Enron_project_submission2

August 11, 2021

1 Identify Fraud from Enron Email

Machine Learning Project — Udacity Data Analyst Nanodegree

1.0.1 Dataset Background

In 2000, Enron was one of the largest companies in the United States. By 2002, it had collapsed into bankruptcy due to widespread corporate fraud. In the resulting Federal investigation, a significant amount of typically confidential information entered into the public record, including tens of thousands of emails and detailed financial data for top executives. This data comes with a hand-generated list of persons of interest in the fraud case, which means individuals who were indicted, reached a settlement or plea deal with the government, or testified in exchange for prosecution immunity. In this project, I will try my best to build a person of interest identifier based on financial and email data made public as a result of the Enron scandal.

Below cell basically consists only of the provided starter code:

1.1 Data Exploration

[1]:
```
import os
os.chdir('C:/Users/Rapha/Documents/Datascience_Nanodegree/Projekte/Project4/
↪For_submission')

import sys
import pickle

sys.path.append(os.getcwd())
sys.path.append('C:/Users/Rapha/Documents/Datascience_Nanodegree/Projekte/
↪Project4/tools')

import pandas as pd
import numpy as np

import matplotlib
import matplotlib.pyplot as plt

from feature_format import featureFormat, targetFeatureSplit
from tester import dump_classifier_and_data
```

```python
import poi_plot, poi_explore

### features_list is a list of strings, each of which is a feature name.
### The first feature must be "poi".

payment_data = ['salary',
                'bonus',
                'long_term_incentive',
                'deferred_income',
                'deferral_payments',
                'loan_advances',
                'other',
                'expenses',
                'director_fees',
                'total_payments',
                'exercised_stock_options',
                'restricted_stock',
                'restricted_stock_deferred',
                'total_stock_value']

email_data = ['to_messages',
              'from_messages',
              'from_poi_to_this_person',
              'from_this_person_to_poi',
              'shared_receipt_with_poi']

features_list = ['poi'] + payment_data + email_data # You will need to use more␣
 ↪features

### Load the dictionary containing the dataset
with open("final_project_dataset.pkl", "r") as data_file:
    data_dict = pickle.load(data_file)

### Store to my_dataset for easy export below.
my_dataset = data_dict
```

```
C:\Users\Rapha\anaconda3\envs\python2\lib\site-
packages\sklearn\cross_validation.py:44: DeprecationWarning: This module was
deprecated in version 0.18 in favor of the model_selection module into which 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. This module will be
removed in 0.20.
  "This module will be removed in 0.20.", DeprecationWarning)
```

The starter code will output the data in the form of a Python dictionary where each key-value pair corresponds to one person. The key is the person's name, and the value is another dictionary.

For easier handling I will convert it to a pandas dataframe.

[2]:
```
#create new dataframe from dict
df = pd.DataFrame.from_dict(data_dict, orient='index')
#parse 'NaN' values as np.nan
df = df.replace('NaN', np.nan)
```

To get a view on the size of our data we can either just call the general info or specifically query the number of persons and features:

[3]:
```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Index: 146 entries, ALLEN PHILLIP K to YEAP SOON
Data columns (total 21 columns):
salary                       95 non-null float64
to_messages                  86 non-null float64
deferral_payments            39 non-null float64
total_payments               125 non-null float64
exercised_stock_options      102 non-null float64
bonus                        82 non-null float64
restricted_stock             110 non-null float64
shared_receipt_with_poi      86 non-null float64
restricted_stock_deferred    18 non-null float64
total_stock_value            126 non-null float64
expenses                     95 non-null float64
loan_advances                4 non-null float64
from_messages                86 non-null float64
other                        93 non-null float64
from_this_person_to_poi      86 non-null float64
poi                          146 non-null bool
director_fees                17 non-null float64
deferred_income              49 non-null float64
long_term_incentive          66 non-null float64
email_address                111 non-null object
from_poi_to_this_person      86 non-null float64
dtypes: bool(1), float64(19), object(1)
memory usage: 24.1+ KB
```

From the info query I can see that all values are parsed in floating point format except from "email_address" and "POI", with the latter being a boolean.

In addition to that one can notice that the dataset contains many missing 'null'/'nan' values. In the next chapter I will elaborate on how to interpret and treat these.

[4]:
```
print 'Number of people in the Enron dataset: {0}'.format(len(df))
print 'Number of features for each person in the Enron dataset: {0}'.
↪format(len(df.iloc[0]))
```

```
Number of people in the Enron dataset: 146
Number of features for each person in the Enron dataset: 21
```

There are 146 rows in the dataset which correspond to 146 individuals and 21 features.

By overwriting the dataframe with only the features list I deliberately disregard the column "email_address" since this will not be of value. After that we will be left with 20 features.

[5]:
```
df = df[features_list]
```

[6]:
```
print 'Number of features for each person in the Enron dataset: {0}'.
↪format(len(df.iloc[0]))
```

```
Number of features for each person in the Enron dataset: 20
```

[7]:
```
pois = df['poi'].loc[df['poi'] == True]
print 'Number of POI\'s: {0}'.format(len(pois))
```

```
Number of POI's: 18
```

1.1.1 NaN Value Treatment

Taking a look into the original Pdf-file for the financial data my interpretation is that empty fields do not stand for unknown quantities but represent "0". However for the e-mail data NaNs are unknown information.

For that reason I will replace any financial data which is NaN with a "0" whereas for the e-mail data I will replace NaN values with the mean of the respective column grouped by POIs and Non-POIS. In other words if a NaN-value corresponds to a POI it will be filled with the mean of the POIs in that column and if a NaN value correspsonds to a Non-POI it will be filled with the mean of the Non-POIs in that column. If I chose to drop all NaNs it would reduce the size of what is already a small dataset. Since the perfomance of a machine learning algorithm is proportional to the amount of data fed into it, I am hesitant to remove any information that could possibly be of use.

[8]:
```
df.isnull().sum(axis = 0)
```

[8]:
```
poi                           0
salary                       51
bonus                        64
long_term_incentive          80
deferred_income              97
deferral_payments           107
loan_advances               142
other                        53
expenses                     51
director_fees               129
total_payments               21
exercised_stock_options      44
restricted_stock             36
restricted_stock_deferred   128
total_stock_value            20
to_messages                  60
from_messages                60
```

```
from_poi_to_this_person      60
from_this_person_to_poi      60
shared_receipt_with_poi      60
dtype: int64
```

[9]:
```
# Fill in the NaN payment and stock values with zero
df[payment_data] = df[payment_data].fillna(0)
```

[10]:
```
from sklearn.preprocessing import Imputer

# Fill in the NaN email data with the mean of column grouped by poi/ non_poi
imp = Imputer(missing_values='NaN', strategy = 'mean', axis=0)

df_poi = df[df['poi'] == True];
df_nonpoi = df[df['poi']==False]

df_poi.loc[:, email_data] = imp.fit_transform(df_poi.loc[:,email_data]);
df_nonpoi.loc[:, email_data] = imp.fit_transform(df_nonpoi.loc[:,email_data]);
df = df_poi.append(df_nonpoi)
```

```
C:\Users\Rapha\anaconda3\envs\python2\lib\site-
packages\pandas\core\indexing.py:517: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: http://pandas.pydata.org/pandas-
docs/stable/indexing.html#indexing-view-versus-copy
  self.obj[item] = s
```

[11]:
```
df.isnull().sum(axis = 0)
```

[11]:
```
poi                         0
salary                      0
bonus                       0
long_term_incentive         0
deferred_income             0
deferral_payments           0
loan_advances               0
other                       0
expenses                    0
director_fees               0
total_payments              0
exercised_stock_options     0
restricted_stock            0
restricted_stock_deferred   0
total_stock_value           0
to_messages                 0
from_messages               0
```

```
from_poi_to_this_person      0
from_this_person_to_poi      0
shared_receipt_with_poi      0
dtype: int64
```

[12]:
```
df.describe()
```

[12]:

```
             salary         bonus  long_term_incentive  deferred_income  \
count  1.460000e+02  1.460000e+02         1.460000e+02     1.460000e+02
mean   3.658114e+05  1.333474e+06         6.646839e+05    -3.827622e+05
std    2.203575e+06  8.094029e+06         4.046072e+06     2.378250e+06
min    0.000000e+00  0.000000e+00         0.000000e+00    -2.799289e+07
25%    0.000000e+00  0.000000e+00         0.000000e+00    -3.792600e+04
50%    2.105960e+05  3.000000e+05         0.000000e+00     0.000000e+00
75%    2.708505e+05  8.000000e+05         3.750648e+05     0.000000e+00
max    2.670423e+07  9.734362e+07         4.852193e+07     0.000000e+00

       deferral_payments  loan_advances         other      expenses  \
count       1.460000e+02   1.460000e+02  1.460000e+02  1.460000e+02
mean        4.387965e+05   1.149658e+06  5.854318e+05  7.074827e+04
std         2.741325e+06   9.649342e+06  3.682345e+06  4.327163e+05
min        -1.025000e+05   0.000000e+00  0.000000e+00  0.000000e+00
25%         0.000000e+00   0.000000e+00  0.000000e+00  0.000000e+00
50%         0.000000e+00   0.000000e+00  9.595000e+02  2.018200e+04
75%         9.684500e+03   0.000000e+00  1.506065e+05  5.374075e+04
max         3.208340e+07   8.392500e+07  4.266759e+07  5.235198e+06

       director_fees  total_payments  exercised_stock_options  \
count   1.460000e+02    1.460000e+02             1.460000e+02
mean    1.942249e+04    4.350622e+06             4.182736e+06
std     1.190543e+05    2.693448e+07             2.607040e+07
min     0.000000e+00    0.000000e+00             0.000000e+00
25%     0.000000e+00    9.394475e+04             0.000000e+00
50%     0.000000e+00    9.413595e+05             6.082935e+05
75%     0.000000e+00    1.968287e+06             1.714221e+06
max     1.398517e+06    3.098866e+08             3.117640e+08

       restricted_stock  restricted_stock_deferred  total_stock_value  \
count      1.460000e+02               1.460000e+02       1.460000e+02
mean       1.749257e+06               2.051637e+04       5.846018e+06
std        1.089995e+07               1.439661e+06       3.624681e+07
min       -2.604490e+06              -7.576788e+06      -4.409300e+04
25%        8.115000e+03               0.000000e+00       2.288695e+05
50%        3.605280e+05               0.000000e+00       9.659550e+05
75%        8.145280e+05               0.000000e+00       2.319991e+06
max        1.303223e+08               1.545629e+07       4.345095e+08
```

```
        to_messages  from_messages  from_poi_to_this_person  \
count    146.000000     146.000000               146.000000
mean    2057.662970     623.343879                63.343444
std     1978.612966    1410.919321                66.918580
min       57.000000      12.000000                 0.000000
25%      904.250000      36.000000                25.750000
50%     2007.111111     392.178571                58.500000
75%     2007.111111     668.763889                58.500000
max    15149.000000   14368.000000               528.000000

       from_this_person_to_poi  shared_receipt_with_poi
count               146.000000               146.000000
mean                 40.030224              1147.846271
std                  76.789203               910.277086
min                   0.000000                 2.000000
25%                   6.000000               591.500000
50%                  36.277778              1058.527778
75%                  36.277778              1117.500000
max                 609.000000              5521.000000
```

1.1.2 Check for errors in dataset

We can make a validity check errors in the financial data by adding up all payment data for each person and check if this equals the total payment for that person.

