Improved_Models

November 5, 2020

1 Improved Model

1.1 Data Preparation

1.1.1 Import Modified Feature Matrix

A modification has been made to the feature matrix extracted in "Data Preparation" module. The changes include:

(1) Corrected a mistake in function that calculates the ignition temperature.
(2) Baseline correction now only incorporate flattening and smoothing the curve, the minor peaks are no longer removed. This change is trying to keep the baseline correction result as close as the commercialized software.

The feature new matrix is stored in a .csv file, which contains features extracted from raw data based on physical meanings, as well as the labels indicating whether the material passes FR tests or not. A total of 41 observations and 5 features were included. Specifically, the output consists of 3 labels, where 0=fail, 1=pass, 2=hard to determine.

We start by importing the .csv file. Appropriate libraries are imported.

[1]:
```
# Read in the data
import numpy as np
import pandas as pd
import pylab as plt
data = pd.read_csv("feature_matrix.csv")
data.head()
```

[1]:

	Total Heat Release	Burning Temperature	Ignition Temperature	Heat Release Capacity	Fire Growth Capacity	FR_labels
0	24722.818517	482.246	350.805	25955.104346	134.021649	2
1	14879.480392	537.858	438.643	15591.943456	120.959219	2
2	16584.116501	515.457	366.537	17369.365738	77.548988	1
3	20246.452607	482.774	396.996	21344.250614	191.805110	0
4	26622.142067	472.215	388.929			

```
4            28036.752193            260.118532          0
```

1.1.2 Scale Data

Based on simple observation on the raw features, it is not suprised to see there are magnitude difference among all features. To eliminate the weight bias caused by descrepancy with units, standard scaling is applied and all analysis will be performed on top of the scaled dataset.

[2]:
```
# import standard scaler
from sklearn.preprocessing import StandardScaler

# scale the data (excluding labels)
scaler = StandardScaler()
scaled = scaler.fit_transform(data.drop(columns='FR_labels'))
scaled = pd.DataFrame(scaled)
scaled['FR_labels'] = data.loc[:,'FR_labels']    # add FR_labels to new␣
↪dataframe
scaled.columns = data.columns    # add column headers back to new dataframe
scaled.head()
```

[2]:

	Total Heat Release	Burning Temperature	Ignition Temperature	\
0	1.808411	-0.424203	-0.990329	
1	-0.335103	0.879587	0.744864	
2	0.036103	0.354409	-0.679551	
3	0.833624	-0.411824	-0.077850	
4	2.222013	-0.659374	-0.237209	

	Heat Release Capacity	Fire Growth Capacity	FR_labels
0	1.778631	-0.202424	2
1	-0.365567	-0.258909	2
2	0.002192	-0.446622	1
3	0.824619	0.047441	0
4	2.209336	0.342840	0

###Baseline Model Pipeline Diagram

1.2 SVC Baseline Model

According to the pipeline diagram in our description file, a 90% train-test split will be performed to the scaled dataset. Support Vector Classifier (SVC) is selected as our baseline model. GridSearchCV is used for determining the optimal hyperparameters (C and γ) with a 3-fold cross-validation. At the end, the accuracy, precision and recall scores are printed as benchmark metrics with other potential models.

Our Support Vector Classifier (SVC) baseline model will not consider previously discussed issues of multicollinearity and outliers with the data but will establish the baseline performance for a classification model. Because dropping the outlier at index=2 made a significant difference, we will be dropping that data point for the baseline but further exploring its significance in the future.

[3]:
```
# imports
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score, recall_score, precision_score
from sklearn.model_selection import GridSearchCV
from sklearn.svm import SVC

# final outlier
origin_feature=scaled

# perform a train-test split. 90% of original data will be used for training
X_svc = origin_feature.drop(columns='FR_labels').values
y_svc = origin_feature['FR_labels'].values
X_train_svc, X_test_svc, y_train_svc, y_test_svc = train_test_split(X_svc,␣
 ↪y_svc, test_size = 0.10)

# define support vector model with rbf kernel
svc = SVC(kernel = 'rbf')

# build up parameter grid and perform GridSearchCV to find the best estimator
alphas = np.array([1e-6, 1e-5, 1e-4, 1e-3, 1e-2, 1e-1, 1])
Cs = 1 / alphas
sigmas = np.array([1e-3, 1e-2, 1e-1, 1, 10, 100])
gammas = 1. / 2 / sigmas**2

param_grid_svc = {'C': Cs,'gamma': gammas}

svc_search = GridSearchCV(svc, param_grid_svc, cv = 3)
svc_search.fit(X_train_svc,y_train_svc)

# resulting predictions
predict_svc = svc_search.best_estimator_.predict(X_test_svc)
full_predict_svc = svc_search.best_estimator_.predict(X_svc)

# note: we have 3 labels, so we use average='macro' to find the average metric␣
 ↪for each
#       label summed. This augments penalized performance caused by class␣
 ↪imbalance.
# print out the accuracy, precison and recall score for the prediction on␣
 ↪validation set
print('Accuracy for validation set: {}'.format(accuracy_score(y_test_svc,␣
 ↪predict_svc)))
print('Precision for validation set: {}'.format(precision_score(y_test_svc,␣
 ↪predict_svc, average='macro')))
print('Recall for validation set: {}\n'.format(recall_score(y_test_svc,␣
 ↪predict_svc, average='macro')))
```

```
# print out the accuracy, precison and recall score for the prediction on full␣
 ↪dataset
print('Accuracy for full dataset: {}'.format(accuracy_score(y_svc,␣
 ↪full_predict_svc)))
print('Precision for full dataset: {}'.format(precision_score(y_svc,␣
 ↪full_predict_svc, average='macro')))
print('Recall for full dataset: {}'.format(recall_score(y_svc,␣
 ↪full_predict_svc, average='macro')))
```

```
Accuracy for validation set: 0.4
Precision for validation set: 0.625
Recall for validation set: 0.625

Accuracy for full dataset: 0.6585365853658537
Precision for full dataset: 0.4380952380952381
Recall for full dataset: 0.47222222222222215

C:\Users\cjher\anaconda3\lib\site-
packages\sklearn\metrics\_classification.py:1221: UndefinedMetricWarning:
Precision is ill-defined and being set to 0.0 in labels with no predicted
samples. Use `zero_division` parameter to control this behavior.
  _warn_prf(average, modifier, msg_start, len(result))
```

Baseline Model Discussion:
After running the above cell a few times, we notice that the score changes drastically based on the random set of X_train, y_train chosen. This is caused by our small data set and should be addressed in future models by generating or obtaining additional data. Additionally, due to the same problem, sometimes the model is unable to predict the borderline class (label 2) shown in the warning above, which is composed of materials that do not have a fixed flame retardant test result (sometimes pass and sometimes fail).

With regards to scores of the validation set and the full dataset, it seems that the data is not overfitting much and seems to generalize well when applied to the larger data set.

#Improved Models

[4]:
```
# Read in the data
import numpy as np
import pandas as pd
import pylab as plt
data = pd.read_csv("feature_matrix.csv")
y_label=data['FR_labels'].values
data.head()
```

[4]:

	Total Heat Release	Burning Temperature	Ignition Temperature	\
0	24722.818517	482.246	350.805	
1	14879.480392	537.858	438.643	
2	16584.116501	515.457	366.537	
3	20246.452607	482.774	396.996	

```
4        26622.142067              472.215               388.929
```

```
   Heat Release Capacity  Fire Growth Capacity  FR_labels
0           25955.104346            134.021649          2
1           15591.943456            120.959219          2
2           17369.365738             77.548988          1
3           21344.250614            191.805110          0
4           28036.752193            260.118532          0
```

##PCA (Principal Component Analysis)

Principal Component Analysis (PCA) will be performed on the original MCC dataset, which includes raw data and curve-flattened data. 10 most important PCs will be extracted from each dataset and return a (41*10) feature matrix. This matrix, itself, will be used as the input for the prediction model. In addition, the PCA extracted matrix will be combined with the original feature matrix for prediction.

