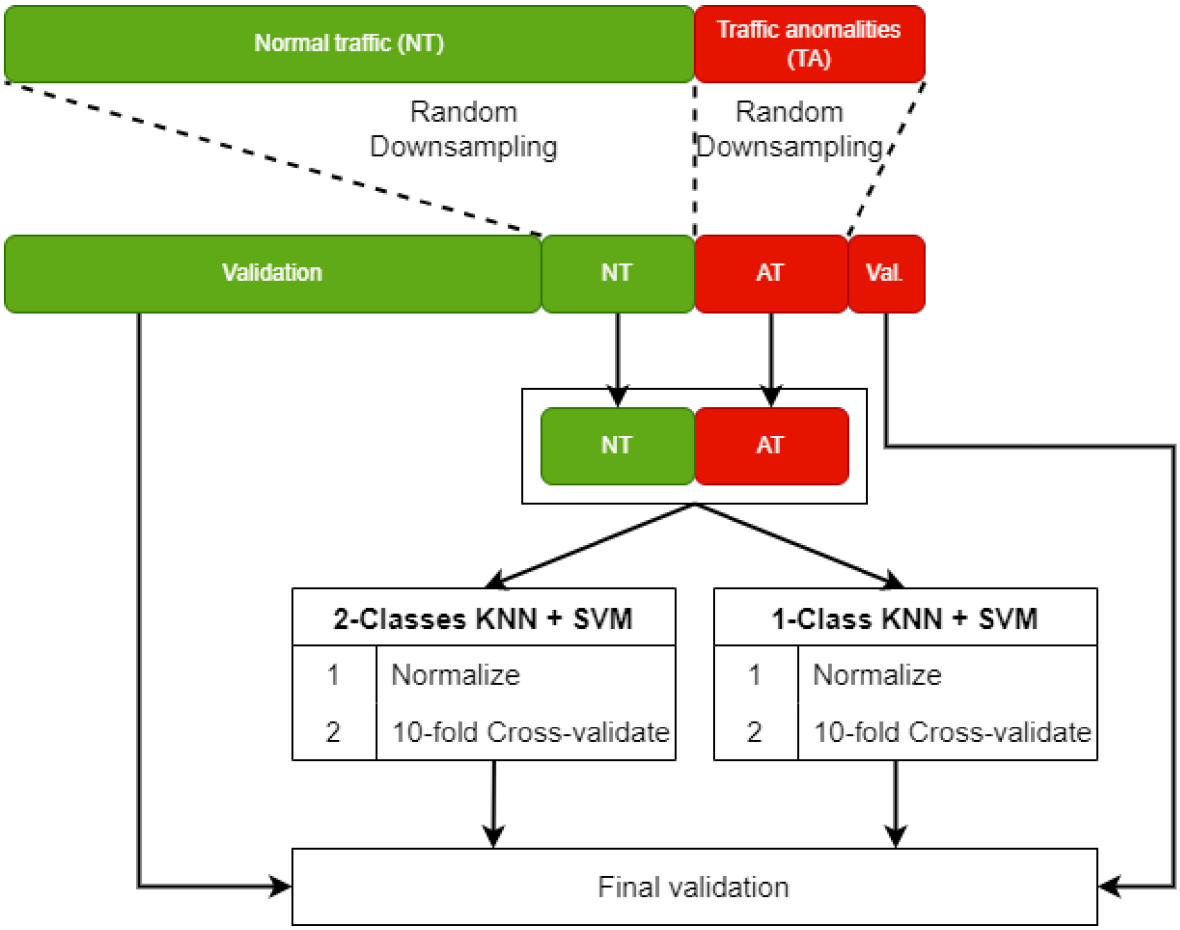
Binary Classification vs. Anomaly Detection with KNN and SVM

Description of experiment:

- dataset contains two classes (normal=-1, abnormal=+1)
- 2000 rows of normal data, 200 rows of abnormal data
- The procedure is shown in the graphic below. Both the normal traffic and the anomaly traffic data are downsampled to, on the one hand, keep some anomaly traffic for the final validation stage; on the second hand, the downsampling allows us to obtain a balanced data set for training the two-classes problems.
- The remaining data not used in the training and testing of the models is preserved for the final validation stage.
- Once the data is downsampled, it is normalized and a 10-fold cross validation is carried out independently for the two-classes problem and for the one-class problem, although the same random seed is used to obtain the same partitions in each case for comparison reasons.
- In the two-classes problem, all the partitions may include normal and anomaly instances. However, in the one-class problem, the partitions are prepared only with the normal traffic instances; the anomaly instances are used to measure the performance of the models obtained for each fold. Interestingly, the normalization for the one-class problem is determined exclusively with data from normal traffic only.
- A final validation stage includes all the data that has not been used in training and testing; this is an unbalanced data set containing instances from normal traffic and from anomalies.
- The aim of this validation stage is to compare the behavior of the different modeling techniques included in this comparison, so conclusions could be extracted.
- the "normal" traffic (2000 lines) is the "negative class", while the "abnormal" traffic (200 lines) is the "positive class"

Design of experiment



In [1]:
```
# This jupyter notebook is based on # Stat479: Machine Learning -- L02: kNN in Python
# https://github.com/rasbt/stat479-machine-learning-fs18/blob/master/02_knn/02_knn_dem
```

1 - choose the learning algorithm (KNN, SVM)

In [2]:
```
# adjust the modeltype=KNN|SVM variable to run different algorithms

#modeltype="OneClassKNN"  #adjust this variable to run the subsequent steps using the
modeltype="OneClassSVM"  #adjust this variable to run the subsequent steps using the S
#modeltype="TwoClassKNN"   #adjust this variable to run the subsequent steps using the
#modeltype="TwoClassSVM"  #adjust this variable to run the subsequent steps using the



#The entire dataset is heavily skewed towards the negative class, with only a small am
#In other words, the entire dataset is "unbalanced".
#You can set dataset_type=balanced   to artificially balance the negative/positive cla
#Setting     dataset_type=unbalanced will use the dataset as-is, with approx 10x more
#Using balanced vs unbalanced data can affect the accuracy of the learning models beca

dataset_type="balanced"
#dataset_type="unbalanced"

print ("The subsequent steps in this jupyter notebook will use the", modeltype,"algori
```

The subsequent steps in this jupyter notebook will use the OneClassSVM algorithm with a dataset that is balanced

2 - Import required packages

In [3]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import math  #get square root function


from sklearn.neighbors import KNeighborsClassifier  #2-class (supervised, with labels)
from sklearn import svm                             #2-class (supervised, with labels)
from sklearn.svm import OneClassSVM                 #1-class (unsupervised, no labels)
from sklearn.neighbors import NearestNeighbors      #1-class (unsupervised, no labels)

from sklearn.preprocessing   import MinMaxScaler
from sklearn.metrics         import confusion_matrix
from sklearn.model_selection import StratifiedKFold    #for cross-validation
from sklearn.model_selection import GridSearchCV       #for cross-validation
```

3 - Load Dataset into a Pandas DataFrame

In [4]:
```
#df_data = pd.read_csv('c:/temp/data7.csv')  # this data has not been scaled/normalize
df_data = pd.read_csv('https://raw.githubusercontent.com/nickjeffrey/sklearn/master/da
```

In [5]:
```
# look at the top few rows of the data (should show the abnormal class in column 35)
df_data.head()
```

Out[5]:

	seconds_since_epoch	datestamp	sp1_watts_generated	sp2_watts_generated	sp3_watts_generated	i
0	1673334002	1/10/2023 0:00	0.0	0.0	0.0	
1	1673334062	1/10/2023 0:01	0.0	0.0	0.0	
2	1673334122	1/10/2023 0:02	0.0	0.0	0.0	
3	1673334182	1/10/2023 0:03	0.0	0.0	0.0	
4	1673334242	1/10/2023 0:04	0.0	0.0	0.0	

5 rows × 35 columns

In [6]:
```
# look at the bottom few rows of the data (should show the normal class in column 35)
df_data.tail()
```

Out[6]:

	seconds_since_epoch	datestamp	sp1_watts_generated	sp2_watts_generated	sp3_watts_generate
2195	1673453753	9:15	32.72	32.85	32.2
2196	1673453813	9:16	27.34	30.48	29.7
2197	1673453873	9:17	27.96	28.65	28.0
2198	1673453933	9:18	33.00	30.94	29.7
2199	1673453993	9:19	31.08	32.72	31.6

5 rows × 35 columns

In [7]:
```
# show number of rows in dataset
print ("Rows in dataset:", len(df_data))
```