[13]:
```
#Cross-check by adding up all of payment related columns
errors_payment = (df[df[payment_data[:-5]].sum(axis='columns') !=
 ↪df['total_payments']])
errors_payment
```

[13]:
```
                     poi  salary  bonus  long_term_incentive  deferred_income  \
BELFER ROBERT      False     0.0    0.0                  0.0              0.0
BHATNAGAR SANJAY   False     0.0    0.0                  0.0              0.0

                  deferral_payments  loan_advances     other  expenses  \
BELFER ROBERT             -102500.0            0.0       0.0       0.0
BHATNAGAR SANJAY                0.0            0.0  137864.0       0.0

                  director_fees  total_payments  exercised_stock_options  \
BELFER ROBERT            3285.0        102500.0                   3285.0
BHATNAGAR SANJAY       137864.0      15456290.0                2604490.0

                  restricted_stock  restricted_stock_deferred  \
BELFER ROBERT                  0.0                    44093.0
BHATNAGAR SANJAY        -2604490.0                 15456290.0

                  total_stock_value  to_messages  from_messages  \
```

```
BELFER ROBERT                -44093.0  2007.111111     668.763889
BHATNAGAR SANJAY                  0.0   523.000000      29.000000

                  from_poi_to_this_person  from_this_person_to_poi  \
BELFER ROBERT                        58.5                36.277778
BHATNAGAR SANJAY                      0.0                 1.000000

                  shared_receipt_with_poi
BELFER ROBERT                 1058.527778
BHATNAGAR SANJAY               463.000000
```

Indeed there are two individuals for which the sum of their payment data does not add up to the alleged total payment. The errors are already present in the original Pdf-File and seem to be caused by a misalignment between the columns. For Robert Belfer the financial data has been shifted one column to the right, whereas for Sanjay Bhatnagar the data has been shifted one column to the left. I will fix that issue by shifting the columns and then check again if the payment data add up correctly to the respective "total_payment" and "total_stock_value".

[14]:
```python
# Retrieve the incorrect data for Belfer
belfer_financial = df.loc['BELFER ROBERT','salary':'total_stock_value'].tolist()
# Delete the first element to shift left and add on a 0 to end as indicated in␣
↪financial data
belfer_financial.pop(0)
belfer_financial.append(0.)
# Reinsert corrected data
df.loc['BELFER ROBERT','salary':'total_stock_value'] = belfer_financial

# Retrieve the incorrect data for Bhatnagar
bhatnagar_financial = df.loc['BHATNAGAR SANJAY','salary':'total_stock_value'].
↪tolist()
# Delete the last element to shift right and add on a 0 to beginning
bhatnagar_financial.pop(-1)
bhatnagar_financial = [0] + bhatnagar_financial
# Reinsert corrected data
df.loc['BHATNAGAR SANJAY','salary':'total_stock_value'] = bhatnagar_financial
```

[15]:
```python
#Check if errors in payment data are solved
df[df[payment_data[:-5]].sum(axis='columns') != df['total_payments']]
```

[15]:
```
Empty DataFrame
Columns: [poi, salary, bonus, long_term_incentive, deferred_income,
deferral_payments, loan_advances, other, expenses, director_fees,
total_payments, exercised_stock_options, restricted_stock,
restricted_stock_deferred, total_stock_value, to_messages, from_messages,
from_poi_to_this_person, from_this_person_to_poi, shared_receipt_with_poi]
Index: []
```

[16]:
```
#Check if errors in stock data are solved
df[df[payment_data[10:-1]].sum(axis='columns') != df['total_stock_value']]
```

[16]:
```
Empty DataFrame
Columns: [poi, salary, bonus, long_term_incentive, deferred_income,
deferral_payments, loan_advances, other, expenses, director_fees,
total_payments, exercised_stock_options, restricted_stock,
restricted_stock_deferred, total_stock_value, to_messages, from_messages,
from_poi_to_this_person, from_this_person_to_poi, shared_receipt_with_poi]
Index: []
```

As I was screening the Pdf-file more closely I stumbled upon an individual called "THE TRAVEL AGENCY IN THE PARK". Obviously this is not the name of an employee but according to documentation was a company owned by Enron's former Chairman's sister and is therefore clearly not a data point which should be included in the data set.

[17]:
```
df.drop(axis=0, labels=['THE TRAVEL AGENCY IN THE PARK'], inplace=True)
```

1.2 Outliers

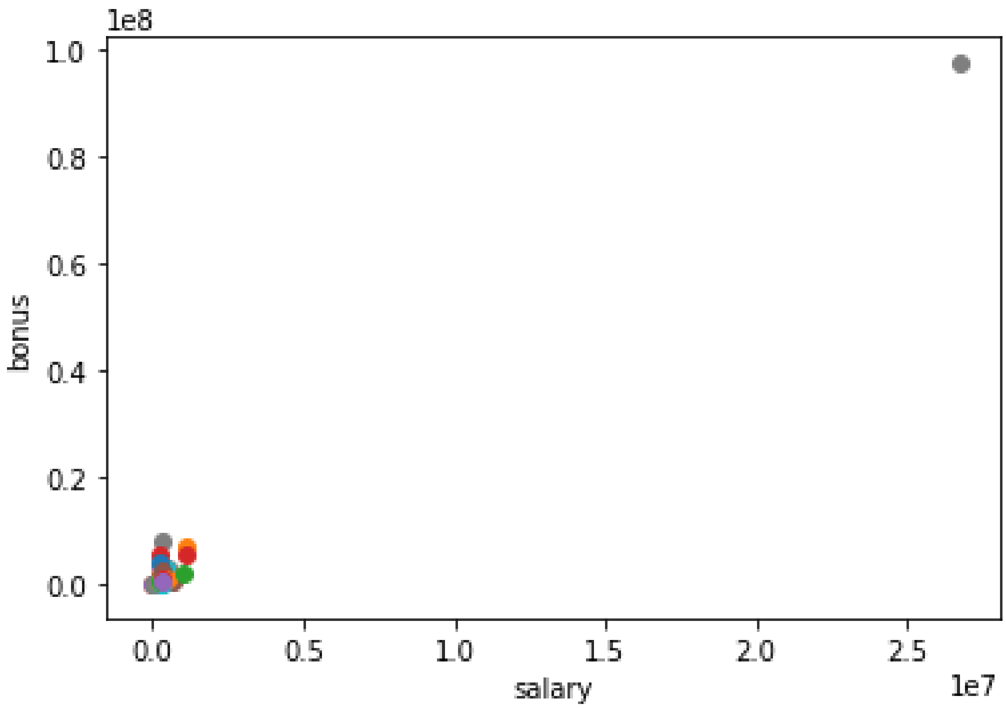
The outlier explorations starts by plotting two of the most telling features when it comes to uncover the relation between the data and POIs: Salary & Bonus

To be able to reuse the scatterplot-code from the Udacity lessons, first I will have to convert the dataframe back to a Python dictionary.

[18]:
```
my_dataset = df.to_dict(orient='index')
```

Scatterplot of Salary vs. Bonus

[19]:
```
poi_plot.scatterplot(my_dataset, "salary", "bonus")
```



[20]:
```
# Find the outlier with the highest salary
outlier = poi_explore.sort_data(my_dataset, "salary", 1, reverse=True)
outlier_name = poi_explore.get_name(my_dataset, "salary", outlier[0])
print 'Outlier name: {0}'.format(outlier_name)
```

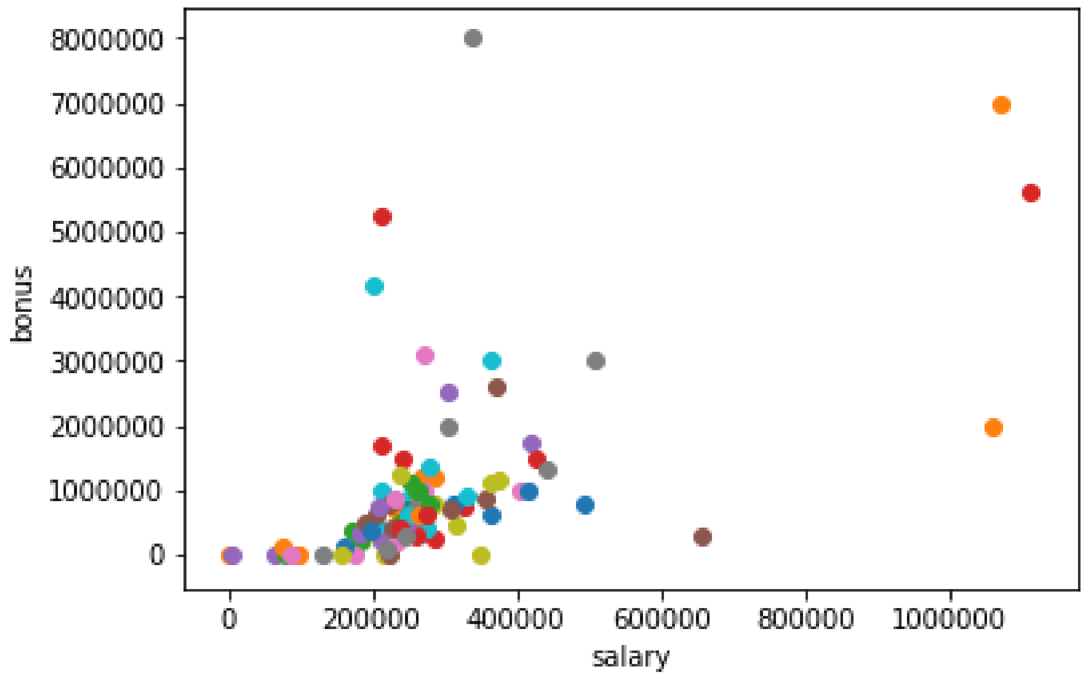
```
Outlier name: TOTAL
```

The plot clearly shows an outlier in the top right of the plot. Ordering the list by salary, the outlier is called "TOTAL", which represents the sum of all the salaries as shown in the Pdf. Since this entry does not represent a person it is invalid and is therefore removed.

