Train / Test Predictive Analytics

This section introduces the predictive analytics technique of splitting data into random subsets for **training and testing** a predictive model. In order to perform unbiased assessment of the classification model. This is illustrated for ROC analysis where the sensitivities and specificities of the training model are estimated from the held out testing data.

Training/Testing for unbiased sensitivity/specificity analysis

Thus far, we have considered examples in which the sensitivy, specificity and ROC curves are calculated on the same data as used for model development. In other words, they are applied to the same data as used for training. This tends to produce optimistic estimates of the error probabilities and adjustment is needed. The situation is analogous to the degree of freedom adjustments in computing the error variance in linear regression.

A general approach to this problem is to randomly subdivide the available data into two subsets:

- **Training data:** These data will be used for model building only and not for predictive assessment.
- **Test data:** These data will not be used for model building; they will only be used for predictive assessment.

This general approach requires that we have enough data that the subsets are large enough to provide adequate power. The general approach will be applied to logistic regression classification here, and applied later to other predictive analytics approaches.

Python libraries:

```
statsmodels.api, statsmodels.formula.api, scikit-learn
```

If you need to install these on your computer enter the following commands from a terminal or anaconda window:

```
conda install scikit-learn
conda install -c conda-forge statsmodels
```

Example: binary response data split into train and test subsets

To illustrate the methods in a known context, we generate binary data from a logistic regression model. We import the functions needed to generate the simulated data.

In [1]:

```
import numpy as np
import pandas as pd
from scipy.stats import bernoulli, norm
```

In [2]:
```
# set the coefficient values
b0, b1 = -0.7, 2.1
#
# set sample size
n = 400
#
# generate exogenous variable
X = norm.rvs(size=n, random_state=1)
odds = np.exp(b0 + b1*X)   # odds depend on x
#
# convert odds to probabilities and generate response y
y = bernoulli.rvs(p=odds/(1+odds), size=n, random_state=12347)
dat = pd.DataFrame({'X':X, 'y':y})
dat.head(10)
```

Out[2]:

	X	y
0	1.624345	1
1	-0.611756	0
2	-0.528172	0
3	-1.072969	0
4	0.865408	1
5	-2.301539	0
6	1.744812	1
7	-0.761207	0
8	0.319039	0
9	-0.249370	0

Random split into train and test sets

Next we split the data into train and test data sets for modeling and evaluation. To do this we import several modules from sklearn.

In [3]:
```
from sklearn.datasets import make_classification
from sklearn.model_selection import train_test_split
from sklearn.metrics import roc_curve
from sklearn.metrics import roc_auc_score
```

Here we specify that the training data should be 80% of the data, with 20% held out as testing data.

In [4]:
```
dat_train, dat_test = \
train_test_split(dat, test_size=0.20, random_state=123457)
```

Compare the shapes of the original, training and testing data frames:

In [5]:
```
dat.shape, dat_train.shape, dat_test.shape
```

Out[5]:
```
((400, 2), (320, 2), (80, 2))
```

Here are the first few rows of the training data. Note that the data splitting is random, not systematic, so as to avoid any biases.

In [6]:
```
dat_train.head()
```

Out[6]:

	X	y
303	-0.880578	0
273	0.884909	1
119	0.408901	1
60	-0.754398	0
121	-0.775162	0

Train the model

In this simple setting, training the model simply means fitting the logistic regression model to **training data** only.

In [7]:
```
import statsmodels.api as sm
import statsmodels.formula.api as smf
```

In [8]:
```python
mod_train = smf.logit('y ~ X', data=dat_train).fit()
mod_train.summary()
```

```
Optimization terminated successfully.
         Current function value: 0.417736
         Iterations 7
```

Out[8]:

Logit Regression Results

Dep. Variable:	y	**No. Observations:**	320
Model:	Logit	**Df Residuals:**	318
Method:	MLE	**Df Model:**	1
Date:	Wed, 15 Apr 2020	**Pseudo R-squ.:**	0.3793
Time:	11:28:39	**Log-Likelihood:**	-133.68
converged:	True	**LL-Null:**	-215.36
		LLR p-value:	2.070e-37

	coef	std err	z	P>|z|	[0.025	0.975]
Intercept	-0.8534	0.167	-5.121	0.000	-1.180	-0.527
X	2.4172	0.273	8.840	0.000	1.881	2.953

Test the model

To evaluate the accuracy of the model as a classifier, we use the **training data model** to compute predictive probabilities for the **test data**. Then we will compare the thresholded classifications based on test data X variable only, to the actual responses y in the test data. Here are the first 10 predictive probabilities.