```
Rows in dataset: 2200
```

In [8]:
```
#view dimensions of dataset (rows and columns)
print ("Rows,columns in dataset:", df_data.shape)
```

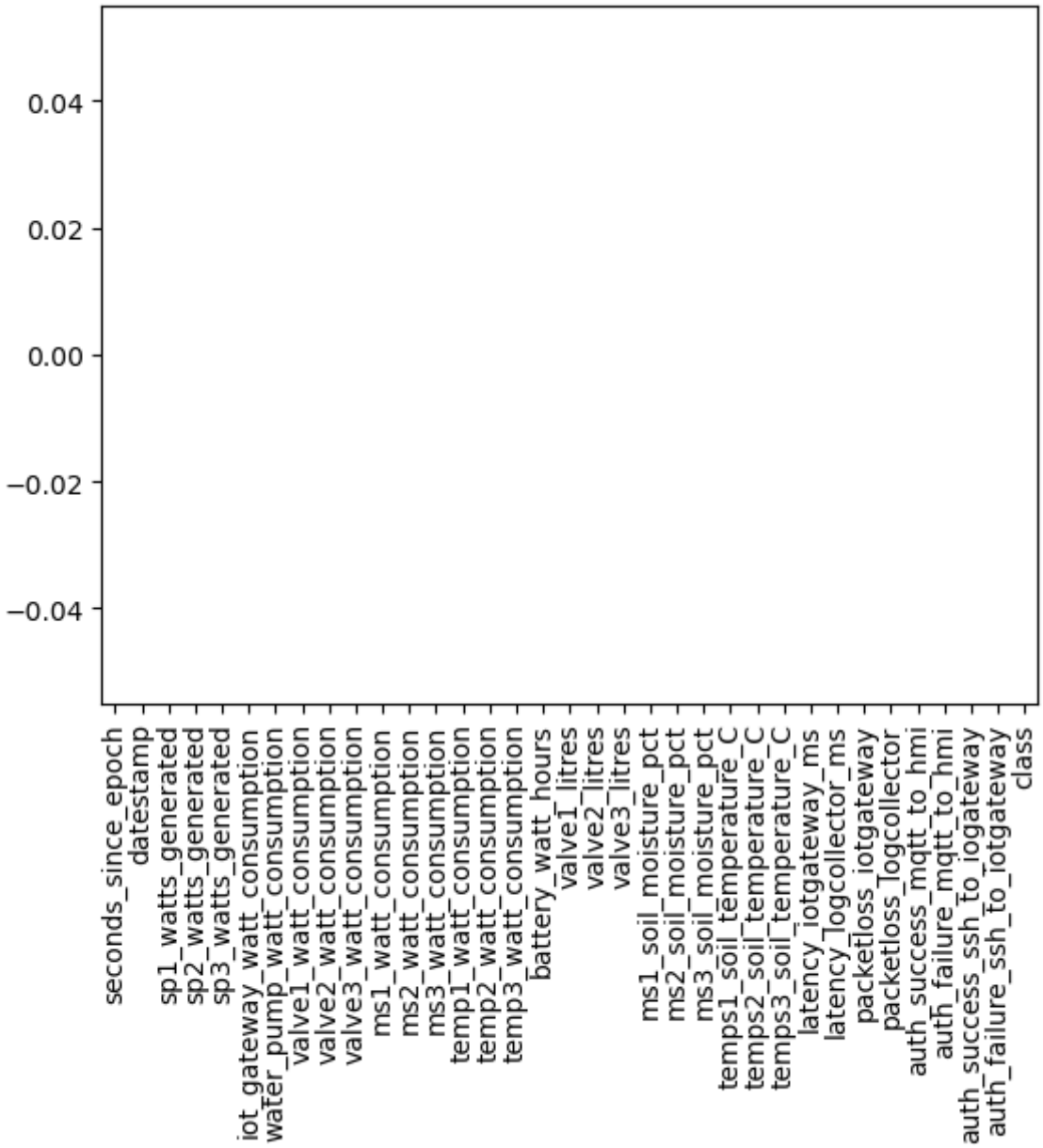
```
Rows,columns in dataset: (2200, 35)
```

In [9]:
```
# check to see if there are any missing values from the dataset

# all of the results should be zero, which would indicate there are not any null value
# if there are any results greater than zero, it would indicate that some pieces of da
df_data.isnull().sum()
```

Out[9]:
```
seconds_since_epoch               0
datestamp                         0
sp1_watts_generated               0
sp2_watts_generated               0
sp3_watts_generated               0
iot_gateway_watt_consumption      0
water_pump_watt_consumption       0
valve1_watt_consumption           0
valve2_watt_consumption           0
valve3_watt_consumption           0
ms1_watt_consumption              0
ms2_watt_consumption              0
ms3_watt_consumption              0
temp1_watt_consumption            0
temp2_watt_consumption            0
temp3_watt_consumption            0
battery_watt_hours                0
valve1_litres                     0
valve2_litres                     0
valve3_litres                     0
ms1_soil_moisture_pct             0
ms2_soil_moisture_pct             0
ms3_soil_moisture_pct             0
temps1_soil_temperature_C         0
temps2_soil_temperature_C         0
temps3_soil_temperature_C         0
latency_iotgateway_ms             0
latency_logcollector_ms           0
packetloss_iotgateway             0
packetloss_logcollector           0
auth_success_mqtt_to_hmi          0
auth_failure_mqtt_to_hmi          0
auth_success_ssh_to_iogateway     0
auth_failure_ssh_to_iotgateway    0
class                             0
dtype: int64
```

In [10]:
```
# show frequency distribution of values in variables
# this shows how many different values are in each feature
# HINT: this would be more useful to display in a histogram.  For example, bin values

#for var in df_data.columns:
#    print(df_data[var].value_counts())
```

In [11]:
```
# visualize any missing values from the dataset in a histogram
# you want all the bars in the graph to be empty, which would indicate zero missing va

df_data.isnull().sum().plot.bar()
plt.show()
```



In [12]:
```python
# another method to visalize missing values from dataset

print ("Checking for missing values in data set")

import matplotlib.pyplot as plt
def plot_nas(df_data: pd.DataFrame):
    if df_data.isnull().sum().sum() != 0:
        na_df = (df_data.isnull().sum() / len(df)) * 100
        na_df = na_df.drop(na_df[na_df == 0].index).sort_values(ascending=False)
        missing_data = pd.DataFrame({'Missing Ratio %' :na_df})
        missing_data.plot(kind = "barh")
        plt.show()
    else:
        print('No NAs found')
plot_nas(df_data)
```

```
Checking for missing values in data set
No NAs found
```

In [13]:
```python
#show the names of the columns (also called feature names)
df_data.columns
```

Out[13]:
```
Index(['seconds_since_epoch', 'datestamp', 'sp1_watts_generated',
       'sp2_watts_generated', 'sp3_watts_generated',
       'iot_gateway_watt_consumption', 'water_pump_watt_consumption',
       'valve1_watt_consumption', 'valve2_watt_consumption',
       'valve3_watt_consumption', 'ms1_watt_consumption',
       'ms2_watt_consumption', 'ms3_watt_consumption',
       'temp1_watt_consumption', 'temp2_watt_consumption',
       'temp3_watt_consumption', 'battery_watt_hours', 'valve1_litres',
       'valve2_litres', 'valve3_litres', 'ms1_soil_moisture_pct',
       'ms2_soil_moisture_pct', 'ms3_soil_moisture_pct',
       'temps1_soil_temperature_C', 'temps2_soil_temperature_C',
       'temps3_soil_temperature_C', 'latency_iotgateway_ms',
       'latency_logcollector_ms', 'packetloss_iotgateway',
       'packetloss_logcollector', 'auth_success_mqtt_to_hmi',
       'auth_failure_mqtt_to_hmi', 'auth_success_ssh_to_iogateway',
       'auth_failure_ssh_to_iotgateway', 'class'],
      dtype='object')
```

In [14]:
```
#show summary info about dataset
df_data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 2200 entries, 0 to 2199
Data columns (total 35 columns):
 #   Column                          Non-Null Count  Dtype  
---  ------                          --------------  -----  
 0   seconds_since_epoch             2200 non-null   int64  
 1   datestamp                       2200 non-null   object 
 2   sp1_watts_generated             2200 non-null   float64
 3   sp2_watts_generated             2200 non-null   float64
 4   sp3_watts_generated             2200 non-null   float64
 5   iot_gateway_watt_consumption    2200 non-null   float64
 6   water_pump_watt_consumption     2200 non-null   float64
 7   valve1_watt_consumption         2200 non-null   float64
 8   valve2_watt_consumption         2200 non-null   float64
 9   valve3_watt_consumption         2200 non-null   float64
 10  ms1_watt_consumption            2200 non-null   float64
 11  ms2_watt_consumption            2200 non-null   float64
 12  ms3_watt_consumption            2200 non-null   float64
 13  temp1_watt_consumption          2200 non-null   float64
 14  temp2_watt_consumption          2200 non-null   float64
 15  temp3_watt_consumption          2200 non-null   float64
 16  battery_watt_hours              2200 non-null   float64
 17  valve1_litres                   2200 non-null   float64
 18  valve2_litres                   2200 non-null   float64
 19  valve3_litres                   2200 non-null   float64
 20  ms1_soil_moisture_pct           2200 non-null   float64
 21  ms2_soil_moisture_pct           2200 non-null   float64
 22  ms3_soil_moisture_pct           2200 non-null   float64
 23  temps1_soil_temperature_C       2200 non-null   float64
 24  temps2_soil_temperature_C       2200 non-null   float64
 25  temps3_soil_temperature_C       2200 non-null   float64
 26  latency_iotgateway_ms           2200 non-null   float64
 27  latency_logcollector_ms         2200 non-null   float64
 28  packetloss_iotgateway           2200 non-null   float64
 29  packetloss_logcollector         2200 non-null   float64
 30  auth_success_mqtt_to_hmi        2200 non-null   int64  
 31  auth_failure_mqtt_to_hmi        2200 non-null   int64  
 32  auth_success_ssh_to_iogateway   2200 non-null   int64  
 33  auth_failure_ssh_to_iotgateway  2200 non-null   int64  
 34  class                           2200 non-null   object 
dtypes: float64(28), int64(5), object(2)
memory usage: 601.7+ KB
```

In [15]:
```
# show data types
df_data.dtypes
```

Out[15]:
```
seconds_since_epoch                int64
datestamp                         object
sp1_watts_generated              float64
sp2_watts_generated              float64
sp3_watts_generated              float64
iot_gateway_watt_consumption     float64
water_pump_watt_consumption      float64
valve1_watt_consumption          float64
valve2_watt_consumption          float64
valve3_watt_consumption          float64
ms1_watt_consumption             float64
ms2_watt_consumption             float64
ms3_watt_consumption             float64
temp1_watt_consumption           float64
temp2_watt_consumption           float64
temp3_watt_consumption           float64
battery_watt_hours               float64
valve1_litres                    float64
valve2_litres                    float64
valve3_litres                    float64
ms1_soil_moisture_pct            float64
ms2_soil_moisture_pct            float64
ms3_soil_moisture_pct            float64
temps1_soil_temperature_C        float64
temps2_soil_temperature_C        float64
temps3_soil_temperature_C        float64
latency_iotgateway_ms            float64
latency_logcollector_ms          float64
packetloss_iotgateway            float64
packetloss_logcollector          float64
auth_success_mqtt_to_hmi           int64
auth_failure_mqtt_to_hmi           int64
auth_success_ssh_to_iogateway      int64
auth_failure_ssh_to_iotgateway     int64
class                             object
dtype: object
```

4 - dimensionality reduction by removing features without predictive value

In [16]:
```
# drop any redundant columns from the dataset which does not have any predictive power