[5]:
```
# run if rampy is not installed
%pip install rampy
```

```
Requirement already satisfied: rampy in c:\users\cjher\anaconda3\lib\site-
packages (0.4.5)
Note: you may need to restart the kernel to use updated packages.Requirement
already satisfied: pandas in c:\users\cjher\anaconda3\lib\site-packages (from
rampy) (1.0.5)
Requirement already satisfied: scipy in c:\users\cjher\anaconda3\lib\site-
packages (from rampy) (1.5.0)
Requirement already satisfied: numpy>=1.12 in c:\users\cjher\anaconda3\lib\site-
packages (from rampy) (1.18.5)
Requirement already satisfied: scikit-learn in
c:\users\cjher\anaconda3\lib\site-packages (from rampy) (0.23.1)
Requirement already satisfied: python-dateutil>=2.6.1 in
c:\users\cjher\anaconda3\lib\site-packages (from pandas->rampy) (2.8.1)

Requirement already satisfied: pytz>=2017.2 in
c:\users\cjher\anaconda3\lib\site-packages (from pandas->rampy) (2020.1)
Requirement already satisfied: joblib>=0.11 in
c:\users\cjher\anaconda3\lib\site-packages (from scikit-learn->rampy) (0.16.0)
Requirement already satisfied: threadpoolctl>=2.0.0 in
c:\users\cjher\anaconda3\lib\site-packages (from scikit-learn->rampy) (2.1.0)
Requirement already satisfied: six>=1.5 in c:\users\cjher\anaconda3\lib\site-
packages (from python-dateutil>=2.6.1->pandas->rampy) (1.15.0)
```

[6]:
```
#
# params: x, array of temperature values; y, array of HRR values
# returns: y_corrected_filtered, flattened and smoothed arrays;
# https://github.com/charlesll/rampy
# https://github.com/charlesll/rampy/blob/master/examples/baseline_fit.ipynb
```

```
import rampy as rp
from scipy.signal import savgol_filter

def baseflatten(x,y):
    bir = np.array([[0,800]])
    y_corrected, background = rp.baseline(x,y,bir,"arPLS",lam=10**10) #flatten␣
 ↪the curve
    y_corrected_filtered=savgol_filter(y_corrected.flatten(),15,3) #smooth the␣
 ↪gradient curve
    return y_corrected_filtered
```

Principal Component Analysis (PCA) will be performed on the original MCC dataset, which includes raw data and curve-flattened data. 5 most important PCs will be extracted from each dataset and return a (41*10) feature matrix. This matrix, itself, will be used as the input for the prediction model. In addition, the PCA extracted matrix will combine with the feature matrix extracted based on physical meanings.

[7]:
```
# Read in the raw data
df = pd.read_csv("./MCC_raw.csv")
data_raw = df.drop([0]).astype(float)
data_raw[data_raw.columns[::3]].head(5)
```

[7]:

	Adhesive-1-1	Adhesive-2-1	Adhesive-3-1	Adhesive-4-1	Adhesive-5-1	\
1	73.744	74.630	74.621	74.539	74.815	
2	73.711	74.653	74.683	74.552	74.815	
3	73.749	74.659	74.715	74.519	74.893	
4	73.741	74.688	74.724	74.498	74.904	
5	73.780	74.745	74.745	74.478	74.951	

	Adhesive-6-1	Adhesive-7-1	Adhesive-8-1	Adhesive-9-1	Adhesive-10-1	…	\
1	75.161	75.574	74.589	75.411	75.404	…	
2	75.181	75.580	74.628	75.390	75.352	…	
3	75.207	75.582	74.650	75.376	75.345	…	
4	75.236	75.617	74.704	75.397	75.335	…	
5	75.237	75.603	74.720	75.365	75.320	…	

	Fiber-FR-10	Fiber-FR-11	Fiber-FR-12	Fiber-FR-13	Fiber-FR-14	\
1	74.736	75.393	74.683	73.755	74.602	
2	74.719	75.416	74.691	73.679	74.588	
3	74.678	75.360	74.725	73.665	74.604	
4	74.652	75.418	74.756	73.647	74.628	
5	74.669	75.412	74.765	73.607	74.704	

	Fiber-FR-15	Fiber-FR-16	Fiber-17	Fiber-18	Fiber-19
1	74.629	75.068	73.866	74.566	73.599
2	74.670	75.021	73.889	74.599	73.637

```
3       74.699       74.989    73.901    74.622    73.658
4       74.735       74.962    73.928    74.609    73.653
5       74.778       74.959    73.933    74.644    73.733

[5 rows x 41 columns]
```

[8]:
```
# Drop all non-numerical (NaN) values
def is_positive_numeric(x):
    if not np.isreal(x):
        return False
    elif not np.isfinite(x):
        return False
    elif pd.isnull(x):
        return False
    else:
        return True

numeric_map = data_raw.applymap(is_positive_numeric)
data=data_raw[numeric_map.all(axis=1).values]
data.tail(5)
```

[8]:
```
      Adhesive-1-1  Unnamed: 1  Unnamed: 2  Adhesive-2-1  Unnamed: 4  \
1395       737.295      -0.002       1.016       739.624      -5.602
1396       737.805       0.102       1.022       740.144      -5.294
1397       738.282       0.155       0.987       740.684      -5.458
1398       738.803       0.020       0.996       741.150      -5.387
1399       739.309       0.060       1.028       741.652      -5.352

      Unnamed: 5  Adhesive-3-1  Unnamed: 7  Unnamed: 8  Adhesive-4-1  …  \
1395       1.014       739.985      -6.388       1.034       735.241  …
1396       1.021       740.486      -6.147       1.003       735.757  …
1397       1.061       741.009      -6.113       1.025       736.241  …
1398       1.007       741.526      -6.189       1.040       736.738  …
1399       0.969       742.025      -6.322       1.015       737.225  …

      Unnamed: 113  Fiber-17  Unnamed: 115  Unnamed: 116  Fiber-18  \
1395         0.998   737.426        -0.924         1.025   738.191
1396         1.017   737.927        -0.815         1.019   738.698
1397         1.040   738.441        -0.762         1.015   739.192
1398         1.004   738.957        -0.871         1.030   739.718
1399         1.004   739.427        -0.804         0.985   740.200

      Unnamed: 118  Unnamed: 119  Fiber-19  Unnamed: 121  Unnamed: 122
1395         1.522         1.009   737.991         3.252         1.013
1396         1.733         1.001   738.499         3.296         1.025
1397         1.684         1.001   739.003         3.080         1.014
1398         1.605         1.019   739.498         3.180         0.998
```

```
1399         1.433         1.007   740.014         3.073         1.010

[5 rows x 123 columns]
```

In the following cell, two 2-D arrays storing the x values (temperature) and y values (HRR) are created.

1) xy_raw: x & y values for raw data
2) xy_flattened: x & y values for curve flattened data

[9]:
```
import warnings
warnings.filterwarnings("ignore")
xy_raw=[]
xy_flattened=[]
xy_corrected=[]
for i in range(0, data.shape[1], 3):
    # extract values for x and y and HR
    select = data.iloc[:,i:i+3]
    x = select.iloc[:,0].values
    xy_raw.append(x)
    xy_flattened.append(x)

    y = select.iloc[:,1].values
    xy_raw.append(y)

    y_b= baseflatten(x,y) #flatten the curve
    xy_flattened.append(y_b.flatten())

    # Uncomment the codes to check the baseline corrected curves

    #fig, ax=plt.subplots()
    #ax.plot(x,y,label='original data')
    #ax.plot(x,y_b,label='flattened data')
    #ax.legend()

xy_raw=np.array(xy_raw)
xy_flattened=np.array(xy_flattened)
```

y values (HRR values) will be used for PCA, the following cells will extract two matrices with 41 rows (observations) and 1399 columns (y values as features).

