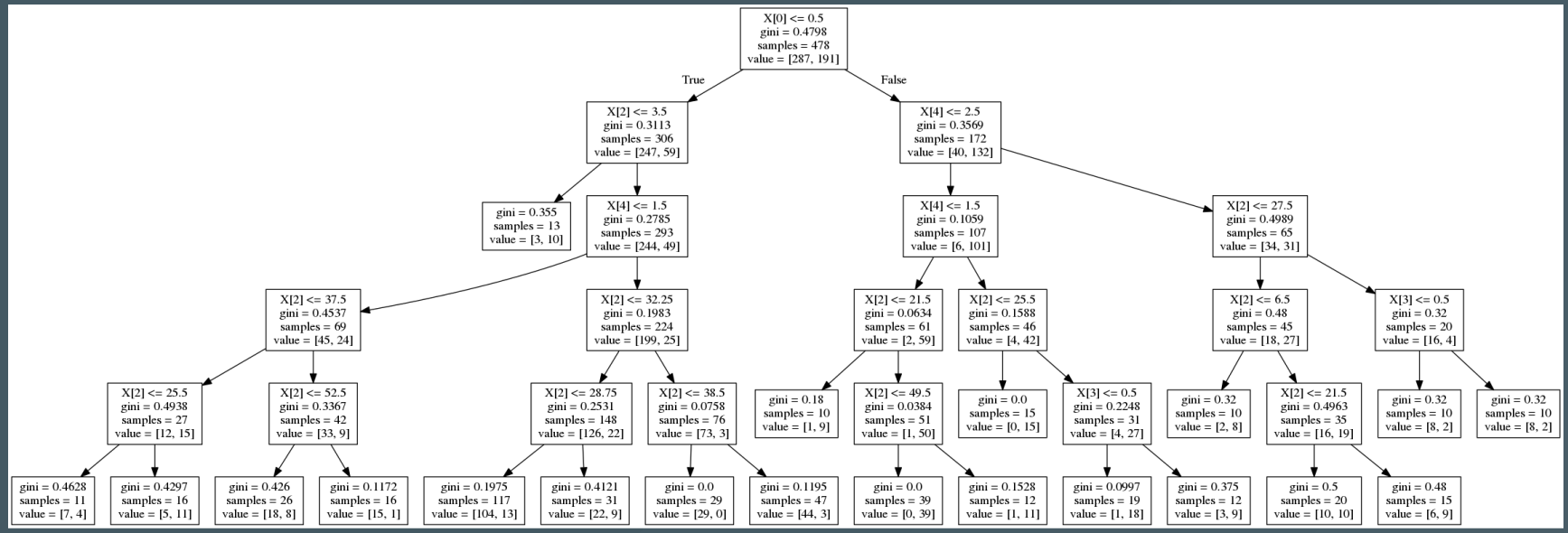
```
model = DecisionTreeClassifier(max_depth=5,
        min_samples_leaf=10)
```

In-sample accuracy: 84.52%

Out-of-sample accuracy: 78.39%

Again, we simplify and do **better** out of sample!

The Tree



It's small on the slide, but it is now a reasonably readable algorithm. At most, you have to ask 5 questions to arrive at an answer.

Overfitting

Overfitting is when we allow our model to overemphasize the random variation between observations in our sample. This practice will lead to higher in-sample accuracy (frequently 100% accuracy), but reduce our accuracy out of sample.

In Lab Today

Using the student data from our logit lab, located in `passFailTrain.csv`, work with your group to construct a Decision Tree to accurately predict which students will receive a passing grade. Use the entire file as training data, and then use `passFailTest.csv` to check your accuracy out-of-sample.

- How deep is your ideal tree?
- How many samples should each leaf contain?
- How accurate can you make your model out-of-sample?