Cycle Data Evaluating a classification model

Declaration: The central idea and coding is abstract from Kevin mark ham youtube video seriese, Introduction to machine learning with scikit-learn video series. You can find link under resources section.

What are the features?

- trip_id: A unique number to identify each trip
- From station Number: From station number where the trip Start
- Day: Day of the trip for example Monday, Tuesday etc.
- Month: Which month trip took place
- Duration: Total trip duration in minutes
- · birthyear: Birth year of user
- · Sex: Gender identification of user
- · age: Current age of user

What is the response?

• Station Number: To Station Number where the trip ends

Question: Can we predict the End station of a bicycle trip by given trip dataset?

Purpose of model evaluation

- Need a way to choose between models: different model types, tuning parameters, and features
- Use a model evaluation procedure to estimate how well a model will generalize to out-ofsample data
- Requires a model evaluation metric to quantify the model performance

Model evaluation procedures

- 1. Training and testing on the same data
 - Rewards overly complex models that "overfit" the training data and won't necessarily generalize

2. Train/test split

- Split the dataset into two pieces, so that the model can be trained and tested on different data
- Better estimate of out-of-sample performance, but still a "high variance" estimate
- · Useful due to its speed, simplicity, and flexibility

3. K-fold cross-validation

Svetamatically create "K" train/test enlits and average the results together

- Systematically create is traininest splits and average the results together
- Even better estimate of out-of-sample performance
- Runs "K" times slower than train/test split

Model evaluation metrics

- Regression problems: Mean Absolute Error, Mean Squared Error, Root Mean Squared Error
- Classification problems: Classification accuracy

Classification accuracy

Libraries used

```
In [2]:
```

```
import os,csv,io,mapsplotlib,time,folium,googlemaps,geopy,zipfile,requests,
warnings
import numpy as np
import pandas as pd
import datetime as dt
import seaborn as sns
import geopandas as gpd
from shapely.geometry import Point
import statsmodels.formula.api as smf
import matplotlib.pyplot as plt
import mysql.connector as sql
from sklearn.linear model import LinearRegression
model = LinearRegression()
from sklearn import metrics
from sklearn.cross validation import train test split
import numpy as np
warnings.simplefilter('ignore')
C:\Users\mrferozi\Anaconda\lib\site-
packages\sklearn\cross validation.py:44: DeprecationWarning: This module wa
s deprecated in version 0.18 in favor of the model selection module into wh
ich all the refactored classes and functions are moved. Also note that the
interface of the new CV iterators are different from that of this module. T
his module will be removed in 0.20.
  "This module will be removed in 0.20.", DeprecationWarning)
```

In [3]:

```
# display plots in the notebook %matplotlib inline
```

In [4]:

```
#where from_station_id_num in(22,31,15,1,25,14,16,37,4,9) or to_station_id
_num in(6,7,9,25,30,34,35,36,37,38,39,42)
#
#importing data from database
db_connection = sql.connect(host='localhost', database='bike', user='root',
password='none')
```

Out[4]:

	trip_id	Duration	from_station_id_num	to_station_id_num	to_station_id	Day	Month
10420	255018	8.0	17	37	SLU-07	6	8
10421	255026	11.0	20	36	SLU-04	6	8
10422	255030	5.0	19	37	SLU-07	6	8
10423	255036	6.0	13	37	SLU-07	6	8
10424	255085	11.0	7	37	SLU-07	6	8
4							·····•

In [5]:

```
# create the 'label' dummy variable using the 'map' method
df['label'] = df.to_station_id.map({'SLU-07':1, 'SLU-04':0})
```

In [6]:

```
df.tail()
```

Out[6]:

	trip_id	Duration	from_station_id_num	to_station_id_num	to_station_id	Day	Month		
10420	255018	8.0	17	37	SLU-07	6	8		
10421	255026	11.0	20	36	SLU-04	6	8		
10422	255030	5.0	19	37	SLU-07	6	8		
10423	255036	6.0	13	37	SLU-07	6	8		
10424	255085	11.0	7	37	SLU-07	6	8		

What is the response?

Station Number: To Station Number where the trip ends

Question: Can we predict the End station of a bicycle trip by given trip dataset?

In [7]:

```
# define X and y
feature_cols = ['trip_id','Duration','from_station_id_num','Day','Month','A
```

```
ge','Gender','Hours']
X = df[feature cols]
y = df.label
In [8]:
# train/test split
from sklearn.cross validation import train test split
X_train, X_test, y_train, y test = train test split(X, y, random state=1)
In [9]:
# train a logistic regression model on the training set
from sklearn.linear model import LogisticRegression
logreg = LogisticRegression()
logreg.fit(X_train, y_train)
Out[9]:
LogisticRegression(C=1.0, class weight=None, dual=False,
fit intercept=True,
          intercept scaling=1, max iter=100, multi class='ovr', n jobs=1,
          penalty='12', random state=None, solver='liblinear', tol=0.0001,
          verbose=0, warm start=False)
In [10]:
# make class predictions for the testing set
y pred class = logreg.predict(X test)
y pred class
Out[10]:
array([1, 0, 1, ..., 0, 0, 1], dtype=int64)
Classification accuracy: percentage of correct predictions
In [11]:
# calculate accuracy
from sklearn import metrics
a =metrics.accuracy_score(y_test, y_pred_class)
print(metrics.accuracy score(y test, y pred class))
0.621787495205
Null accuracy: accuracy that could be achieved by always predicting the most frequent class
In [12]:
# examine the class distribution of the testing set (using a Pandas Series
method)
y test.value counts()
Out[12]:
    1343
     1264
Name: label, dtype: int64
In [13]:
```

```
# calculate the percentage of ones
y_test.mean()

Out[13]:
0.515151515151515151

In [14]:

# calculate the percentage of zeros
1 - y_test.mean()

Out[14]:
0.48484848484848486

In [15]:

# calculate null accuracy (for multi-class classification problems)
y_test.value_counts().head(1) / len(y_test)*100

Out[15]:
1 51.515152
Name: label, dtype: float64
```

Comparing the true and predicted response values

```
In [16]:
```

Classification accuracy: percentage of correct predictions

```
In [17]:
```

```
# calculate accuracy
from sklearn import metrics
a =metrics.accuracy_score(y_test, y_pred_class)
print((metrics.accuracy_score(y_test, y_pred_class))*100)
```

62.1787495205

Classification accuracy or percentage of correct predictions is **62.17** Percent is bad.

Conclusion:

- · Classification accuracy is the easiest classification metric to understand
- But, it does not tell you the **underlying distribution** of response values
- And, it does not tell you what "types" of errors your classifier is making

Confusion matrix

Table that describes the performance of a classification model

```
In [18]:
```

```
# IMPORTANT: first argument is true values, second argument is predicted va
lues
print(metrics.confusion_matrix(y_test, y_pred_class))
[[887 377]
  [609 734]]
```

The bottom right is called the true positive. It is indicate that 734 cases the classifier identified correctly predicted the to_station number (end station). Upper left is called true negative in 887 cases the classifier correctly predicted. The upper right is called false positive indicate the 377 cases the classifier incorrectly predicted when in-fact they do not. The bottom left is called the false negative which indicated from the 609 cases the classifier predicted incorrectly.

Basic terminology

- True Positives (TP): we *correctly* predicted that they *do* fall between End station (To station)
- True Negatives (TN): we *correctly* predicted that they *don't* fall between End station (To_station)
- False Positives (FP): we *incorrectly* predicted that they *do* fall between End station (To_station) (a "Type I error")
- False Negatives (FN): we *incorrectly* predicted that they *don't* have fall between End station (To_station) (a "Type II error")

```
In [19]:
```

```
In [21]:
```

Where 1 represent positive and 0 present negative.

```
In [22]:
```

#Where 1 represent positive and 0 present negative.

```
TP = confusion[1, 1]
TN = confusion[0, 0]
FP = confusion[0, 1]
FN = confusion[1, 0]
```

Metrics computed from a confusion matrix

Classification Accuracy: Overall, how often is the classifier correct?

```
In [23]:
```

```
print (((TP + TN) / float(TP + TN + FP + FN))*100,' ','Percent')
print ((metrics.accuracy_score(y_test, y_pred_class))*100,' ','Percent')
62.1787495205    Percent
62.1787495205    Percent
```

Classification Error: Overall, how often is the classifier incorrect?

Also known as "Misclassification Rate"

In [24]:

```
print (((FP + FN) / float(TP + TN + FP + FN))*100,' ','Percent')
print ((1 - metrics.accuracy_score(y_test, y_pred_class))*100,' ','Percent')
37.8212504795    Percent
37.8212504795    Percent
```

Sensitivity: When the actual value is positive, how often is the prediction correct?

- How "sensitive" is the classifier to detecting positive instances?
- Also known as "True Positive Rate" or "Recall"

In [25]:

```
Sensitivity = ((TP / float(TP + FN))*100)
print ((TP / float(TP + FN))*100,' ','Percent')
```

54.6537602383 Percent

Specificity: When the actual value is negative, how often is the prediction correct?

How "specific" (or "selective") is the classifier in predicting positive instances?

In [26]:

```
specificity=((TN / float(TN + FP))*100)
print((TN / float(TN + FP))*100,' ','Percent')
```

70.1740506329 Percent

Precision: When a positive value is predicted, how often is the prediction correct?

• How "precise" is the classifier when predicting positive instances?

```
In [27]:
print((TP / float(TP + FP))*100,' ','Percent')
66.066606607 Percent
```

Conclusion:

- Confusion matrix gives us a more complete picture of how our classifier is performing
- Also allows us to compute various classification metrics, and these metrics can guide model model selection

Adjusting the classification threshold

```
In [28]:
# print the first 10 predicted responses
logreg.predict(X test)[0:10]
Out[28]:
array([1, 0, 1, 1, 0, 0, 0, 1, 1, 0], dtype=int64)
In [29]:
# print the first 10 predicted probabilities of class membership
logreg.predict proba(X test)[0:10, :]
Out [29]:
array([[ 0.41726387, 0.58273613],
      [ 0.52979737, 0.47020263],
       [ 0.44199653, 0.55800347],
       [ 0.46377986, 0.53622014],
      [ 0.99563954, 0.00436046],
      [ 0.63714538, 0.36285462],
      [ 0.66322039, 0.33677961],
      [ 0.1904182 , 0.8095818 ],
      [ 0.483926 , 0.516074 ],
       [ 0.62262909, 0.37737091]])
In [30]:
# print the first 10 predicted probabilities for class 1
logreg.predict proba(X test)[0:10, 1]
Out[30]:
array([ 0.58273613, 0.47020263, 0.55800347, 0.53622014, 0.00436046,
        0.36285462, 0.33677961, 0.8095818, 0.516074, 0.37737091])
In [31]:
# store the predicted probabilities for class 1
y pred prob = logreg.predict proba(X test)[:, 1]
In [32]:
# allow plots to appear in the notebook
```

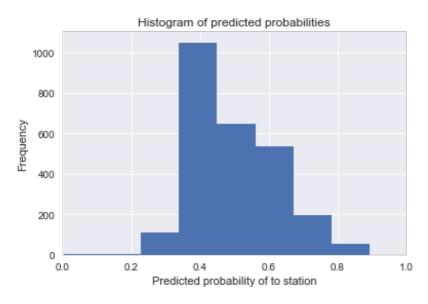
```
%matplotlib inline
import matplotlib.pyplot as plt
plt.rcParams['font.size'] = 14
```

In [33]:

```
# histogram of predicted probabilities
plt.hist(y_pred_prob, bins=8)
plt.xlim(0, 1)
plt.title('Histogram of predicted probabilities')
plt.xlabel('Predicted probability of to station')
plt.ylabel('Frequency')
```

Out[33]:

<matplotlib.text.Text at 0x227ed276ef0>



Histogram show us the distribution of numerical variable we can see the height of the third bar for example 1100 percent of the observations had values between 0.3 and 0.4 given the 0.5 classification threshold as above mention we can see from the histogram the end station 37 is rarely predicted. Since only the small minority of the testing set observation had a predicted probability above the threshold. For better specificity and sensitivity, we will adjust the threshold from 0.5 to 0.3.

Decrease the threshold for predicting to station in order to increase the sensitivity of the classifier

In [34]:

```
# predict to station if the predicted probability is greater than 0.3
from sklearn.preprocessing import binarize
y_pred_class = binarize([y_pred_prob], 0.4)[0]
```

In [35]:

```
# print the first 10 predicted probabilities
y_pred_prob[0:10]
```

Out[35]:

```
array([ 0.58273613,  0.47020263,  0.55800347,  0.53622014,  0.00436046,  0.36285462,  0.33677961,  0.8095818,  0.516074,  0.37737091])
```

In [36]:

The bottom right is called the true positive. It is indicating that 1128 cases the classifier identified correctly predicted and which is 53.67 percent increased. The Upper left is called true negative is now 446 cases the classifier correctly predicted, and which is decrease 49.71 percent. The upper right is called false positive indicate the 818 cases the classifier incorrectly predicted the journey which is 117 percent increased. The bottom left is called the false negative which indicated from the 215 cases which is decreased by 65 percent.

Basic terminology

- **True Positives (TP):** we *correctly* predicted that they *do* fall between End station (To station)
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- False Positives (FP): we *incorrectly* predicted that they *do* fall between End station (To_station) (a "Type I error")
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Our main purpose of the exercise to increase the True positive which is increased by 53.67 and decrease the true negative which is decrease 49.71 percent. It is not the great result but this study decides to use Linear support vector for further classification model evaluation to obtain a better result and to find better model.

Sensitivity: When the actual value is positive, how often is the prediction correct?

```
In [39]:
print('Previouse Sensitivity', Sensitivity)
Previouse Sensitivity 54.6537602383
In [40]:
# sensitivity has increased (used to be 0.24)
```

```
Present_Sensitivity=((46 / float(46 + 16))*100)

print((46 / float(46 + 16))*100)

74.19354838709677

In [41]:

print ('sensitivity has increased:',Present_Sensitivity - Sensitivity,'Percent')

sensitivity has increased: 19.5397881488 Percent
```

Specificity: When the actual value is negative, how often is the prediction correct?

```
In [42]:

print('Previouse specificity','', specificity)

Previouse specificity 70.1740506329

In [43]:

# specificity has decreased (used to be 0.91)

Present_specificity=((80 / float(80 + 50))*100)

print((80 / float(80 + 50))*100)

61.53846153846154

In [44]:

print ('Specificity has decreased:', specificity - Present_specificity,'Percent')
```

Since the observation move from left column to right column that guarantee that number of false positive will increase and true negative will decreased which decreases the specificity.

Conclusion:

- Threshold of 0.5 is used by default (for binary problems) to convert predicted probabilities into class predictions
- Threshold can be **adjusted** to increase sensitivity or specificity
- Sensitivity and specificity have an inverse relationship

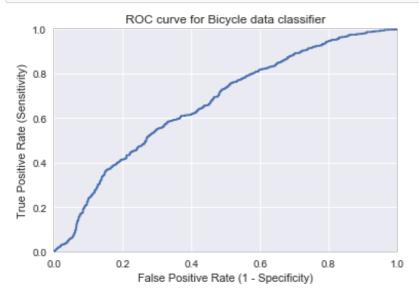
Specificity has decreased: 8.63558909445 Percent

ROC Curves and Area Under the Curve (AUC)

By, using ROC Curves and Area Under the Curve (AUC). We could see how sensitivity and specificity are affected by various thresholds, without actually changing the threshold

```
In [45]:
# IMPORTANT: first argument is true values, second argument is predicted pr
obabilities
fpr, tpr, thresholds = metrics.roc_curve(y_test, y_pred_prob)
plt.plot(fpr, tpr)
plt.xlim([0.0, 1.0])
```

```
plt.ylim([0.0, 1.0])
plt.title('ROC curve for Bicycle data classifier')
plt.xlabel('False Positive Rate (1 - Specificity)')
plt.ylabel('True Positive Rate (Sensitivity)')
plt.grid(True)
```



- ROC curve can help us to choose a threshold that balances sensitivity and specificity in a
 way that makes sense for your particular context
- We can't actually see the thresholds used to generate the curve on the ROC curve itself

In [46]:

```
# define a function that accepts a threshold and prints sensitivity and
specificity
def evaluate_threshold(threshold):
   print('Sensitivity:', tpr[thresholds > threshold][-1])
   print('Specificity:', 1 - fpr[thresholds > threshold][-1])
```

In [47]:

```
evaluate_threshold(0.5)
```

Sensitivity: 0.546537602383 Specificity: 0.701740506329

In [48]:

```
evaluate_threshold(0.3)
```

Sensitivity: 0.997021593448 Specificity: 0.0110759493671

AUC is the **percentage** of the ROC plot that is **underneath the curve**:

In [49]:

```
# IMPORTANT: first argument is true values, second argument is predicted pr
obabilities
print(metrics.roc_auc_score(y_test, y_pred_prob))
```

0.665956035515

- AUC is useful as a **single number summary** of classifier performance.
- If we randomly chose one positive and one negative observation, AUC represents the likelihood that our classifier will assign a higher predicted probability to the positive observation
- AUC is useful even when there is high class imbalance (unlike classification accuracy).

```
In [50]:
```

```
# calculate cross-validated AUC
from sklearn.cross_validation import cross_val_score
cross_val_score(logreg, X, y, cv=10, scoring='roc_auc').mean()
```

Out[50]:

0.65329949441385016

Confusion matrix advantages:

- Allows us to calculate a variety of metrics
- Useful for multi-class problems (more than two response classes)

ROC/AUC advantages:

- Does not require us to set a classification threshold
- Still useful when there is high class imbalance

Resources

References: From the video series: Introduction to machine learning with scikit-learn

- scikit-learn documentation: Cross-validation, Model evaluation
- scikit-learn issue on GitHub: MSE is negative when returned by cross val score
- Section 5.1 of <u>An Introduction to Statistical Learning</u> (11 pages) and related videos: <u>K-fold</u>
 and leave-one-out cross-validation (14 minutes), <u>Cross-validation the right and wrong ways</u>
 (10 minutes)
- Scott Fortmann-Roe: <u>Accurately Measuring Model Prediction Error</u>
- Machine Learning Mastery: <u>An Introduction to Feature Selection</u>
- Harvard CS109: Cross-Validation: The Right and Wrong Way
- Journal of Cheminformatics: <u>Cross-validation pitfalls when selecting and assessing</u> regression and classification models