In [9]:
```python
phat = mod_train.predict(exog=dict(X=dat_test['X']))
phat.head(10)
```

Out[9]:
```
323    0.054672
222    0.948561
11     0.002920
346    0.220987
223    0.356884
139    0.322830
376    0.986799
12     0.163461
55     0.637519
171    0.790127
dtype: float64
```

To help visualize training versus testing, we plot the actual responses y in the test set versus their predicted or estimated probabiliites based on the training model and their correpsonding X values.

In [10]:
```python
import matplotlib.pyplot as plt
import seaborn as sns
sns.set()
```

In [11]:
```python
thresh = 0.5
sns.scatterplot(x=phat, y=dat_test['y'], hue=1*(phat > thresh))
plt.legend(loc='center right')
plt.xlabel('phat')
plt.vlines(x=thresh, ymin=0, ymax=1)
plt.title('Actual y_test versus phat_train(X_test)')
plt
plt.show()
```

Function to compute sensitivity and specificity for a given threshold.

In [12]:
```python
from sklearn.metrics import confusion_matrix, roc_curve, roc_auc_score
```

In [13]:
```python
def senspec(y, score, thresh):
    yhat = 1*(score >= thresh)
    tn, fp, fn, tp = confusion_matrix(y_true=y, y_pred=yhat).ravel()
    sens = tp / (fn + tp)
    spec = tn / (fp + tn)
    return pd.DataFrame({'tn':[tn],
                         'fp':[fp],
                         'fn':[fn],
                         'tp':[tp],
                         'sens':[sens],
                         'spec':[spec]})
```

Test results based on current threshold:

In [14]:
```
senspec(dat_test['y'], phat, thresh)
```

Out[14]:

	tn	fp	fn	tp	sens	spec
0	38	5	12	25	0.675676	0.883721

Comparison with naive training data results

In [15]:
```
senspec(dat_train['y'], mod_train.fittedvalues, thresh)
```

Out[15]:

	tn	fp	fn	tp	sens	spec
0	175	17	46	82	0.640625	0.911458

Test results with different threshold:

In [16]:
```
senspec(dat_test['y'], phat, 0.33)
```

Out[16]:

	tn	fp	fn	tp	sens	spec
0	36	7	5	32	0.864865	0.837209

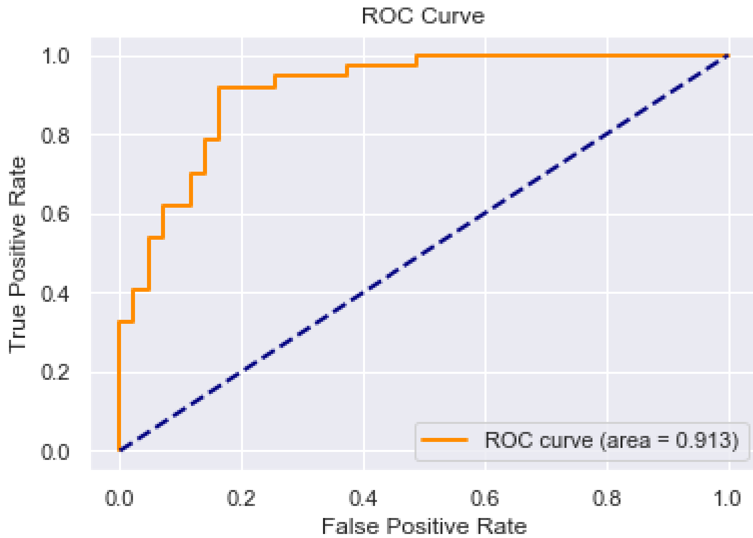
In this example using 0.33 gives considerably higher sensitivity at a small cost in specificity.

ROC curve for test data

In [17]:
```
fpr, tpr, score = roc_curve(y_true=dat_test['y'], y_score=phat)
auc = roc_auc_score(y_true=dat_test['y'], y_score=phat)
```

In [18]:
```
def plot_roc(fpr, tpr, auc, lw=2):
    plt.plot(fpr, tpr, color='darkorange', lw=lw,
             label='ROC curve (area = '+str(round(auc,3))+')')
    plt.plot([0, 1], [0, 1], color='navy', lw=lw, linestyle='--')
    plt.xlabel('False Positive Rate')
    plt.ylabel('True Positive Rate')
    plt.title('ROC Curve')
    plt.legend(loc="lower right")
    plt.show()
```

In [19]:
```
plot_roc(fpr, tpr, auc)
```



The AUC performance (0.913) is high. If we were to select a threshold minimizing distance to tehupper left corner, the ROC curve suggests that it may be possible to achieve a sensitivity (= true positive rate) of around 0.92 and specifity (= 1 - false positive rate) of around 0.84.

In [20]:
```
senspec(dat_test['y'], phat, 0.30)
```

Out[20]:

	tn	fp	fn	tp	sens	spec
0	36	7	3	34	0.918919	0.837209

Example: Train/Test ROC analysis for Pew Research Data

Preprocessing:

In [21]:
```
import zipfile as zp
```

In [22]:
```
zf = zp.ZipFile('../data/Feb17-public.zip')
missing_values = ["NaN", "nan", "Don't know/Refused (VOL.)"]
df = pd.read_csv(zf.open('Feb17public.csv'),
                 na_values=missing_values)[['age', 'sex', \
                                            'q52', 'party']]
```

In [23]:
```
# reduce q52 responses to two categories and
# create binary reponse variable
df['q52'][df['q52']!='Favor'] = 'Not_favor'
df['y'] = df['q52'].map({'Not_favor':0,'Favor':1})
#
# use cleaned data without records that have missing values
dfclean = df.dropna()
dfclean.head()
```

Out[23]:

	age	sex	q52	party	y
0	80.0	Female	Not_favor	Independent	0
1	70.0	Female	Not_favor	Democrat	0
2	69.0	Female	Not_favor	Independent	0
3	50.0	Male	Favor	Republican	1
4	70.0	Female	Not_favor	Democrat	0

1. Split the data into train and test data sets.

In [24]:
```
df_train, df_test = train_test_split(dfclean,
                                     test_size=0.20,
                                     random_state=1)
```

In [25]:
```
display("Training data", df_train.shape, df_train.head(),\
        "Testing data", df_test.shape, df_test.head())
```

```
'Training data'
```

```
(1172, 5)
```

	age	sex	q52	party	y
49	86.0	Male	Favor	Independent	1
1075	69.0	Female	Not_favor	Democrat	0
102	63.0	Male	Favor	Republican	1
1296	19.0	Male	Not_favor	Independent	0
338	60.0	Male	Not_favor	Democrat	0

```
'Testing data'
```

```
(293, 5)
```

	age	sex	q52	party	y
1032	50.0	Male	Not_favor	Democrat	0
671	40.0	Female	Not_favor	Republican	0
639	27.0	Male	Not_favor	Independent	0
943	43.0	Male	Not_favor	Independent	0
882	20.0	Male	Favor	No preference (VOL.)	1

2. Fit the model to training data only.

In [26]:
```
pewmod = smf.logit('y ~ party + age + sex',\
    data=df_train).fit()
pewmod.summary()
```

```
Optimization terminated successfully.
         Current function value: 0.454704
         Iterations 7
```

Out[26]:

Logit Regression Results

Dep. Variable:	y	**No. Observations:**	1172
Model:	Logit	**Df Residuals:**	1165
Method:	MLE	**Df Model:**	6
Date:	Wed, 15 Apr 2020	**Pseudo R-squ.:**	0.2818
Time:	11:28:41	**Log-Likelihood:**	-532.91
converged:	True	**LL-Null:**	-742.00
		LLR p-value:	3.438e-87

	coef	std err	z	P>|z|	[0.025	0.975]
Intercept	-3.7460	0.324	-11.564	0.000	-4.381	-3.111
party[T.Independent]	1.8242	0.223	8.173	0.000	1.387	2.262
party[T.No preference (VOL.)]	1.8553	0.415	4.475	0.000	1.043	2.668
party[T.Other party (VOL.)]	2.1395	1.249	1.713	0.087	-0.308	4.587
party[T.Republican]	3.7061	0.239	15.537	0.000	3.239	4.174
sex[T.Male]	0.4678	0.155	3.015	0.003	0.164	0.772
age	0.0170	0.004	3.860	0.000	0.008	0.026

3. Get the predictive probabilities for the test data.

The predict function uses the fitted model to extract any exogenous variables it needs from the test data. We do not have to specify which variables. We just provide the whole test data frame. Compare the following two code cells and results.