[21]:
```
# Remove outlier TOTAL from dict and from df
my_dataset.pop('TOTAL', None);
df.drop(axis=0, labels=['TOTAL'], inplace=True)
```

Scatterplot of Salary vs. Bonus of original dataset after removal of outlier

[22]:
```
poi_plot.scatterplot(my_dataset, "salary", "bonus")
```



[23]:
```
#Entries in Dict & Dataframe after Cleaning and outlier removal
print (len(my_dataset))
print (len(df))
```

```
144
144
```

After cleaning and outlier removal the data set is left with 144 entries that all represent valid Enron employees.

1.3 Pick Algorithms and first shot performances

The first training and testing runs will be to assess the out-of-the-box performance of several algorithms using all of the 20 features. For this initial step I selected 6 algorithms: GaussianNB, DecisionTreeClassifier, SVC, KMeans, AdaBoostClassifier and RandomForestClassifier.

I will run the algorithms with the default parameters except I will alter the kernel used in the Support Vector Machine to be linear and I will select the number of clusters = 2 for KMeans as I know in advance that the targets are only two categories that should be classified.

Concerning algorithm performance I will base my assessment on the F1-score. Since the F1-score is a combined measure of precision and recall I think it will serve best our aim to achieve both a good Recall and Precision. For this project the minimum requirement is a precision and recall score of at least 0.3.

[24]:
```python
from sklearn.naive_bayes import GaussianNB
from sklearn.tree import DecisionTreeClassifier
from sklearn.svm import SVC
from sklearn.cluster import KMeans
from sklearn.ensemble import AdaBoostClassifier
from sklearn.ensemble import RandomForestClassifier

import tester

# Create and test the Gaussian Naive Bayes Classifier
clf = GaussianNB()
tester.dump_classifier_and_data(clf, my_dataset, features_list)
tester.main();
```

```
GaussianNB(priors=None)
        Accuracy: 0.77220       Precision: 0.25991      Recall: 0.38350 F1:
0.30984     F2: 0.35020
        Total predictions: 15000        True positives:  767    False positives:
2184    False negatives: 1233   True negatives: 10816
```

[25]:
```python
# Create and test the Decision Tree Classifier
clf = DecisionTreeClassifier()
tester.dump_classifier_and_data(clf, my_dataset, features_list)
tester.main();
```

```
DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=None,
            max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            presort=False, random_state=None, splitter='best')
        Accuracy: 0.81547       Precision: 0.31538      Recall: 0.32800 F1:
0.32157     F2: 0.32540
        Total predictions: 15000        True positives:  656    False positives:
1424    False negatives: 1344   True negatives: 11576
```

[26]:
```python
# Create and test the Support Vector Classifier
clf = SVC(kernel='linear', max_iter=1000)
tester.dump_classifier_and_data(clf, my_dataset, features_list)
tester.main();
```

```
C:\Users\Rapha\anaconda3\envs\python2\lib\site-packages\sklearn\svm\base.py:220:
ConvergenceWarning: Solver terminated early (max_iter=1000).  Consider pre-
processing your data with StandardScaler or MinMaxScaler.
  % self.max_iter, ConvergenceWarning)
```

```
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma='auto', kernel='linear',
```

```
  max_iter=1000, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
        Accuracy: 0.48540       Precision: 0.14027      Recall: 0.55750 F1:
0.22414     F2: 0.34955
        Total predictions: 15000        True positives: 1115    False positives:
6834   False negatives:  885   True negatives: 6166
```

[27]:
```
# Create and test the K Means clustering classifier
clf = KMeans(n_clusters=2)
tester.dump_classifier_and_data(clf, my_dataset, features_list)
tester.main();
```

```
KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=300,
    n_clusters=2, n_init=10, n_jobs=1, precompute_distances='auto',
    random_state=None, tol=0.0001, verbose=0)
        Accuracy: 0.82960       Precision: 0.20921      Recall: 0.10000 F1:
0.13532     F2: 0.11166
        Total predictions: 15000        True positives:  200    False positives:
756   False negatives: 1800   True negatives: 12244
```

[28]:
```
# Create and test the AdaBoost classifier
clf = AdaBoostClassifier()
tester.dump_classifier_and_data(clf, my_dataset, features_list)
tester.main();
```

```
AdaBoostClassifier(algorithm='SAMME.R', base_estimator=None,
          learning_rate=1.0, n_estimators=50, random_state=None)
        Accuracy: 0.86307       Precision: 0.48133      Recall: 0.34800 F1:
0.40395     F2: 0.36841
        Total predictions: 15000        True positives:  696    False positives:
750   False negatives: 1304   True negatives: 12250
```

[29]:
```
# Create and test the RandomForest classifier
clf = RandomForestClassifier()
tester.dump_classifier_and_data(clf, my_dataset, features_list)
tester.main();
```

```
RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
            max_depth=None, max_features='auto', max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            n_estimators=10, n_jobs=1, oob_score=False, random_state=None,
            verbose=0, warm_start=False)
        Accuracy: 0.86987       Precision: 0.53715      Recall: 0.17350 F1:
0.26228     F2: 0.20067
        Total predictions: 15000        True positives:  347    False positives:
```

```
299   False negatives: 1653   True negatives: 12701
```

Both GaussianNB and DecisionTreeClassifier achieved a good result in F1-score even exceeding the required 0.3 just out-of-the-box. Also AdaBoostClassifier did a decent job.

1.3.1 Cross-validation

By making use of the tester.py script provided from Udacity I could run these training and testing runs with minimal code here. What the tester.py script does, it uses StatifiedShuffleSPlit to split the data into labels and features sets with which the classifier is being trained and tested and then randomly shuffles the data before splitting it again into training and testing sets. This process is being repeated several times. In our case 1000 times since this is the value provided in the tester.py script. This iterative shuffling and splitting is one possible form of what is being referred to as cross-validation.

Cross-validation prevents one from making the classic mistake of training an algoithm on the same data used to test the algorithm. If this happens, the test results may show that the classifier is accurate, but that is only because the algorithm has seen the testing data before. When the classifier is deployed on new samples, the performance may be poor because it was trained and tuned for a very specific set of instances. The classifier will not be able to generalize to new cases because it is only fit and tuned to the specific samples it is tested on. Cross-validation solves this issue by training and testing on multiple different subsets of the features and labels and is ideal for use on small datasets to avoid overfitting.

1.4 Scaling

Scaling of some sort whether that is Normalization (MinMax scaling) or Standardization is usually necessary because there are different units for the features in the dataset. Scaling creates non-dimensional features such that those features with a larger range of values do not have an undue influence on the classifier. For example, many classifiers calculate the distance between two points by the Euclidean distance. If one of the features has a broad range of values, the distance will be governed by this particular feature. Therefore, the range of all features should be normalized so that each feature contributes approximately proportionately to the final distance.

In the following I will test if feature scaling has a positive effect on the overall algorithm performance. This is not required as per project specifications but rather I will do this out of curiosity. Instead I could have just applied scaling only for algorithms that utilize Euclidian distances which is how one would usually handle it (will be explained at the end of chapter scaling).

I will run the algorithms as I did before only this time with standardized values. Feature standardization makes the values of each feature in the data have zero-mean and unit-variance. Sklearn's preprocessing module provides a scale function which I will use to generate a new dataset with scaled values.

There is also another method from Scikitlearn called 'StandardScaler' which according to the docs is actually the preferred method. The problem with scaling a dataset before splitting it into training and testing sets is that it will bias the model evaluation because information would have leaked from the test set into the training set. This is a common mistake which is why the use of StandardScaler is recommended. In the following I will try both so I can make a cross check between the two methods.

[30]:
```python
# Scale the dataset and send it back to a dictionary
from sklearn.preprocessing import scale

scaled_df = df.copy()
scaled_df.ix[:,1:] = scale(scaled_df.ix[:,1:])
my_dataset_scaled = scaled_df.to_dict(orient='index')
```

```
C:\Users\Rapha\anaconda3\envs\python2\lib\site-packages\ipykernel_launcher.py:5:
DeprecationWarning:
.ix is deprecated. Please use
.loc for label based indexing or
.iloc for positional indexing

See the documentation here:
http://pandas.pydata.org/pandas-docs/stable/indexing.html#deprecate_ix
  """
```

[31]:
```python
# Create and test the Gaussian Naive Bayes Classifier with scaled data
clf = GaussianNB()
tester.dump_classifier_and_data(clf, my_dataset_scaled, features_list)
tester.main();
```

```
GaussianNB(priors=None)
        Accuracy: 0.40013       Precision: 0.16003      Recall: 0.82350 F1:
0.26798     F2: 0.45020
        Total predictions: 15000        True positives: 1647    False positives:
8645   False negatives:  353   True negatives: 4355
```

[32]:
```python
# Crosscheck with StandardScaler in a pipeline

from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler

clf = Pipeline([('scaler', StandardScaler()),('classify', GaussianNB())])

tester.dump_classifier_and_data(clf, my_dataset, features_list)
tester.main()
```

```
Pipeline(steps=[('scaler', StandardScaler(copy=True, with_mean=True,
with_std=True)), ('classify', GaussianNB(priors=None))])
        Accuracy: 0.39780       Precision: 0.15981      Recall: 0.82600 F1:
0.26781     F2: 0.45046
        Total predictions: 15000        True positives: 1652    False positives:
8685   False negatives:  348   True negatives: 4315
```

Using 'Standard Scaler' within a Pipeline produces nearly the same results. Therefore I conclude that both methods produce valid results. I assume it will be the case also for the other classifiers…

[33]:
```
# Create and test the Decision Tree Classifier with scaled data
clf = DecisionTreeClassifier()
tester.dump_classifier_and_data(clf, my_dataset_scaled, features_list)
tester.main();
```

```
DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=None,
            max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            presort=False, random_state=None, splitter='best')
        Accuracy: 0.81593       Precision: 0.32060      Recall: 0.34000 F1:
0.33002     F2: 0.33594
        Total predictions: 15000        True positives:  680    False positives:
1441    False negatives: 1320   True negatives: 11559
```

[34]:
```
# Create and test the Support Vector Classifier with scaled data
clf = SVC(kernel='linear', max_iter=1000)
tester.dump_classifier_and_data(clf, my_dataset_scaled, features_list)
tester.main();
```

```
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma='auto', kernel='linear',
  max_iter=1000, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
        Accuracy: 0.87080       Precision: 0.54247      Recall: 0.19800 F1:
0.29011     F2: 0.22680
        Total predictions: 15000        True positives:  396    False positives:
334   False negatives: 1604   True negatives: 12666
```

[35]:
```
# Create and test the K Means clustering classifier with scaled data
clf = KMeans(n_clusters=2)
tester.dump_classifier_and_data(clf, my_dataset_scaled, features_list)
tester.main();
```

```
KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=300,
    n_clusters=2, n_init=10, n_jobs=1, precompute_distances='auto',
    random_state=None, tol=0.0001, verbose=0)
        Accuracy: 0.80860       Precision: 0.15464      Recall: 0.09750 F1:
0.11960     F2: 0.10528
        Total predictions: 15000        True positives:  195    False positives:
1066    False negatives: 1805   True negatives: 11934
```

[36]:
```
# Create and test the AdaBoost classifier with scaled data
clf = AdaBoostClassifier()
tester.dump_classifier_and_data(clf, my_dataset_scaled, features_list)
tester.main();
```

```
AdaBoostClassifier(algorithm='SAMME.R', base_estimator=None,
          learning_rate=1.0, n_estimators=50, random_state=None)
        Accuracy: 0.86327       Precision: 0.48233      Recall: 0.34800 F1:
0.40430     F2: 0.36853
        Total predictions: 15000        True positives:  696    False positives:
747   False negatives: 1304   True negatives: 12253
```

[37]:
```python
# Create and test the RandomForest classifier with scaled data
clf = RandomForestClassifier()
tester.dump_classifier_and_data(clf, my_dataset_scaled, features_list)
tester.main();
```

```
RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
            max_depth=None, max_features='auto', max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            n_estimators=10, n_jobs=1, oob_score=False, random_state=None,
            verbose=0, warm_start=False)
        Accuracy: 0.86927       Precision: 0.53033      Recall: 0.17050 F1:
0.25804     F2: 0.19727
        Total predictions: 15000        True positives:  341    False positives:
302   False negatives: 1659   True negatives: 12698
```

1.5 Results from first shots

Unscaled:

Classifier	Accuracy	Precision	Recall	F1 Score
GaussianNB	0.772	0.260	0.384	0.310
DecisionTree	0.815	0.315	0.328	0.322
SVC (kernel='linear')	0.485	0.140	0.558	0.224
KMeans (n_clusters=2)	0.829	0.209	0.100	0.135
Adaboost	0.863	0.481	0.348	0.404
Random Forest	0.870	0.537	0.174	0.262

Scaled:

Classifier	Accuracy	Precision	Recall	F1 Score
GaussianNB	0.400	0.160	0.824	0.268
DecisionTree	0.816	0.321	0.340	0.330
SVC (kernel='linear')	0.871	0.542	0.198	0.290
KMeans (n_clusters=2)	0.809	0.154	0.098	0.120
Adaboost	0.863	0.482	0.348	0.404
Random Forest	0.869	0.530	0.171	0.258

The results are mixed. For GaussianNB and DecisionTree the scaled data does not bring an improvement whereas for SVC the performance improved considerably. The performances of Random Forest and KMeans improved a little. AdaBoosts' performance did not change at all.

In a way these results confirm kind of what one would already expect. Algorithms where feature scaling matters are ones that utilize Euclidean distances, like K-means or K-nearest neighbors, logistic regression, SVMs, perceptrons, neural networks, etc. For ensemble algorithms like AdaBoost, XGBoost, etc. they depend on the base_classifier. In Sklearn it uses DecisionTree by default thus scaling isn't needed. The DecisionTree itself does not utilize Euclidian distances either.

However one may have expected a visible performance improvement for the KMeans-Algorithm. This I could not observe.

The fact that RandomForest has improved in performance by a minimal fraction is not reason enough for me to apply scaling. Since RF is an ensemble algorithm it normally doens not require scaling. So I won't do it either.

1.6 Feature Engineering

The aim of feature engineering is to increase algorithm performance by creating new features out of existing information. In this case I try to combine existing features with each other in such way that it has a positive effect on the algorithms performance.

For example the ratios between the email features 'from_poi_to_this_person' and 'to_messages' or 'from_messages' might be a useful combination for the creation of a new feature as it could be the case that somebody went unnoticed with lower email volume, but almost all of it directed to or coming from a POI. I could imagine that in contrast to total numbers these new features based on the percentage of emails to or from POIs will do a better job in revealing the persons with higher communication to POIs. It seems evident that individuals who interact more with a POI are themselves more likely to be a POI.

[38]:
```
# Add the new email features to the dataframe
df['to_poi_ratio'] = df['from_poi_to_this_person'] / df['to_messages']
df['from_poi_ratio'] = df['from_this_person_to_poi'] / df['from_messages']

features_list.append('to_poi_ratio')
features_list.append('from_poi_ratio')
```

In addition I will create two new financial features that are also a combination from already existing features. Namely the fraction of bonus&salary and bonus&total_payments. The reason for choosing these combinations are primarily because I suspect that persons receiving very large bonuses compared to their usual annual income are more likely to be involved in fraudulent activities and therefore be POIs.

[39]:
```
# Add the new financial features to the dataframe
df['bonus_to_salary'] = df['bonus'] / df['salary']
df['bonus_to_total'] = df['bonus'] / df['total_payments']

features_list.append('bonus_to_salary')
features_list.append('bonus_to_total')
```

[40]:
```
print 'Number of features with newly engineered features: {0}'.format(len(df.
↪iloc[0]))
```

```
Number of features with newly engineered features: 24
```

[41]:
```
# Fill any NaN financial data with a 0
df.fillna(value= 0, inplace=True)
```

[42]:
```
my_dataset = df.to_dict(orient='index')
```

[43]:
```
#update 'scaled_df', and 'my_dataset_scaled' with new enineered features
scaled_df = df.copy()
scaled_df.ix[:,1:] = scale(scaled_df.ix[:,1:])

my_dataset_scaled = scaled_df.to_dict(orient='index')
```

```
C:\Users\Rapha\anaconda3\envs\python2\lib\site-packages\ipykernel_launcher.py:3:
DeprecationWarning:
.ix is deprecated. Please use
.loc for label based indexing or
.iloc for positional indexing

See the documentation here:
http://pandas.pydata.org/pandas-docs/stable/indexing.html#deprecate_ix
  This is separate from the ipykernel package so we can avoid doing imports
until
```

There are now a total number of 24 features of which I do not yet know if I produced some unnecessary redundancies. Let's test the performances using the tester.py script and see if the newly engineered features bring some improvement.

[44]:
```
clf = GaussianNB()
tester.dump_classifier_and_data(clf, my_dataset, features_list)
tester.main();
```

```
GaussianNB(priors=None)
        Accuracy: 0.77220       Precision: 0.25991      Recall: 0.38350 F1:
0.30984     F2: 0.35020
        Total predictions: 15000        True positives:  767    False positives:
2184   False negatives: 1233   True negatives: 10816
```

[45]:
```
clf = DecisionTreeClassifier()
tester.dump_classifier_and_data(clf, my_dataset, features_list)
tester.main();
```

```
DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=None,
            max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
```

```
            presort=False, random_state=None, splitter='best')
        Accuracy: 0.89847       Precision: 0.61955      Recall: 0.61800 F1:
0.61877     F2: 0.61831
        Total predictions: 15000        True positives: 1236    False positives:
759   False negatives:  764   True negatives: 12241
```

[107]:
```
clf = SVC(kernel='linear', max_iter=1000)
tester.dump_classifier_and_data(clf, my_dataset_scaled, features_list)
tester.main();
```

```
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma='auto', kernel='linear',
  max_iter=1000, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
        Accuracy: 0.85960       Precision: 0.44894      Recall: 0.23300 F1:
0.30678     F2: 0.25780
        Total predictions: 15000        True positives:  466    False positives:
572   False negatives: 1534   True negatives: 12428
```

[47]:
```
clf = KMeans(n_clusters=2)
tester.dump_classifier_and_data(clf, my_dataset, features_list)
tester.main();
```

```
KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=300,
    n_clusters=2, n_init=10, n_jobs=1, precompute_distances='auto',
    random_state=None, tol=0.0001, verbose=0)
        Accuracy: 0.83047       Precision: 0.21807      Recall: 0.10500 F1:
0.14175     F2: 0.11715
        Total predictions: 15000        True positives:  210    False positives:
753   False negatives: 1790   True negatives: 12247
```

[48]:
```
clf = AdaBoostClassifier()
tester.dump_classifier_and_data(clf, my_dataset, features_list)
tester.main();
```

```
AdaBoostClassifier(algorithm='SAMME.R', base_estimator=None,
          learning_rate=1.0, n_estimators=50, random_state=None)
        Accuracy: 0.88000       Precision: 0.56068      Recall: 0.46200 F1:
0.50658     F2: 0.47886
        Total predictions: 15000        True positives:  924    False positives:
724   False negatives: 1076   True negatives: 12276
```

[49]:
```
clf = RandomForestClassifier()
tester.dump_classifier_and_data(clf, my_dataset, features_list)
tester.main();
```

```
RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
            max_depth=None, max_features='auto', max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            n_estimators=10, n_jobs=1, oob_score=False, random_state=None,
            verbose=0, warm_start=False)
        Accuracy: 0.88073       Precision: 0.63937      Recall: 0.24200 F1:
0.35111     F2: 0.27635
        Total predictions: 15000        True positives:  484    False positives:
273   False negatives: 1516   True negatives: 12727
```

After adding the new features, the scores for all algorithms have improved or at least remained the same. KMeans still performes very poorly regarding F1-score and recall so I will drop it for further investigation.

1.7 Results with engineered features

Unscaled:

Classifier	Accuracy	Precision	Recall	F1 Score
GaussianNB	0.772	0.260	0.384	0.310
DecisionTree	0.898	0.620	0.618	0.619
SVC (kernel='linear')	0.860	0.449	0.233	0.307
KMeans (n_clusters=2)	0.837	0.219	0.088	0.126
Adaboost	0.880	0.561	0.462	0.507
Random Forest	0.881	0.639	0.242	0.351

Based on the F1-score the DecisionTree is now leading the pack followed by AdaBoost.

1.8 Feature Selection

With overall 24 features this is quite a number. By creating new features I was able to improve performance but I do not yet know if all of the features are really necessary or if I can remove some of them. Having less but important features is not only to be considered as "nice to have" but really an important step to tuning algorithm performance.

One way to perform feature selection is to query the feature importances for a classifier and then modifiy the features list manually to exlude the ones below a certain threshold. In the following I will query the feature importances at the example of DecisionTreeClassifier and AdaBoostClassifier. For each I will print a features list ordered by importance.

[50]:
```python
clf_tree = DecisionTreeClassifier()
tester.test_classifier(clf_tree, my_dataset, features_list)
```

```
DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=None,
            max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
```

```
            presort=False, random_state=None, splitter='best')
        Accuracy: 0.89620       Precision: 0.61159      Recall: 0.60700 F1:
0.60928     F2: 0.60791
        Total predictions: 15000        True positives: 1214    False positives:
771   False negatives:  786   True negatives: 12229
```

[51]:
```python
# Get the feature importances of the DecisionTree Classifier
tree_feature_importances = (clf_tree.feature_importances_)
tree_features = zip(tree_feature_importances, features_list[1:])
tree_features = sorted(tree_features, key= lambda x:x[0], reverse=True)

# Display the feature names with 10 highest importance values
print('Tree Feature Importances:\n')
for i in range(10):
    print('{} : {:.4f}'.format(tree_features[i][1], tree_features[i][0]))
```

```
Tree Feature Importances:

from_poi_ratio : 0.3521
shared_receipt_with_poi : 0.2094
other : 0.1693
expenses : 0.1469
to_poi_ratio : 0.0688
from_messages : 0.0535
salary : 0.0000
bonus : 0.0000
long_term_incentive : 0.0000
deferred_income : 0.0000
```

[52]:
```python
clf_ada = AdaBoostClassifier()
tester.test_classifier(clf_ada, my_dataset, features_list);
```

```
AdaBoostClassifier(algorithm='SAMME.R', base_estimator=None,
          learning_rate=1.0, n_estimators=50, random_state=None)
        Accuracy: 0.88013       Precision: 0.56114      Recall: 0.46350 F1:
0.50767     F2: 0.48021
        Total predictions: 15000        True positives:  927    False positives:
725   False negatives: 1073   True negatives: 12275
```

[53]:
```python
# Get the feature importances for the AdaBoost Classifier
ada_feature_importances = clf_ada.feature_importances_
ada_features = zip(ada_feature_importances, features_list[1:])

# Display the feature names with 10 highest importance values
print('Ada Boost Feature Importances:\n')
ada_features = sorted(ada_features, key=lambda x:x[0], reverse=True)
```

```python
for i in range(10):
    print('{} : {:.4f}'.format(ada_features[i][1], ada_features[i][0]))
```

```
Ada Boost Feature Importances:

total_payments : 0.1400
to_poi_ratio : 0.1400
exercised_stock_options : 0.1200
other : 0.1000
from_this_person_to_poi : 0.1000
shared_receipt_with_poi : 0.0800
expenses : 0.0600
from_poi_to_this_person : 0.0600
from_poi_ratio : 0.0600
deferred_income : 0.0400
```

An interesting observation is that the top 10 features do not really conform. So feature importances can vary quite considerably between different algorithms.

1.9 Evaluation Metrics

When it comes to evaluate an algorithm, there are several evaluation metrics at our disposal, as seen during the whole project. Each of them is a perfectly valid means for evaluation but also typcially favors one type of error which is why we should use different metrics if we want our classifier to be able to generalize on the data.

Accuracy It describes the ratio between the items labeled correctly and all items. In the Enron case, the ratio between correctly identified POIs and all persons. The difficulty we face in the Enron data is that there are many more non-POIs than POI. This poses the problem that one could simply assign the more common label for all data points and still reach a pretty high Accuracy.

Recall Recall is intuitively the ability of the classifier to find all the positive samples. In the Enron case, Recall describes the ability of the algorithm to correctly identify a POI provided that the person is a POI. Boosting the Recall metric has the affect that the classifier is correctly identifying every single POI. The tradeoff is that the algorithm will be biased towards identifying POIs. In this case this is rather what we want - better make sure no POI gues unnoticed and later declare the misclassified individuals innocent.

Precision Intuitively, precision is the ability of the classifier not to label as positive a sample that is negative. In the Enron case, if the classifier doesn't have great Recall, but it does have good Precision, it means that whenever a POI gets flagged in the test set, there is good confidence that it is a real POI and not a false alarm. The tradeoff is that sometimes real POIs are missed, which in the case of Enron is definitely something we do not want.

F1-Score The F1 score can be interpreted as a weighted average of the precision and recall. The relative contribution of precision and recall to the F1 score are equal. In some way, the F1 score can be thought of "the best of both worlds". It will probably serve as a good metric for most problems and deliver a relatively balanced model. In the Enron case, I would argue that actually a good

Recall is more important even at the cost of a lower Precision. But for the purpose of this project I think that optimizing on the F1-score should serve me well. This is accounted for in the code by "scoring='f1' ".

1.10 GridSearchCV with SelectKBest

Another means for feature selection is to use SelectKBest which removes all but the k highest scoring features. Only the problem is that we don't yet know the value of k, i.e. the optimal number of features. I could manually play around with k until I assume having found the optimal number but there is a better way…

Namely, what I can do is to combine SelektKBest with GridSearchCV in order to identify the highest scoring features and at the same time find the optimal number of features. To combine these two functions one can use another tool called Pipeline. Pipeline can be used to chain multiple estimators into one. This is useful as there is often a fixed sequence of steps in processing the data, for example in feature selection. Using a pipeline one can perform a Grid Search over parameters of all estimators in the pipeline at once.

[54]:
```
#splitting data with feature_format.py
from feature_format import featureFormat, targetFeatureSplit

data_dict = featureFormat(my_dataset, features_list)
labels, features = targetFeatureSplit(data_dict)
```

[55]:
```
data_dict_scaled = featureFormat(my_dataset_scaled, features_list)
labels_scaled, features_scaled = targetFeatureSplit(data_dict)
```

Since I do not want to use the tester.py script like I did before but still need to split my data in labels and features, I can use the *featureFormat*- as well as *targetFeatureSplit*-fuctions from the feature_format.py script to format and split the data.

Grid Search with SelektKBest for DecisionTreeClassifier The pipeline can be used like any other estimator and avoids leaking the test set into the train set.

[56]:
```
from sklearn.model_selection import GridSearchCV, RandomizedSearchCV
from sklearn.pipeline import Pipeline
from sklearn.feature_selection import SelectKBest

# Create a pipeline with feature selection and classification
estimators = [
    ('select_features', SelectKBest()),
    ('classify', DecisionTreeClassifier())
]

n_features = np.arange(1, len(features_list))

param_grid = [{'select_features__k': n_features}]

pipe = Pipeline(estimators)
```

[57]:
```
grid_search_tree = GridSearchCV(pipe, param_grid=param_grid, scoring='f1', cv =␣
↪10)
grid_search_tree.fit(features_scaled, labels_scaled)
```

```
C:\Users\Rapha\anaconda3\envs\python2\lib\site-
packages\sklearn\metrics\classification.py:1113: UndefinedMetricWarning: F-score
is ill-defined and being set to 0.0 due to no predicted samples.
  'precision', 'predicted', average, warn_for)
```

[57]:
```
GridSearchCV(cv=10, error_score='raise',
       estimator=Pipeline(steps=[('select_features', SelectKBest(k=10,
score_func=<function f_classif at 0x000000000C4FB5F8>)), ('classify',
DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=None,
            max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            presort=False, random_state=None, splitter='best'))]),
       fit_params={}, iid=True, n_jobs=1,
       param_grid=[{'select_features__k': array([ 1,  2,  3,  4,  5,  6,  7,  8,
9, 10, 11, 12, 13, 14, 15, 16, 17,
       18, 19, 20, 21, 22, 23])}],
       pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
       scoring='f1', verbose=0)
```

[58]:
```
grid_search_tree.best_params_
```

[58]:
```
{'select_features__k': 18}
```

[59]:
```
grid_search_tree.best_score_
```

[59]:
```
0.67245370370370372
```

The GridSearch with SelectKBest states that the optimal number of features for the DecisionTreeClassifier is 18 out of 24 that we have at our disposal. The corresponding score that was achieved with the 18 best features is not too bad either.

Randomized Search with SelektKBest for DecisionTreeClassifier When tuning the hyperparameters of an estimator, Grid Search and Random Search are both popular methods. According to some publications random search is even perceived as the better method depending on the type of problem. That is why I wanted to see how it performs in direct comparison although the requirement for this project is to use GridSearch.

[60]:
```
param_dist = {'select_features__k': n_features}
```

[61]:
```
random_search_tree = RandomizedSearchCV(pipe, param_dist, scoring='f1', cv = 10)
random_search_tree.fit(features, labels)
```

[61]:
```
RandomizedSearchCV(cv=10, error_score='raise',
          estimator=Pipeline(steps=[('select_features', SelectKBest(k=10,
score_func=<function f_classif at 0x000000000C4FB5F8>)), ('classify',
DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=None,
            max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            presort=False, random_state=None, splitter='best'))]),
          fit_params={}, iid=True, n_iter=10, n_jobs=1,
          param_distributions={'select_features__k': array([ 1,  2,  3,  4,  5,
6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16, 17,
       18, 19, 20, 21, 22, 23])},
          pre_dispatch='2*n_jobs', random_state=None, refit=True,
          return_train_score=True, scoring='f1', verbose=0)
```

[62]:
```
random_search_tree.best_params_
```

[62]:
```
{'select_features__k': 21}
```

[63]:
```
random_search_tree.best_score_
```

[63]:
```
0.65509259259259267
```

RandomSearch returns a k-value of 21 resulting in a lower F1-score than with the 18 features that GridSearch identified as best. So in this case GridSearch returns a better result.

Grid Search with SelektKBest for AdaBoost Classifier Same as we just did for DecisionTree now for AdaBosst

[64]:
```
# Create a pipeline with feature selection and classification for AdaBoost
estimators = [
    ('select_features', SelectKBest()),
    ('classify', AdaBoostClassifier())
]

n_features = np.arange(1, len(features_list))

param_grid = [{'select_features__k': n_features}]

pipe = Pipeline(estimators)
```

[65]:
```
grid_search_ada = GridSearchCV(pipe, param_grid=param_grid, scoring='f1', cv=10)
grid_search_ada.fit(features, labels)
```

[65]:
```
GridSearchCV(cv=10, error_score='raise',
       estimator=Pipeline(steps=[('select_features', SelectKBest(k=10,
score_func=<function f_classif at 0x000000000C4FB5F8>)), ('classify',
```

```
AdaBoostClassifier(algorithm='SAMME.R', base_estimator=None,
          learning_rate=1.0, n_estimators=50, random_state=None))]),
       fit_params={}, iid=True, n_jobs=1,
       param_grid=[{'select_features__k': array([ 1,  2,  3,  4,  5,  6,  7,  8,
9, 10, 11, 12, 13, 14, 15, 16, 17,
       18, 19, 20, 21, 22, 23])}],
       pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
       scoring='f1', verbose=0)
```

[66]:
```
grid_search_ada.best_params_
```

[66]:
```
{'select_features__k': 16}
```

[67]:
```
grid_search_ada.best_score_
```

[67]:
```
0.62152777777777779
```

Randomized Search with SelectKBest for AdaBoostClassifier

[68]:
```
param_dist = {'select_features__k': n_features}
```

[69]:
```
random_search_ada = RandomizedSearchCV(pipe, param_dist, scoring='f1', cv = 10)
random_search_ada.fit(features, labels)
```

[69]:
```
RandomizedSearchCV(cv=10, error_score='raise',
          estimator=Pipeline(steps=[('select_features', SelectKBest(k=10,
score_func=<function f_classif at 0x000000000C4FB5F8>)), ('classify',
AdaBoostClassifier(algorithm='SAMME.R', base_estimator=None,
          learning_rate=1.0, n_estimators=50, random_state=None))]),
          fit_params={}, iid=True, n_iter=10, n_jobs=1,
          param_distributions={'select_features__k': array([ 1,  2,  3,  4,  5,
6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16, 17,
       18, 19, 20, 21, 22, 23])},
          pre_dispatch='2*n_jobs', random_state=None, refit=True,
          return_train_score=True, scoring='f1', verbose=0)
```

[70]:
```
random_search_ada.best_params_
```

[70]:
```
{'select_features__k': 16}
```

[71]:
```
random_search_ada.best_score_
```

[71]:
```
0.62152777777777779
```

For AdaBoost however GridSearchCV and RandomSearch deliver the same results. The optimal number of features found by SelectKBest for the AdaBoostClassifier is 16.

For the following RandomForest and GaussianNB I will be running SelectKBest in combination with GridSearch since this is actually the requirement for this project and in the previous cases performed best, or at least equally well.

Grid Search with SelektKBest for RandomForest

[72]:
```
estimators = [
    ('select_features', SelectKBest()),
    ('classify', RandomForestClassifier())
]

n_features = np.arange(1, len(features_list))

param_grid = [{'select_features__k': n_features}]

pipe = Pipeline(estimators)
```

[73]:
```
grid_search_rf = GridSearchCV(pipe, param_grid=param_grid, scoring='f1', cv =10)
grid_search_rf.fit(features, labels)
```

[73]:
```
GridSearchCV(cv=10, error_score='raise',
       estimator=Pipeline(steps=[('select_features', SelectKBest(k=10,
score_func=<function f_classif at 0x000000000C4FB5F8>)), ('classify',
RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
            max_depth=None, max_features='auto', max_leaf_nodes=None,
            min_impu…mators=10, n_jobs=1, oob_score=False, random_state=None,
            verbose=0, warm_start=False))]),
       fit_params={}, iid=True, n_jobs=1,
       param_grid=[{'select_features__k': array([ 1,  2,  3,  4,  5,  6,  7,  8,
9, 10, 11, 12, 13, 14, 15, 16, 17,
       18, 19, 20, 21, 22, 23])}],
       pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
       scoring='f1', verbose=0)
```

[74]:
```
grid_search_rf.best_params_
```

[74]:
```
{'select_features__k': 6}
```

[75]:
```
grid_search_rf.best_score_
```

[75]:
```
0.53356481481481477
```

For the GridSearch of the RandomForestClassifier I chose to apply scaling since I want to use scaled data also for the final testing. For Random Forest the optimal number of features is 21.

Grid Search with SelektKBest for SVM

[76]:
```
# Create a pipeline with feature selection and classification for SVC

estimators = [
    ('select_features', SelectKBest()),
    ('scaler', StandardScaler()),
    ('classify', SVC()),
]
```

```
n_features = np.arange(1, len(features_list))

param_grid = [{'select_features__k': n_features}]

pipe = Pipeline(estimators)

grid_search_svc = GridSearchCV(pipe, param_grid=param_grid, scoring='f1', cv␣
↪=10)
grid_search_svc.fit(features, labels)
```

[76]:
```
GridSearchCV(cv=10, error_score='raise',
       estimator=Pipeline(steps=[('select_features', SelectKBest(k=10,
score_func=<function f_classif at 0x000000000C4FB5F8>)), ('scaler',
StandardScaler(copy=True, with_mean=True, with_std=True)), ('classify',
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma='auto', kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False))]),
       fit_params={}, iid=True, n_jobs=1,
       param_grid=[{'select_features__k': array([ 1,  2,  3,  4,  5,  6,  7,  8,
9, 10, 11, 12, 13, 14, 15, 16, 17,
       18, 19, 20, 21, 22, 23])}],
       pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
       scoring='f1', verbose=0)
```

[77]:
```
grid_search_svc.best_params_
```

[77]:
```
{'select_features__k': 3}
```

[78]:
```
grid_search_svc.best_score_
```

[78]:
```
0.13425925925925924
```

Unfortunately using SelectKBest on SVC did not return a valid result. At least for me 3 features do not really make sense. Therefore I will not do feature selection and run the final classifier with the complete set of features

Grid Search with SelektKBest for GaussianNB

[79]:
```
# Create a pipeline with feature selection and classification for SVC

estimators = [
    ('select_features', SelectKBest()),
    ('classify', GaussianNB()),
]

n_features = np.arange(1, len(features_list))
```

```
param_grid = [{'select_features__k': n_features}]

pipe = Pipeline(estimators)

grid_search_gnb = GridSearchCV(pipe, param_grid=param_grid, scoring='f1', cv␣
 ↪=10)
grid_search_gnb.fit(features, labels)
```

[79]:
```
GridSearchCV(cv=10, error_score='raise',
       estimator=Pipeline(steps=[('select_features', SelectKBest(k=10,
score_func=<function f_classif at 0x000000000C4FB5F8>)), ('classify',
GaussianNB(priors=None))]),
       fit_params={}, iid=True, n_jobs=1,
       param_grid=[{'select_features__k': array([ 1,  2,  3,  4,  5,  6,  7,  8,
9, 10, 11, 12, 13, 14, 15, 16, 17,
       18, 19, 20, 21, 22, 23])}],
       pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
       scoring='f1', verbose=0)
```

[80]:
```
grid_search_gnb.best_params_
```

[80]:
```
{'select_features__k': 22}
```

[81]:
```
grid_search_gnb.best_score_
```

[81]:
```
0.37638888888888888
```

For GaussionNB the optimal number of features is 22.

1.11 Testing the classifiers with optimal number of features

Now that I know the optimal number of features for each individual classifier I want to test the classifiers with their respective best number of features using the tester.py script.

[89]:
```
# Create the classifier with the optimal hyperparameters as found by␣
 ↪GridSearchCV
tree_clf_kbest = Pipeline([
    ('select_features', SelectKBest(k=18)),
    ('classify', DecisionTreeClassifier()),
])
# Test the classifier using tester.py
tester.dump_classifier_and_data(tree_clf_kbest, my_dataset, features_list)
tester.main()
```

```
Pipeline(steps=[('select_features', SelectKBest(k=18, score_func=<function
f_classif at 0x000000000C4FB5F8>)), ('classify',
DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=None,
            max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
```

```
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            presort=False, random_state=None, splitter='best'))])
        Accuracy: 0.89927       Precision: 0.62367      Recall: 0.61650 F1:
0.62007     F2: 0.61792
        Total predictions: 15000        True positives: 1233    False positives:
744   False negatives:  767   True negatives: 12256
```

For the DecisionTree again I took the unscaled data. I tried both but the unscaled yielded a higher performance here even though in the out-of-the-box run it performed better with the scaled data.

[90]:

```
# Create the classifier with the optimal hyperparameters as found by␣
 ↪GridSearchCV
ada_clf_kbest = Pipeline([
    ('select_features', SelectKBest(k=16)),
    ('classify', AdaBoostClassifier()),
])
# Test the classifier using tester.py
tester.dump_classifier_and_data(ada_clf_kbest, my_dataset, features_list)
tester.main()
```

```
Pipeline(steps=[('select_features', SelectKBest(k=16, score_func=<function
f_classif at 0x000000000C4FB5F8>)), ('classify',
AdaBoostClassifier(algorithm='SAMME.R', base_estimator=None,
          learning_rate=1.0, n_estimators=50, random_state=None))])
        Accuracy: 0.88927       Precision: 0.60180      Recall: 0.50100 F1:
0.54679     F2: 0.51837
        Total predictions: 15000        True positives: 1002    False positives:
663   False negatives:  998   True negatives: 12337
```

[91]:

```
# Create the classifier with the optimal hyperparameters as found by␣
 ↪GridSearchCV
rf_clf_kbest = Pipeline([
    ('select_features', SelectKBest(k=6)),
    ('classify', RandomForestClassifier()),
])
# Test the classifier using tester.py
tester.dump_classifier_and_data(rf_clf_kbest, my_dataset, features_list)
tester.main()
```

```
Pipeline(steps=[('select_features', SelectKBest(k=6, score_func=<function
f_classif at 0x000000000C4FB5F8>)), ('classify',
RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
            max_depth=None, max_features='auto', max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            n_estimators=10, n_jobs=1, oob_score=False, random_state=None,
            verbose=0, warm_start=False))])
```

```
        Accuracy: 0.86853       Precision: 0.51333      Recall: 0.26950 F1:
0.35344     F2: 0.29779
        Total predictions: 15000        True positives:  539    False positives:
511   False negatives: 1461   True negatives: 12489
```

[94]:
```
# Create the classifier with the optimal hyperparameters as found by␣
 ↪GridSearchCV
gnb_clf_kbest = Pipeline([
    ('select_features', SelectKBest(k=22)),
    ('classify', GaussianNB()),
])
# Test the classifier using tester.py
tester.dump_classifier_and_data(gnb_clf_kbest, my_dataset, features_list)
tester.main()
```

```
Pipeline(steps=[('select_features', SelectKBest(k=22, score_func=<function
f_classif at 0x000000000C4FB5F8>)), ('classify', GaussianNB(priors=None))])
        Accuracy: 0.77707       Precision: 0.26569      Recall: 0.38100 F1:
0.31306     F2: 0.35057
        Total predictions: 15000        True positives:  762    False positives:
2106   False negatives: 1238   True negatives: 10894
```

1.12 Hyperparameter Tuning

https://en.wikipedia.org/wiki/Hyperparameter_optimization

In machine learning, hyperparameter optimization or tuning is the problem of choosing a set of optimal hyperparameters for a learning algorithm. A hyperparameter is a parameter whose value is used to control the learning process. The same kind of machine learning model can require different constraints, weights or learning rates to generalize different data patterns. These measures are called hyperparameters, and have to be tuned so that the model can optimally solve the machine learning problem.Cross-validation is often used to estimate this generalization performance. The traditional way of performing hyperparameter optimization is grid search or randomized search. Grid search is simply an exhaustive searching through a manually specified subset of the hyperparameter space of a learning algorithm. A grid search algorithm must be guided by some performance metric, typically measured by cross-validation on the training set or evaluation on a held-out validation set. Random Search replaces the exhaustive enumeration of all combinations by selecting them randomly. It can outperform Grid search, especially when only a small number of hyperparameters affects the final performance of the machine learning algorithm.

Decision Tree

[95]:
```
# Create a pipeline with feature selection and classifier

tree_pipe = Pipeline([
    ('select_features', SelectKBest(k=18)),
    ('classify', DecisionTreeClassifier()),
])
```

```python
# Define the configuration of parameters to test with the
# Decision Tree Classifier
param_grid = dict(classify__criterion = ['gini', 'entropy'],
                  classify__splitter = ['best', 'random'],
                  classify__max_depth = [None, 5, 10, 15, 20],
                  classify__min_samples_split = [2, 4, 6, 8, 10, 20, 40],
                  classify__min_samples_leaf = [2, 4, 6, 8, 10, 20, 40],
                  classify__max_features = [None, 'sqrt', 'log2', 'auto'])

# Use GridSearchCV to find the optimal hyperparameters for the classifier
tree_clf_tuned = GridSearchCV(tree_pipe, param_grid = param_grid, scoring='f1',␣
 ↪cv=10)
tree_clf_tuned.fit(features, labels)
```

[95]:
```
GridSearchCV(cv=10, error_score='raise',
       estimator=Pipeline(steps=[('select_features', SelectKBest(k=18,
score_func=<function f_classif at 0x000000000C4FB5F8>)), ('classify',
DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=None,
            max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            presort=False, random_state=None, splitter='best'))]),
       fit_params={}, iid=True, n_jobs=1,
       param_grid={'classify__splitter': ['best', 'random'],
'classify__criterion': ['gini', 'entropy'], 'classify__min_samples_split': [2,
4, 6, 8, 10, 20, 40], 'classify__max_depth': [None, 5, 10, 15, 20],
'classify__max_features': [None, 'sqrt', 'log2', 'auto'],
'classify__min_samples_leaf': [2, 4, 6, 8, 10, 20, 40]},
       pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
       scoring='f1', verbose=0)
```

[96]:
```python
tree_clf_tuned.best_score_
```

[96]:
```
0.7592592592592593
```

[97]:
```python
tree_clf_tuned.best_params_
```

[97]:
```
{'classify__criterion': 'entropy',
 'classify__max_depth': None,
 'classify__max_features': None,
 'classify__min_samples_leaf': 2,
 'classify__min_samples_split': 20,
 'classify__splitter': 'best'}
```

AdaBoost

[98]:
```
from sklearn.ensemble import RandomForestClassifier

# Create the pipeline with feature selection and AdaBoostClassifier
ada_pipe = Pipeline([('select_features', SelectKBest(k=16)),
                     ('classify', AdaBoostClassifier())
                    ])

# Define the parameter configurations to test with GridSearchCV
param_grid = dict(classify__base_estimator=[DecisionTreeClassifier(),␣
↪RandomForestClassifier(), GaussianNB()],
                  classify__n_estimators = [50, 100, 150, 200],
                  classify__learning_rate = [0.5, 1, 1.5, 2, 4])

# Use GridSearchCV to automate the process of finding the optimal parameters
ada_clf_tuned = GridSearchCV(ada_pipe, param_grid=param_grid, scoring='f1',␣
↪cv=10)
ada_clf_tuned.fit(features, labels)
```

```
C:\Users\Rapha\anaconda3\envs\python2\lib\site-
packages\sklearn\naive_bayes.py:232: RuntimeWarning: invalid value encountered
in divide
  new_mu = np.average(X, axis=0, weights=sample_weight / n_new)
C:\Users\Rapha\anaconda3\envs\python2\lib\site-
packages\sklearn\naive_bayes.py:234: RuntimeWarning: invalid value encountered
in divide
  weights=sample_weight / n_new)
C:\Users\Rapha\anaconda3\envs\python2\lib\site-
packages\sklearn\naive_bayes.py:427: RuntimeWarning: divide by zero encountered
in log
  jointi = np.log(self.class_prior_[i])
C:\Users\Rapha\anaconda3\envs\python2\lib\site-
packages\sklearn\ensemble\weight_boosting.py:288: RuntimeWarning: invalid value
encountered in less
  proba[proba < np.finfo(proba.dtype).eps] = np.finfo(proba.dtype).eps
C:\Users\Rapha\anaconda3\envs\python2\lib\site-
packages\sklearn\ensemble\weight_boosting.py:603: RuntimeWarning: invalid value
encountered in greater
  return self.classes_.take(pred > 0, axis=0)
C:\Users\Rapha\anaconda3\envs\python2\lib\site-
packages\sklearn\ensemble\weight_boosting.py:519: RuntimeWarning: invalid value
encountered in less
  proba[proba < np.finfo(proba.dtype).eps] = np.finfo(proba.dtype).eps
C:\Users\Rapha\anaconda3\envs\python2\lib\site-
packages\sklearn\ensemble\weight_boosting.py:531: RuntimeWarning: invalid value
encountered in less
  (estimator_weight < 0)))
C:\Users\Rapha\anaconda3\envs\python2\lib\site-
packages\sklearn\ensemble\weight_boosting.py:530: RuntimeWarning: invalid value
```

```
encountered in greater
  ((sample_weight > 0) |
```

[98]:
```
GridSearchCV(cv=10, error_score='raise',
       estimator=Pipeline(steps=[('select_features', SelectKBest(k=16,
score_func=<function f_classif at 0x000000000C4FB5F8>)), ('classify',
AdaBoostClassifier(algorithm='SAMME.R', base_estimator=None,
          learning_rate=1.0, n_estimators=50, random_state=None))]),
       fit_params={}, iid=True, n_jobs=1,
       param_grid={'classify__learning_rate': [0.5, 1, 1.5, 2, 4],
'classify__n_estimators': [50, 100, 150, 200], 'classify__base_estimator':
[DecisionTreeClassifier(class_weight=None, criterion='gini', max_depth=None,
            max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07…_score=False, random_state=None,
            verbose=0, warm_start=False), GaussianNB(priors=None)]},
       pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
       scoring='f1', verbose=0)
```

[99]:
```python
ada_clf_tuned.best_score_
```

[99]:
```
0.66435185185185186
```

[100]:
```python
ada_clf_tuned.best_params_
```

[100]:
```
{'classify__base_estimator': DecisionTreeClassifier(class_weight=None,
criterion='gini', max_depth=None,
             max_features=None, max_leaf_nodes=None,
             min_impurity_split=1e-07, min_samples_leaf=1,
             min_samples_split=2, min_weight_fraction_leaf=0.0,
             presort=False, random_state=None, splitter='best'),
 'classify__learning_rate': 4,
 'classify__n_estimators': 200}
```

RandomForest

[101]:
```python
# Create a pipeline with feature selection and classifier
rf_pipe = Pipeline([
    ('select_features', SelectKBest(k=6)),
    ('classify', RandomForestClassifier()),
])

# Define the configuration of parameters to test with the
# Random Forest Classifier
param_grid = dict(classify__n_estimators = [5, 10, 50, 100, 200],
                  classify__criterion = ['gini', 'entropy'],
                  classify__max_depth = [None, 4, 5, 6, 7, 8],
#                  classify__min_samples_split = [2, 4, 6, 8, 10, 20],
#                  classify__min_samples_leaf = [2, 4, 6, 8, 10, 20],
#                  classify__max_features = [None, 'sqrt', 'log2', 'auto']
```

```
                 )

# Use GridSearchCV to find the optimal hyperparameters for the classifier
rf_clf_tuned = GridSearchCV(rf_pipe, param_grid = param_grid, scoring='f1',␣
 ↪cv=10)
rf_clf_tuned.fit(features, labels)
```

[101]:
```
GridSearchCV(cv=10, error_score='raise',
       estimator=Pipeline(steps=[('select_features', SelectKBest(k=6,
score_func=<function f_classif at 0x000000000C4FB5F8>)), ('classify',
RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
            max_depth=None, max_features='auto', max_leaf_nodes=None,
            min_impur…mators=10, n_jobs=1, oob_score=False, random_state=None,
            verbose=0, warm_start=False))]),
       fit_params={}, iid=True, n_jobs=1,
       param_grid={'classify__n_estimators': [5, 10, 50, 100, 200],
'classify__criterion': ['gini', 'entropy'], 'classify__max_depth': [None, 4, 5,
6, 7, 8]},
       pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
       scoring='f1', verbose=0)
```

[102]:
```
rf_clf_tuned.best_score_
```

[102]:
```
0.5185185185185185
```

[103]:
```
rf_clf_tuned.best_params_
```

[103]:
```
{'classify__criterion': 'entropy',
 'classify__max_depth': 6,
 'classify__n_estimators': 10}
```

Random Forest comes with a bunch of parameters. I opted for *'criterion'*, *'max_depth'*, *'n_estimator'*. When I select more than that(like the ones that are commented out in above code) the process would take unreasonably long or would not terminate at all.

SVC

[104]:
```
#Using scaling on SVC-classifier since I already saw in chapter "Scaling" that␣
 ↪it tends to improve performance on SVC
# Create a pipeline with feature selection and classifier
svm_pipe = Pipeline(steps=[
    ('scaler', StandardScaler()),
    ('classify', SVC()),
])

# Define the configuration of parameters to test with the SVC Classifier
param_grid = ([{'classify__C': [1, 50, 100, 1000],
                'classify__gamma': [0.5, 0.1, 0.01],
                'classify__degree': [1, 2],
```

```
                'classify__kernel': ['rbf', 'poly', 'linear'],
                'classify__max_iter': [1, 100, 1000]}])

# Use GridSearchCV to find the optimal hyperparameters for the classifier
svm_clf_tuned = GridSearchCV(svm_pipe, param_grid = param_grid, scoring='f1',␣
 ↪cv=10)
svm_clf_tuned.fit(features, labels)
```

```
C:\Users\Rapha\anaconda3\envs\python2\lib\site-packages\sklearn\svm\base.py:220:
ConvergenceWarning: Solver terminated early (max_iter=1).  Consider pre-
processing your data with StandardScaler or MinMaxScaler.
  % self.max_iter, ConvergenceWarning)
C:\Users\Rapha\anaconda3\envs\python2\lib\site-packages\sklearn\svm\base.py:220:
ConvergenceWarning: Solver terminated early (max_iter=100).  Consider pre-
processing your data with StandardScaler or MinMaxScaler.
  % self.max_iter, ConvergenceWarning)
```

[104]:
```
GridSearchCV(cv=10, error_score='raise',
       estimator=Pipeline(steps=[('scaler', StandardScaler(copy=True,
with_mean=True, with_std=True)), ('classify', SVC(C=1.0, cache_size=200,
class_weight=None, coef0=0.0,
  decision_function_shape=None, degree=3, gamma='auto', kernel='rbf',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False))]),
       fit_params={}, iid=True, n_jobs=1,
       param_grid=[{'classify__C': [1, 50, 100, 1000], 'classify__degree': [1,
2], 'classify__max_iter': [1, 100, 1000], 'classify__gamma': [0.5, 0.1, 0.01],
'classify__kernel': ['rbf', 'poly', 'linear']}],
       pre_dispatch='2*n_jobs', refit=True, return_train_score=True,
       scoring='f1', verbose=0)
```

[105]:
```
svm_clf_tuned.best_score_
```

[105]:
```
0.574074074074074
```

[106]:
```
svm_clf_tuned.best_params_
```

[106]:
```
{'classify__C': 1000,
 'classify__degree': 1,
 'classify__gamma': 0.01,
 'classify__kernel': 'rbf',
 'classify__max_iter': 100}
```

GaussianNB For GaussianNB there are no hyperparameters avaiable to tune.

Here is a summary of the hyperparameters obtained from GridSearch and SelectKBest:

Decision Tree Classifier:

Parameter	SelectKBest	criterion	max_depth	max_features	min_samples_split	min_samples_leaf	splitter
Optimal Value	18	'entropy'	None	None	20	2	best

AdaBoost Classifier:

Parameter	SelectKBest	base_estimator	learning_rate	n_estimators
Optimal Value	16	DecisionTreeClassifier	4	200

Random Forest Classifier:

Parameter	SelectKBest	criterion	max_depth	n_estimators
Optimal Value	6	'entropy'	6	10

SVC Classifier:

Parameter	'C'	degree	gamma	kernel	max_iter
Optimal Value	1000	1	0.01	rbf	100

Gaussian Naive Bayes:

Parameter	SelectKBest
Optimal Value	22

1.13 Final Test

The final step is to implement the optimal hyper parameters into the models and to finally test the classifiers with that configuration using the provided tester function.

Decision Tree

[108]:
```
tester.dump_classifier_and_data(tree_clf_tuned.best_estimator_, my_dataset,␣
 ↪features_list)
tester.main()
```

```
Pipeline(steps=[('select_features', SelectKBest(k=18, score_func=<function
f_classif at 0x000000000C4FB5F8>)), ('classify',
DecisionTreeClassifier(class_weight=None, criterion='entropy', max_depth=None,
            max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=2,
            min_samples_split=20, min_weight_fraction_leaf=0.0,
            presort=False, random_state=None, splitter='best'))])
        Accuracy: 0.92333       Precision: 0.68398      Recall: 0.79000 F1:
```

```
0.73318      F2: 0.76625
        Total predictions: 15000        True positives: 1580    False positives:
730   False negatives:  420   True negatives: 12270
```

Cross Check: In above cell I queried the results from the DecisionTreeClassifier with the optimal parameters found by grid search using ".best_estimator_". As a cross check I will again build a classifier manually with these exact parameters. The results should be identical. And indeed they are.

[109]:
```
# Implement the Decision Tree Classifier with the optimal parameters
tree_clf_final = Pipeline([
    ('select_features', SelectKBest(k=18)),
    ('classify', DecisionTreeClassifier(criterion='entropy', splitter='best',␣
 ↪,max_depth=None, max_features=None, min_samples_leaf=2,␣
 ↪min_samples_split=20))
])

# Test the classifier with cross-validation
tester.dump_classifier_and_data(tree_clf_final, my_dataset, features_list)
tester.main()
```

```
Pipeline(steps=[('select_features', SelectKBest(k=18, score_func=<function
f_classif at 0x000000000C4FB5F8>)), ('classify',
DecisionTreeClassifier(class_weight=None, criterion='entropy', max_depth=None,
            max_features=None, max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=2,
            min_samples_split=20, min_weight_fraction_leaf=0.0,
            presort=False, random_state=None, splitter='best'))])
        Accuracy: 0.92240       Precision: 0.68017      Recall: 0.78900 F1:
0.73056      F2: 0.76453
        Total predictions: 15000        True positives: 1578    False positives:
742   False negatives:  422   True negatives: 12258
```

AdaBoost

[110]:
```
# Test the classifier with cross-validation
tester.dump_classifier_and_data(ada_clf_tuned.best_estimator_, my_dataset,␣
 ↪features_list)
tester.main()
```

```
Pipeline(steps=[('select_features', SelectKBest(k=16, score_func=<function
f_classif at 0x000000000C4FB5F8>)), ('classify',
AdaBoostClassifier(algorithm='SAMME.R',
          base_estimator=DecisionTreeClassifier(class_weight=None,
criterion='gini', max_depth=None,
            max_features=None, max_leaf_node…ndom_state=None,
splitter='best'),
          learning_rate=4, n_estimators=200, random_state=None))])
```

```
        Accuracy: 0.89887       Precision: 0.62391      Recall: 0.60800 F1:
0.61585     F2: 0.61112
        Total predictions: 15000        True positives: 1216    False positives:
733   False negatives:  784   True negatives: 12267
```

Random Forest

[111]:
```
tester.dump_classifier_and_data(rf_clf_tuned.best_estimator_, my_dataset,␣
 ↪features_list)
tester.main()
```

```
Pipeline(steps=[('select_features', SelectKBest(k=6, score_func=<function
f_classif at 0x000000000C4FB5F8>)), ('classify',
RandomForestClassifier(bootstrap=True, class_weight=None, criterion='entropy',
            max_depth=6, max_features='auto', max_leaf_nodes=None,
            min_impurity_split=1e-07, min_samples_leaf=1,
            min_samples_split=2, min_weight_fraction_leaf=0.0,
            n_estimators=10, n_jobs=1, oob_score=False, random_state=None,
            verbose=0, warm_start=False))])
        Accuracy: 0.86600       Precision: 0.49545      Recall: 0.27200 F1:
0.35119     F2: 0.29897
        Total predictions: 15000        True positives:  544    False positives:
554   False negatives: 1456   True negatives: 12446
```

SVC

[112]:
```
tester.dump_classifier_and_data(svm_clf_tuned.best_estimator_, my_dataset,␣
 ↪features_list)
tester.main()
```

```
Pipeline(steps=[('scaler', StandardScaler(copy=True, with_mean=True,
with_std=True)), ('classify', SVC(C=1000, cache_size=200, class_weight=None,
coef0=0.0,
  decision_function_shape=None, degree=1, gamma=0.01, kernel='rbf',
  max_iter=100, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False))])
        Accuracy: 0.89020       Precision: 0.60376      Recall: 0.51350 F1:
0.55499     F2: 0.52933
        Total predictions: 15000        True positives: 1027    False positives:
674   False negatives:  973   True negatives: 12326
```

In case of the SVC I applied standard scaling since SVMs require standardized data.

GaussianNB No parameter tuning performed. Hence, same results as in chapter "Testing the classifiers with optimal number of features".

[113]:
```
tester.dump_classifier_and_data(gnb_clf_kbest, my_dataset, features_list)
tester.main()
```

```
Pipeline(steps=[('select_features', SelectKBest(k=22, score_func=<function
f_classif at 0x000000000C4FB5F8>)), ('classify', GaussianNB(priors=None))])
        Accuracy: 0.77707       Precision: 0.26569      Recall: 0.38100 F1:
0.31306     F2: 0.35057
        Total predictions: 15000        True positives:  762    False positives:
2106   False negatives: 1238   True negatives: 10894
```

At last here is a summary of my final results:

Algorithm	Accuracy	Precision	Recall	F1 Score
DecisionTree	0.923	0.684	0.790	0.733
AdaBoost	0.899	0.624	0.608	0.616
RandomForest	0.866	0.495	0.272	0.351
SVC	0.890	0.604	0.514	0.555
GaussianNB	0.777	0.266	0.381	0.313

The best performing algorithm is pretty clearly the DecisionTreeClassifier. No huge surprise though, since it has already ranged among the best algorithms in the out-of-the-box runs. So if I were to build up a model to identify POIs with machine learning the DecisionTreeClassifier would be the algorithm of my choice.

The weakest performance delivered GaussianNB and RandomForest not even reaching the minimum requirements of this project of 0.3 for precision respectively recall. GaussianNB did not perform too bad in the initial runs but due to the fact that it does not come with any hyperparameter tuning options I was not able to enhance the performance. RandomForest is said to be a very powerful ensemble-algorithm, which is why I did not want to give up on it until the very end hoping that hyperparameter tuning would have a significant effect, but unfortunately not.

1.14 Conclusion

In the process of the project I happened to mix up the terms 'Overfitting' and 'Data Leakage'. Maybe because I didn't fully understand the difference. I thought all of this is kind of what is being referred to as 'Overfitting'. Maybe because both classic overfitting and data leakage will result in a model performing well on training data but poorly on unseen 'real world' data. But nevertheless I think one needs to distinguish between the two.

Overfitting is a complex issue of which every aspiring machine learner should be aware. That is why I want to dedicate my conclusion to this topic.

What is Overfitting? In order to evaluate the performance of a particular ML model, we invariably split the data into two sets including training and testing subsets. The algorithm is trained on the training dataset and evaluated/tested on the test dataset, then it is applied to make predictions on new (unseen) data points. Overfitting occurs when the model performs too well on the training data but poorly on the new data points while the goal is to maximize its accuracy on the unseen data points. This means that the model fails to generalize to unseen data.

I would describe classic overfitting at following example:

For example, in its fundamental nature, an SVC classifier works by recursively drawing a boundary between different classes on the data, that maximizes the distance to the nearest point, also called the margin.

On the one hand this boundary can be as simplistic as a straight line, which generalizes well but doesn't yield optimal results out of a particular situation. On the other hand it can be a twisted, wiggled boundary with an exceptional fit for that situation, but it wouldn't fit other situations. In this case our classifier would be somehow biased by the data and that's a clear example of overfitting.

To avoid such an overfit situation but still yield a good performance we have to find the optimal hyperparameters. This can for example be done using GridSearch or Random Search, as we did in our project.

How to avoid Overfitting: Source: https://elitedatascience.com/overfitting-in-machine-learning

1. Perform Cross Validation
2. Train with more data
3. Remove features
4. Early stopping
5. Regularization
6. Ensembling

What is Data Leakage? When the data you are using to train a machine learning algorithm happens to have the information you are trying to predict.

Overfitting vs. Data Leakage When data leakage occurs, it may lead to overfitting (overly optimistic training accuracy) but the model also performs too well on the test data. As we mentioned, data points are leaked from test set into training set, which means the model will predict something it learned/saw (but we think it is unseen data points) while overfitting may lead to poor generalization performance of a predictive model.

How to avoid Data Leackage: Source: https://machinelearningmastery.com/data-leakage-machine-learning/

1. Perform data preparation within cross validation folds
2. Hold back a validation dataset

Generally, it is good practice to use both of these techniques.

1. Perform Data Preparation Within Cross Validation Folds You can easily leak information when preparing your data for machine learning. The effect is overfitting your training data and having an overly optimistic evaluation of your models performance on unseen data. For example, if you normalize or standardize your entire dataset, then estimate the performance of your model using cross validation, you have committed the sin of data leakage.The data rescaling process that you performed had knowledge of the full distribution of data in the training dataset when calculating the scaling factors (like min and max or mean and standard deviation). This knowledge was stamped into the rescaled values and exploited by all algorithms in your cross validation test harness. A non-leaky evaluation of machine learning

algorithms in this situation would calculate the parameters for rescaling data within each fold of the cross validation and use those parameters to prepare the data on the held out test fold on each cycle.

2. Hold Back a Validation Dataset Another, perhaps simpler approach is to split your training dataset into train and validation sets, and store away the validation dataset. Once you have completed your modeling process and actually created your final model, evaluate it on the validation dataset. This can give you a sanity check to see if your estimation of performance has been overly optimistic and has leaked.