[10]:
```
features_raw=xy_raw[1::2,:]
print(features_raw.shape)
features_flattened=xy_flattened[1::2,:]
print(features_flattened.shape)
```

```
(41, 1399)
(41, 1399)
```

Because the x values deviate slightly among each observation, it might lead to error if we use original y values directly. Therefore, for each observation, a linear interpolation will be performed and all y values will be re-calculated based on the same x values. Aligned feature matrices and heatmap for correlation matrices are printed below

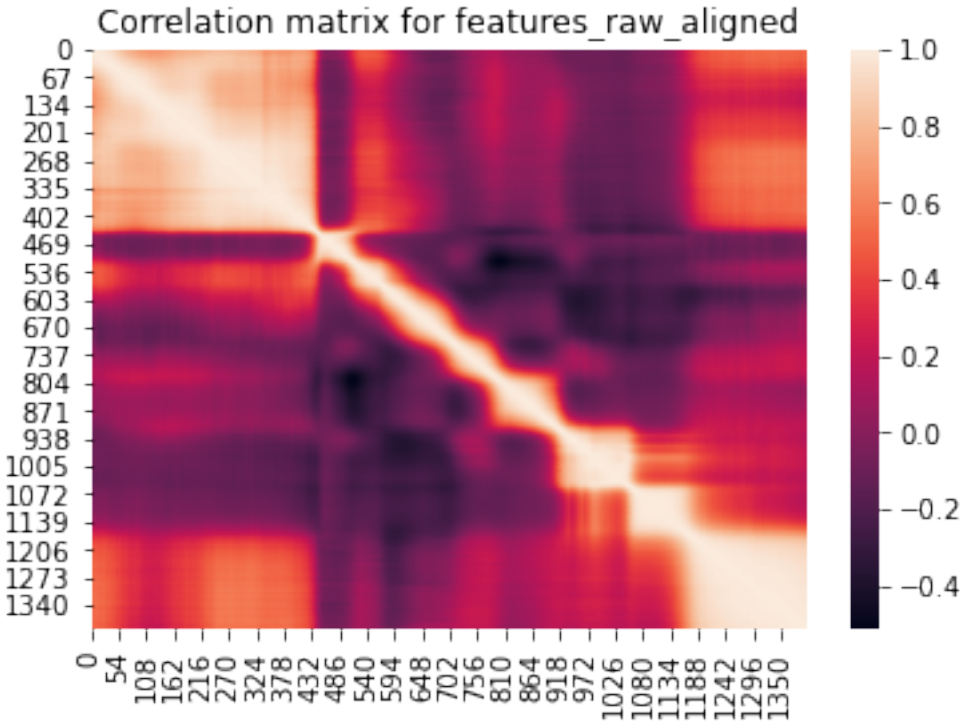
[11]:
```
from scipy import interpolate
# define new aligned x values
x_aligned=np.linspace(max(xy_raw[::2,1]),min(xy_raw[::2,-1]),num=1400)

# function interpolating each observations, and return a new feature matrix␣
↪with aligned x values
def align_data(xy_inp):
    features_inp_aligned=[]
    for i in range(0,41):
        x = xy_inp[2*i,:]
        y=xy_inp[2*i+1,:]

        # interpolate the curve
        interp = interpolate.interp1d(x, y)
        y_aligned=interp(x_aligned)
        features_inp_aligned.append(y_aligned)

        # Uncomment the codes to check the interpolation results

        #fig, ax=plt.subplots()
        #ax.plot(x,y,label='original data')
        #ax.plot(x_aligned,y_aligned,label='interpolated data')
        #ax.legend()
    features_inp_aligned=np.array(features_inp_aligned)
    return features_inp_aligned
```

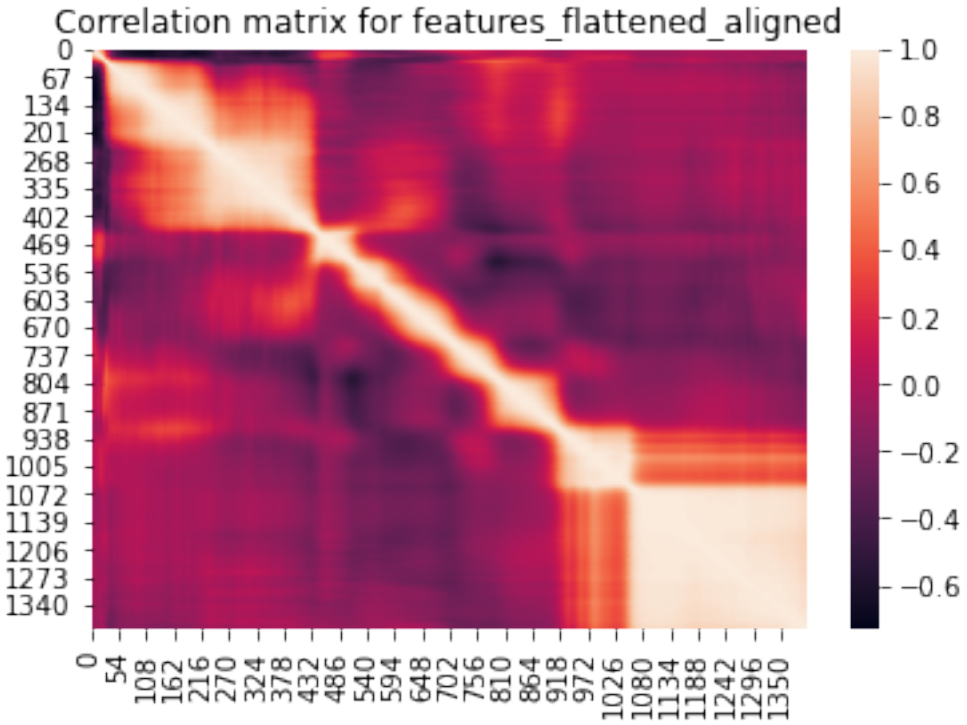
[12]:
```
# Calculate feature matrices with aligned data
features_raw_aligned=align_data(xy_raw)
features_flattened_aligned=align_data(xy_flattened)
print(features_raw_aligned.shape)
print(features_flattened_aligned.shape)
```

```
(41, 1400)
(41, 1400)
```

[13]:
```
import seaborn as sns
corr_raw_aligned=np.corrcoef(features_raw_aligned.T)
hm1=sns.heatmap(corr_raw_aligned).set_title('Correlation matrix for␣
↪features_raw_aligned')

plt.figure()
corr_flattened_aligned=np.corrcoef(features_flattened_aligned.T)
```

```
hm2=sns.heatmap(corr_flattened_aligned).set_title('Correlation matrix for␣
↪features_flattened_aligned')
```





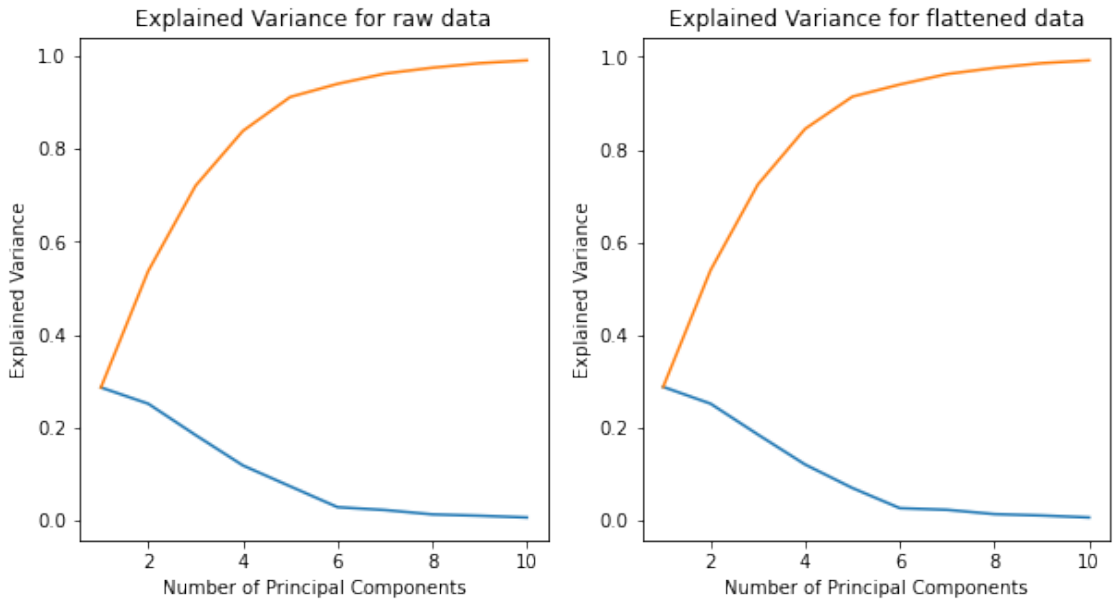
Find the first 10 PCs based on aligned features

[14]:
```
from sklearn.decomposition import PCA
k=10
pca_raw=PCA(n_components=k)
pca_flattened=PCA(n_components=k)
pca_corrected=PCA(n_components=k)

raw_pc=pca_raw.fit_transform(features_raw_aligned)
print(raw_pc[0,:])

flattened_pc=pca_flattened.fit_transform(features_flattened_aligned)
print(flattened_pc[0,:])
```

```
[-686.42103209  311.84630269  710.71679886 -241.66235881  837.55141237
  -73.54494024   35.39005441  -50.01410212  132.44691814 -177.28925658]
[-675.35973346  297.70606542  709.67295662 -210.1040181   880.6852894
   14.376059     74.34795734   49.63853734  170.4150219  -148.95422749]
```