In [27]:
```
# predictive probabilities - explicit method
phat_test = pewmod.predict(exog=df_test[['age', 'sex', 'party']])
phat_test.head(10)
```

Out[27]:
```
1032    0.080907
671     0.654430
639     0.269731
943     0.326381
882     0.252808
1228    0.079654
1179    0.288219
591     0.077712
550     0.413034
443     0.654430
dtype: float64
```

In [28]:
```
# predictive probabilities - implicit method
phat_test = pewmod.predict(exog=df_test)
phat_test.head(10)
```

Out[28]:
```
1032    0.080907
671     0.654430
639     0.269731
943     0.326381
882     0.252808
1228    0.079654
1179    0.288219
591     0.077712
550     0.413034
443     0.654430
dtype: float64
```

4a. Evaluation: Test data sensitivity and specificity

In [29]:
```
# Using a probability threshold of 0.5
senspec(df_test['y'], phat_test, 0.5)
```

Out[29]:

	tn	fp	fn	tp	sens	spec
0	162	16	50	65	0.565217	0.910112

In [30]:
```
# Using a probability threshold of 0.33
senspec(df_test['y'], phat_test, 0.3)
```

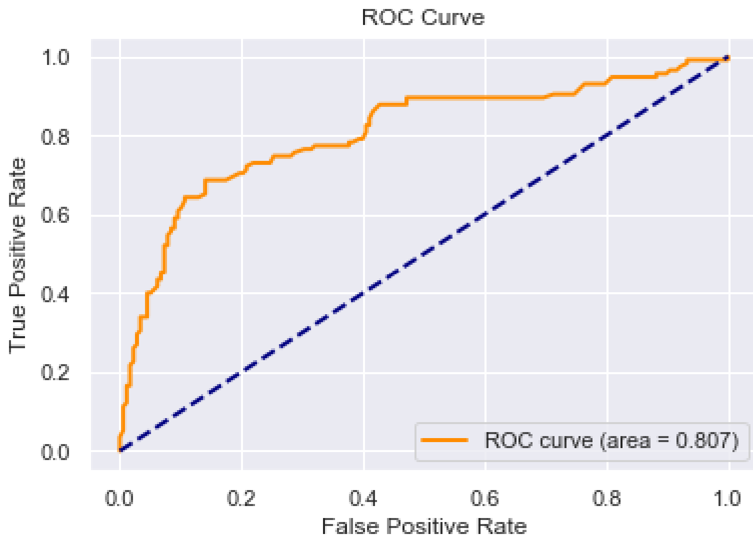
Out[30]:

	tn	fp	fn	tp	sens	spec
0	128	50	29	86	0.747826	0.719101

4b. Evaluation: Test data ROC curve

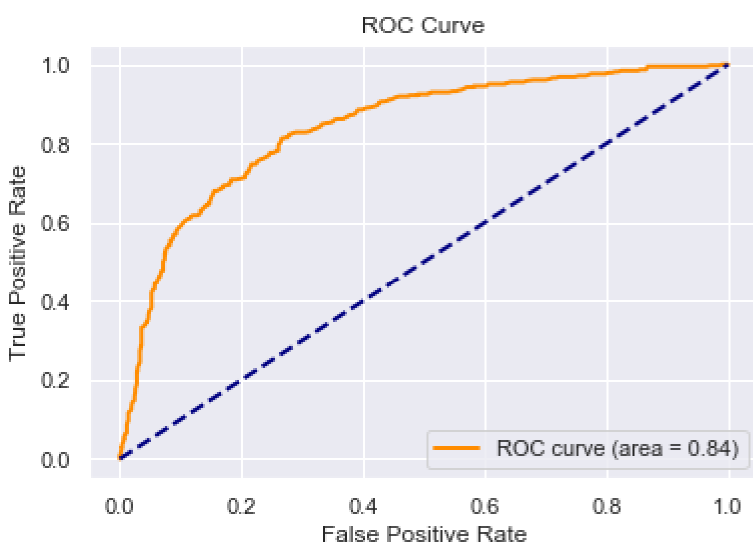
In [31]:
```
fpr_pew, tpr_pew, score_pew = roc_curve(y_true=df_test['y'], y_score=phat_test
)
auc_pew = roc_auc_score(y_true=df_test['y'], y_score=phat_test)
```

In [32]:
```
plot_roc(fpr_pew, tpr_pew, auc_pew)
```



For comparison, here is the naive ROC curve for the training data

In [33]:
```
fpr_pew0, tpr_pew0, score_pew0 = roc_curve(y_true=df_train['y'], y_score=pewmo
d.fittedvalues)
auc_pew0 = roc_auc_score(y_true=df_train['y'], y_score=pewmod.fittedvalues)
plot_roc(fpr_pew0, tpr_pew0, auc_pew0)
```



In this example the training data AUC = 0.84, which is optimistic compared with unbiased test data AUC of 0.81.