#In this example, seconds_since_epoch and datestamp do not have any predictive value b
df_data.drop('seconds_since_epoch', axis=1, inplace=True)
df_data.drop('datestamp', axis=1, inplace=True)

# the water pump only runs for a brief period once per day, filling up a reservoir hol
# the values are zero for most of the day, so this feature has limited predictive valu
df_data.drop('water_pump_watt_consumption', axis=1, inplace=True)


# These columns are for ping packet loss.
# If the value is ever >0, the data will be in the "abnormal" class.
# In other words, this allows the learning model to "cheat" by ignoring all the other
# So, this particular data feature should be tracked not with machine learning, but wi
df_data.drop('packetloss_iotgateway', axis=1, inplace=True)
df_data.drop('packetloss_logcollector', axis=1, inplace=True)
```

```
# Same issue as the previous ping features.
# These colums are for machine-to-machine data transfers, if the authentication failur
# In other words, this allows the learning model to "cheat" by ignoring all the other
# So, this particular data feature should be tracked not with machine learning, but wi
df_data.drop('auth_failure_mqtt_to_hmi', axis=1, inplace=True)
df_data.drop('auth_failure_ssh_to_iotgateway', axis=1, inplace=True)
```

In [17]:
```
#Look at the dataset again, you should see several columns have been dropped
df_data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 2200 entries, 0 to 2199
Data columns (total 28 columns):
 #   Column                          Non-Null Count  Dtype
---  ------                          --------------  -----
 0   sp1_watts_generated             2200 non-null   float64
 1   sp2_watts_generated             2200 non-null   float64
 2   sp3_watts_generated             2200 non-null   float64
 3   iot_gateway_watt_consumption    2200 non-null   float64
 4   valve1_watt_consumption         2200 non-null   float64
 5   valve2_watt_consumption         2200 non-null   float64
 6   valve3_watt_consumption         2200 non-null   float64
 7   ms1_watt_consumption            2200 non-null   float64
 8   ms2_watt_consumption            2200 non-null   float64
 9   ms3_watt_consumption            2200 non-null   float64
 10  temp1_watt_consumption          2200 non-null   float64
 11  temp2_watt_consumption          2200 non-null   float64
 12  temp3_watt_consumption          2200 non-null   float64
 13  battery_watt_hours              2200 non-null   float64
 14  valve1_litres                   2200 non-null   float64
 15  valve2_litres                   2200 non-null   float64
 16  valve3_litres                   2200 non-null   float64
 17  ms1_soil_moisture_pct           2200 non-null   float64
 18  ms2_soil_moisture_pct           2200 non-null   float64
 19  ms3_soil_moisture_pct           2200 non-null   float64
 20  temps1_soil_temperature_C       2200 non-null   float64
 21  temps2_soil_temperature_C       2200 non-null   float64
 22  temps3_soil_temperature_C       2200 non-null   float64
 23  latency_iotgateway_ms           2200 non-null   float64
 24  latency_logcollector_ms         2200 non-null   float64
 25  auth_success_mqtt_to_hmi        2200 non-null   int64
 26  auth_success_ssh_to_iogateway   2200 non-null   int64
 27  class                           2200 non-null   object
dtypes: float64(25), int64(2), object(1)
memory usage: 481.4+ KB
```

In [18]:
```
# look at the dimensions (rows and columns) of the dataset again after removing a few
#view dimensions of dataset (rows and columns)
print ("Rows,columsn in dataset:")
df_data.shape
```

```
Rows,columsn in dataset:
```

Out[18]:
```
(2200, 28)
```

5 - Get Features into a NumPy Array

In [19]:
```
#X = df_data[['latency_iotgateway_ms', 'latency_logcollector_ms']].values
X = df_data.values  #assign the entire dataframe to X

# Drop the "class" column from this array because we only want the data with predictiv
# and the "class" column is the binary classifier

# [rows,colums], so in this example, do nothing with the rows (before the first comma)
# use negative indexing -1 to drop the last column
X = X[:,:-1]
```

In [20]:
```
# sanity check, look at the first 1 rows, all columns
# since the data has not been scaled/normalized yet, you will see values larger than 1
#X[:1, :]  #slicing
#X[0]  #indexing
X
```

Out[20]:
```
array([[0.0, 0.0, 0.0, ..., 0.527, 11, 4],
       [0.0, 0.0, 0.0, ..., 1.117, 15, 11],
       [0.0, 0.0, 0.0, ..., 0.187, 3, 8],
       ...,
       [27.96, 28.65, 28.04, ..., 0.567, 1, 1],
       [33.0, 30.94, 29.79, ..., 0.641, 1, 3],
       [31.08, 32.72, 31.65, ..., 0.465, 1, 3]], dtype=object)
```

6 - perform feature scaling with MinMaxScaler

In [21]:
```
# take all the values in the X array and scale them to values between 0 and 1
# https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.MinMaxScaler
# https://scikit-learn.org/stable/auto_examples/applications/plot_digits_denoising.htm

X = MinMaxScaler(feature_range=(0,1)).fit_transform(X)
```

In [22]:
```
# sanity check, look at the first 1 rows, all columns
# since the data has been scaled/normalized, all the values will be between 0 and 1
X[:1, :]  #slicing a 2-dimensional array (keeps the shape)
```

Out[22]:
```
array([[0.        , 0.        , 0.        , 0.98717949, 0.96969697,
        0.375     , 0.3030303 , 0.42857143, 0.14285714, 0.28571429,
        0.28571429, 0.71428571, 0.42857143, 0.47031739, 0.57697121,
        0.34230288, 0.31308704, 0.75488163, 0.78494168, 0.43921038,
        0.65853659, 0.24944568, 0.81634938, 0.91806452, 0.27349081,
        0.58823529, 0.36363636]])
```

Alternatively, instead of using MinMaxScaler, you can use StandardScaler, which creates a mean of 0, standard deviation of 1, with normal distribution. https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.StandardScaler.html

In [ ]:

7 - Get Class Labels into a NumPy array

In [23]:
```
# This will add a new column called "ClassLabel", which converts the "normal|abnormal"
# alphabetic content of the "class" column to an integer
# 2-class models do not assume discrete values for each class, often normal=0, abnorma
# but we will use -1 and 1 because the unsupervised class wants those values
# 1-class models assume normal=-1, abnormal=1  (but these values also work for supervi

label_dict = {'normal': 1, 'abnormal': -1}

df_data['ClassLabel'] = df_data['class'].map(label_dict)
```

In [24]:
```
# look at the top few rows of the data (should show the abnormal class in the last col
df_data.head()
```

Out[24]:

	sp1_watts_generated	sp2_watts_generated	sp3_watts_generated	iot_gateway_watt_consumption	val
0	0.0	0.0	0.0	1.63	
1	0.0	0.0	0.0	1.12	
2	0.0	0.0	0.0	0.28	
3	0.0	0.0	0.0	1.16	
4	0.0	0.0	0.0	0.97	

5 rows × 29 columns

In [25]:
```
# look at the bottom few rows of the data (should show the normal class in the last co
df_data.tail()
```

Out[25]:

	sp1_watts_generated	sp2_watts_generated	sp3_watts_generated	iot_gateway_watt_consumption
2195	32.72	32.85	32.22	0.90
2196	27.34	30.48	29.71	0.78
2197	27.96	28.65	28.04	0.78
2198	33.00	30.94	29.79	0.89
2199	31.08	32.72	31.65	0.76

5 rows × 29 columns

In [26]:
```
# define the Class Labels (should be -1 normal or 1 for abnormal)
y = df_data['ClassLabel'].values