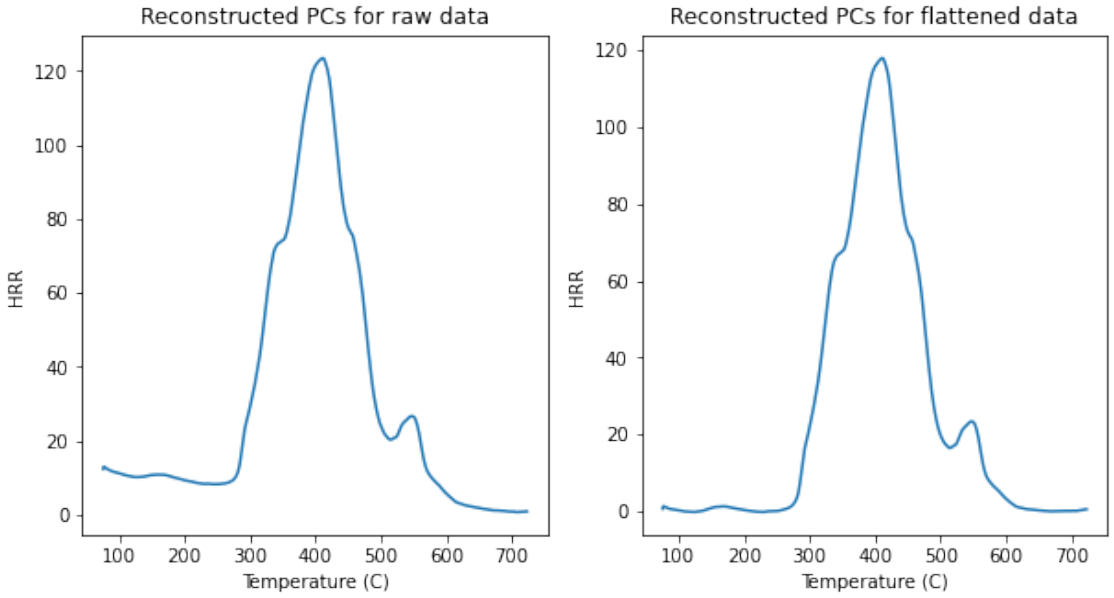
[15]:
```
raw_mean=raw_pc.mean(axis=0)
flattened_mean=flattened_pc.mean(axis=0)

fig,axes=plt.subplots(1,2,figsize=(10,5))
axes[0].plot(range(1,len(raw_mean)+1),pca_raw.explained_variance_ratio_)
axes[0].plot(range(1,len(raw_mean)+1),np.cumsum(pca_raw.
 ↪explained_variance_ratio_))
axes[0].set_xlabel('Number of Principal Components')
axes[0].set_ylabel('Explained Variance')
axes[0].set_title('Explained Variance for raw data')

axes[1].plot(range(1,len(flattened_mean)+1),pca_flattened.
 ↪explained_variance_ratio_)
axes[1].plot(range(1,len(flattened_mean)+1),np.cumsum(pca_flattened.
 ↪explained_variance_ratio_))
axes[1].set_xlabel('Number of Principal Components')
axes[1].set_ylabel('Explained Variance')
axes[1].set_title('Explained Variance for flattened data')
```

[15]:
```
Text(0.5, 1.0, 'Explained Variance for flattened data')
```



[16]:
```
raw_reconstructed=pca_raw.inverse_transform(raw_mean)
flattened_reconstructed=pca_flattened.inverse_transform(flattened_mean)

fig,axes=plt.subplots(1,2,figsize=(10,5))
axes[0].plot(x_aligned,raw_reconstructed)
axes[0].set_xlabel('Temperature (C)')
axes[0].set_ylabel('HRR')
axes[0].set_title('Reconstructed PCs for raw data')

axes[1].plot(x_aligned,flattened_reconstructed)
axes[1].set_xlabel('Temperature (C)')
axes[1].set_ylabel('HRR')
axes[1].set_title('Reconstructed PCs for flattened data')
```

[16]:
```
Text(0.5, 1.0, 'Reconstructed PCs for flattened data')
```



1.2.1 Forward selection to determine most predictive PCs???

[17]:
```
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score, recall_score, precision_score
from sklearn.model_selection import GridSearchCV
from sklearn.svm import SVC

def baseline_predict(X_svc,y_svc):
    # perform a train-test split. 90% of original data will be used for training
    X_train_svc, X_test_svc, y_train_svc, y_test_svc = train_test_split(X_svc,␣
 ↪y_svc, test_size = 0.10)

    # define support vector model with rbf kernel
    svc = SVC(kernel = 'rbf')

    # build up parameter grid and perform GridSearchCV to find the best␣
 ↪estimator
    alphas = np.array([1e-6, 1e-5, 1e-4, 1e-3, 1e-2, 1e-1, 1])
    Cs = 1 / alphas
    sigmas = np.array([1e-3, 1e-2, 1e-1, 1, 10, 100])
    gammas = 1. / 2 / sigmas**2

    param_grid_svc = {'C': Cs,'gamma': gammas}

    svc_search = GridSearchCV(svc, param_grid_svc, cv = 3)
    svc_search.fit(X_train_svc,y_train_svc)
```

```
    # resulting predictions
    predict_svc = svc_search.best_estimator_.predict(X_test_svc)
    full_predict_svc = svc_search.best_estimator_.predict(X_svc)

    test_accuracy=accuracy_score(y_test_svc, predict_svc)
    test_precision=precision_score(y_test_svc, predict_svc, average='macro')
    test_recall=recall_score(y_test_svc, predict_svc, average='macro')

    full_accuracy=accuracy_score(y_svc, full_predict_svc)
    full_precision=precision_score(y_svc, full_predict_svc, average='macro')
    full_recall=recall_score(y_svc, full_predict_svc, average='macro')

    return␣
↪test_accuracy,test_precision,test_recall,full_accuracy,full_precision,full_recall
```

1.3 Generative Model

Due to the small size of our dataset, it is n

[18]:
```
feature_matrix = pd.read_csv("feature_matrix.csv")
feature_matrix['PC1'] = flattened_pc[:,0]
feature_matrix['PC2'] = flattened_pc[:,1]
feature_matrix['PC3'] = flattened_pc[:,2]
feature_matrix.head(10)
```

[18]:

	Total Heat Release	Burning Temperature	Ignition Temperature	\
0	24722.818517	482.246	350.805	
1	14879.480392	537.858	438.643	
2	16584.116501	515.457	366.537	
3	20246.452607	482.774	396.996	
4	26622.142067	472.215	388.929	
5	12581.675639	488.529	292.177	
6	27364.231613	468.963	377.870	
7	14539.335519	469.506	384.928	
8	15665.463662	437.267	334.539	
9	13535.355054	461.318	343.769	

	Heat Release Capacity	Fire Growth Capacity	FR_labels	PC1	\
0	25955.104346	134.021649	2	-675.359733	
1	15591.943456	120.959219	2	909.690756	
2	17369.365738	77.548988	1	63.184583	
3	21344.250614	191.805110	0	785.952883	
4	28036.752193	260.118532	0	-1375.196882	
5	13257.707466	36.933912	1	312.467042	
6	28900.669510	238.762552	0	-1823.270549	
7	15291.533325	139.195486	1	-673.781301	
8	16466.951534	114.496239	1	-534.780041	

```
9           14282.096095             84.124726          1  -613.962631
```

```
           PC2         PC3
0   297.706065  709.672957
1   342.229152   38.531590
2  -388.364571  435.757401
3  1344.401661  280.523465
4  1562.118158  335.994645
5  -994.660995 -171.510404
6  1123.422047  811.066965
7   -70.424838   63.789101
8 -1735.166316   67.101112
9 -1013.199055  282.618485
```

[19]:
```
data = feature_matrix
# import standard scaler
from sklearn.preprocessing import StandardScaler

# scale the data (excluding labels)
scaler = StandardScaler()
scaled = scaler.fit_transform(data.drop(columns='FR_labels'))
scaled = pd.DataFrame(scaled)
scaled.columns = data.drop(columns='FR_labels').columns
scaled['FR_labels'] = data.loc[:,'FR_labels']    # add FR_labels to new␣
↪dataframe
scaled.head()
origin_feature_matrix=scaled
origin_feature_matrix.shape
```

[19]:
```
(41, 9)
```

[20]:
```
# plot
import seaborn as sns
sns.pairplot(scaled,hue='FR_labels')
```

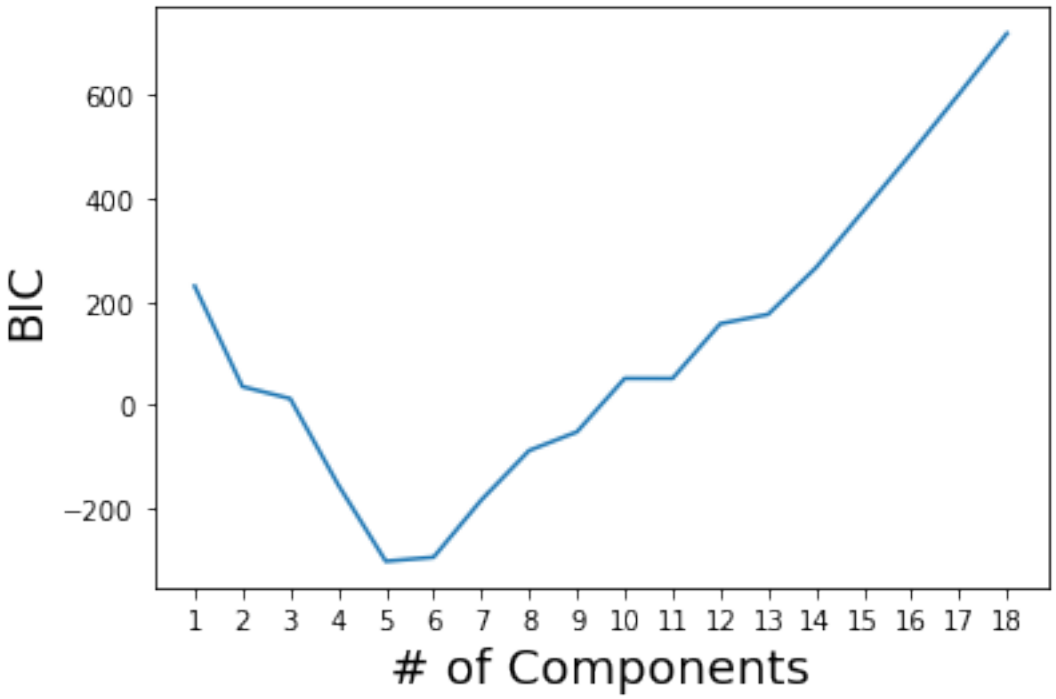
[20]:
```
<seaborn.axisgrid.PairGrid at 0x1da30125670>
```

###Gaussian Mixture

[21]:
```
y = scaled['FR_labels']
from sklearn.mixture import GaussianMixture

X = scaled.drop(columns='FR_labels')[y == 0].values
n_components = np.arange(1, 19)

BICs = []
models = []
for n in n_components:
    gmm_n =  GaussianMixture(n, covariance_type = 'full').fit(X)
    bic = gmm_n.bic(X)
    BICs.append(bic)
```

```
    models.append(gmm_n)


fig, ax = plt.subplots()
ax.plot(n_components, BICs)
ax.set_xlabel('# of Components', size = 18);
ax.set_ylabel('BIC', size = 18)
ax.set_xticks(n_components);
best_n=[]
best_n.append(n_components[BICs == min(BICs)][0])
print(best_n)
```

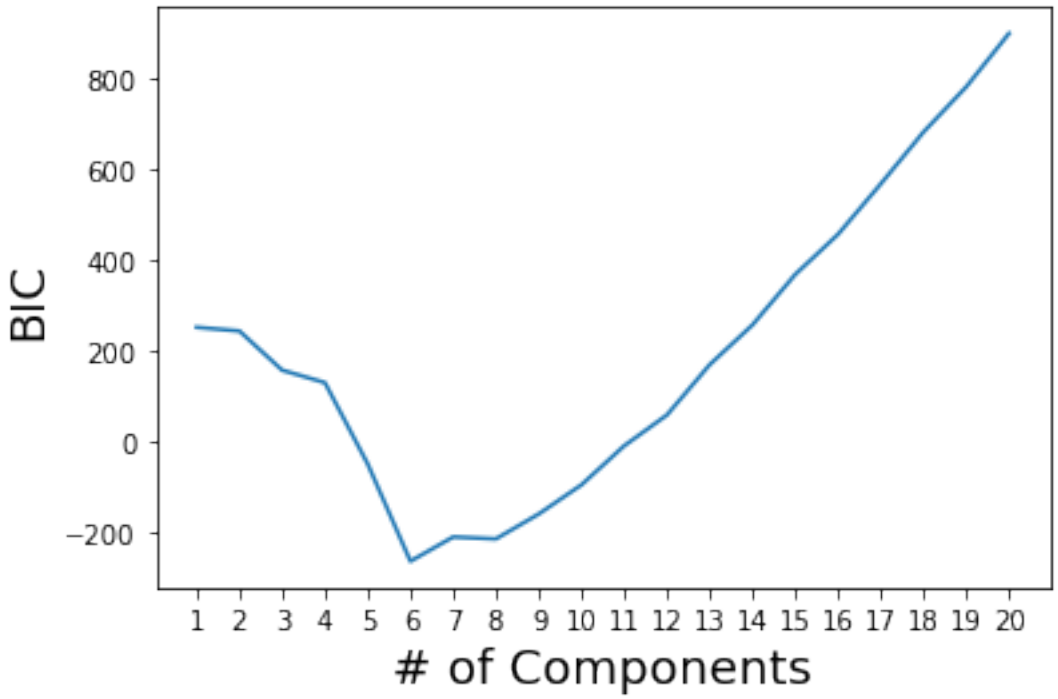
[5]



[22]:
```
y = scaled['FR_labels']
from sklearn.mixture import GaussianMixture

X = scaled.drop(columns='FR_labels')[y == 1].values
n_components = np.arange(1, 21)

BICs = []
models = []
for n in n_components:
    gmm_n =  GaussianMixture(n, covariance_type = 'full').fit(X)
```

```
    bic = gmm_n.bic(X)
    BICs.append(bic)
    models.append(gmm_n)


fig, ax = plt.subplots()
ax.plot(n_components, BICs)
ax.set_xlabel('# of Components', size = 18);
ax.set_ylabel('BIC', size = 18)
ax.set_xticks(n_components);
best_n.append(n_components[BICs == min(BICs)][0])
print(best_n)
```

```
[5, 6]
```



[23]:
```
vals = []
for i in range(0,2):
  X = scaled.drop(columns='FR_labels')[y == i].values
  gmm = GaussianMixture(n_components = 5, covariance_type = 'full')
  gmm.fit(X)
  new = gmm.sample(100)
  vals.append(new[0])
```

[24]:
```
new0 = pd.DataFrame(vals[0])
new0['FR_labels'] = np.zeros(100).astype(int)
new0.columns = scaled.columns
new1 = pd.DataFrame(vals[1])
new1['FR_labels'] = np.ones(100).astype(int)
new1.columns = scaled.columns
final = scaled.append(new0)
final = final.append(new1)
final
```

[24]:

	Total Heat Release	Burning Temperature	Ignition Temperature	\
0	1.808411	-0.424203	-0.990329	
1	-0.335103	0.879587	0.744864	
2	0.036103	0.354409	-0.679551	
3	0.833624	-0.411824	-0.077850	
4	2.222013	-0.659374	-0.237209	
..	…	…	…	
95	-1.081838	0.224518	1.123469	
96	-0.510300	0.109623	0.655658	
97	-0.077270	0.667905	0.413082	
98	-0.682197	0.255999	0.562615	
99	-0.509503	0.540363	0.933226	

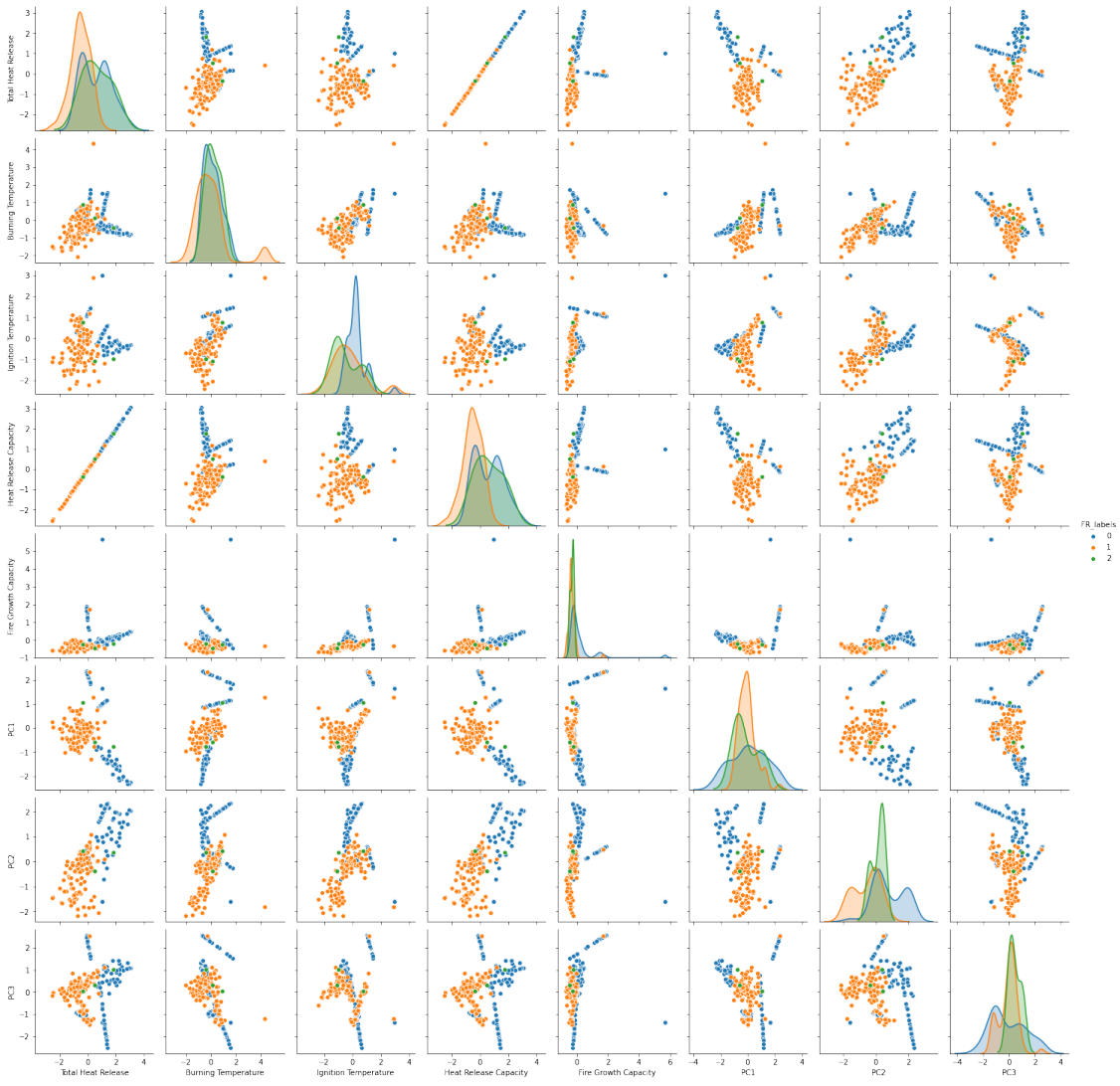
	Heat Release Capacity	Fire Growth Capacity	PC1	PC2	PC3	\
0	1.778631	-0.202424	-0.780066	0.367749	1.022207	
1	-0.365567	-0.258909	1.050728	0.422747	0.055501	
2	0.002192	-0.446622	0.072981	-0.479737	0.627661	
3	0.824619	0.047441	0.907806	1.660705	0.404063	
4	2.209336	0.342840	-1.588405	1.929644	0.483964	
..	…	…	…	…	…	
95	-1.085874	-0.012660	0.706580	-0.133468	0.858272	
96	-0.490908	-0.065789	0.236920	0.120113	0.023390	
97	-0.069270	-0.264607	0.160714	0.625354	-0.822917	
98	-0.656169	-0.160562	0.267802	-0.090997	-0.167082	
99	-0.504532	-0.067655	0.765922	0.313542	0.012615	

	FR_labels
0	2
1	2
2	1
3	0
4	0
..	…
95	1
96	1
97	1
98	1

```
99          1

[241 rows x 9 columns]
```

[25]:
```
sns.pairplot(final,hue='FR_labels')
```

[25]:
```
<seaborn.axisgrid.PairGrid at 0x1da2a6b3fd0>
```



This actually doesn't look too bad. It seems to preserve the distribution of the original data, even with the addition of 100 points. I did not add points for FR_label=2 class because it is sparse to begin with.

###Kernel Density Estimation

[26]:
```
from sklearn.neighbors import KernelDensity
from sklearn.model_selection import GridSearchCV
```

[27]:
```
vals = []
for i in range(0,2):
  X = scaled.drop(columns='FR_labels')[y == i].values

  # use grid search cross-validation to optimize the bandwidth
  params = {'bandwidth': np.logspace(-1, 1, 20)}
  grid = GridSearchCV(KernelDensity(kernel='gaussian'), params)
  grid.fit(X)

  print("best bandwidth: {0}".format(grid.best_estimator_.bandwidth))
  print(grid.best_estimator_.score(X))

  # use the best estimator to compute the kernel density estimate
  kde = KernelDensity(bandwidth = .54, kernel = 'gaussian')
  kde.fit(X)
  print(np.logspace(-1, 1, 20))
  print(kde.score(X))
  new = kde.sample(100)
  vals.append(new)
```

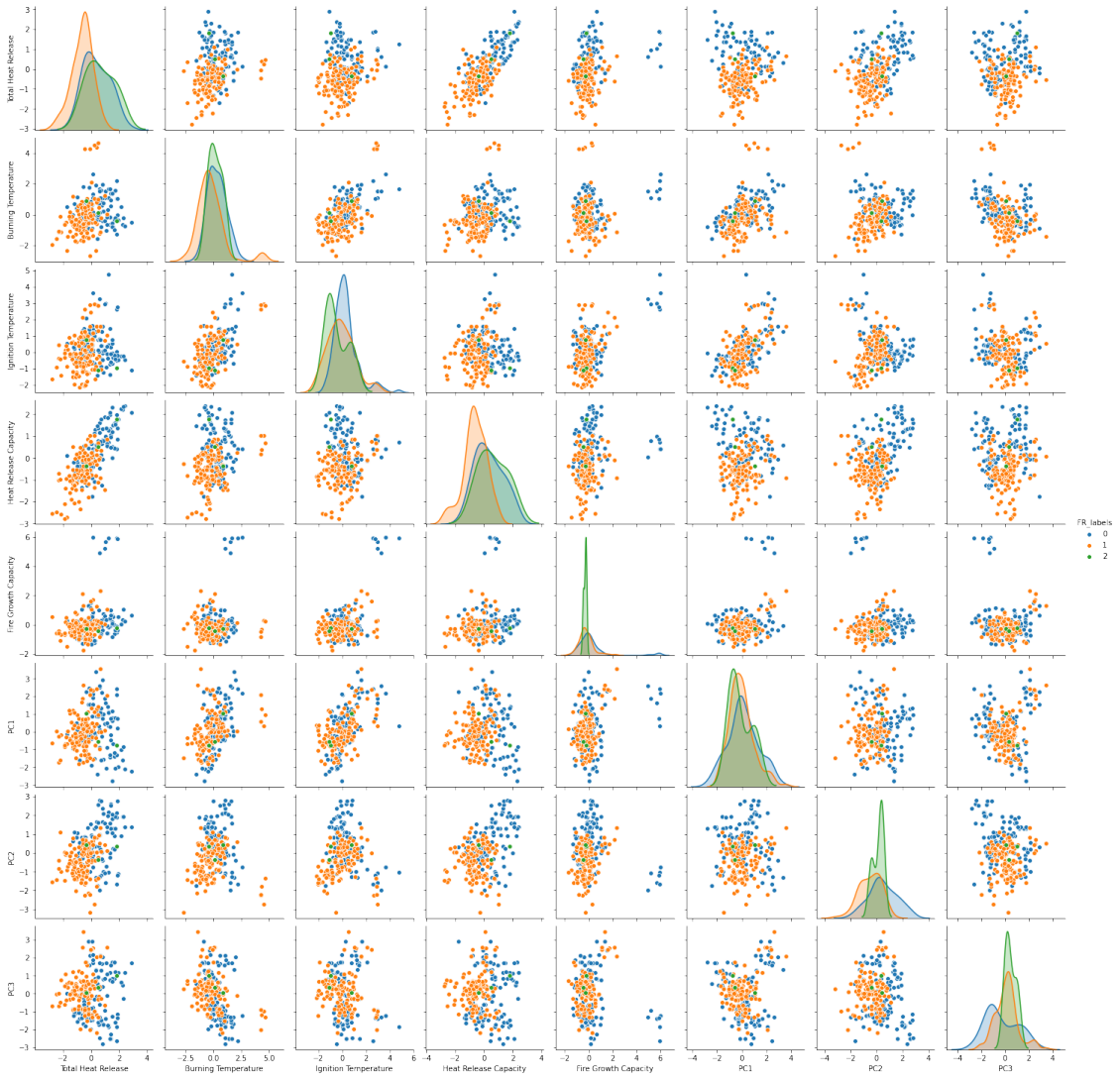
```
best bandwidth: 0.6951927961775606
-117.70908947368294
[ 0.1         0.1274275   0.16237767  0.20691381  0.26366509  0.33598183
  0.42813324  0.54555948  0.6951928   0.88586679  1.12883789  1.43844989
  1.83298071  2.33572147  2.97635144  3.79269019  4.83293024  6.15848211
  7.8475997  10.        ]
-83.34054583333229
best bandwidth: 0.6951927961775606
-136.85204064684024
[ 0.1         0.1274275   0.16237767  0.20691381  0.26366509  0.33598183
  0.42813324  0.54555948  0.6951928   0.88586679  1.12883789  1.43844989
  1.83298071  2.33572147  2.97635144  3.79269019  4.83293024  6.15848211
  7.8475997  10.        ]
-100.98346153566186
```

[28]:
```
new0 = pd.DataFrame(vals[0])
new0['FR_labels'] = np.zeros(100).astype(int)
new0.columns = scaled.columns
new1 = pd.DataFrame(vals[1])
new1['FR_labels'] = np.ones(100).astype(int)
new1.columns = scaled.columns
final = scaled.append(new0)
final = final.append(new1)
final
```

[28]:
```
    Total Heat Release  Burning Temperature  Ignition Temperature  \
0             1.808411            -0.424203             -0.990329
1            -0.335103             0.879587              0.744864
2             0.036103             0.354409             -0.679551
3             0.833624            -0.411824             -0.077850
4             2.222013            -0.659374             -0.237209
..                 …                   …                     …
95           -0.662276             0.455443              0.575375
96           -1.212980            -0.655079             -1.953262
97           -1.405636            -0.472365              0.574471
98           -0.583222            -1.688204             -0.885139
99           -0.438033             0.439771              1.278297

    Heat Release Capacity  Fire Growth Capacity       PC1       PC2       PC3  \
0                1.778631             -0.202424 -0.780066  0.367749  1.022207
1               -0.365567             -0.258909  1.050728  0.422747  0.055501
2                0.002192             -0.446622  0.072981 -0.479737  0.627661
3                0.824619              0.047441  0.907806  1.660705  0.404063
4                2.209336              0.342840 -1.588405  1.929644  0.483964
..                    …                     …       …         …         …
95              -1.039101             -0.368334  1.675698 -0.934325  1.177548
96              -1.265756             -0.464628  0.370434 -1.385647  0.177019
97              -1.904052             -0.719317  0.514430  0.012650  0.604339
98              -0.377791             -1.735399  0.139514 -1.019283  0.736869
99               0.251828              0.217014 -1.312832  0.217401 -0.103642

    FR_labels
0           2
1           2
2           1
3           0
4           0
..        …
95          1
96          1
97          1
98          1
99          1

[241 rows x 9 columns]
```

[29]:
```
sns.pairplot(final,hue='FR_labels')
```

[29]:
```
<seaborn.axisgrid.PairGrid at 0x1da449d2cd0>
```



##Classifiers

[30]:
```
X_ori=origin_feature_matrix.drop(columns='FR_labels').values
y_ori=origin_feature_matrix['FR_labels'].values
X_ori.shape
```

[30]: (41, 8)

SVC (Baseline model)

[31]:
```
# perform a train-test split. 90% of original data will be used for training
X_svc = final.drop(columns='FR_labels').values
y_svc = final['FR_labels'].values
```

```
X_train_svc, X_test_svc, y_train_svc, y_test_svc = train_test_split(X_svc,␣
↪y_svc, test_size = 0.25)

# define support vector model with rbf kernel
svc = SVC(kernel = 'rbf')

# build up parameter grid and perform GridSearchCV to find the best estimator
alphas = np.array([1e-6, 1e-5, 1e-4, 1e-3, 1e-2, 1e-1, 1])
Cs = 1 / alphas
sigmas = np.array([1e-3, 1e-2, 1e-1, 1, 10, 100])
gammas = 1. / 2 / sigmas**2

param_grid_svc = {'C': Cs,'gamma': gammas}

svc_search = GridSearchCV(svc, param_grid_svc, cv = 5)
svc_search.fit(X_train_svc,y_train_svc)

# resulting predictions
predict_svc = svc_search.best_estimator_.predict(X_test_svc)
full_predict_svc = svc_search.best_estimator_.predict(X_svc)
origin_predict_svc = svc_search.best_estimator_.predict(X_ori)
# note: we have 3 labels, so we use average='macro' to find the average metric␣
↪for each
#       label summed. This augments penalized performance caused by class␣
↪imbalance.
# print out the accuracy, precison and recall score for the prediction on␣
↪validation set
print('Accuracy for validation set: {}'.format(accuracy_score(y_test_svc,␣
↪predict_svc)))
print('Precision for validation set: {}'.format(precision_score(y_test_svc,␣
↪predict_svc, average='macro')))
print('Recall for validation set: {}\n'.format(recall_score(y_test_svc,␣
↪predict_svc, average='macro')))

# print out the accuracy, precison and recall score for the prediction on full␣
↪dataset
print('Accuracy for full dataset: {}'.format(accuracy_score(y_svc,␣
↪full_predict_svc)))
print('Precision for full dataset: {}'.format(precision_score(y_svc,␣
↪full_predict_svc, average='macro')))
print('Recall for full dataset: {}'.format(recall_score(y_svc,␣
↪full_predict_svc, average='macro')))

# print out the accuracy, precison and recall score for the prediction on␣
↪original dataset (before data generation)
```

```
print('Accuracy for original dataset: {}'.format(accuracy_score(y_ori,␣
 ↪origin_predict_svc)))
print('Precision for original dataset: {}'.format(precision_score(y_ori,␣
 ↪origin_predict_svc, average='macro')))
print('Recall for original dataset: {}'.format(recall_score(y_ori,␣
 ↪origin_predict_svc, average='macro')))
```

```
Accuracy for validation set: 0.7868852459016393
Precision for validation set: 0.7981283422459893
Recall for validation set: 0.7511261261261262

Accuracy for full dataset: 0.9377593360995851
Precision for full dataset: 0.959494927998865
Recall for full dataset: 0.9581920903954803
Accuracy for original dataset: 0.9024390243902439
Precision for original dataset: 0.9393939393939394
Recall for original dataset: 0.9333333333333332
```

####Decision Tree

[32]:
```
from sklearn.tree import DecisionTreeClassifier

X_DT = final.drop(columns='FR_labels').values
y_DT = final['FR_labels'].values
X_train_DT, X_test_DT, y_train_DT, y_test_DT = train_test_split(X_DT, y_DT,␣
 ↪test_size = 0.25)

# Create dtree instance
dtree = DecisionTreeClassifier()

# Create parameter grid - currently just max depth
max_depths = [2,3,5,10,15,20, 100]
criterions = ['gini', 'entropy']
param_grid_dtree = {'max_depth': max_depths, 'criterion': criterions}
print(X_DT.shape)
print(y_DT.shape)
```

```
(241, 8)
(241,)
```

[33]:
```
# GridSearch Hyperparameter Tuning
DT_search = GridSearchCV(dtree, param_grid_dtree, cv=5)
DT_search.fit(X_train_DT, y_train_DT)

# Predict both the testing set and the full data set
dtree_prediction = DT_search.best_estimator_.predict(X_test_DT)
dtree_full_prediction = DT_search.best_estimator_.predict(X_DT)
dtree_origin_prediction = DT_search.best_estimator_.predict(X_ori)
```

```
# note: we have 3 labels, so we use average='macro' to find the average metric␣
 ↪for each
#       label summed. This augments penalized performance caused by class␣
 ↪imbalance.
# print out the accuracy, precison and recall score for the prediction on␣
 ↪validation set
print('Accuracy for validation set: {}'.format(accuracy_score(y_test_DT,␣
 ↪dtree_prediction)))
print('Precision for validation set: {}'.format(precision_score(y_test_DT,␣
 ↪dtree_prediction, average='macro')))
print('Recall for validation set: {}\n'.format(recall_score(y_test_DT,␣
 ↪dtree_prediction, average='macro')))

# print out the accuracy, precison and recall score for the prediction on full␣
 ↪dataset
print('Accuracy for full dataset: {}'.format(accuracy_score(y_DT,␣
 ↪dtree_full_prediction)))
print('Precision for full dataset: {}'.format(precision_score(y_DT,␣
 ↪dtree_full_prediction, average='macro')))
print('Recall for full dataset: {}\n'.format(recall_score(y_DT,␣
 ↪dtree_full_prediction, average='macro')))

# print out the accuracy, precison and recall score for the prediction on␣
 ↪original dataset (before data generation)
print('Accuracy for original dataset: {}'.format(accuracy_score(y_ori,␣
 ↪dtree_origin_prediction)))
print('Precision for original dataset: {}'.format(precision_score(y_ori,␣
 ↪dtree_origin_prediction, average='macro')))
print('Recall for original dataset: {}'.format(recall_score(y_ori,␣
 ↪dtree_origin_prediction, average='macro')))
```

```
Accuracy for validation set: 0.7704918032786885
Precision for validation set: 0.5241301907968574
Recall for validation set: 0.5132616487455196

Accuracy for full dataset: 0.8464730290456431
Precision for full dataset: 0.7945893719806763
Recall for full dataset: 0.7885122410546139

Accuracy for original dataset: 0.8292682926829268
Precision for original dataset: 0.8944444444444445
Recall for original dataset: 0.7888888888888889
```

###Random Forest

[34]:
```
from sklearn.ensemble import RandomForestClassifier


X_RF = final.drop(columns='FR_labels').values
y_RF = final['FR_labels'].values
X_train_RF, X_test_RF, y_train_RF, y_test_RF = train_test_split(X_RF, y_RF,␣
 ↪test_size = 0.25)

# Instantiate random forest model
ranfor = RandomForestClassifier()

# Create parameter grid
# We are searching over two hyperparameters for our Random Forest model


n_estimators = [3, 5, 7, 10, 15, 20, 25, 50, 100]
maximum_feats = ['auto', 'log2']
max_depths = [2,3,5,10,15,20, 100]
criterions = ['gini', 'entropy']
param_grid_ranfor = {'n_estimators': n_estimators, 'criterion': criterions,␣
 ↪'max_features': maximum_feats,'max_depth': max_depths}
```

[35]:
```
# GridSearch Hyperparameter Tuning
RF_search = GridSearchCV(ranfor, param_grid_ranfor, cv=5)
RF_search.fit(X_train_RF, y_train_RF)

# Predict both the testing set and the full data set
ranfor_prediction = RF_search.best_estimator_.predict(X_test_RF)
ranfor_full_prediction = RF_search.best_estimator_.predict(X_RF)
ranfor_origin_prediction = RF_search.best_estimator_.predict(X_ori)

# note: we have 3 labels, so we use average='macro' to find the average metric␣
 ↪for each
#       label summed. This augments penalized performance caused by class␣
 ↪imbalance.
# print out the accuracy, precison and recall score for the prediction on␣
 ↪validation set
print('Accuracy for validation set: {}'.format(accuracy_score(y_test_RF,␣
 ↪ranfor_prediction)))
print('Precision for validation set: {}'.format(precision_score(y_test_RF,␣
 ↪ranfor_prediction, average='macro')))
print('Recall for validation set: {}\n'.format(recall_score(y_test_RF,␣
 ↪ranfor_prediction, average='macro')))

# print out the accuracy, precison and recall score for the prediction on full␣
 ↪dataset
```

```
print('Accuracy for full dataset: {}'.format(accuracy_score(y_RF,␣
 ↪ranfor_full_prediction)))
print('Precision for full dataset: {}'.format(precision_score(y_RF,␣
 ↪ranfor_full_prediction, average='macro')))
print('Recall for full dataset: {}\n'.format(recall_score(y_RF,␣
 ↪ranfor_full_prediction, average='macro')))

# print out the accuracy, precison and recall score for the prediction on␣
 ↪original dataset (before data generation)
print('Accuracy for original dataset: {}'.format(accuracy_score(y_ori,␣
 ↪ranfor_origin_prediction)))
print('Precision for original dataset: {}'.format(precision_score(y_ori,␣
 ↪ranfor_origin_prediction, average='macro')))
print('Recall for original dataset: {}'.format(recall_score(y_ori,␣
 ↪ranfor_origin_prediction, average='macro')))
```

```
Accuracy for validation set: 0.6721311475409836
Precision for validation set: 0.6726190476190477
Recall for validation set: 0.671505376344086

Accuracy for full dataset: 0.9128630705394191
Precision for full dataset: 0.9414553267012283
Recall for full dataset: 0.8328154425612052

Accuracy for original dataset: 0.9024390243902439
Precision for original dataset: 0.9324561403508772
Recall for original dataset: 0.837037037037037
```

###KNN

[36]:
```
from sklearn.neighbors import KNeighborsClassifier

X_KNN = final.drop(columns='FR_labels').values
y_KNN = final['FR_labels'].values
X_train_KNN, X_test_KNN, y_train_KNN, y_test_KNN = train_test_split(X_KNN,␣
 ↪y_KNN, test_size = 0.25)

KNN = KNeighborsClassifier()
# neighbors = np.array([2,4,6,8,10,12,15,18,20,15])
neighbors = np.array([2,3])
KNN_param_grid = {'n_neighbors': neighbors}
```

[37]:
```
# Hyperparameter tunning
KNN_search = GridSearchCV(KNN, KNN_param_grid, cv=5)
KNN_search.fit(X_train_KNN, y_train_KNN)

# resulting predictions
```

```
predict_KNN = KNN_search.best_estimator_.predict(X_test_KNN)
full_predict_KNN = KNN_search.best_estimator_.predict(X_KNN)
origin_predict_KNN = KNN_search.best_estimator_.predict(X_ori)

# note: we have 3 labels, so we use average='macro' to find the average metric␣
 ↪for each
#       label summed. This augments penalized performance caused by class␣
 ↪imbalance.
# print out the accuracy, precison and recall score for the prediction on␣
 ↪validation set
print('Accuracy for validation set: {}'.format(accuracy_score(y_test_KNN,␣
 ↪predict_KNN)))
print('Precision for validation set: {}'.format(precision_score(y_test_KNN,␣
 ↪predict_KNN, average='macro')))
print('Recall for validation set: {}\n'.format(recall_score(y_test_KNN,␣
 ↪predict_KNN, average='macro')))

# print out the accuracy, precison and recall score for the prediction on full␣
 ↪dataset
print('Accuracy for full dataset: {}'.format(accuracy_score(y_KNN,␣
 ↪full_predict_KNN)))
print('Precision for full dataset: {}'.format(precision_score(y_KNN,␣
 ↪full_predict_KNN, average='macro')))
print('Recall for full dataset: {}\n'.format(recall_score(y_KNN,␣
 ↪full_predict_KNN, average='macro')))

# print out the accuracy, precison and recall score for the prediction on␣
 ↪original dataset (before data generation)
print('Accuracy for original dataset: {}'.format(accuracy_score(y_ori,␣
 ↪origin_predict_KNN)))
print('Precision for original dataset: {}'.format(precision_score(y_ori,␣
 ↪origin_predict_KNN, average='macro')))
print('Recall for original dataset: {}'.format(recall_score(y_ori,␣
 ↪origin_predict_KNN, average='macro')))
```

```
Accuracy for validation set: 0.7704918032786885
Precision for validation set: 0.5132902298850575
Recall for validation set: 0.5306513409961685

Accuracy for full dataset: 0.8755186721991701
Precision for full dataset: 0.5839307048984468
Recall for full dataset: 0.5911487758945386

Accuracy for original dataset: 0.8292682926829268
Precision for original dataset: 0.5531746031746031
Recall for original dataset: 0.5981481481481481
```

[ ]: