Group7_Final_Codes

November 26, 2020

0.1 Accessing Data in Google Collab

[ ]:
```
# Mount Drive
from google.colab import drive
drive.mount('/content/drive')
```

```
Mounted at /content/drive
```

[ ]:
```
# Move to where Data is located
%cd 'drive/My Drive/ChBE 6745 Project/Data'
```

```
/content/drive/.shortcut-targets-by-id/1C8dheEq3N-3FxfXYpvTW6P2eth8rAiLm/ChBE
6745 Project/Data
```

1 1. Data Preparation

1.0.1 1.1 Read Original Data

[1]:
```
# Read in the data
import numpy as np
import pandas as pd
import pylab as plt
df = pd.read_csv("data/MCC_raw.csv")
data = df.drop([0]).astype(float)
data.head()
```

[1]:
```
   Adhesive-1-1  Unnamed: 1  Unnamed: 2  Adhesive-2-1  Unnamed: 4  Unnamed: 5  \
1        73.744       4.570       0.084        74.630       5.286       0.067
2        73.711       6.830       0.024        74.653       7.127       0.055
3        73.749       8.960       0.005        74.659       8.873       0.029
4        73.741       9.812       0.030        74.688      10.275       0.035
5        73.780      10.874       0.031        74.745      11.123       0.086

   Adhesive-3-1  Unnamed: 7  Unnamed: 8  Adhesive-4-1  …  Unnamed: 113  \
1        74.621       4.898       0.061        74.539  …        -0.034
2        74.683       6.988       0.139        74.552  …        -0.066
3        74.715       8.493       0.094        74.519  …        -0.079
4        74.724       9.658       0.041        74.498  …        -0.059
```

```
5        74.745      10.535       0.030        74.478  …         -0.029

   Fiber-17  Unnamed: 115  Unnamed: 116  Fiber-18  Unnamed: 118  Unnamed: 119  \
1    73.866         4.474         0.016    74.566         5.061         0.040
2    73.889         6.175         0.020    74.599         6.919         0.037
3    73.901         7.630         0.035    74.622         8.775         0.056
4    73.928         8.643         0.040    74.609        10.098         0.010
5    73.933         9.300         0.032    74.644        10.662         0.023

   Fiber-19  Unnamed: 121  Unnamed: 122
1    73.599         5.051        -0.007
2    73.637         6.740         0.037
3    73.658         7.944         0.059
4    73.653         9.038         0.016
5    73.733         9.599         0.076

[5 rows x 123 columns]
```

[2]:
```
# Read in Flame Retardant Test Results
df = pd.read_csv("data/FR_results.csv")
FR_labels = df.iloc[:,1]
df.head()
```

[2]:
```
     Material  Result
0  Adhesive-1       2
1  Adhesive-2       2
2  Adhesive-3       1
3  Adhesive-4       0
4  Adhesive-5       0
```

1.1 1.2 Extract physical features

1.1.1 Baseline correction

To calculate most accurate features, the baseline corrected curve should be flat (no slope for the area before and after main peaks) and smooth (with no small peaks before 300C). Therefore, the baseline correction function can be divided into three steps, including (1) curve flattening

(1) curve flattening:

the original dataset might result in a slope (can be either descending or ascending) before and after the main peaks. To obtain accurate results, the slope area must be flattened. A library called Rampy, which was developed by Charles, et. al. from the Australian National University, was applied to flatten the tilt area.

[3]:
```
# run if rampy is not installed
%pip install rampy
# imports
import rampy as rp
```

```python
from scipy.signal import savgol_filter
```

```
Requirement already satisfied: rampy in
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-packages (0.4.5)
Requirement already satisfied: scipy in
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-packages (from rampy)
(1.5.0)
Requirement already satisfied: scikit-learn in
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-packages (from rampy)
(0.23.1)
Requirement already satisfied: numpy>=1.12 in
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-packages (from rampy)
(1.18.5)
Requirement already satisfied: pandas in
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-packages (from rampy)
(1.0.5)
Requirement already satisfied: joblib>=0.11 in
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-packages (from scikit-
learn->rampy) (0.16.0)
Requirement already satisfied: threadpoolctl>=2.0.0 in
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-packages (from scikit-
learn->rampy) (2.1.0)
Requirement already satisfied: python-dateutil>=2.6.1 in
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-packages (from
pandas->rampy) (2.8.1)
Requirement already satisfied: pytz>=2017.2 in
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-packages (from
pandas->rampy) (2020.1)
Requirement already satisfied: six>=1.5 in
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-packages (from python-
dateutil>=2.6.1->pandas->rampy) (1.15.0)
Note: you may need to restart the kernel to use updated packages.
```

[4]:
```python
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
```

1.1.2 Total Heat Release Rate (THR)

Total Heat Release Rate (THR) is the area under the curve

[5]:
```python
# imports
import scipy
```

```python
from scipy import integrate

# Calculates the area under the curve
#
# params: x, array of temperature values; y, array of HRR values
# returns: THR, the value for total heat release rate

def calculate_THR(Temp,HRR):
    return np.trapz(HRR,Temp)
```

1.1.3 Burning Temperature

$T_{burning}$ = The temperature when 95% of the heat is released for the material

[6]:
```python
# Finds the temperature corresponding to the highest peak
#
# params: x, array of temperature values; y, array of HRR values
# returns: Tb, the burning temperature
def calculate_Tb(Temp,HRR):
    THR = calculate_THR(Temp, HRR)
    for i in range(len(Temp)):
      #print(np.trapz(HRR[:i]))
      #if np.trapz(HRR[:i],Temp) >= 0.50*THR:
        if np.trapz(HRR[:i],Temp[:i]) >= 0.95*THR:
            break
    # return Temp[np.argmax(HRR)]
    return Temp[i]
```

1.1.4 Ignition Temperature

$T_{ignition}$ = The temperature at peak HRR

[7]:
```python
# Finds the temperature corresponding to start of the highest peak
#
# params: x, array of temperature values; y, array of HRR values
# returns: Tign, the ignition temperature
def calculate_Tign(Temp,HRR):
    return Temp[np.argmax(HRR)]
```

1.1.5 Heat Release Capacity (HRC)

HRC $= \frac{PeakHeatReleased}{HeatofPyrolysis} = \frac{HRRpeak}{HR_{average}}$

[8]:
```python
# Calculates HRC using THR and heat of pyrolysis (Q/HR_average)
#
# params: THR, the total heat release; Tign, ignition temperature; Tinf, final␣
↪temperature?
```

```
# returns: HRC, the heat release capacity
def calculate_HRC(HRR,HR):
    HR_average = np.average(HR)
    HRC = HRR.max()/HR_average
    return HRC
```

1.1.6 Fire Growth Capacity (FGC)

$\text{FGC} = (\frac{THR}{T_{burning}-T_{ignition}})(\frac{T_{burning}-T_0}{T_{ignition}-T_0})$
$(T_0 = 25°\text{C})$

[9]:
```
# Calculates the FGC using THR, ignition temperature, and burning temperature
#
# params: THR, the total heat release; Tign, ignition temperature; Tb, burning␣
↪temperature
# returns: FGC, the fire growth capacity
def calculate_FGC(THR, Tb, Tign):
    FGC = (THR/(Tb - Tign))/((Tb - 25)/(Tign - 25))
    return FGC
```

1.1.7 *Generation of physical feature matrix*

[10]:
```
# setup lists to store desired features
THRs = []
Tbs = []
Tigns = []
HRCs = []
FGCs = []

# Iterate and generate arrays for desired features
for i in range(0, data.shape[1], 3):
    # extract values for x and y and HR
    select = data.iloc[:,i:i+3]
    select = select.dropna()
    x = select.iloc[:,0].values
    y = select.iloc[:,1].values
    HR = select.iloc[:,2].values

    # perform data manipulation to get desired features
    x_b=x
    y_b= baseflatten(x,y)
    #x_b, y_b=x,y
    y_b = y_b.reshape(-1)
    THR = calculate_THR(x_b,y_b)
    Tb = calculate_Tb(x_b,y_b)
    Tign = calculate_Tign(x_b,y_b)
    HRC = calculate_HRC(y_b,HR)
```

```python
    FGC = calculate_FGC(THR, Tb, Tign)
    THRs.append(THR)
    Tbs.append(Tb)
    Tigns.append(Tign)
    HRCs.append(HRC)
    FGCs.append(FGC)

# setup dataframe for feature matrix
feature_matrix = pd.DataFrame()
feature_matrix['Total Heat Release'] = THRs
feature_matrix['Burning Temperature'] = Tbs
feature_matrix['Ignition Temperature'] = Tigns
feature_matrix['Heat Release Capacity'] = HRCs
feature_matrix['Fire Growth Capacity'] = FGCs

# Add column for FR test result labels
feature_matrix['FR_labels'] = FR_labels

feature_matrix
```

```
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-
packages/rampy/baseline.py:239: RuntimeWarning: overflow encountered in exp
  wt = 1.0/(1 + np.exp( 2* (d-(2*s-m))/s ) )
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-
packages/rampy/baseline.py:239: RuntimeWarning: overflow encountered in exp
  wt = 1.0/(1 + np.exp( 2* (d-(2*s-m))/s ) )
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/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-
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/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-
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packages/rampy/baseline.py:239: RuntimeWarning: overflow encountered in exp
  wt = 1.0/(1 + np.exp( 2* (d-(2*s-m))/s ) )
```

```
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-
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  wt = 1.0/(1 + np.exp( 2* (d-(2*s-m))/s ) )
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-
packages/rampy/baseline.py:239: RuntimeWarning: overflow encountered in exp
  wt = 1.0/(1 + np.exp( 2* (d-(2*s-m))/s ) )
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-
packages/rampy/baseline.py:239: RuntimeWarning: overflow encountered in exp
  wt = 1.0/(1 + np.exp( 2* (d-(2*s-m))/s ) )
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-
packages/rampy/baseline.py:239: RuntimeWarning: overflow encountered in exp
  wt = 1.0/(1 + np.exp( 2* (d-(2*s-m))/s ) )
/Users/jonathanhsu/opt/anaconda3/lib/python3.8/site-
packages/rampy/baseline.py:239: RuntimeWarning: overflow encountered in exp
  wt = 1.0/(1 + np.exp( 2* (d-(2*s-m))/s ) )
```

[10]:

	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	
10	14178.259539	467.231	343.069	
11	13733.818919	464.270	347.173	
12	18800.523850	505.251	345.554	
13	10108.881613	474.260	377.459	
14	22676.186701	472.709	362.218	
15	13508.735381	521.542	448.094	
16	23939.831693	487.407	383.850	
17	19294.516971	486.116	386.766	
18	17128.294361	499.631	392.544	
19	16829.480496	478.397	347.196	
20	9445.812630	454.495	392.153	
21	11476.936168	445.633	387.507	
22	22108.366774	546.075	423.090	
23	15417.243257	507.836	414.242	
24	13964.145848	496.518	413.977	
25	14476.838576	507.520	413.363	
26	14478.490807	494.518	405.179	
27	13639.171927	505.809	414.222	
28	17033.998777	556.337	471.337	
29	12297.810335	502.143	444.366	

30	13716.011922	523.783	412.512
31	13502.303067	523.608	410.299
32	13943.630835	527.438	413.512
33	16571.160297	529.889	412.938
34	14221.581910	513.213	406.528
35	5167.263519	434.635	353.822
36	22097.573589	546.599	423.916
37	17043.636116	487.803	460.072
38	16193.419580	485.731	457.009
39	18308.441157	685.511	547.126
40	21107.867542	565.899	552.126

	Heat Release Capacity	Fire Growth Capacity	FR_labels
0	226.086018	134.021649	2
1	167.301374	120.959219	2
2	115.388857	77.548988	1
3	234.511889	191.805110	0
4	403.934907	260.118532	0
5	287.523491	36.933912	1
6	444.419598	238.762552	0
7	187.059855	139.195486	1
8	424.940076	114.496239	1
9	223.623054	84.124726	1
10	229.024328	82.130862	1
11	235.366359	86.020734	1
12	149.574676	78.578931	2
13	153.645265	81.928333	1
14	301.383347	154.581687	0
15	128.401428	156.716815	1
16	340.662241	179.403199	0
17	289.134535	152.364431	0
18	161.619850	123.859865	1
19	167.595632	91.153861	1
20	173.072118	129.523200	1
21	197.996460	170.164352	1
22	456.031261	137.336364	0
23	230.140251	132.794096	0
24	212.654901	139.563000	0
25	222.966686	123.749555	0
26	222.792879	131.225454	0
27	195.231834	120.553261	0
28	326.030189	168.341238	0
29	156.057762	187.075736	1
30	182.071574	95.767770	0
31	174.158642	92.083557	1
32	182.349082	94.640055	0
33	246.269663	108.871797	1

```
34         193.413740        104.174547          1
35          86.277692         51.326682          1
36         458.908800        137.754218          0
37         414.906734        577.778918          1
38         413.971806        528.651235          0
39         208.517584        104.582162          1
40         483.335487       1493.530418          0
```

1.2 1.3 Extract Principal component features

###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.

[11]:
```python
# Read in the raw data
df = pd.read_csv("data/MCC_raw.csv")
data_raw = df.drop([0]).astype(float)
data_raw[data_raw.columns[::3]].head(5)
```

[11]:
```
   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]
```

[12]:
```python
# 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)
```

[12]:
```
      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

[13]:
```
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).

[14]:
```
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

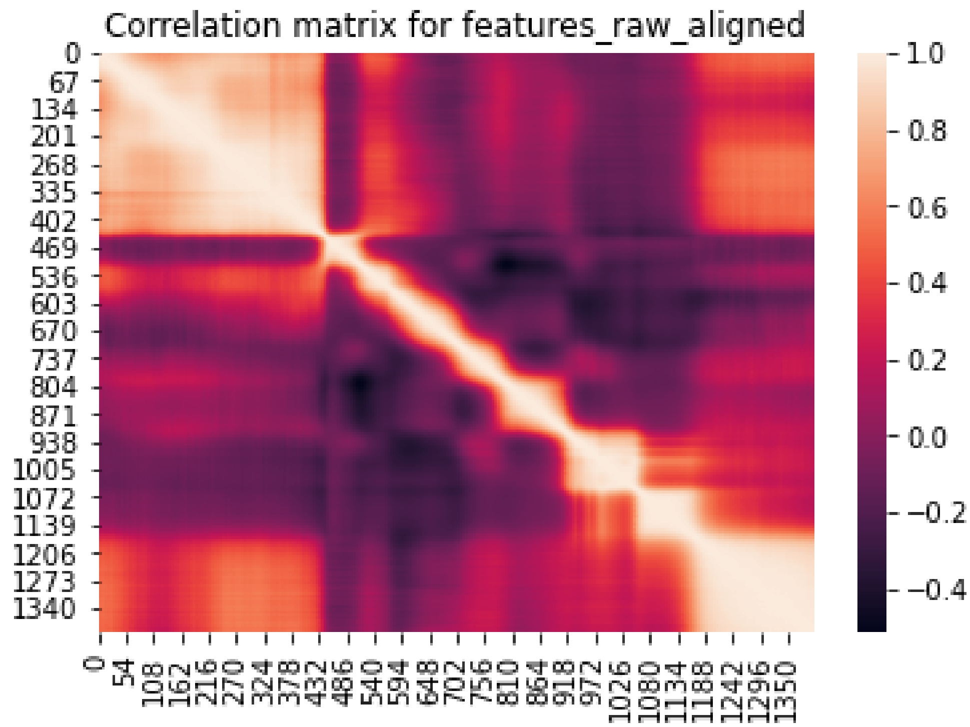
[15]:
```
from scipy import interpolate
# define new aligned x values
x_aligned=np.linspace(max(xy_raw[::2,1]),min(xy_raw[::2,-1]),num=1400)

# 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
```

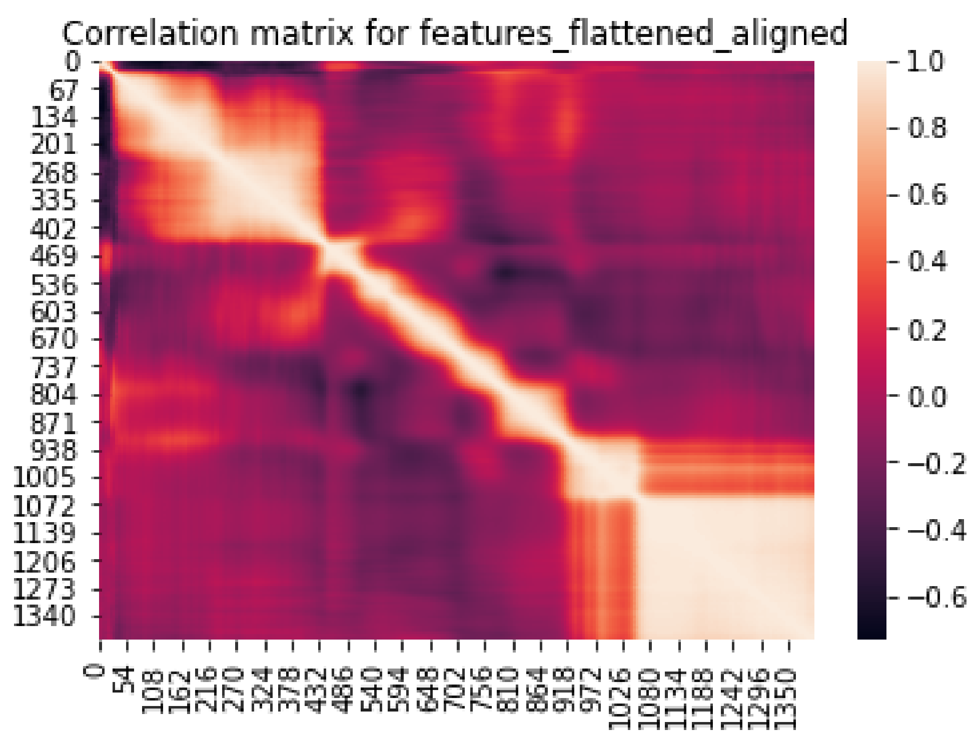
[16]:
```
# Calculate feature matrices with aligned data
features_raw_aligned=align_data(xy_raw)
features_flattened_aligned=align_data(xy_flattened)
print(features_raw_aligned.shape)
print(features_flattened_aligned.shape)
```

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

[17]:
```
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')
```





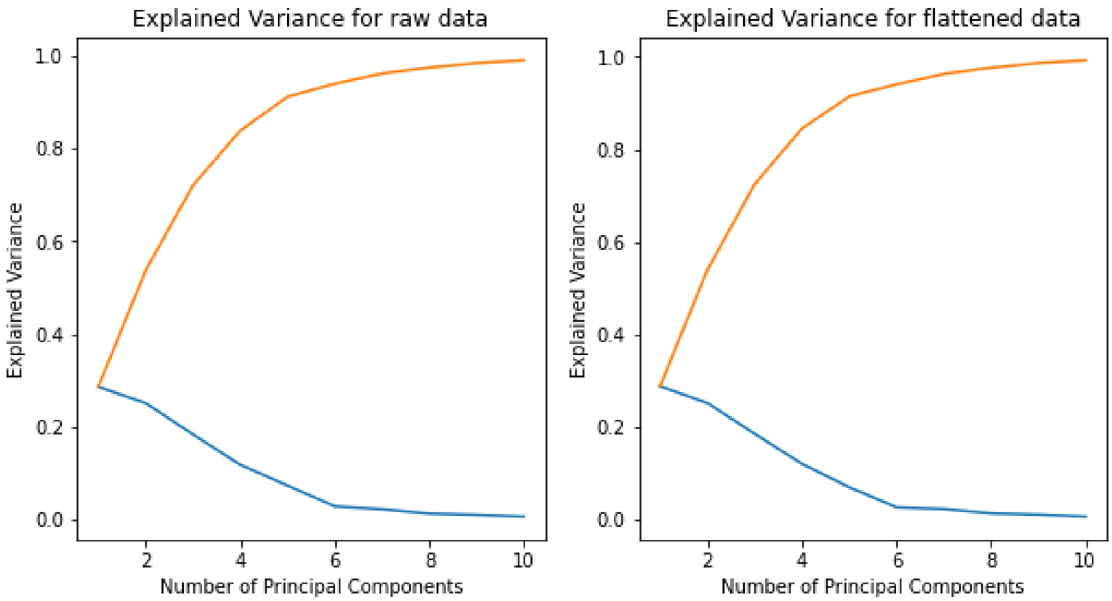
Find the first 10 PCs based on aligned features

[18]:
```
from sklearn.decomposition import PCA
k=10
pca_raw=PCA(n_components=k)
pca_flattened=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  -50.01410213  132.44691814 -177.28925653]
[-675.35966478  297.70609534  709.67296853 -210.10418253  880.68519073
   14.37603541   74.34793143   49.63832081  170.41499748 -148.95424958]
```

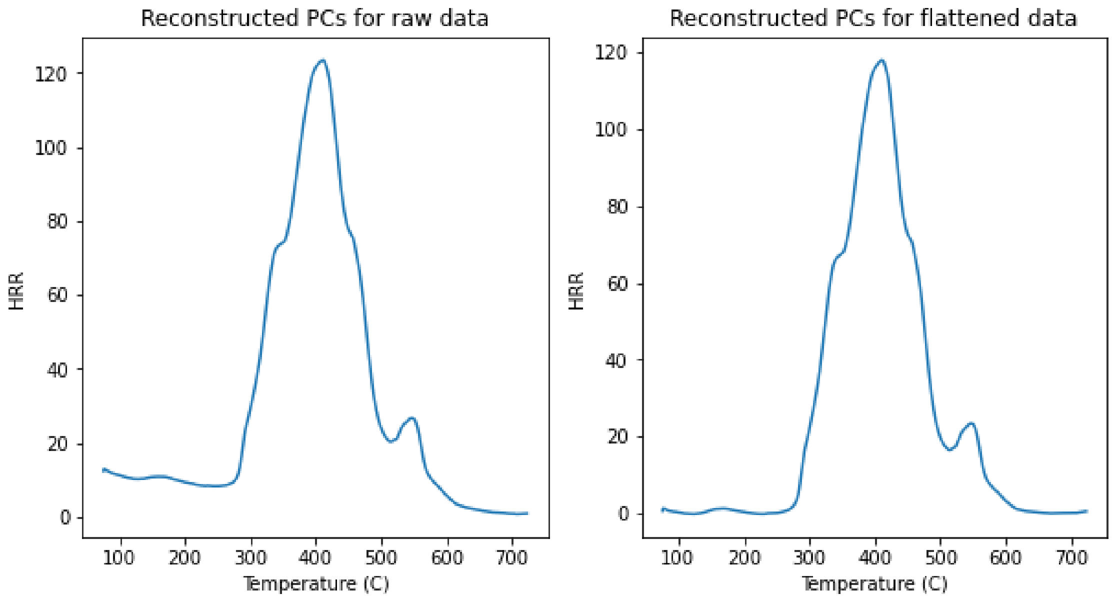
[19]:
```
raw_mean=raw_pc.mean(axis=0)
flattened_mean=flattened_pc.mean(axis=0)

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')
```

[19]:
```
Text(0.5, 1.0, 'Explained Variance for flattened data')
```



[20]:
```python
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')
```

[20]:
```
Text(0.5, 1.0, 'Reconstructed PCs for flattened data')
```



2 2. Baseline Model

2.0.1 2.1 Import Modified Feature Matrix

Only physical features are accounted for the baseline model.

The feature matrixcontains 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.

[21]:
```
# Read in the data
import numpy as np
import pandas as pd
import pylab as plt
data=feature_matrix
data.head()
```

[21]:
```
   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             226.086018            134.021649          2
1             167.301374            120.959219          2
```

```
2          115.388857          77.548988          1
3          234.511889         191.805110          0
4          403.934907         260.118532          0
```

2.0.2 2.2 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.

[22]:
```python
# 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()
```

[22]:
```
   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              -0.240135             -0.202424          2
1              -0.797272             -0.258909          2
2              -1.289277             -0.446622          1
3              -0.160279              0.047441          0
4               1.445442              0.342840          0
```

2.1 2.3 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.

[23]:
```python
# 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: 0.6
Precision for validation set: 0.5
Recall for validation set: 0.38888888888888884

Accuracy for full dataset: 0.926829268292683
Precision for full dataset: 0.8849206349206349
Recall for full dataset: 0.9462962962962962
```

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.

3 3. Improved Models

[24]:
```
# Read in the data
import numpy as np
import pandas as pd
import pylab as plt
#data = pd.read_csv("feature_matrix.csv")
data = feature_matrix
y_label=data['FR_labels'].values
data.head()
```

[24]:
```
   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          226.086018          134.021649          2
1          167.301374          120.959219          2
2          115.388857           77.548988          1
3          234.511889          191.805110          0
4          403.934907          260.118532          0
```

3.1 3.1 Generative Model

[25]:
```python
#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)
```

[25]:
```
   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             226.086018            134.021649          2  -675.359665
1             167.301374            120.959219          2   909.690780
2             115.388857             77.548988          1    63.184653
3             234.511889            191.805110          0   785.953021
4             403.934907            260.118532          0 -1375.196724
5             287.523491             36.933912          1   312.466980
6             444.419598            238.762552          0 -1823.270483
7             187.059855            139.195486          1  -673.781299
8             424.940076            114.496239          1  -534.780150
9             223.623054             84.124726          1  -613.962714

           PC2         PC3
0   297.706095  709.672969
1   342.229118   38.531565
2  -388.364698  435.757341
3  1344.401641  280.523430
4  1562.118235  335.994676
5  -994.661003 -171.510428
6  1123.422331  811.067096
7   -70.424785   63.789112
```

```
8 -1735.166289   67.101104
9 -1013.198967  282.618511
```

[26]:
```
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
```

[26]:
```
(41, 9)
```

[27]:
```
# plot
import seaborn as sns
sns.pairplot(scaled,hue='FR_labels')
```

[27]:
```
<seaborn.axisgrid.PairGrid at 0x7f93b6ba34c0>
```

[28]:
```python
from sklearn.model_selection import train_test_split
X = scaled.drop(columns='FR_labels').values
y = scaled['FR_labels'].values
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.25,␣
↪random_state=3)
```

[29]:
```python
train = pd.DataFrame(X_train)
train.columns = data.drop(columns='FR_labels').columns
train['FR_labels'] = y_train
sns.pairplot(train,hue='FR_labels')
```

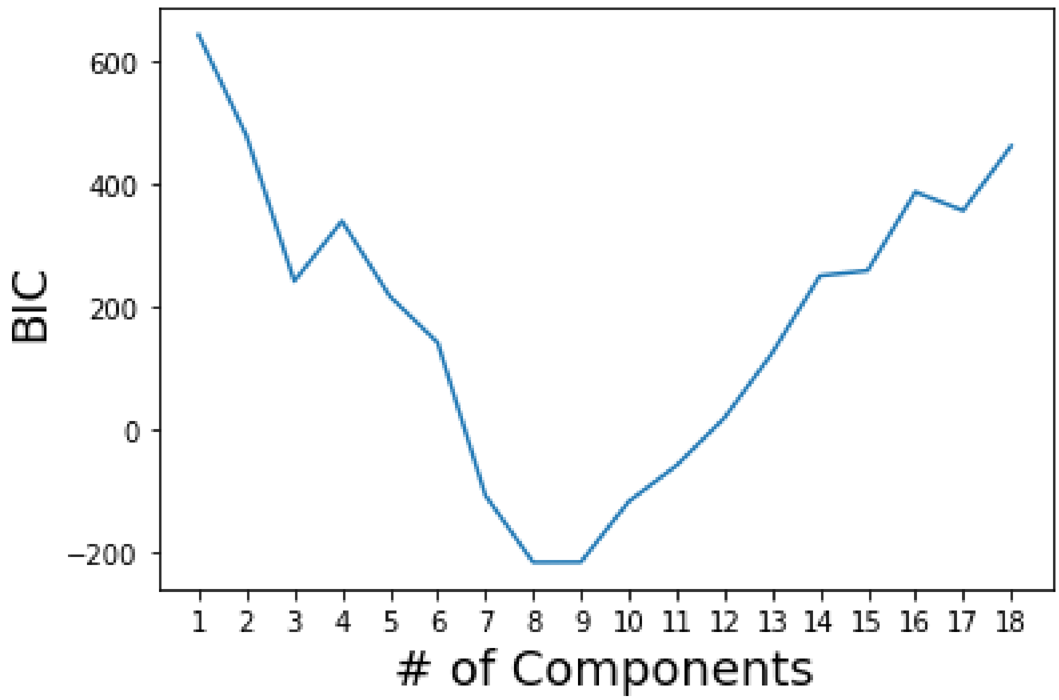
[29]:
```
<seaborn.axisgrid.PairGrid at 0x7f93b3b21af0>
```

3.1.1 Gaussian Mixture Method

[30]:
```
#y = scaled['FR_labels']
y = y_train
from sklearn.mixture import GaussianMixture

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

BICs = []
models = []
for n in n_components:
    gmm_n =  GaussianMixture(n, covariance_type = 'full',random_state=0).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)
```

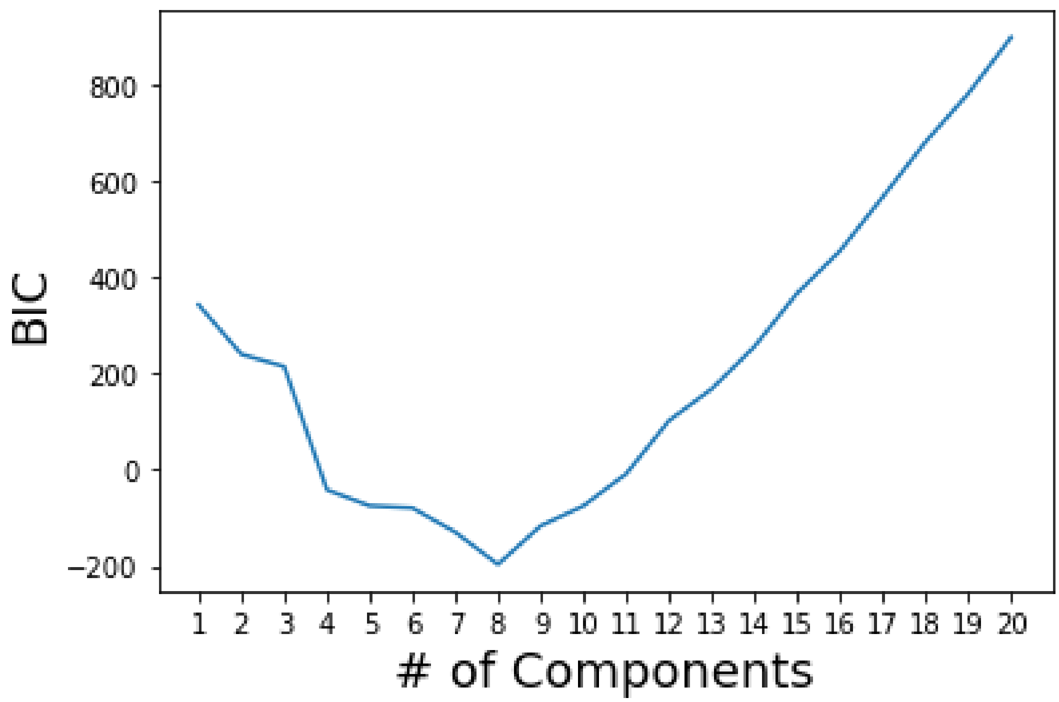
[8]



[31]:
```
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',random_state=0).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)
```

```
[8, 8]
```



[32]:
```
vals = []
for i in range(0,2):
  X = scaled.drop(columns='FR_labels')[y == i].values
  gmm = GaussianMixture(n_components = best_n[i], covariance_type =␣
 ↪'full',random_state=0)
  gmm.fit(X)
  new = gmm.sample(100)
  vals.append(new[0])
```

[33]:
```
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 = train.append(new0)
final = final.append(new1)
final.shape
```

[33]:
```
(230, 9)
```

[34]:
```
sns.pairplot(final,hue='FR_labels')
```

[34]:
```
<seaborn.axisgrid.PairGrid at 0x7f93b70bc520>
```

3.1.2 Kernel Density Estimation

[35]:
```
from sklearn.neighbors import KernelDensity

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

  # use the best estimator to compute the kernel density estimate
  kde = KernelDensity(kernel='gaussian', bandwidth=.5)
  kde.fit(X)

  new = kde.sample(100)
  vals.append(new)
```

[36]:
```
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
kde_plot = train.append(new0)
kde_plot = kde_plot.append(new1)
sns.pairplot(kde_plot,hue='FR_labels')
```

[36]:
```
<seaborn.axisgrid.PairGrid at 0x7f93be74bbe0>
```

3.2 3.2 Classifiers

[37]:
```
#X_ori=origin_feature_matrix.drop(columns='FR_labels').values
#y_ori=origin_feature_matrix['FR_labels'].values
X_ori = X_test
y_ori = y_test
X_ori.shape
```

[37]: (11, 8)

3.2.1 SVC (Baseline model)

[38]:
```
# perform a train-test split. 90% of original data will be used for training
X_svc = final.drop(columns='FR_labels').values
print(X_svc.shape)
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)

# Get best estimator and use hyperparameters to fit best_svc model

print(svc_search.best_estimator_)

best_svc = SVC(kernel = 'rbf',C=100,gamma=0.5)
%time best_svc.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: {}\n'.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')))
```

```
(230, 8)
SVC(C=1000000.0, gamma=0.5)
CPU times: user 1.31 ms, sys: 159 µs, total: 1.47 ms
Wall time: 1.22 ms
Accuracy for validation set: 0.896551724137931
Precision for validation set: 0.9142857142857144
Recall for validation set: 0.896551724137931

Accuracy for full dataset: 0.9739130434782609
Precision for full dataset: 0.9834710743801653
Recall for full dataset: 0.9821428571428571

Accuracy for original dataset: 0.9090909090909091
Precision for original dataset: 0.9166666666666667
Recall for original dataset: 0.9166666666666667
```

3.2.2 Decision Tree

[39]:
```
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)
```

```
(230, 8)
(230,)
```

[40]:
```
# GridSearch Hyperparameter Tuning
DT_search = GridSearchCV(dtree, param_grid_dtree, cv=5)
DT_search.fit(X_train_DT, y_train_DT)

print(DT_search.best_estimator_)

best_DT = DecisionTreeClassifier(max_depth=10)

%time best_DT.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')))
```

```
DecisionTreeClassifier(max_depth=10)
CPU times: user 1.34 ms, sys: 276 µs, total: 1.62 ms
Wall time: 1.41 ms
Accuracy for validation set: 0.8793103448275862
Precision for validation set: 0.5880952380952381
Recall for validation set: 0.60125

Accuracy for full dataset: 0.9695652173913043
Precision for full dataset: 0.9802469135802468
Recall for full dataset: 0.8711093857832988

Accuracy for original dataset: 0.8181818181818182
Precision for original dataset: 0.8166666666666667
Recall for original dataset: 0.8166666666666667
```

3.2.3 Random Forest

[41]:
```
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}
```

[42]:
```
# GridSearch Hyperparameter Tuning
RF_search = GridSearchCV(ranfor, param_grid_ranfor, cv=5)
RF_search.fit(X_train_RF, y_train_RF)

print(RF_search.best_estimator_)

best_RF = RandomForestClassifier(max_depth=20,n_estimators=10)

%time best_RF.fit(X_train_DT, y_train_DT)
best_RF.predict(X_ori)


# 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')))

# I have noticed that the accuracy for the validation set changes pretty wildly␣
↪each time I re-run the previous block with the test_train_split
```

```
RandomForestClassifier(criterion='entropy', max_depth=15, n_estimators=5)
CPU times: user 12.2 ms, sys: 524 µs, total: 12.8 ms
Wall time: 12.9 ms
Accuracy for validation set: 0.9827586206896551
Precision for validation set: 0.9838709677419355
Recall for validation set: 0.9821428571428572

Accuracy for full dataset: 0.991304347826087
Precision for full dataset: 0.9941520467836257
Recall for full dataset: 0.8859903381642512

Accuracy for original dataset: 1.0
Precision for original dataset: 1.0
Recall for original dataset: 1.0
```

3.2.4 KNN

[43]:
```
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}
```

[44]:
```
# Hyperparameter tunning
KNN_search = GridSearchCV(KNN, KNN_param_grid, cv=5)
#KNN_search.fit(X_train_KNN, y_train_KNN)
KNN_search.fit(X_train_KNN, y_train_KNN)

print(KNN_search.best_estimator_)

best_KNN = KNeighborsClassifier(n_neighbors=2)

%time best_KNN.fit(X_train_DT, y_train_DT)
```

```
# 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')))
```

```
KNeighborsClassifier(n_neighbors=2)
CPU times: user 1.02 ms, sys: 196 µs, total: 1.22 ms
Wall time: 1.19 ms
Accuracy for validation set: 1.0
Precision for validation set: 1.0
Recall for validation set: 1.0

Accuracy for full dataset: 0.9695652173913043
Precision for full dataset: 0.6465219474069032
```

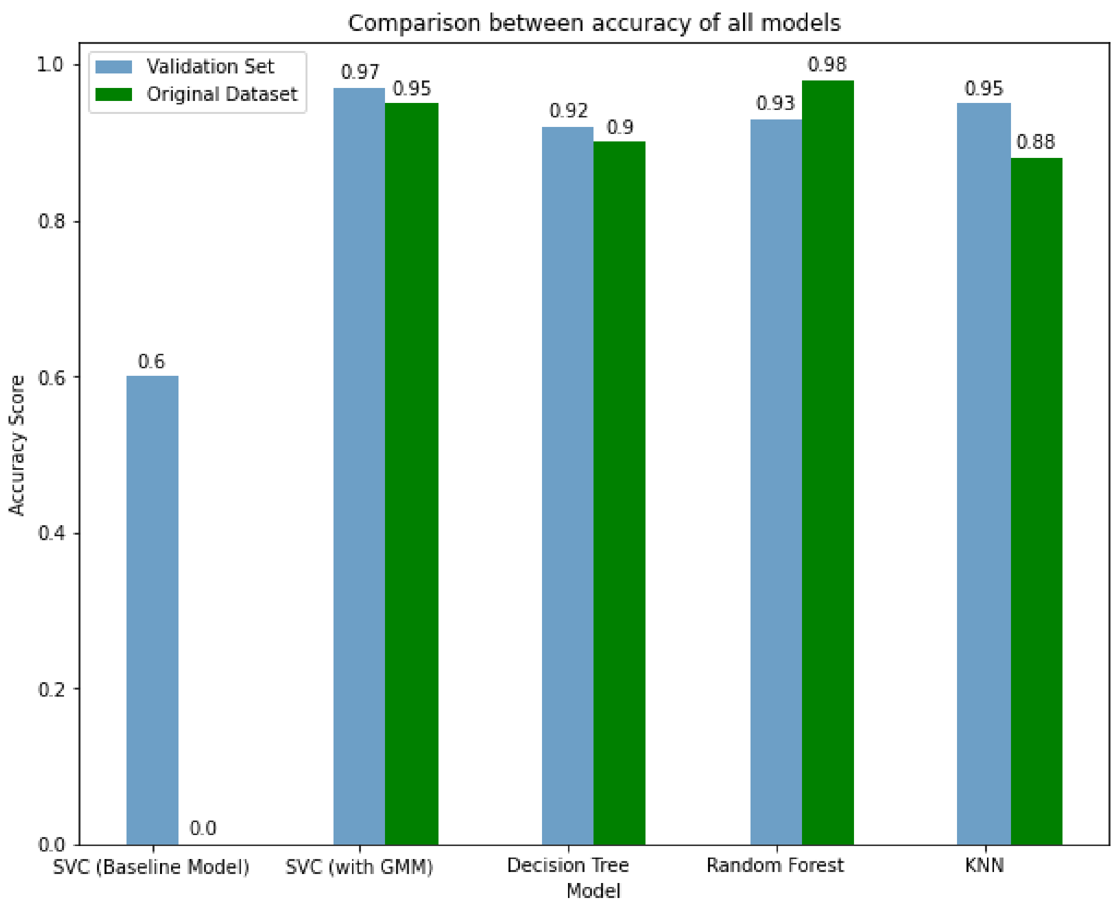
```
Recall for full dataset: 0.6550724637681159

Accuracy for original dataset: 1.0
Precision for original dataset: 1.0
Recall for original dataset: 1.0
```

3.3 3.3 Model Comparison

[47]:

```
from matplotlib.pyplot import figure
labels = ['SVC (Baseline Model)', 'SVC (with GMM)', 'Decision Tree', 'Random␣
 ↪Forest', 'KNN']
physical = (0.60, 0.97, 0.92, 0.93, 0.95)
pca = (0, 0.95, 0.90, 0.98, 0.88)
n_groups = 5
x = np.arange(len(labels))  # the label locations
width = 0.25  # the width of the bars
index = np.arange(n_groups)
bar_width = 0.25

fig, ax = plt.subplots(figsize=(10,8))

rects1 = plt.bar(index, physical, bar_width,
alpha=0.8,
color='#4887b8',
label='Validation Set')

rects2 = plt.bar(index + bar_width, pca, bar_width,
alpha=1,
color='g',
label='Original Dataset')

# Add some text for labels, title and custom x-axis tick labels, etc.
ax.set_ylabel('Accuracy Score')
ax.set_xlabel('Model')
ax.set_title('Comparison between accuracy of all models')
ax.set_xticks(x)
ax.set_xticklabels(labels)


def autolabel(rects):
    """Attach a text label above each bar in *rects*, displaying its height."""
    for rect in rects:
        height = rect.get_height()
        ax.annotate('{}'.format(height),
                    xy=(rect.get_x() + rect.get_width() / 2, height),
                    xytext=(0, 3),  # 3 points vertical offset
                    textcoords="offset points",
```

```
                    ha='center', va='bottom')

autolabel(rects1)
autolabel(rects2)
plt.legend()

plt.show()
```



[48]:
```
labels = ['SVC (Baseline Model)', 'SVC (with GMM)', 'Decision Tree', 'Random␣
 ↪Forest', 'KNN']
physical = (969, 1990, 968, 11000, 0)

x = np.arange(len(labels))  # the label locations
width = 0.5  # the width of the bars

fig, ax = plt.subplots(figsize=(10,8))
rects1 = ax.bar(x, physical, width, label='Men')
```

```
# Add some text for labels, title and custom x-axis tick labels, etc.
ax.set_ylabel('Wall Clock Times (\N{greek small letter mu}s)')
ax.set_xlabel('Model')
ax.set_title('Comparison between speed of all models')
ax.set_xticks(x)
ax.set_xticklabels(labels)

def autolabel(rects):
    """Attach a text label above each bar in *rects*, displaying its height."""
    for rect in rects:
        height = rect.get_height()
        ax.annotate('{}'.format(height),
                    xy=(rect.get_x() + rect.get_width() / 2, height),
                    xytext=(0, 3),  # 3 points vertical offset
                    textcoords="offset points",
                    ha='center', va='bottom')

autolabel(rects1)

plt.show()
```