#show the first 5 rows of the y array (which holds the classifier -1 or 1)
y[:5]
```

Out[26]:
```
array([-1, -1, -1, -1, -1], dtype=int64)
```

In [27]:
```
#show the last 5 rows of the y array (which holds the classifier -1 or 1)
y[-5:]
```

Out[27]:
```
array([1, 1, 1, 1, 1], dtype=int64)
```

8 - Shuffle Dataset and Create Training and Test Subsets

In [28]:
```
# count the size of the dataset (number of rows)

indices = np.arange(y.shape[0])
indices
```

Out[28]:
```
array([   0,    1,    2, ..., 2197, 2198, 2199])
```

In [29]:
```
# randomize the dataset before splitting
# this is a seeded deterministic shuffle
# in this example, a seed value of 123 is given, which makes the output deterministic,
# any seed value can be chosen, but it should remain consistent so the results can be

rnd = np.random.RandomState(123)
shuffled_indices = rnd.permutation(indices)
shuffled_indices
```

Out[29]:
```
array([ 809,  403,  304, ..., 1766, 1122, 1346])
```

In [30]:
```
# before we shuffle the data, downsample the "abnormal" or "positive" class down,
# by splitting the 200 lines to 160/40 (aka 80%/20%)

# shuffle within the positive and negative classes to avoid bias
# create a new array that only includes the first 200 rows
X_pos = X[:200]  #implies from beginning up to (but not including) 200
X_neg = X[200:]  #implies from 200 to end
y_pos = y[:200]  #contains the "ClassLabel" feature which will be -1 for negative clas
y_neg = y[200:]  #contains the "ClassLabel" feature which will be -1 for negative clas

# or use this shortcut, more readable version of the above
#X_pos,y_pos = X[:200],y[:200]
#X_neg,y_neg = X[200:],y[200:]


# shuffle the positive indices (this is the "anomaly" data)
indices_pos = np.arange(X_pos.shape[0])  # or use the len function to get the number o
pos_shuffled_indices = rnd.permutation(indices_pos)
X_pos_shuffled = X_pos[pos_shuffled_indices]
y_pos_shuffled = y_pos[pos_shuffled_indices]


# shuffle the negative indices (this is the "normal" data)
indices_neg = np.arange(X_neg.shape[0])
neg_shuffled_indices = rnd.permutation(indices_neg)
X_neg_shuffled = X_neg[neg_shuffled_indices]
y_neg_shuffled = y_neg[neg_shuffled_indices]


# split the data between test and train
# grab the first 40 lines (20%) of the abormal (positive) class for test data
X_test_pos, y_test_pos = X_pos_shuffled[:40],y_pos_shuffled[:40]
```

```
# grab the last 160 lines (80%) of the abnormal (positive) class for training data
X_train_pos, y_train_pos = X_pos_shuffled[40:],y_pos_shuffled[40:]  #only the starting

if (dataset_type == "balanced"):
    # we want the abnormal/normal classes to be balanced, so grab the same amount of d
    # rows 0 to 160 will be the first 160 lines of the "normal" or negative class
    # first value is included, last value is not included :160 means 0 is implied, 160
    X_train_neg, y_train_neg = X_neg_shuffled[:160],y_neg_shuffled[:160]
    # the remaining lines are for test
    X_test_neg, y_test_neg = X_neg_shuffled[160:],y_neg_shuffled[160:]
elif (dataset_type == "unbalanced"):
    # the source dataset is unbalanced, with 10x as much data from the negative class
    # This option will split the 2000 rows of negative class data into 400 rows (20%)
    X_train_neg, y_train_neg = X_neg_shuffled[:1600],y_neg_shuffled[:1600]
    X_test_neg,  y_test_neg  = X_neg_shuffled[1600:],y_neg_shuffled[1600:]
else:
    print ("ERROR: Please set dataset_type=balanced|unbalanced at the beginning of thi
```

In [31]:

```
# sanity check to verify the sizes of the test and train data
if (dataset_type == "balanced"):
    print ("This model is using a balanced dataset, so the amount of training data wil
if (dataset_type == "unbalanced"):
    print ("This model is using an unbalanced dataset, so the amount of training data

print ("")
print ("Total size of negative/normal   class rows,columns:", X_neg.shape)
print ("Total size of positive/abnormal class rows,columns:", X_pos.shape)
print ("")
print ("Test data:")
print("Rows,columns of X_test_pos: ", X_test_pos.shape)
print("Rows,columns of X_test_neg: ", X_test_neg.shape)
print ("")
print ("Training data:")
print("Rows,columns of X_train_pos:", X_train_pos.shape)
print("Rows,columns of X_train_neg:", X_train_neg.shape)
print ("")
print ("Class labels with single column:")
print("Rows of y_test_pos: ", y_test_pos.shape)
print("Rows of y_test_neg: ", y_test_neg.shape)
print("Rows of y_train_pos:", y_train_pos.shape)
print("Rows of y_train_neg:", y_train_neg.shape)
```

```
This model is using a balanced dataset, so the amount of training data will be the sa
me for the negative and postive classes.

Total size of negative/normal   class rows,columns: (2000, 27)
Total size of positive/abnormal class rows,columns: (200, 27)

Test data:
Rows,columns of X_test_pos:  (40, 27)
Rows,columns of X_test_neg:  (1840, 27)

Training data:
Rows,columns of X_train_pos: (160, 27)
Rows,columns of X_train_neg: (160, 27)

Class labels with single column:
Rows of y_test_pos:  (40,)
Rows of y_test_neg:  (1840,)
Rows of y_train_pos: (160,)
Rows of y_train_neg: (160,)
```

In [32]:

```
# sanity check to visualize the labels, make sure the classLabel boundaries are correc
# this confirms that we split up the data correcly into training data and test data ir

print ("y testing data for positive/abnormal class, should be all -1:")
print (y_test_pos)   # should output all 1
print ("")
print ("y testing data for negative/normal class, should be all +1:")
print (y_test_neg)   # should output all 0
print ("")
print ("y training data for positive/abnormal class, should be all -1:")
print (y_train_pos)  # should output all 1
print ("")
print ("y training data for negative/normal class, should be all +1:")
print (y_train_neg)  # should output all 0
```

```
y testing data for positive/abnormal class, should be all -1:
[-1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1]

y testing data for negative/normal class, should be all +1:
[1 1 1 ... 1 1 1]

y training data for positive/abnormal class, should be all -1:
[-1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1]

y training data for negative/normal class, should be all +1:
[1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 1 1 1 1 1 1 1 1 1 1 1 1]
```

In [33]:

```
# create the training set and test set
```

```
#concatentate the 2 python arrays of positive and negative classes into a single array
X_train = np.concatenate((X_train_pos,X_train_neg))
y_train = np.concatenate((y_train_pos,y_train_neg))

X_test = np.concatenate((X_test_pos,X_test_neg))
y_test = np.concatenate((y_test_pos,y_test_neg))
```

In [34]:

```
# sanity check, look at the "train" and "test" data
print ("\n X_train data:\n", X_train)
print ("\n y_train data:\n", y_train)
print ("\n X_test data:\n" , X_test)
print ("\n y_test data:\n" , y_test)
```

```
 X_train data:
 [[0.         0.         0.         ... 0.232021   0.         0.45454545]
 [0.         0.         0.         ... 0.15170604 0.05882353 0.36363636]
 [0.         0.         0.         ... 0.41049869 0.05882353 0.18181818]
 ...
 [0.         0.         0.         ... 0.25301837 0.         0.        ]
 [0.59803565 0.54128774 0.55347399 ... 0.26771654 0.         0.45454545]
 [0.55165515 0.58475809 0.57675518 ... 0.232021   0.         0.18181818]]

 y_train data:
 [-1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  1  1  1  1  1  1  1  1]

 X_test data:
 [[0.         0.         0.         ... 0.34225722 0.         0.36363636]
 [0.         0.         0.         ... 0.2855643  0.         0.36363636]
 [0.         0.         0.         ... 0.33595801 0.         0.18181818]
 ...
 [0.49036013 0.43288469 0.45416515 ... 0.30341207 0.         0.45454545]
 [0.84849036 0.88359403 0.89687159 ... 0.23779528 0.         0.54545455]
 [0.18061113 0.18879593 0.18897781 ... 0.21994751 0.         0.18181818]]

 y_test data:
 [-1 -1 -1 ...  1  1  1]
```

9 - perform cross-validation (10-fold)

In [35]:

```
# create a custom class based on BaseEstimator
# We have to do this because the unsupervised KNN model does not include a "predict" f
# which will be required when we want to calculate accuracy scores.

import sklearn
#define a custom class based on the BaseEstimator class
```

```
#based on paper at https://doi.org/10.1109/TKDE.2018.2806975
class NearestNeighborPredict(sklearn.base.BaseEstimator):
    def __init__(self,n_neighbors,threshold):
        self.clf = NearestNeighbors(n_neighbors=n_neighbors)
        self.n_neighbors = n_neighbors
        self.threshold = threshold

    def set_params(self, **params):
        self.n_neighbors = params["n_neighbors"]
        self.threshold = params["threshold"]
        #re-initialize the classifier because we changed the values
        self.clf = NearestNeighbors(n_neighbors=self.n_neighbors)
        return self

    def get_params(self, deep = True):
        return {'n_neighbors':self.n_neighbors, 'threshold':self.threshold}

    def predict(self, X):
        distances, indices = self.clf.kneighbors(X)
        #print ("DEBUG: indices.shape is:",indices.shape)
        DJ = distances.mean(axis=1)  #average of distances from test sample to nearest
        #print ("DEBUG: DJ.shape is:",DJ.shape)
        DK = np.zeros(len(X))  #initialize array with a zero value for every example
        for j in range(self.n_neighbors):
            X_nbrs = self.X_train[indices[:,j]]
            #print ("DEBUG: X_nbrs.shape is:",X_nbrs.shape)
            distances, indices = self.clf.kneighbors(X_nbrs)  #distances and indexes c
            DKj = distances.mean(axis=1)
            DK += DKj
        return (DJ < self.threshold * DK) * 2 - 1

    def fit(self, X, y, **kwargs):
        self.clf.fit(X)  #unsupervised, so only X. y is not used
        self.X_train = X
        #print ("DEBUG: self.threshold,self.n_neighbors:", self.threshold,self.n_neigh
```

In [36]:

```
# sklearn has a cross-validation function that we will use here
# this function will combine your datasets and perform cross-validation
from sklearn.model_selection import cross_val_score


if (modeltype == "TwoClassKNN"):
    #use KNN, start with sklearn default n_neighbors=2, will tune later
    # clf is short for classifier, which refers to the algorithm being used KNN, SVM,
    clf = KNeighborsClassifier(n_neighbors=2)
elif (modeltype == "TwoClassSVM"):
    # the random_state is a seed value that we use for reproducability
    #use SVM algorithm, start with default C=1, will tune later
    clf = svm.SVC(kernel='linear', C=1, random_state=42)
elif (modeltype == "OneClassSVM"):
    # the random_state is a seed value that we use for reproducability
    #use OneClassSVM algorithm, start with default kernel=linear, will try to tune lat
    clf = OneClassSVM(kernel='linear')
elif (modeltype == "OneClassKNN"):
    # create a custom scoring function because OneClassKNN does not have a "predict" c
    clf = NearestNeighborPredict(n_neighbors=2,threshold=1)
else:
   print ("ERROR: Please set modeltype variable at the top of this notebook to the des
```

In [ ]:

In [ ]:

In [37]:
```
# this where all the training and validation happens
# cv=number of cross-validations you want to do
# this folds the data cv times, then returns the accuracy of each fold, showing averag

if (modeltype == "TwoClassKNN" or modeltype == "TwoClassSVM"):    #supervised learning
    scores = cross_val_score(clf, X_train, y_train, cv=10)
elif (modeltype == "OneClassSVM" or modeltype == "OneClassKNN"):  #unsupervised learni
    #OneClassKNN does not have a predict function,
    # which is required by cross_val_score, so we manually defined earlier
    # needs scoring attribute to be defined
    scores = cross_val_score(clf, X_train, y_train, scoring='accuracy', cv=10)
```

In [ ]:

10 - check initial algorithm accuracy before hyperparameter tuning

In [38]:
```
# print the scores for every cross-validation fold (cv=10)
# this will output an array containing the score for each fold
# the default output of the cross validation function is accuracy,
# so the output of this command will show the accuracy of each fold

print ("Scores for each cross-validation fold for",modeltype,"model before hyperparame
scores
```

Out[38]:
```
Scores for each cross-validation fold for OneClassSVM model before hyperparameter opt
imization:
array([0.71875, 0.8125 , 0.6875 , 0.65625, 0.75   , 0.78125, 0.6875 ,
       0.6875 , 0.6875 , 0.59375])
```

In [39]:
```
# mean average of the scores of each cross-validation fold
scores_average = np.mean(scores)
print ("Mean average score using", modeltype, "model before hyperparameter optimizatio
```

```
Mean average score using OneClassSVM model before hyperparameter optimization: 0.7062
5
```

In [40]:
```
# median average of the scores of each cross-validation fold
scores_median = np.median(scores)
print ("Median average score using", modeltype, "model before hyperparameter optimizat
```

```
Median average score using OneClassSVM model before hyperparameter optimization: 0.68
75
```

In [41]:
```
# standard deviation of the scores of each cross-validation fold
scores_stddev = np.std(scores)
print ("Standard deviation across scores using", modeltype, "model before hyperparamet
```

```
Standard deviation across scores using OneClassSVM model before hyperparameter optimi
zation: 0.059621200088559104
```

In [42]:
```
# train the function with the entire training set (without any splitting)
# the .fit function finds the parameter of the model that best fits the dataset
# parameters are the values found during the .fit, hyperparameters are what we refine
# this step trains the model
clf.fit (X_train,y_train)
```

Out[42]:
```
OneClassSVM(kernel='linear')
```

In [43]:
```
# evaluate on the test set using the score function
# this returns a really high accuracy value, because this particular dataset is "unbal
# because there is way more of the negative class than the positive class.
# In other words, because this dataset is unbalanced, this accuracy result is misleadi
# HINT: in this example, the "test" dataset is unbalance, the "train" data is balanced

# this is the score of the test data before tuning
if (modeltype == "TwoClassKNN" or modeltype == "TwoClassSVM"):   #for supervised learn
    clf.score (X_test,y_test)
elif (modeltype == "OneClassSVM" or modeltype == "OneClassKNN"):  #unsupervised learni
    print ("Accuracy for", modeltype , "before optimization is:",(clf.predict (X_test)
```

```
Accuracy for OneClassSVM before optimization is: 0.6803191489361702
```

11 - find optimal hyperparameters

In [44]:
```
# perform a GridSearchCV function to find the optimal hyperparameter (K in KNN or C fo

# define the grid we are going to search
if (modeltype == "TwoClassKNN"):
    parameters = {"n_neighbors":range(1,50)}   #find an optimal value for n_neighbors
    knn =  KNeighborsClassifier()  #instance of base classifier we want to search
    clf = GridSearchCV(knn, parameters)
elif (modeltype == "TwoClassSVM"):
    parameters = {'kernel':('linear', 'rbf'), 'C':range(1,11)}  #last element in range
    # combine the classifer model with the GridSearchCV classifier to calculate accura
    svc = svm.SVC()  #instance of base classifier we want to search
    clf = GridSearchCV(svc, parameters)
elif (modeltype == "OneClassSVM"):
    #parameters = {'kernel':('linear', 'poly', 'rbf', 'sigmoid', 'precomputed')}
    parameters = {'kernel':('linear', 'poly', 'rbf', 'sigmoid')}
    onesvm = OneClassSVM()
    clf = GridSearchCV(onesvm, parameters, scoring='accuracy')
elif (modeltype == "OneClassKNN"):
    parameters = {"n_neighbors":range(1,10),"threshold":np.arange(0,10,0.1)}   #start,
    knn = NearestNeighborPredict(n_neighbors=2,threshold=1)  #use the custom class we
    clf = GridSearchCV(knn, parameters,scoring='accuracy')
else:
   print ("ERROR: Please set modeltype variable at the top of this notebook to the des
```

In [ ]:

In [45]:
```
# fit the model against the train data
print ("Performing GridSearchCV to find optimal hyperparameter within this range:")
if (modeltype == "TwoClassKNN" or modeltype == "TwoClassSVM"):
    clf.fit (X_train,y_train)
elif (modeltype == "OneClassSVM" or modeltype == "OneClassKNN"):
    clf.fit (X_train,y_train)
```

```
Performing GridSearchCV to find optimal hyperparameter within this range:
```

In [46]:
```
# for OneClassKNN, show the classifier inside the custom class
if (modeltype == "OneClassKNN"):
    clf.best_estimator_.clf.get_params()
    print ("best_estimator for",modeltype)
    print (clf.best_estimator_.clf.get_params())
```

In [ ]:
```

```

In [47]:
```
# figure out the optimal hyperparameters

if (modeltype == "TwoClassKNN"):
    # for KNN, we are most interested in the value of n_neighbors and metric
    # the output of this command will show all parameters used by the algorithm
    print ("Using 2-class KNN algorithm, parameters shown below:\n", clf.get_params())
elif (modeltype == "TwoClassSVM"):
    # for SVM, we are most interested in the value of param_C and param_kernel
    # this output shows all the possibilities for C (coefficient)
    print ("\nUsing 2-class SVM algorithm, parameters shown below:\n")
    print ("\nAll keys from clf.cv_results_ \n" , sorted(clf.cv_results_.keys()))
    print ("\nparam_C \n", clf.cv_results_["param_C"])
    print ("\nparam_kernel \n", clf.cv_results_["param_kernel"])
    print ("\nparams \n", clf.cv_results_["params"])
elif (modeltype == "OneClassSVM"):
    #print ("Using OneClassSVM algorithm, parameters shown below:\n", clf.get_params()
    print ("Using OneClassSVMN algorithm, optimal parameters shown below:\n", clf.best
elif (modeltype == "OneClassKNN"):
    print ("Using OneClassKNN algorithm, optimal parameters shown below:\n", clf.best_
else:
    print ("ERROR: Please set modeltype variable at the top of this notebook to OneCla
```

```
Using OneClassSVMN algorithm, optimal parameters shown below:
 {'cache_size': 200, 'coef0': 0.0, 'degree': 3, 'gamma': 'scale', 'kernel': 'linear',
'max_iter': -1, 'nu': 0.5, 'shrinking': True, 'tol': 0.001, 'verbose': False}
```

In [48]:
```
# show all parameters of the classifier
print ("all parameters for classifier using model",modeltype)
clf.get_params()
```

```
all parameters for classifier using model OneClassSVM
```

Out[48]:
```
{'cv': None,
 'error_score': nan,
 'estimator__cache_size': 200,
 'estimator__coef0': 0.0,
 'estimator__degree': 3,
 'estimator__gamma': 'scale',
 'estimator__kernel': 'rbf',
 'estimator__max_iter': -1,
 'estimator__nu': 0.5,
 'estimator__shrinking': True,
 'estimator__tol': 0.001,
 'estimator__verbose': False,
 'estimator': OneClassSVM(),
 'n_jobs': None,
 'param_grid': {'kernel': ('linear', 'poly', 'rbf', 'sigmoid')},
 'pre_dispatch': '2*n_jobs',
 'refit': True,
 'return_train_score': False,
 'scoring': 'accuracy',
 'verbose': 0}
```

12 - recalculate scores after hyperparameter tuning to see if the scores improve

In [49]:
```
# recalculate the scores after the hyperparameter tuning to see if the scores improve
# this will return the ideal (or optimized) classifier

scores = cross_val_score(clf.best_estimator_, X_train, y_train, scoring='accuracy', cv
scores
```

Out[49]:
```
array([0.71875, 0.8125 , 0.6875 , 0.65625, 0.75   , 0.78125, 0.6875 ,
       0.6875 , 0.6875 , 0.59375])
```

13 - average the scores of each cross-validation fold

In [50]:
```
scores_average = np.mean(scores)
print ("Mean average score using", modeltype, "model after hyperparameter tuning:", sc
```

```
Mean average score using OneClassSVM model after hyperparameter tuning: 0.70625
```

In [51]:
```
# median average of the scores of each cross-validation fold
scores_median = np.median(scores)
print ("Median average score using", modeltype, "model before hyperparameter optimizat
```

```
Median average score using OneClassSVM model before hyperparameter optimization: 0.68
75
```

In [52]:
```
# standard deviation of the scores of each cross-validation fold
scores_stddev = np.std(scores)
print ("Standard deviation of scores using", modeltype, "model before hyperparameter o
```

```
Standard deviation of scores using OneClassSVM model before hyperparameter optimizati
on: 0.059621200088559104
```

In [53]:
```
# perform the final validation

# we have already done this section in a previous step, not needed here
# train the function with the entire training set (without any splitting) using the de
#clf.fit (X_train,y_train)
#print ("\nFit the model with default hyperparameters:\n", clf.fit (X_train,y_train))

# train the function with the entire training set (without any splitting) using the op
clf.best_estimator_.fit (X_train,y_train)
print ("Fit the model with optimized hyperparameters:\n", clf.best_estimator_.fit (X_t
```

```
Fit the model with optimized hyperparameters:
 OneClassSVM(kernel='linear')
```

In [ ]:
```

```

In [54]:
```
# Question: why does the score stay the same after hyperparameter optimization?
# because the clf classifier has been re-trained.  If you want the older value of clf.
# a different variable so it does not get overwritten.

# are we getting overfitting here in the test data?
# threshold is off for this model, because the threshold for unbalanced data is 0.5
# need to come up with a threshold that determines range of data to classify as 0 or 1

# this is the score of the test data after hyperparameter optimization

# evaluate on the test set using the score function
# this returns a really high accuracy value, because this particular dataset is "unbal
# because there is way more of the negative class than the positive class.
# In other words, because this dataset is unbalanced, this accuracy result is misleadi
#clf.score (X_test,y_test)                 #uses the default hyperparameters
#clf.best_estimator_.score (X_test,y_test)  #uses the optimal hyperparameters
#print (modeltype, "score before hyperparameter optimization:", clf.score (X_test,y_te


#***
if (modeltype == "TwoClassKNN" or modeltype == "TwoClassSVM"):   #for supervised learr
    print (modeltype, "score after hyperparameter optimization:")
    print (clf.best_estimator_.score (X_test,y_test))
elif (modeltype == "OneClassSVM" or modeltype == "OneClassKNN"):
    #unsupervised learning models do not have a score, so use accuracy instead
    print ("Accuracy for ",modeltype,"is:",(clf.predict (X_test) == y_test).mean())
```

```
Accuracy for  OneClassSVM is: 0.6803191489361702
```

In [55]:
```
# look in the classification data dictionary to figure out where the optimal hyperparc
# This command outputs a lot of text, look at the next cell for a shortcut
# This shows the entire dictionary (multidimensional array), so it is hard to parse ou
clf.cv_results_
```

Out[55]:
```
{'mean_fit_time': array([0.0017962 , 0.00179501, 0.00299187, 0.00297923]),
 'std_fit_time': array([3.99096732e-04, 3.98731431e-04, 3.16297988e-07, 1.52970371e-0
5]),
 'mean_score_time': array([0.00059738, 0.00039887, 0.0009974 , 0.00101027]),
 'std_score_time': array([4.87763966e-04, 4.88519378e-04, 4.42200589e-07, 1.54554097e
-05]),
 'param_kernel': masked_array(data=['linear', 'poly', 'rbf', 'sigmoid'],
              mask=[False, False, False, False],
        fill_value='?',
             dtype=object),
 'params': [{'kernel': 'linear'},
  {'kernel': 'poly'},
  {'kernel': 'rbf'},
  {'kernel': 'sigmoid'}],
 'split0_test_score': array([0.8125 , 0.8125 , 0.46875, 0.8125 ]),
 'split1_test_score': array([0.703125, 0.703125, 0.59375 , 0.671875]),
 'split2_test_score': array([0.71875 , 0.71875 , 0.546875, 0.734375]),
 'split3_test_score': array([0.6875 , 0.6875 , 0.53125, 0.6875 ]),
 'split4_test_score': array([0.640625, 0.640625, 0.46875 , 0.640625]),
 'mean_test_score': array([0.7125  , 0.7125  , 0.521875, 0.709375]),
 'std_test_score': array([0.05642334, 0.05642334, 0.04800716, 0.05978477]),
 'rank_test_score': array([1, 1, 4, 3])}
```

In [56]:
```
# shortcut for previous step to show the optimal hyperparameter
# for SVM, this gives us a value of C=8, which is right near the middle of the CVGridS
# for KNN, this gives us a value of n_neighbors=38, which is within the range of 1-50
clf.best_estimator_
print ("The optimized hyperparameter for", modeltype, "model is:", clf.best_estimator_
```

```
The optimized hyperparameter for OneClassSVM model is: OneClassSVM(kernel='linear')
```

In [57]:
```
# Show optimized hyperparameters
print ("Optimized hyperparameters for",modeltype,"model are:")
clf.best_estimator_.get_params()
```

```
Optimized hyperparameters for OneClassSVM model are:
```

Out[57]:
```
{'cache_size': 200,
 'coef0': 0.0,
 'degree': 3,
 'gamma': 'scale',
 'kernel': 'linear',
 'max_iter': -1,
 'nu': 0.5,
 'shrinking': True,
 'tol': 0.001,
 'verbose': False}
```

14 - Confusion Matrix for entire test set

In [58]:
```
# Confusion Matrix

# A confusion matrix is a table that is often used to describe the performance of a
# classification model (or "classifier") on a set of test data for which the true valu
# Scikit-learn provides facility to calculate confusion matrix using the confusion_mat

# this output shows a FP as a bit high, probably due to the threshold on this unbalanc
# could probably be improved by adding another hyperparameter for threshold.
```

```
# Evaluate model
y_pred = clf.best_estimator_.predict(X_test)  #use the optimal hyperparameter calculat
cm = confusion_matrix(y_test*-1, y_pred*-1)   #flip the classes by multiplying by -1

TN, FP, FN, TP = cm.ravel() #use the .ravel function to pull out TN,TP,FN,TP

print('Confusion matrix\n\n', cm)
print('\nTrue Negatives  (TN) = ', TN)
print('False Positives (FP) = ', FP)
print('False Negatives (FN) = ', FN)
print('True Positives  (TP) = ', TP)
```

```
Confusion matrix

 [[1254  586]
 [  15   25]]

True Negatives  (TN) =  1254
False Positives (FP) =  586
False Negatives (FN) =  15
True Positives  (TP) =  25
```

15 - visualize confusion matrix

In [59]:
```
# visualize confusion matrix with a heatmap
import seaborn as sns
import matplotlib.pyplot as plt
```

In [60]:
```
## very simple graph of confusion matrix
#sns.heatmap(cm, annot=True,cmap='summer',cbar=False)
#plt.show()

## add details below graph to help interpret results
#print('Confusion matrix\n\n', cm)
#print('\nTrue Negatives  (TN) = ', TN)
#print('False Positives (FP) = ', FP)
#print('False Negatives (FN) = ', FN)
#print('True Positives  (TP) = ', TP)
```

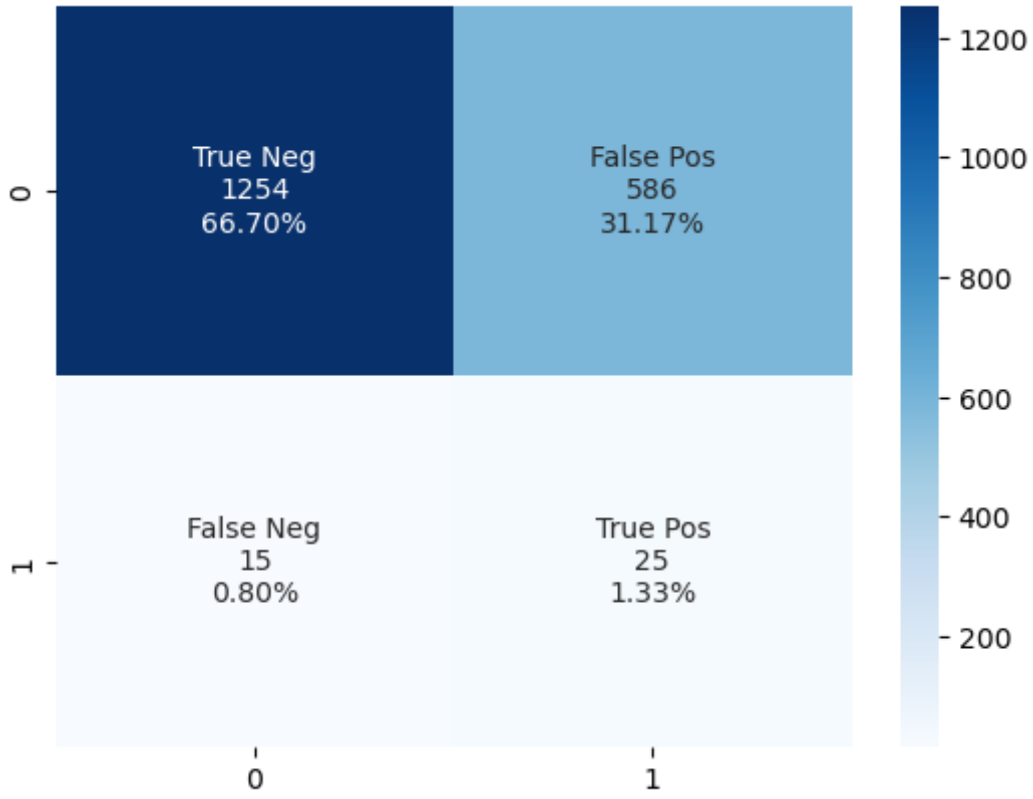
In [61]:
```
## visualize confusion matrix with slightly more detailed graph
## Example from https://proclusacademy.com/blog/practical/confusion-matrix-accuracy-sk

#import seaborn as sns


## Change figure size and increase dpi for better resolution
#plt.figure(figsize=(8,6), dpi=100)
## Scale up the size of all text
#sns.set(font_scale = 1.1)

## Plot Confusion Matrix using Seaborn heatmap()
## Parameters:
## first param - confusion matrix in array format
## annot = True: show the numbers in each heatmap cell
## fmt = 'd': show numbers as integers.
#ax = sns.heatmap(cm, annot=True, fmt='d', )
```

```
## set x-axis label and ticks.
#ax.set_xlabel("Predicted Result", fontsize=14, labelpad=20)
#ax.xaxis.set_ticklabels(['Negative', 'Positive'])

## set y-axis label and ticks
#ax.set_ylabel("Actual Result", fontsize=14, labelpad=20)
#ax.yaxis.set_ticklabels(['Negative', 'Positive'])

## set plot title
#ax.set_title("Confusion Matrix", fontsize=14, pad=20)

#plt.show()


## add details below graph to help interpret results
#print('Confusion matrix\n\n', cm)
#print('\nTrue Negatives  (TN) = ', TN)
#print('False Positives (FP) = ', FP)
#print('False Negatives (FN) = ', FN)
#print('True Positives  (TP) = ', TP)
```

In [62]:

```
# visualize confusion matrix with more detailed labels
# https://medium.com/@dtuk81/confusion-matrix-visualization-fc31e3f30fea

group_names = ['True Neg','False Pos','False Neg','True Pos']
group_counts = ["{0:0.0f}".format(value) for value in cm.flatten()]
group_percentages = ["{0:.2%}".format(value) for value in cm.flatten()/np.sum(cm)]
labels = [f"{v1}\n{v2}\n{v3}" for v1, v2, v3 in zip(group_names,group_counts,group_per
labels = np.asarray(labels).reshape(2,2)
sns.heatmap(cm, annot=labels, fmt='', cmap='Blues')

# add details below graph to help interpret results
print('Confusion matrix\n\n', cm)
print('\nTrue Negatives  (TN) = ', TN)
print('False Positives (FP) = ', FP)
print('False Negatives (FN) = ', FN)
print('True Positives  (TP) = ', TP)
```

```
Confusion matrix

 [[1254  586]
 [  15   25]]

True Negatives  (TN) =  1254
False Positives (FP) =  586
False Negatives (FN) =  15
True Positives  (TP) =  25
```



16 - Accuracy of model for entire training dataset

In [63]:
```
# Assign values from confusion matrix to True Positive, True Negative, False Positive,

print ("True Negatives: ", TN)
print ("False Positives:", FP)
print ("False Negatives:", FN)
print ("True Positives: ", TP)

Accuracy = (( TP + TN) / ( TP + TN + FP + FN))
Sensitivity = TP / (TP + FN)
Specificity = TN / (TN + FP)
GeometricMean = math.sqrt(Sensitivity * Specificity)

print ("")
print ("Accuracy:       ", Accuracy)
print ("Sensitivity:    ", Sensitivity)
print ("Specificity:    ", Specificity)
print ("Geometric Mean: ", GeometricMean)
```

```
True Negatives:  1254
False Positives: 586
False Negatives: 15
True Positives:  25

Accuracy:        0.6803191489361702
Sensitivity:     0.625
Specificity:     0.6815217391304348
Geometric Mean:  0.652649283272817
```

17 - Confusion matrix for each cross validation fold

In [64]:
```
# define a function to perform a stratified cross validation
# in this context, "stratified" means that for each split performed by the cross-valid
# the distribution is preserved in a consistent manner for each split.
# This makes the splits for each CV more consistent with each other, reducing variabli

def cv_confusion_matrix(clf, X, y, folds=10):
    skf = StratifiedKFold(n_splits=folds)
    cv_iter = skf.split(X, y)
    cms = []   #instantiate an empty list
    for train, test in cv_iter:
        clf.fit(X[train,], y[train])
        #multiply the inputs in the following line by -1 to flip the positive/negative
        cm = confusion_matrix(y[test]*-1, clf.predict(X[test])*-1, labels=clf.classes_
        cms.append(cm)
    #return np.mean(np.array(cms), axis=0)  #just show average of each run
    return (np.array(cms))                  #show the confusion matrix for each fold
```

In [65]:
```
# xxx
# call the above function
#run the function using the optimal hyperparameter with the training data and target w
#this returns a 3-dimensional matrix
if (modeltype == "TwoClassSVM" or modeltype == "TwoClassKNN"):
    cv_confusion_matrix(clf.best_estimator_,X_train,y_train,10)
elif (modeltype == "OneClassSVM" or modeltype == "OneClassKNN"):
    #manually create the "classes" attribute for unsupervised models, does not exist b
    clf.best_estimator_.classes_ = [-1,1]
    # now you can run the custom function cv_confusion_matrix after defining the "cl
    cv_confusion_matrix(clf.best_estimator_,X_train,y_train,10)
```

In [ ]:
```

```

In [66]:
```
# put the 3-dimensional matrix into a variable so we can parse out each cross-validati
cms = cv_confusion_matrix(clf.best_estimator_,X_train,y_train,10)

# show the confusion matrix for the first fold  (will provide TN,FP,FN,TP for a single
cms[0]
```

Out[66]:
```
array([[13,  3],
       [ 5, 11]], dtype=int64)
```

18 - Accuracy of model for each cross-validation fold

To measure the quality of the models the Accuracy, Sensitivity, Specificity, and the Geometric Mean measurements will be used.

The Accuracy will give some ideas of the performance on the balanced data set, while Sensitivity and Specificity will help in the final validation stage where the data will be clearly unbalanced.

https://lifenscience.com/sensitivity-specificity-accuracy/ Sensitivity, Specificity, and Accuracy are the terms which are most commonly associated with a Binary classification test and they statistically measure the performance of the test. Sensitivity indicates, how well the test predicts one category and Specificity measures how well the test predicts the other category. Whereas Accuracy is expected to measure how well the test predicts both categories.

https://en.wikipedia.org/wiki/Sensitivity_and_specificity Sensitivity and specificity mathematically describe the accuracy of a test which reports the presence or absence of a condition. Individuals for which the condition is satisfied are considered "positive" and those for which it is not are considered "negative".

Sensitivity (true positive rate) refers to the probability of a positive test, conditioned on truly being positive. The range for sensitivity is 0 to 1, with a value of 1 indicating perfect sensitivity (i.e. 100% of positive cases are correctly identified as positive). A value of 0 indicates poor sensitivity (i.e. no positive cases are correctly identified as positive).

Specificity (true negative rate) refers to the probability of a negative test, conditioned on truly being negative. The range for specificity is also 0 to 1, with a value of 1 indicating perfect specificity (i.e. 100% of negative cases are correctly identified as negative). A value of 0 indicates poor specificity (i.e. no negative cases are correctly identified as negative).

Calculate the following for each of the cross-validations: Accuracy, Sensitivity, Specificity, Geometric Mean

TP = True Positive

TN = True Negative

FP = False Positive

FN = False Negative

Formulas:

Accuracy = (TP + TN) / (TP + TN + FP + RN)

Sensitivity = TP / (TP + FN)

Specificity = TN / (TP + FP)

Geometric Mean =

$$\sqrt{Sensitivity * Specificity}$$

In [67]:
```
# show the confusion matrix for each cross-validation fold

for i in range(10):
    #
```

```
    # Capture True Negative, False Positive, False Negative, True Positive for each cr
    #
    #TN = cms[i][0,0]    #obtain True  Negative value from confusion matrix
    #FP = cms[i][0,1]    #obtain False Positive value from confusion matrix
    #FN = cms[i][1,0]    #obtain False Negative value from confusion matrix
    #TP = cms[i][1,1]    #obtain True  Positive value from confusion matrix
    TN, FP, FN, TP = cms[i].ravel() #use the .ravel function to pull out TN,FP,FN,TP f
    #
    # Calculate Accuracy, Sensitivity, Specificity, Geometric Mean for each cross-vali
    # Be careful to avoid divide by zero errors
    #
    if (TP+TN+FP+FN > 0):
        Accuracy = ((TP + TN) / (TP + TN + FP + FN))
    elif (TP+TN+FP+FN == 0):
        Accuracy = 0   #avoid divide by zero error, this should never happen because t

    if (TP > 0 and FN > 0):
        Sensitivity = TP / (TP + FN)  #this is the normal and expected formula
    elif (TP == 0 and FP == 0):       #this CV fold had no instances of the positive c
        Sensitivity = 1               #set to perfect sensitity because there were no
    elif (TP == 0 and FN > 0):
        Sensitivity = 0               #avoid divide by zero error, set to zero (poor s

    if (TN+FP > 0):
        Specificity = TN / (TN + FP)  #this is the normal and expected formula
    elif (TN == 0 and FN == 0):       #this CV fold had no instances of the negative c
        Specificity = 1               #set to perfect specificity 0.0000=poor 1.0000=p

    GeometricMean = math.sqrt(Sensitivity * Specificity)
    #
    # truncate above calculations to 4 decimal places
    #
    Accuracy      = round(Accuracy,4)
    Sensitivity   = round(Sensitivity,4)
    Specificity   = round(Specificity,4)
    GeometricMean = round(GeometricMean,4)
    #
    # print output
    #
    print ("\n-------- Cross Validation Fold", i ,"--------")
    print ("True Negative:  ", TN)
    print ("False Positive: ", FP)
    print ("False Negative: ", FN)
    print ("True Positive:  ", TP)
    print ("Accuracy:       ", Accuracy)
    print ("Sensitivity:    ", Sensitivity)
    print ("Specificity:    ", Specificity)
    print ("Geometric Mean: ", GeometricMean)
```

```
-------- Cross Validation Fold 0 --------
True Negative:   13
False Positive:  3
False Negative:  5
True Positive:   11
Accuracy:        0.75
Sensitivity:     0.6875
Specificity:     0.8125
Geometric Mean:  0.7474

-------- Cross Validation Fold 1 --------
True Negative:   11
False Positive:  5
False Negative:  5
True Positive:   11
Accuracy:        0.6875
Sensitivity:     0.6875
Specificity:     0.6875
Geometric Mean:  0.6875

-------- Cross Validation Fold 2 --------
True Negative:   12
False Positive:  4
False Negative:  4
True Positive:   12
Accuracy:        0.75
Sensitivity:     0.75
Specificity:     0.75
Geometric Mean:  0.75

-------- Cross Validation Fold 3 --------
True Negative:   10
False Positive:  6
False Negative:  3
True Positive:   13
Accuracy:        0.7188
Sensitivity:     0.8125
Specificity:     0.625
Geometric Mean:  0.7126

-------- Cross Validation Fold 4 --------
True Negative:   11
False Positive:  5
False Negative:  7
True Positive:   9
Accuracy:        0.625
Sensitivity:     0.5625
Specificity:     0.6875
Geometric Mean:  0.6219

-------- Cross Validation Fold 5 --------
True Negative:   11
False Positive:  5
False Negative:  6
True Positive:   10
Accuracy:        0.6562
Sensitivity:     0.625
Specificity:     0.6875
Geometric Mean:  0.6555
```

```
-------- Cross Validation Fold 6 --------
True Negative:   11
False Positive:  5
False Negative:  8
True Positive:   8
Accuracy:        0.5938
Sensitivity:     0.5
Specificity:     0.6875
Geometric Mean:  0.5863

-------- Cross Validation Fold 7 --------
True Negative:   11
False Positive:  5
False Negative:  3
True Positive:   13
Accuracy:        0.75
Sensitivity:     0.8125
Specificity:     0.6875
Geometric Mean:  0.7474

-------- Cross Validation Fold 8 --------
True Negative:   9
False Positive:  7
False Negative:  6
True Positive:   10
Accuracy:        0.5938
Sensitivity:     0.625
Specificity:     0.5625
Geometric Mean:  0.5929

-------- Cross Validation Fold 9 --------
True Negative:   10
False Positive:  6
False Negative:  3
True Positive:   13
Accuracy:        0.7188
Sensitivity:     0.8125
Specificity:     0.625
Geometric Mean:  0.7126
```

19 - classification report (f1 score) for entire test dataset

In [68]:

```python
# Classification Report

# Another important report is the Classification report.
# It is a text summary of the precision, recall, F1 score for each class.
# Scikit-learn provides facility to calculate Classification report using the classifi

# F1 is the harmonic mean rather than the geometric mean
# F1 gives you the average that is closest to the worst-case scenario

#import classification_report
from sklearn.metrics import classification_report

print(classification_report(y_test*-1,y_pred*-1))  #multiply by -1 to flip class label
```

	precision	recall	f1-score	support
-1	0.99	0.68	0.81	1840
1	0.04	0.62	0.08	40
accuracy			0.68	1880
macro avg	0.51	0.65	0.44	1880
weighted avg	0.97	0.68	0.79	1880

In [ ]: