Techniques for Feature Selection and Parameter Optimization

In [1]:
```
%pylab inline
```

```
Populating the interactive namespace from numpy and matplotlib
```

In [2]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
```

Import titanic data using pandas

Modified version of the "Titanic" data can be found at: http://facweb.cs.depaul.edu/mobasher/classes/csc478/Data/titanic-trimmed.csv (http://facweb.cs.depaul.edu/mobasher/classes/csc478/Data/titanic-trimmed.csv). Original unmodified Titanic data is available at CMU StatLib (http://lib.stat.cmu.edu/S/Harrell/data/ascii/titanic.txt).

In [3]:
```
url = "http://facweb.cs.depaul.edu/mobasher/classes/csc478/Data/titanic-trim
titanic = pd.read_csv(url)
titanic.head(10)
```

Out[3]:

	pid	pclass	survived	sex	age	sibsp	parch	fare	embarked
0	1	1st	1	female	29.0	0	0	211.337494	Southampton
1	2	1st	1	male	NaN	1	2	151.550003	Southampton
2	3	1st	0	female	2.0	1	2	151.550003	Southampton
3	4	1st	0	male	30.0	1	2	151.550003	Southampton
4	5	1st	0	female	25.0	1	2	151.550003	Southampton
5	6	1st	1	male	48.0	0	0	26.549999	Southampton
6	7	1st	1	female	63.0	1	0	77.958298	Southampton
7	8	1st	0	male	39.0	0	0	0.000000	Southampton
8	9	1st	1	female	53.0	2	0	51.479198	Southampton
9	10	1st	0	male	71.0	0	0	49.504200	Cherbourg

In [4]:
```
titanic.describe(include="all")
```

Out[4]:

	pid	pclass	survived	sex	age	sibsp	parch	
count	1309.000000	1309	1309.000000	1309	1045.000000	1309.000000	1309.000000	1308
unique	NaN	3	NaN	2	NaN	NaN	NaN	
top	NaN	3rd	NaN	male	NaN	NaN	NaN	
freq	NaN	709	NaN	843	NaN	NaN	NaN	
mean	655.000000	NaN	0.381971	NaN	29.908852	0.498854	0.385027	33
std	378.020061	NaN	0.486055	NaN	14.392485	1.041658	0.865560	51
min	1.000000	NaN	0.000000	NaN	0.166700	0.000000	0.000000	0
25%	328.000000	NaN	0.000000	NaN	21.000000	0.000000	0.000000	7
50%	655.000000	NaN	0.000000	NaN	28.000000	0.000000	0.000000	14
75%	982.000000	NaN	1.000000	NaN	39.000000	1.000000	0.000000	31
max	1309.000000	NaN	1.000000	NaN	80.000000	8.000000	9.000000	512

Handling missing variables

In [5]:
```
titanic[titanic.age.isnull()].shape
```

Out[5]:
```
(264, 9)
```

In [6]:
```
age_mean = titanic.age.mean()
titanic.age.fillna(age_mean, axis=0, inplace=True)
titanic.dropna(axis=0, inplace=True)
```

In [7]:
```
titanic.shape
```

Out[7]:
```
(1306, 9)
```

In [8]:
```
titanic.set_index('pid', drop=True, inplace=True)
titanic.head()
```

Out[8]:

	pclass	survived	sex	age	sibsp	parch	fare	embarked
pid								
1	1st	1	female	29.000000	0	0	211.337494	Southampton
2	1st	1	male	29.908852	1	2	151.550003	Southampton
3	1st	0	female	2.000000	1	2	151.550003	Southampton
4	1st	0	male	30.000000	1	2	151.550003	Southampton
5	1st	0	female	25.000000	1	2	151.550003	Southampton

Creating dummy variables for categorical features

In [9]:

```
titanic_ssf = pd.get_dummies(titanic)
titanic_ssf.head(10)
```

Out[9]:

	survived	age	sibsp	parch	fare	pclass_1st	pclass_2nd	pclass_3rd	sex_f
pid									
1	1	29.000000	0	0	211.337494	1	0	0	
2	1	29.908852	1	2	151.550003	1	0	0	
3	0	2.000000	1	2	151.550003	1	0	0	
4	0	30.000000	1	2	151.550003	1	0	0	
5	0	25.000000	1	2	151.550003	1	0	0	
6	1	48.000000	0	0	26.549999	1	0	0	
7	1	63.000000	1	0	77.958298	1	0	0	
8	0	39.000000	0	0	0.000000	1	0	0	
9	1	53.000000	2	0	51.479198	1	0	0	
10	0	71.000000	0	0	49.504200	1	0	0	

In [10]:

```
titanic_names = titanic_ssf.columns.values
print(titanic_names)
```

```
['survived' 'age' 'sibsp' 'parch' 'fare' 'pclass_1st' 'pclass_2nd'
 'pclass_3rd' 'sex_female' 'sex_male' 'embarked_Cherbourg'
 'embarked_Queenstown' 'embarked_Southampton']
```

In [11]:

```
y = titanic_ssf['survived']
X = titanic_ssf[titanic_names[1:]]
X.head()
```

Out[11]:

	age	sibsp	parch	fare	pclass_1st	pclass_2nd	pclass_3rd	sex_female	se:
pid									
1	29.000000	0	0	211.337494	1	0	0	1	
2	29.908852	1	2	151.550003	1	0	0	0	
3	2.000000	1	2	151.550003	1	0	0	1	
4	30.000000	1	2	151.550003	1	0	0	0	
5	25.000000	1	2	151.550003	1	0	0	1	

In [12]:

```
titanic_ssf.describe().T
```

Out[12]:

	count	mean	std	min	25%	50%	75%	
survived	1306.0	0.381317	0.485896	0.0000	0.0000	0.000000	1.000	1
age	1306.0	29.854661	12.812320	0.1667	22.0000	29.908852	35.000	80
sibsp	1306.0	0.500000	1.042580	0.0000	0.0000	0.000000	1.000	8
parch	1306.0	0.385911	0.866357	0.0000	0.0000	0.000000	0.000	9
fare	1306.0	33.223956	51.765986	0.0000	7.8958	14.454200	31.275	512
pclass_1st	1306.0	0.245789	0.430719	0.0000	0.0000	0.000000	0.000	1
pclass_2nd	1306.0	0.212098	0.408950	0.0000	0.0000	0.000000	0.000	1
pclass_3rd	1306.0	0.542113	0.498414	0.0000	0.0000	1.000000	1.000	1
sex_female	1306.0	0.355283	0.478782	0.0000	0.0000	0.000000	1.000	1
sex_male	1306.0	0.644717	0.478782	0.0000	0.0000	1.000000	1.000	1
embarked_Cherbourg	1306.0	0.206738	0.405121	0.0000	0.0000	0.000000	0.000	1
embarked_Queenstown	1306.0	0.094181	0.292192	0.0000	0.0000	0.000000	0.000	1
embarked_Southampton	1306.0	0.699081	0.458833	0.0000	0.0000	1.000000	1.000	1

Build the training and testing dataset

In [13]:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, rar
```

In [14]:

```
# Now let's train the decision tree on the training data

from sklearn import tree
dt = tree.DecisionTreeClassifier(criterion='entropy')
dt = dt.fit(X_train, y_train)
```

A versatile function to measure performance of a calssification model

In [15]:

```
from sklearn import metrics

def measure_performance(X, y, clf, show_accuracy=True, show_classification_r
    y_pred = clf.predict(X)
    if show_accuracy:
         print("Accuracy:{0:.3f}".format(metrics.accuracy_score(y, y_pred)),
    if show_classification_report:
        print("Classification report")
        print(metrics.classification_report(y, y_pred),"\n")

    if show_confussion_matrix:
        print("Confussion matrix")
        print(metrics.confusion_matrix(y, y_pred),"\n")
```

In [16]:

```
from sklearn import metrics
measure_performance(X_test, y_test, dt, show_confussion_matrix=False)
```

```
Accuracy:0.744

Classification report
             precision    recall  f1-score   support

          0       0.79      0.80      0.79       161
          1       0.67      0.66      0.67       101

avg / total       0.74      0.74      0.74       262
```

Feature Selection

Select the top 30% of the most important features, using a chi2 test

In [17]:

```
from sklearn import feature_selection
```

In [18]:

```
fs = feature_selection.SelectPercentile(feature_selection.chi2, percentile=3
X_train_fs = fs.fit_transform(X_train, y_train)
```

In [19]:

```
np.set_printoptions(suppress=True, precision=2, linewidth=120)
print(list(X.columns))
print(fs.get_support())
print(fs.scores_)
```

```
['age', 'sibsp', 'parch', 'fare', 'pclass_1st', 'pclass_2nd', 'pclass_3rd'
[False False False  True  True False False  True  True False False False]
[  17.19    0.     22.34 5185.44   61.98    1.28   35.15  189.1   102.94
```

In [20]:
```
print(X.columns[fs.get_support()].values)
```

```
['fare' 'pclass_1st' 'sex_female' 'sex_male']
```

In [21]:
```
for i in range(len(X.columns.values)):
    if fs.get_support()[i]:
        print("%10s  %3.2f" % (X.columns.values[i], fs.scores_[i]))
```

```
      fare  5185.44
pclass_1st  61.98
sex_female  189.10
  sex_male  102.94
```

In [22]:
```
print(X_train_fs)
```

```
[[31.39  0.    0.    1.  ]
 [15.05  0.    0.    1.  ]
 [91.08  1.    0.    1.  ]
 ...
 [21.    0.    1.    0.  ]
 [31.5   0.    0.    1.  ]
 [ 7.9   0.    0.    1.  ]]
```

Evaluate performance with the new feature set on test data

In [23]:
```
dt = tree.DecisionTreeClassifier(criterion='entropy')
dt.fit(X_train_fs, y_train)
X_test_fs = fs.transform(X_test)
measure_performance(X_test_fs, y_test, dt, show_confussion_matrix=False)
```

```
Accuracy:0.821

Classification report
             precision    recall  f1-score   support

          0       0.86      0.84      0.85       161
          1       0.76      0.78      0.77       101

avg / total       0.82      0.82      0.82       262
```

To do feature selection more systematically, we need to find the best percentile using cross-validation

In [24]:

```
from sklearn.model_selection import cross_val_score
dt = tree.DecisionTreeClassifier(criterion='entropy')

percentiles = range(1, 100, 5)
results = []
for i in range(1, 100, 5):
    fs = feature_selection.SelectPercentile(feature_selection.chi2, percenti
    X_train_fs = fs.fit_transform(X_train, y_train)
    scores = cross_val_score(dt, X_train_fs, y_train, cv=5)
    print("%2d  %0.4f" % (i, scores.mean()))
    results = np.append(results, scores.mean())
```

```
 1  0.7012
 6  0.7012
11  0.7614
16  0.7614
21  0.7614
26  0.7614
31  0.7585
36  0.7585
41  0.7681
46  0.7643
51  0.7643
56  0.7605
61  0.7605
66  0.7529
71  0.7510
76  0.7509
81  0.7528
86  0.7529
91  0.7547
96  0.7519
```

In [25]:

```
optimal_percentile_ind = np.where(results == results.max())[0][0]
print(optimal_percentile_ind)
```

```
8
```

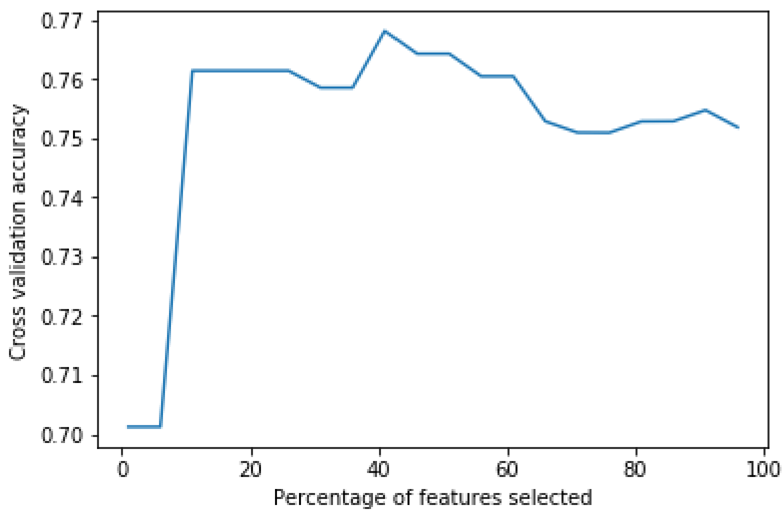
In [26]:

```
optimal_percentile_ind = np.where(results == results.max())[0][0]
print("Optimal percentile of features:{0}".format(percentiles[optimal_percer
optimal_num_features = int(percentiles[optimal_percentile_ind]*len(X.columns
print("Optimal number of features:{0}".format(optimal_num_features), "\n")

# Plot percentile of features VS. cross-validation scores
import pylab as pl
pl.figure()
pl.xlabel("Percentage of features selected")
pl.ylabel("Cross validation accuracy")
pl.plot(percentiles,results)
```

```
Optimal percentile of features:41

Optimal number of features:4
```

Out[26]:

```
[<matplotlib.lines.Line2D at 0x15bb88ccda0>]
```



Evaluate our best number of features on the test set

In [27]:
```
fs = feature_selection.SelectKBest(feature_selection.chi2, optimal_num_featu
X_train_fs = fs.fit_transform(X_train, y_train)
dt = tree.DecisionTreeClassifier(criterion='entropy')
dt.fit(X_train_fs, y_train)
X_test_fs = fs.transform(X_test)
measure_performance(X_test_fs, y_test, dt, show_confussion_matrix=False)
```

```
Accuracy:0.821

Classification report
             precision    recall  f1-score   support

          0       0.86      0.84      0.85       161
          1       0.76      0.78      0.77       101

avg / total       0.82      0.82      0.82       262
```

Model selection

Exploring and comparing model parameters

In [28]:
```
print(dt.get_params())
```

```
{'random_state': None, 'max_depth': None, 'splitter': 'best', 'max_leaf_nc
```

Let's first focus on "criterion' parameter and find the best one

In [29]:
```
dt = tree.DecisionTreeClassifier(criterion='entropy')
scores = cross_val_score(dt, X_train_fs, y_train, cv=5)
print("Entropy criterion accuracy on cv: {0:.3f}".format(scores.mean()))

dt = tree.DecisionTreeClassifier(criterion='gini')
scores = cross_val_score(dt, X_train_fs, y_train, cv=5)
print("Gini criterion accuracy on cv: {0:.3f}".format(scores.mean()))
```

```
Entropy criterion accuracy on cv: 0.759
Gini criterion accuracy on cv: 0.758
```

In [30]:

```
# Now we can fit the model to the full training data usign the optimal featu
# and apply the model to the set-aside test data
dt = tree.DecisionTreeClassifier(criterion='entropy')
dt.fit(X_train_fs, y_train)
X_test_fs = fs.transform(X_test)
measure_performance(X_test_fs, y_test, dt, show_confussion_matrix=False, sho
```

```
Accuracy:0.821

Classification report
             precision    recall  f1-score   support

          0       0.86      0.84      0.85       161
          1       0.76      0.78      0.77       101

avg / total       0.82      0.82      0.82       262
```

Another parameter of decision tree that can have an impact on accuracy is 'max-depth'

In [31]:

```
dt = tree.DecisionTreeClassifier(criterion='entropy')
dt.set_params(max_depth=5)

dt.fit(X_train, y_train)
measure_performance(X_test, y_test, dt, show_confussion_matrix=False, show_c
```

```
Accuracy:0.794
```

But, again, we need a more systematic way to explore the space of values for each parameter. The following is a general function that performs cross-validation using a range of values for a specified parameter of a model

In [32]:

```
from sklearn.model_selection import KFold

def calc_params(X, y, clf, param_values, param_name, K):

    # Convert input to Numpy arrays
    X = np.array(X)
    y = np.array(y)

    # initialize training and testing score arrays with zeros
    train_scores = np.zeros(len(param_values))
    test_scores = np.zeros(len(param_values))

    # iterate over the different parameter values
    for i, param_value in enumerate(param_values):
        print(param_name, ' = ', param_value)

        # set classifier parameters
        clf.set_params(**{param_name:param_value})

        # initialize the K scores obtained for each fold
        k_train_scores = np.zeros(K)
        k_test_scores = np.zeros(K)

        # create KFold cross validation
        cv = KFold(n_splits=K, shuffle=True, random_state=0)

        # iterate over the K folds
        j = 0
        for train, test in cv.split(X):
            # fit the classifier in the corresponding fold
            # and obtain the corresponding accuracy scores on train and test
            clf.fit(X[train], y[train])
            k_train_scores[j] = clf.score(X[train], y[train])
            k_test_scores[j] = clf.score(X[test], y[test])
            j += 1

        # store the mean of the K fold scores
        train_scores[i] = np.mean(k_train_scores)
        test_scores[i] = np.mean(k_test_scores)

    # plot the training and testing scores in a log scale
    plt.plot(param_values, train_scores, label='Train', alpha=0.4, lw=2, c='
    plt.plot(param_values, test_scores, label='X-Val', alpha=0.4, lw=2, c='g
    plt.legend(loc=7)
    plt.xlabel(param_name + " values")
    plt.ylabel("Mean cross validation accuracy")

    # return the training and testing scores on each parameter value
    return train_scores, test_scores
```

Now we can explore the impact of max-depth more systematically

In [33]:

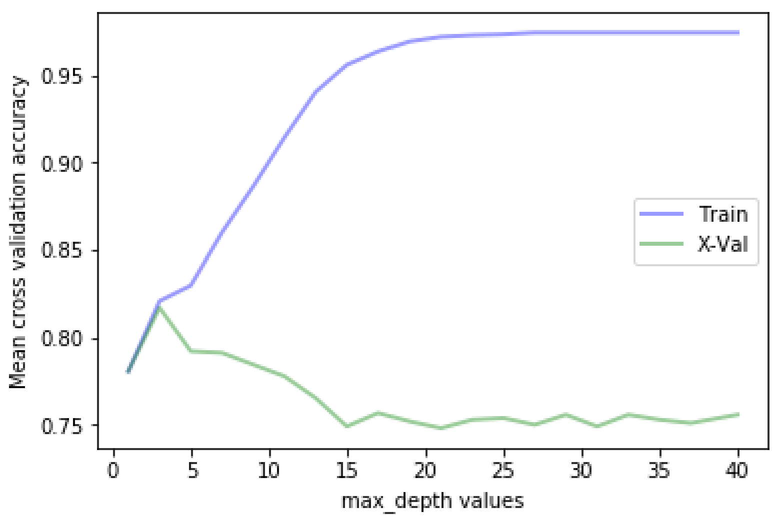
```
# Let's create an evenly spaced range of numbers in a specified interval
md = np.linspace(1, 40, 20)
md = np.array([int(e) for e in md])
print(md)
```

```
[ 1  3  5  7  9 11 13 15 17 19 21 23 25 27 29 31 33 35 37 40]
```

In [34]:

```
train_scores, test_scores = calc_params(X_train, y_train, dt, md, 'max_depth
```

```
max_depth  =  1
max_depth  =  3
max_depth  =  5
max_depth  =  7
max_depth  =  9
max_depth  =  11
max_depth  =  13
max_depth  =  15
max_depth  =  17
max_depth  =  19
max_depth  =  21
max_depth  =  23
max_depth  =  25
max_depth  =  27
max_depth  =  29
max_depth  =  31
max_depth  =  33
max_depth  =  35
max_depth  =  37
max_depth  =  40
```



max_depth = 3 seems to work best; larger values seem to lead to over-fitting.

In [35]:

```
dt = tree.DecisionTreeClassifier(criterion='entropy')
dt.set_params(max_depth=3)

dt.fit(X_train, y_train)
measure_performance(X_test, y_test, dt, show_confussion_matrix=False, show_c
```

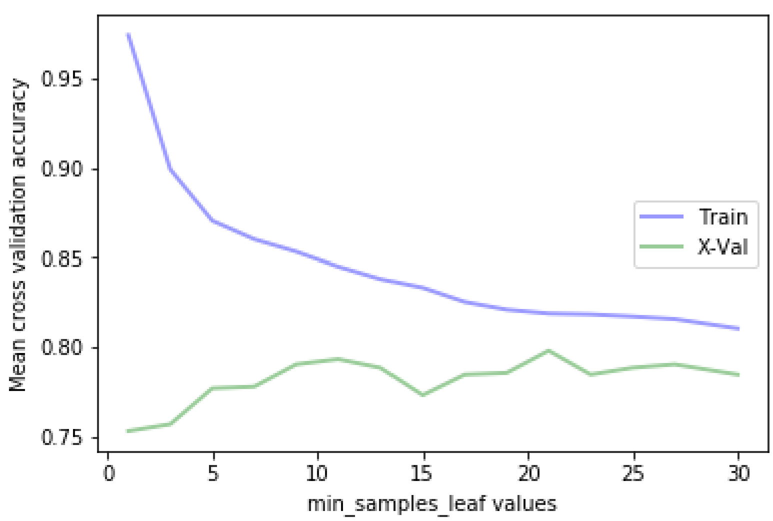
```
Accuracy:0.798
```

Another parameter of decision tree that's important is the min number of samples allowed at a leaf node

In [36]:

```
msl = np.linspace(1, 30, 15)
msl = np.array([int(e) for e in msl])

dt = tree.DecisionTreeClassifier(criterion='entropy')
train_scores, test_scores = calc_params(X_train, y_train, dt, msl, 'min_samp
```

```
min_samples_leaf  =  1
min_samples_leaf  =  3
min_samples_leaf  =  5
min_samples_leaf  =  7
min_samples_leaf  =  9
min_samples_leaf  =  11
min_samples_leaf  =  13
min_samples_leaf  =  15
min_samples_leaf  =  17
min_samples_leaf  =  19
min_samples_leaf  =  21
min_samples_leaf  =  23
min_samples_leaf  =  25
min_samples_leaf  =  27
min_samples_leaf  =  30
```



Looks like min_samples_leaf around 11 seems like a good choice. Let's now combine these optimal parameter values in our final model to fit the full training data.

In [37]:
```
dt = tree.DecisionTreeClassifier(criterion='entropy')
dt.set_params(min_samples_leaf=11, max_depth=3)

dt.fit(X_train, y_train)
measure_performance(X_test, y_test, dt, show_confussion_matrix=False)
```

```
Accuracy:0.798

Classification report
             precision    recall  f1-score   support

          0       0.83      0.85      0.84       161
          1       0.75      0.71      0.73       101

avg / total       0.80      0.80      0.80       262
```

Grid Search allows us to more systematically explore different combinations of multiple parameters

In [38]:
```
from sklearn.model_selection import GridSearchCV

dt = tree.DecisionTreeClassifier()

parameters = {
    'criterion': ['entropy','gini'],
    'max_depth': np.linspace(1, 20, 10, dtype=int),
    'min_samples_leaf': np.linspace(1, 30, 15, dtype=int),
    'min_samples_split': np.linspace(2, 20, 10, dtype=int)
}

gs = GridSearchCV(dt, parameters, verbose=1, cv=5)
```

In [39]:
```
%time _ = gs.fit(X_train, y_train)

gs.best_params_, gs.best_score_
```

```
Fitting 5 folds for each of 3000 candidates, totalling 15000 fits
Wall time: 55.7 s

[Parallel(n_jobs=1)]: Done 15000 out of 15000 | elapsed:   55.5s finished
```

Out[39]:
```
({'criterion': 'gini',
  'max_depth': 3,
  'min_samples_leaf': 3,
  'min_samples_split': 2},
 0.8132183908045977)
```

In [40]:

```
dt = tree.DecisionTreeClassifier(criterion='gini', max_depth=3, min_samples_

dt.fit(X_train, y_train)
measure_performance(X_test, y_test, dt, show_confussion_matrix=False, show_c
```

```
Accuracy:0.798

Classification report
             precision    recall  f1-score   support

          0       0.83      0.85      0.84       161
          1       0.75      0.71      0.73       101

avg / total       0.80      0.80      0.80       262
```

In [ ]: