Homework 5

Shao-Ting Chiu (UIN:433002162)

12/1/22

Table of contents

Description

Problems from the Book

9.8

11.11

Both problems are coding assignments, with starting code provided. Each is worth 40 points.

Problem 9.8

This assignment concerns the application of PCA to the soft magnetic alloy data set (See section A8.5).

(a)

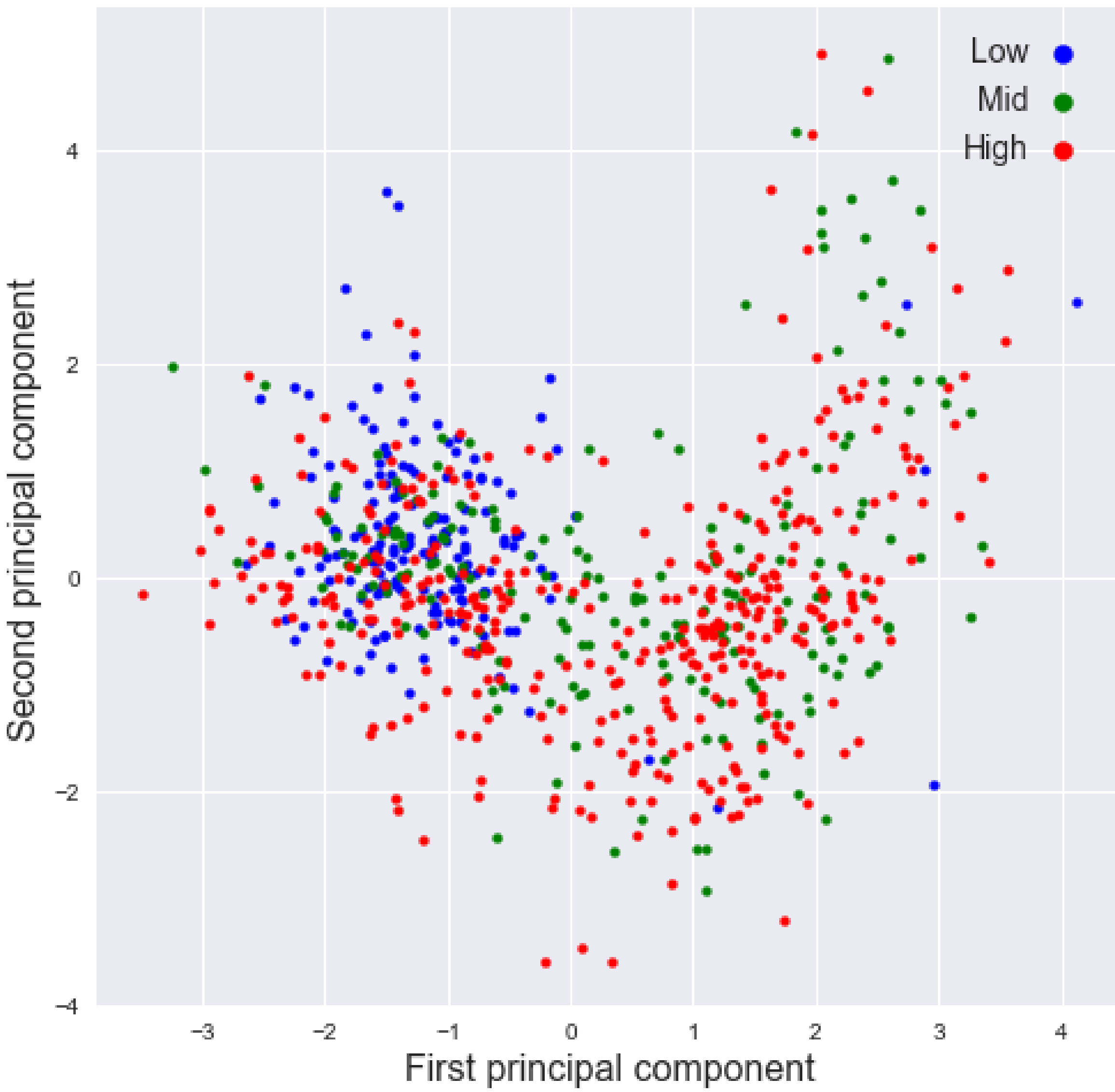
Reproduce the plots in Figure 9.5 by running c09_PCA.py

```
""""
Foundations of Pattern Recognition and Machine Learning
Chapter 9 Figure 9.5
Author: Ulisses Braga-Neto

PCA example using the softt magnetic alloy dataset
"""

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler as ssc
```

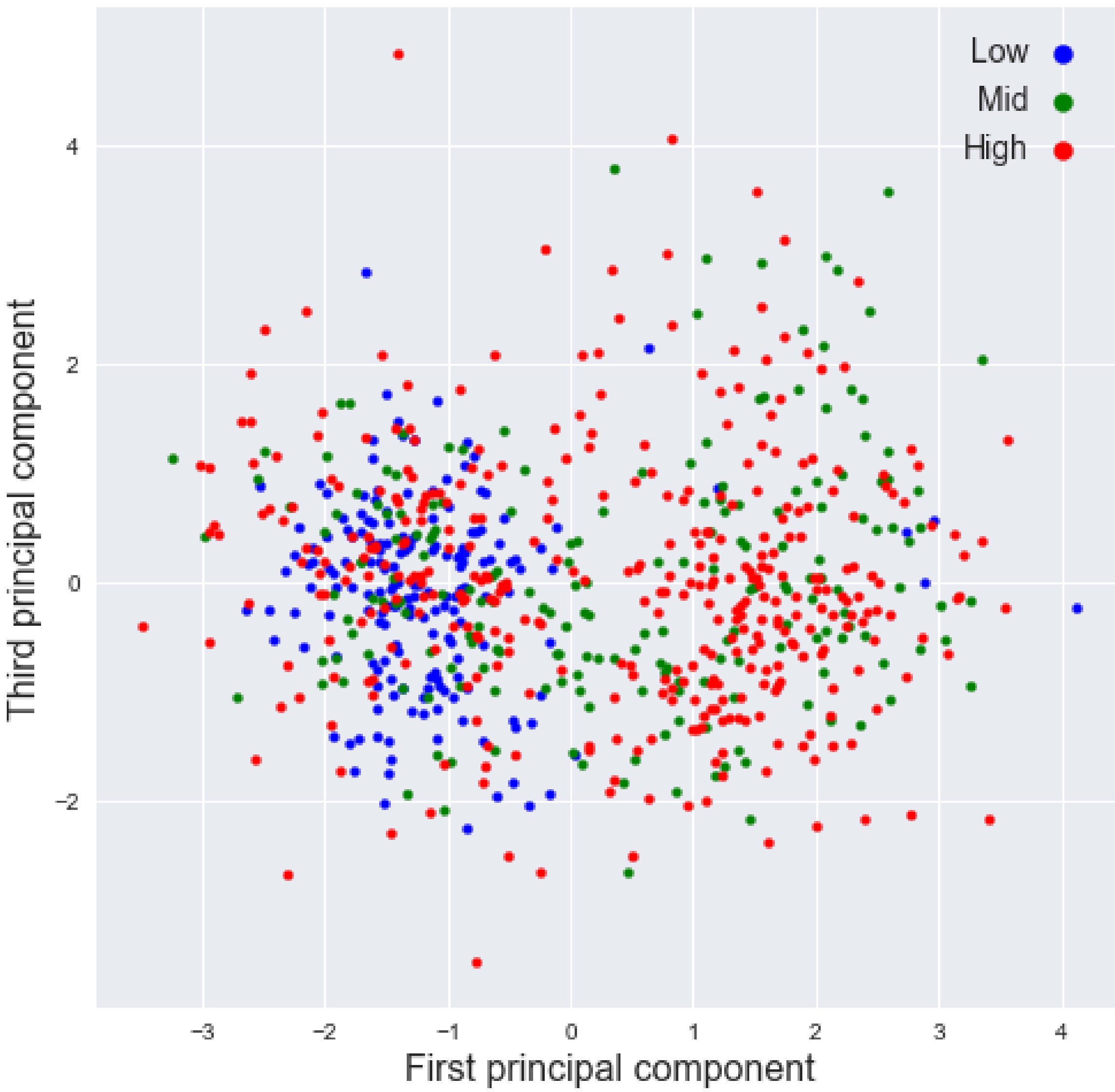
```
# Fix random state for reproducibility
np.random.seed(0)

SMA = pd.read_csv('data/Soft_Magnetic_Alloy_Dataset.csv')

fn0 = SMA.columns[0:26]          # all feature names
fv0 = SMA.values[:,0:26]         # all feature values
rs0 = SMA['Coercivity (A/m)']    # select response
```

```
# pre-process the data
n_orig   = fv0.shape[0]                  # original number of training points
p_orig   = np.sum(fv0>0,axis=0)/n_orig  # fraction of nonzero components for each feature
noMS     = p_orig>0.05
fv1      = fv0[:,noMS]             # drop features with less than 5% nonzero components
noNA     = np.invert(np.isnan(rs0))     # find available response values
SMA_feat = fv1[noNA,:]                   # filtered feature values
SMA_fnam = fn0[noMS]                     # filtered feature names
SMA_resp = rs0[noNA]                     # filtered response values

n,d = SMA_feat.shape # filtered data dimensions

# add random perturbation to the features
sg = 2
```

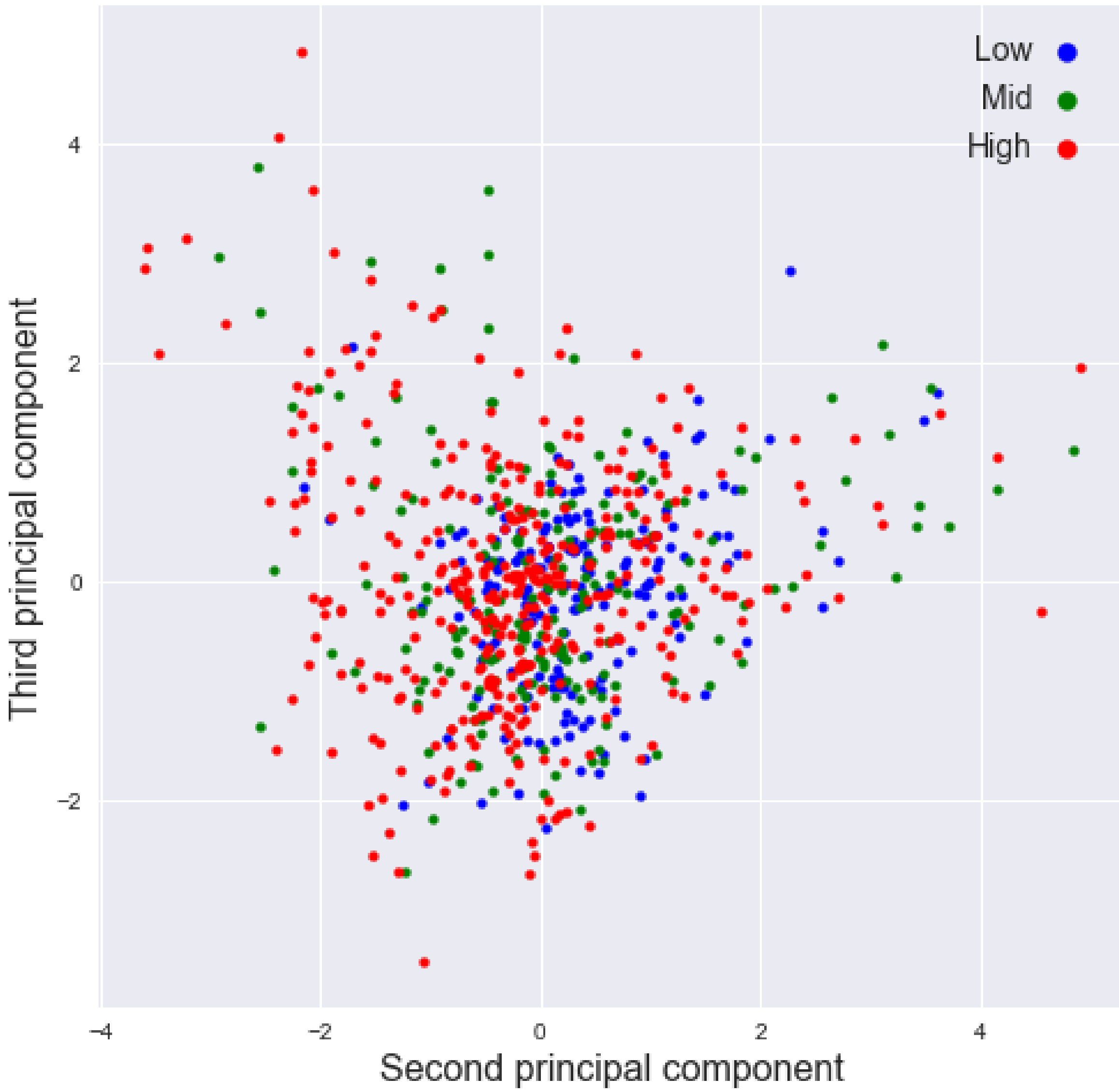
```
SMA_feat_ns = SMA_feat + np.random.normal(0,sg,[n,d])
SMA_feat_ns = (SMA_feat_ns + abs(SMA_feat_ns))/2 # clamp values at zero

# standardize data
SMA_feat_std = ssc().fit_transform(SMA_feat_ns)

# compute PCA
pca = PCA()
pr = pca.fit_transform(SMA_feat_std)

# PCA plots
def plot_PCA(X,Y,resp,thrs,nam1,nam2):
    Ihigh = resp>thrs[1]
    Imid = (resp>thrs[0])&(resp<=thrs[1])
    Ilow = resp<=thrs[0]
    plt.xlabel(nam1+' principal component',fontsize=16)
    plt.ylabel(nam2+' principal component',fontsize=16)
    plt.scatter(X[Ilow],Y[Ilow],c='blue',s=16,marker='o',label='Low')
    plt.scatter(X[Imid],Y[Imid],c='green',s=16,marker='o',label='Mid')
    plt.scatter(X[Ihigh],Y[Ihigh],c='red',s=16,marker='o',label='High')
    plt.xticks(size='medium')
    plt.yticks(size='medium')
    plt.legend(fontsize=14,facecolor='white',markerscale=2,markerfirst=False,handletextpad
    plt.show()

fig=plt.figure(figsize=(8,8))#,dpi=150)
plot_PCA(pr[:,0],pr[:,1],SMA_resp,[2,8],'First','Second')
fig=plt.figure(figsize=(8,8))#,dpi=150)
plot_PCA(pr[:,0],pr[:,2],SMA_resp,[2,8],'First','Third')
fig=plt.figure(figsize=(8,8))#,dpi=150)
plot_PCA(pr[:,1],pr[:,2],SMA_resp,[2,8],'Second','Third')
```



Low
Mid
High
Second principal component
First principal component



Low
Mid
High
Third principal component
First principal component
−3
−2
−1
0
1
2
3
4
−2
0
2
4



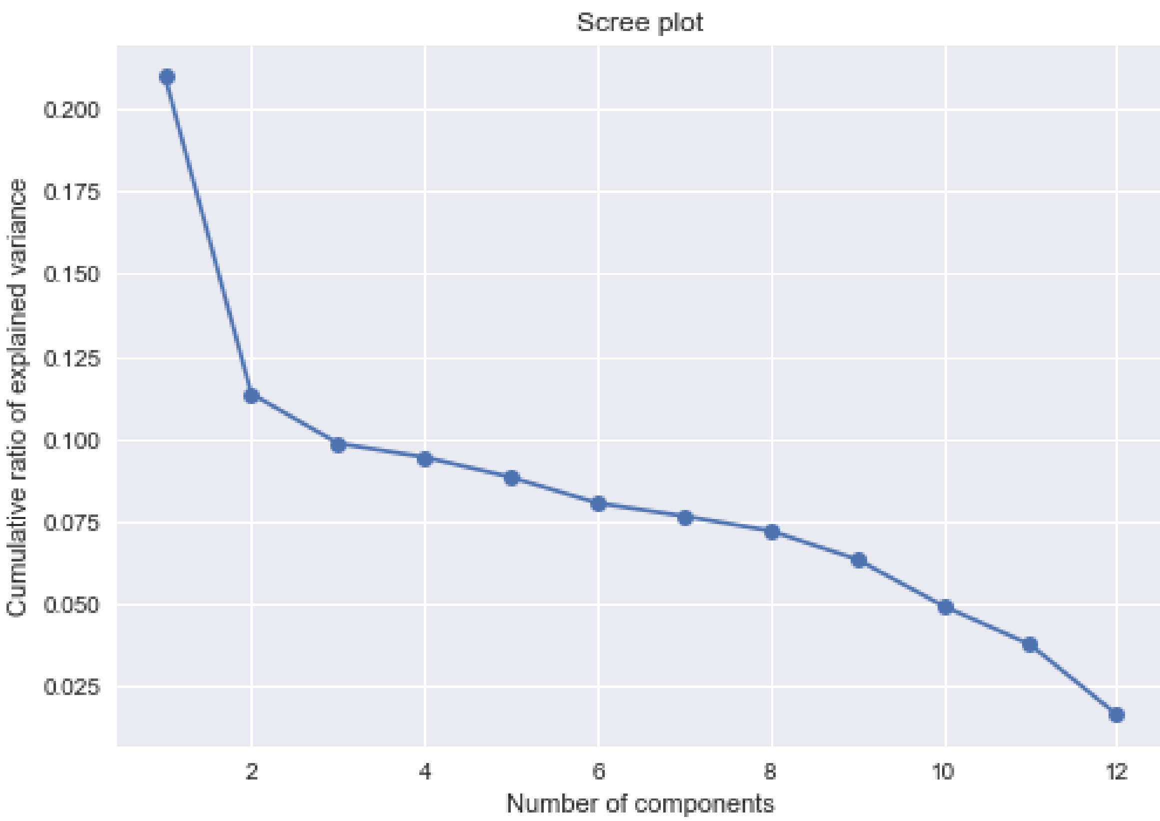
(b)

Plot the percentage of variance explained by each PC as a function of PC number. This is called the *scree plot*. Now plot the cumulative percentage of variance explained by the PCs as a function of PC number. How many PCs are needed to explain 95% of the variance.

Coding hint: use the attribute `explained_variance_ratio_` and the `cumsum()` method.

```
n = len(pca.explained_variance_ratio_)
#plt.plot( np.arange(1, n+1) ,np.cumsum(pca.explained_variance_ratio_))
plt.plot( np.arange(1, n+1) ,pca.explained_variance_ratio_, "-o")
plt.xlabel("Number of components")
plt.ylabel("Cumulative ratio of explained variance")
plt.title("Scree plot")
```

```
Text(0.5, 1.0, 'Scree plot')
```




```
np.cumsum(pca.explained_variance_ratio_)
```

```
array([0.20991838, 0.32353309, 0.42210314, 0.51647789, 0.6047665 ,
       0.68519162, 0.76168501, 0.83369708, 0.89706386, 0.94621316,
       0.98369719, 1.        ])
```

```python
np.where(np.cumsum(pca.explained_variance_ratio_) > 0.95)[0][0] + 1
```

```
11
```

- (2)
  - 11 PCs are needed to explain 95% of the variance.

(c)

Print the loading matrix W (this is the matrix of eigenvectors, ordered by PC number from left to right). The absolute value of the coefficients indicate the relative importance of each original variable (row of W) in the corresponding PC (column of W). [1]

```python
#for i in range(0,n):
#    print("Component", i+1,":",pca.components_[i].T)

wd = pd.DataFrame(pca.components_.T * np.sqrt(pca.explained_variance_ratio_), columns = ["
wd.iloc[:,0:6]
```

	PC1	PC2	PC3	PC4	PC5	PC6
0	0.217429	-0.128414	-0.000768	-0.013032	0.025015	-0.018742
1	-0.231749	0.065983	-0.014794	-0.089591	-0.010017	0.005178
2	0.032908	0.166780	0.078030	0.083952	-0.009801	-0.005831
3	-0.093151	-0.142560	-0.098557	0.086218	0.086567	-0.076516
4	0.198563	0.135102	-0.001895	-0.026140	0.032221	0.055660
5	-0.026492	0.008521	-0.036036	0.214858	-0.108705	-0.008577
6	-0.017498	-0.014458	-0.162399	-0.104232	-0.065114	0.042457
7	0.052591	-0.099443	0.151379	-0.036285	-0.161591	-0.083255
8	-0.157455	0.021118	0.011608	0.081410	-0.001242	0.047744
9	-0.041245	0.059526	0.063562	-0.019442	0.142836	-0.178096
10	-0.010472	-0.101413	0.114606	0.041513	0.123522	0.164500
11	-0.171381	-0.043990	0.121028	-0.062770	-0.033236	0.034567

```python
wd.iloc[:,6:]
```

[1] https://scentellegher.github.io/machine-learning/2020/01/27/pca-loadings-sklearn.html

	PC7	PC8	PC9	PC10	PC11	PC12
0	-0.015495	-0.005038	0.051062	-0.046767	-0.091825	-0.070203
1	-0.023988	-0.035185	-0.063599	0.058694	-0.014704	-0.085907
2	-0.096659	0.160212	-0.048367	-0.038402	-0.047184	-0.010801
3	-0.098246	0.066477	-0.030437	-0.034888	0.084873	-0.020465
4	0.017248	-0.016361	0.043242	-0.027380	0.124907	-0.045211
5	0.141188	-0.028350	-0.034109	-0.016461	0.001849	-0.032101
6	0.098092	0.169961	0.031244	-0.005649	-0.004468	-0.001099
7	-0.013892	0.063737	0.015561	0.073965	0.057188	-0.012833
8	-0.047099	0.012760	0.213021	0.033689	-0.007880	-0.009804
9	0.134329	0.040100	0.041069	0.012429	-0.005979	-0.004630
10	0.070125	0.069752	-0.044561	0.062093	0.007589	-0.009022
11	0.038157	-0.002185	0.012125	-0.170754	0.018848	-0.004422

(d)

Identify which two features contribute the most to the discriminating first PC and plot the data using these top two features. What can you conclude about the effect of these two features on the coercivity? This is an application of PCA to feature selection.

```
most_id = np.abs(wd["PC1"]).argsort()[-2:].to_numpy()
```

```
most_id
```

```
array([0, 1])
```

```
thrs = [2, 8]
id_d = {
    "high": SMA_resp>thrs[1],
    "mid": (SMA_resp>thrs[0])&(SMA_resp<=thrs[1]),
    "low": SMA_resp<=thrs[0]
}
cs = ["blue", "green", "red"]

for i, lb in enumerate(["low", "mid", "high"]):
    plt.scatter(SMA_feat_std[id_d[lb], most_id[1]], SMA_feat_std[id_d[lb], most_id[0]],\
                c= cs[i],s=16,marker='o',label=lb)
```

```
plt.legend(fontsize=14,facecolor='white',markerscale=2,markerfirst=False,handletextpad=0)
plt.xticks(size='medium');
plt.yticks(size='medium');
plt.xlabel(SMA_fnam[most_id[1]])
plt.ylabel(SMA_fnam[most_id[0]])
```

```
Text(0, 0.5, 'Fe')
```

Relations 1. High: -1 ~ 2 in feature 1; -2 ~ 2 in feature 0 2. Mid: -1 ~ 0 in feature 1; -1 ~ 2 in feature 0 3. low: Approximately locates around -1 ~ 2 in feature 1, -3 ~ 1 in feature 0

There values are refferred to the normalized units.

Problem 11.11

Apply linear regression to the stacking fault energy (SFE) data set.

(a)

Modify `c11_SFE.py` to fit a univariate linear regression model (with intercept) separately to each of the seven variables remaining after preprocessing (two of these were already done in Example 11.4. List the fitted coefficients, the normalized RSS, and the R^2 statsitic for each model.

Which one of the seven variables is the best predictor of SFE, according to R^2? Plot the SFE response against each of the seven variables, with regression lines superimposed. How do you interpret these results?

```python
""""
Foundations of Pattern Recognition and Machine Learning
Chapter 11 Figure 11.3
Author: Ulisses Braga-Neto

Regression with a line example with stacking fault energy dataset
"""

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.base import clone
from sklearn.linear_model import LinearRegression
from sklearn.metrics import r2_score
plt.style.use('seaborn')
```

```
MatplotlibDeprecationWarning: The seaborn styles shipped by Matplotlib are deprecated since 3
  plt.style.use('seaborn')
```

```python
def r2(model, x, y):
    y_pred = model.predict(x)
    return r2_score(y, y_pred)

def fitted_coef(model):
    return model.coef_[0]

def fitted_int(model):
    return model.intercept_

def normalized_RSS(model, xrr, yr):
```

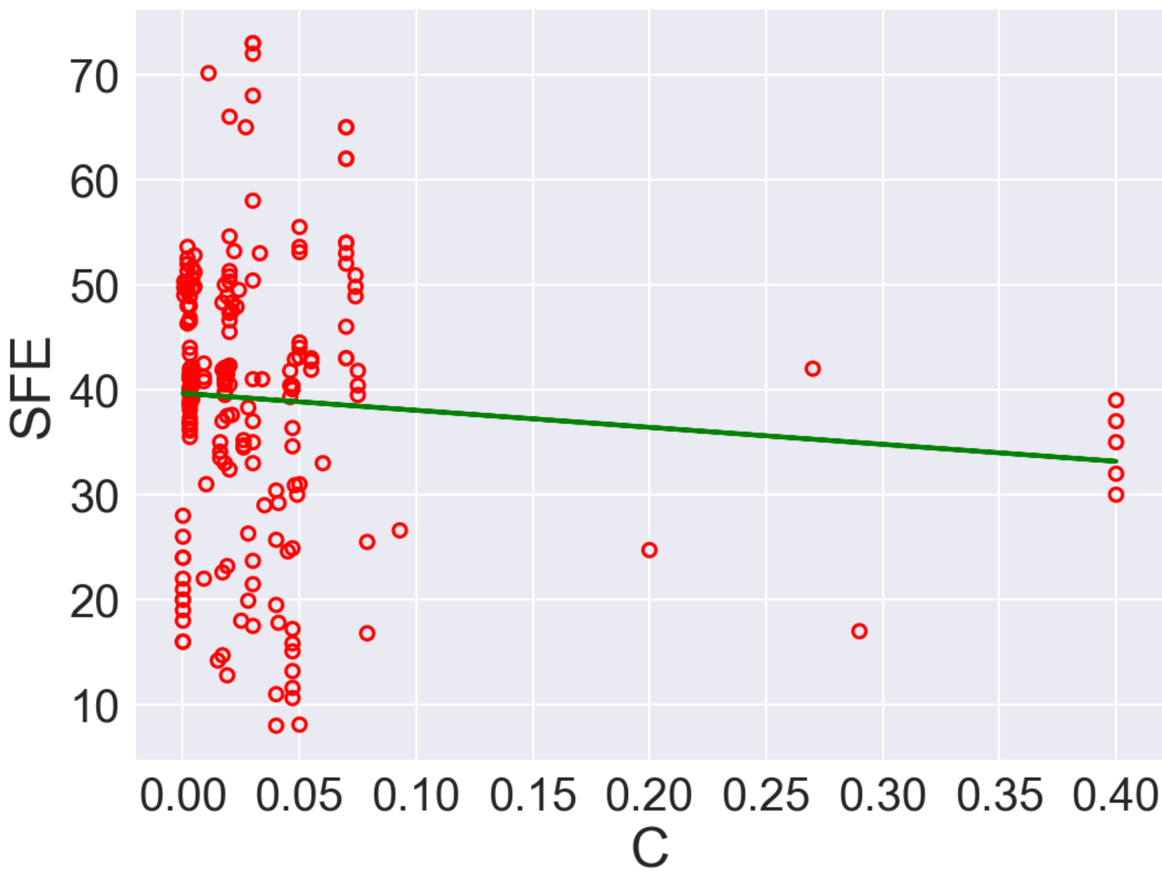
```
    y_pred = model.predict(xrr)
    rss = np.sum(np.square(y_pred - yr)) / len(y_pred)
    return rss
```

```
SFE_orig = pd.read_table('data/Stacking_Fault_Energy_Dataset.txt')
```

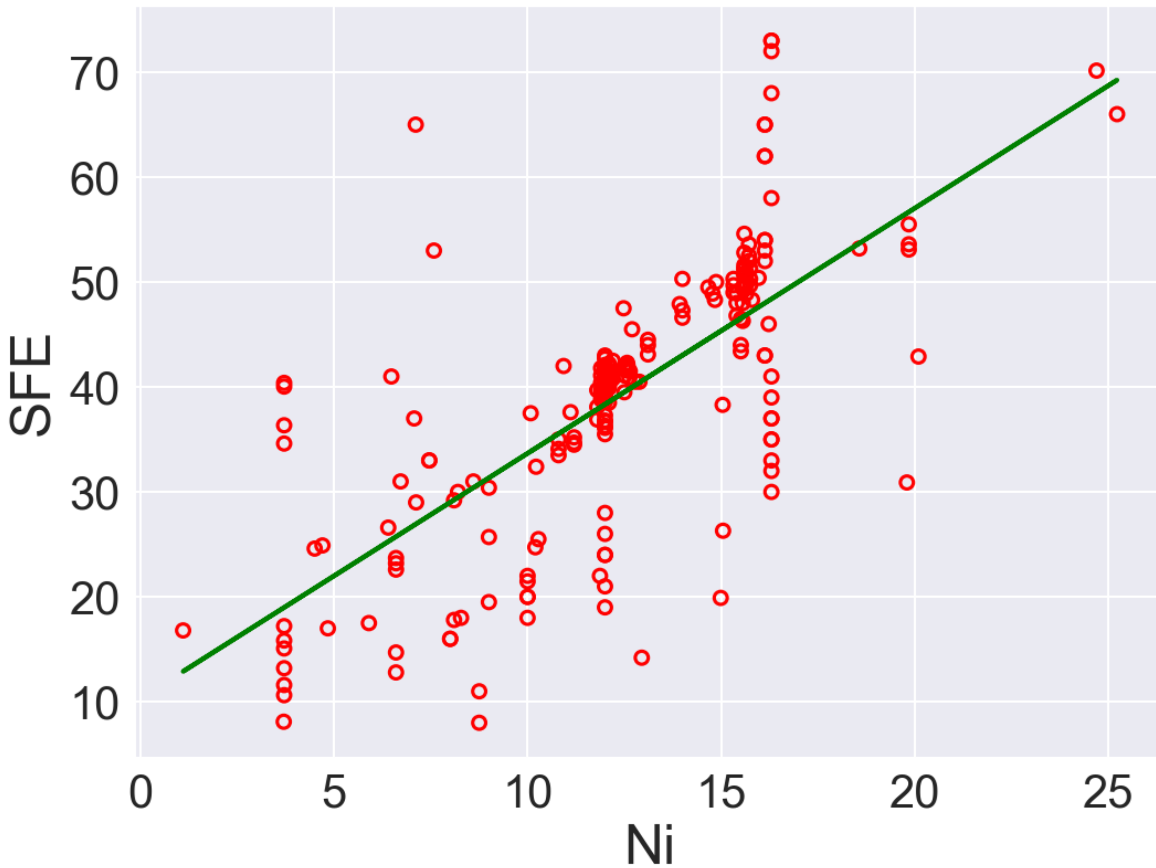
```
# pre-process the data

n_orig = SFE_orig.shape[0]          # original number of rows
p_orig = np.sum(SFE_orig>0)/n_orig  # fraction of nonzero entries for each column
SFE_colnames = SFE_orig.columns[p_orig>0.6]
SFE_col = SFE_orig[SFE_colnames]        # throw out columns with fewer than 60% nonzero en
m_col = np.prod(SFE_col,axis=1)
SFE = SFE_col.iloc[np.nonzero(m_col.to_numpy())] # throw out rows that contain any zero en
```

```
yr = SFE['SFE']
model = LinearRegression()
res = {
    "feature": [],
    "slope": [],
    "intercept": [],
    "Norm RSS":[],
    "R2": []
}

for feat in SFE.keys()[:-1].to_numpy():
    xr = np.array(SFE[feat])
    xrr = xr.reshape((-1,1)) # format xr for Numpy regression code
    model.fit(xrr,yr)

    # Performance
    res["feature"].append(feat)
    res["slope"].append(fitted_coef(model))
    res["intercept"].append(fitted_int(model))
    res["Norm RSS"].append(normalized_RSS(model, xrr, yr))
    res["R2"].append(r2(model, xrr, yr))

    # Plotting
    fig=plt.figure(figsize=(8,6),dpi=150)
    plt.xlabel(feat,size=24)
```

```
    plt.ylabel('SFE',size=24)
    plt.xticks(size=20)
    plt.yticks(size=20)
    plt.scatter(xr,yr,s=32,marker='o',facecolor='none',edgecolor='r',linewidth=1.5)
    ## Plotting regression model
    plt.plot(xrr,model.predict(xrr),c='green',lw=2)
    plt.show()
```

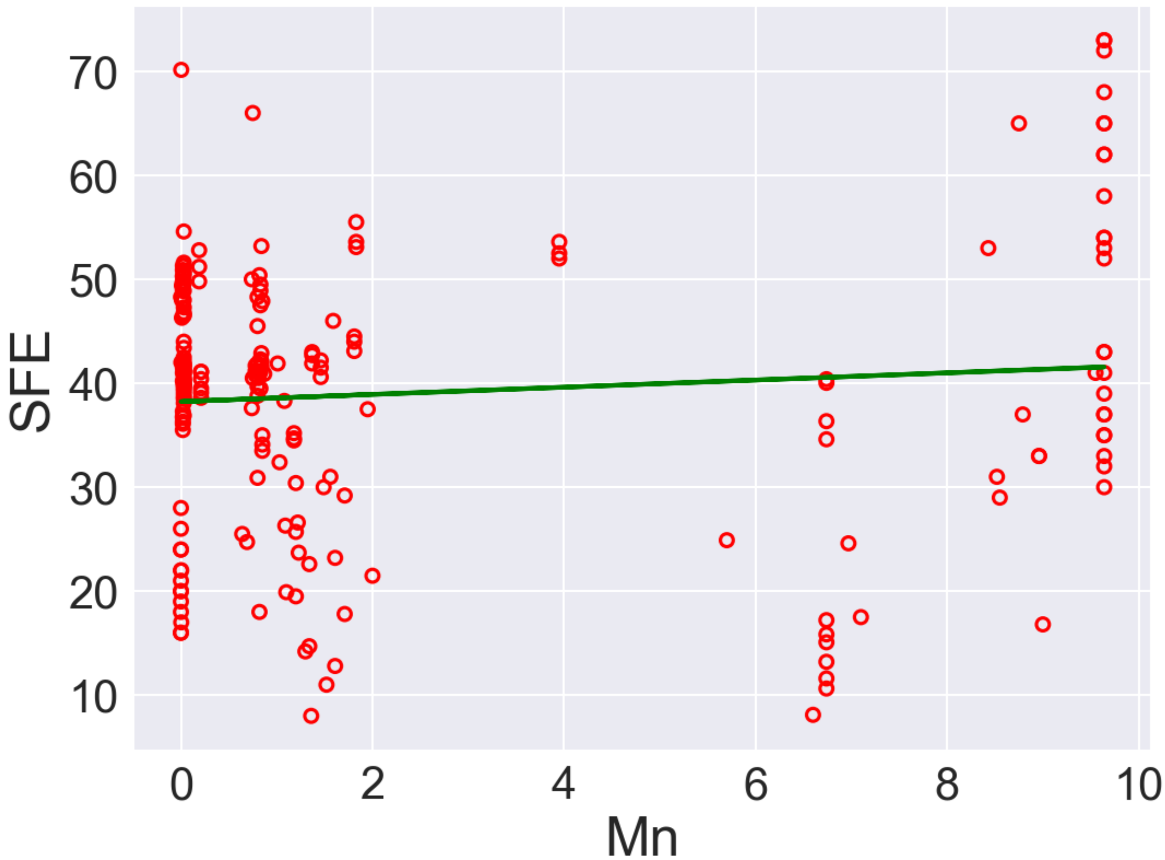



70
60
50
40
30
20
10
SFE
0.0
0.1
0.2
0.3
0.4
0.5
N

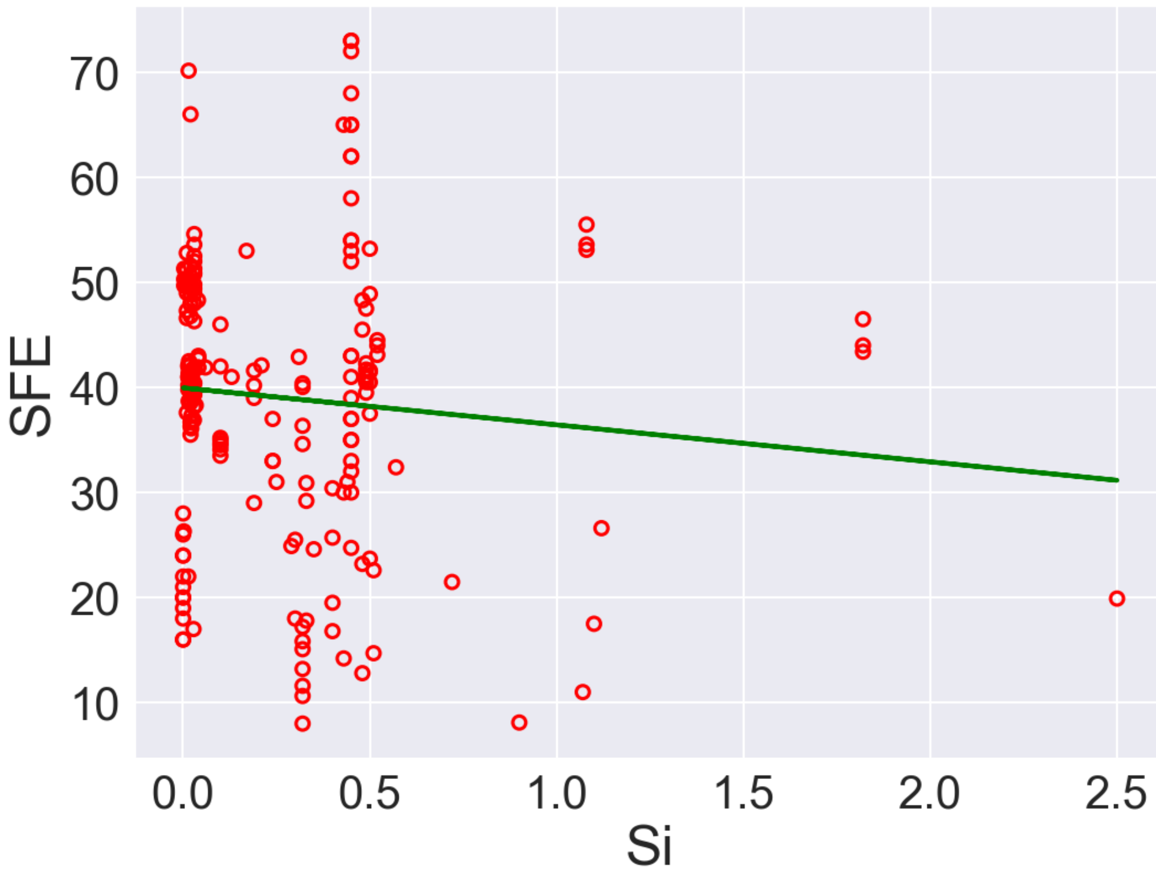


SFE
Ni
70
60
50
40
30
20
10
0
5
10
15
20
25

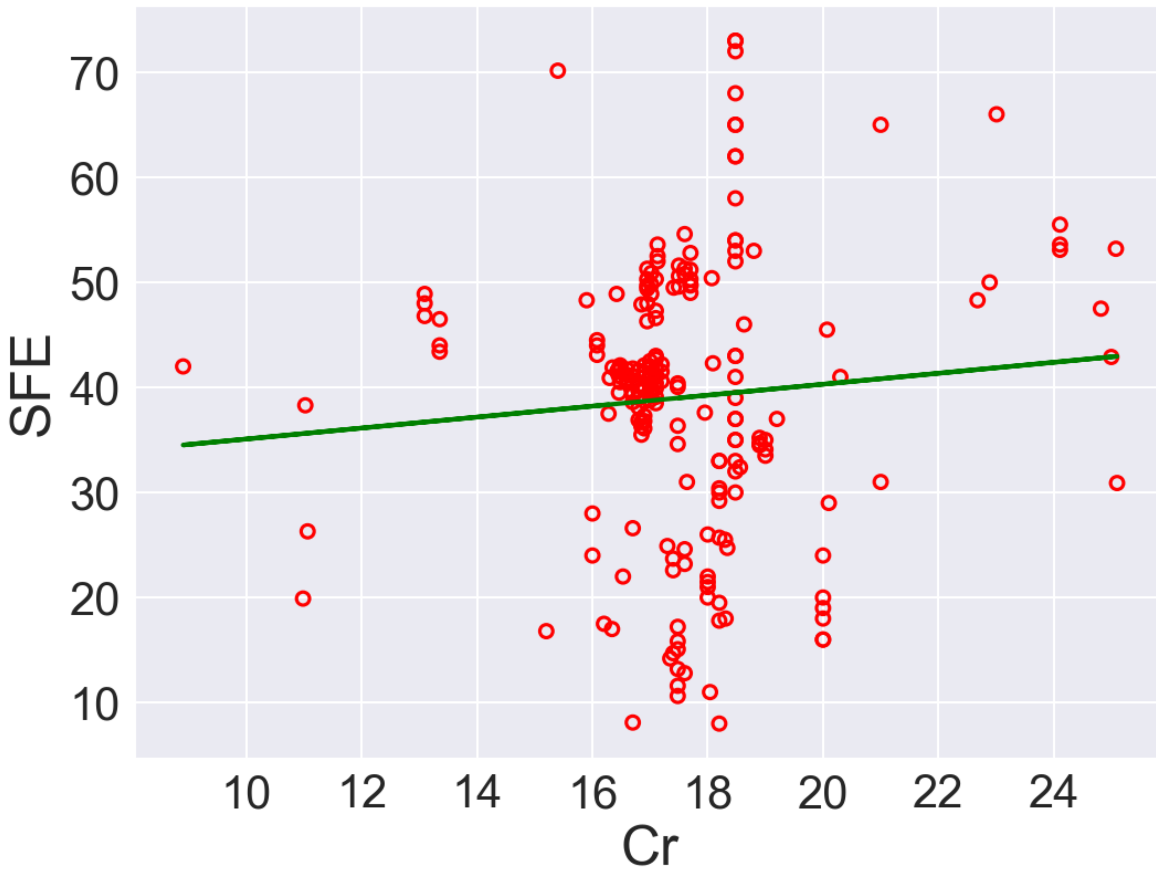
70
60
50
40
30
20
10
SFE
50
55
60
65
70
75
80
Fe



70
60
50
40
30
20
10
SFE
0
2
4
6
8
10
Mn



70
60
50
40
30
20
10
SFE
0.0
0.5
1.0
1.5
2.0
2.5
Si




```
pd.DataFrame(res)
```

	feature	slope	intercept	Norm RSS	R2
0	C	-16.200376	39.658087	167.480699	0.006946
1	N	20.088487	37.447183	162.756200	0.034959
2	Ni	2.335338	10.324642	84.669120	0.497966
3	Fe	-1.440431	134.100015	100.297936	0.405297
4	Mn	0.345602	38.236325	167.230592	0.008429
5	Si	-3.520817	39.959897	167.129698	0.009027
6	Cr	0.521318	29.878868	167.428848	0.007254

According to R^2, `Ni` is the best predictor that has positive linear relation between `SFE`. Also, `Fe` has high correlation coefficient. The rest of the features performs low correlation between `SFE`. As we can see in the linear regression plots.

(b)

> Perform multivariate linear regression with a linear forward wrapper search (for 1 to 5 variables) using the R^2 statistic as the search criterion. List the normalized RSS, the R^2 statistic, and the *adjusted* R^2 statistic for each model. Which would be the most predictive model according to adjusted R^2? How do you compare these results with those of item (a)?

Use the adjusted R^2 formula:

$$R^2_{adj} = 1 - \frac{(1 - R^2)(n-1)}{n-k-1}$$

Ref: Sequential forward search https://vitalflux.com/sequential-forward-selection-python-example/

```
def adr2(model, x, y):
    r = r2(model,x,y)
    N = x.shape[0]
    p = x.shape[1]
    return 1 - (1-r)*(N-1)/(N-p-1)

class SequentialForwardSearch():
    def __init__(self, clf):
        self.clf = clone(clf)

    def search(self, xs, ys):
        unchosen_ids = list(range(xs.shape[1]))
        chosen_ids = []
        self.scores = []
        self.subset = []
        self.r2 = []
        self.rss = []
        self.adr2 = []

        while len(unchosen_ids) > 0:
            scrs = [] #scores record

            for i in unchosen_ids:
                subset = chosen_ids + [i]
                scrs.append( self._score(xs[:, subset], ys))

```

```python

            best_i = np.argmax(scrs) #best base
            chosen_ids.append(unchosen_ids.pop(best_i)) # swap

            # Rcord
            self.scores.append(scrs[best_i])

            # Performance
            self.clf.fit(xs[:, chosen_ids], ys)
            self.r2.append(r2(self.clf, xs[:, chosen_ids], ys))
            self.rss.append(normalized_RSS(self.clf, xs[:, chosen_ids], ys))
            self.adr2.append(adr2(self.clf, xs[:, chosen_ids], ys))

        self.subset = chosen_ids

    def _score(self, xs, ys):
        self.clf.fit(xs, ys)
        return r2(self.clf, xs, ys)

```

```python
# data
xr = SFE.drop("SFE", axis=1).to_numpy()[:, 0:5]
yr = SFE['SFE']

# Search
sh = SequentialForwardSearch(LinearRegression())
sh.search(xr, yr)
ids_sh = sh.subset

## Performance
fts = [ str([res["feature"][j] for j in sh.subset[0:i+1]]) for i in range(0, len(sh.subset
pd.DataFrame({"Feature": fts, "R2": sh.r2, "Norm RSS": sh.rss, "Adjust R2": sh.adr2})
```

	Feature	R2	Norm RSS	Adjust R2
0	['Ni']	0.497966	84.669120	0.495564
1	['Ni', 'N']	0.553514	75.300860	0.549221
2	['Ni', 'N', 'C']	0.572860	72.038072	0.566670
3	['Ni', 'N', 'C', 'Fe']	0.579493	70.919455	0.571328
4	['Ni', 'N', 'C', 'Fe', 'Mn']	0.579832	70.862215	0.569584

If solely depends on R^2, model with 5 is the best option. However, after adding regularization term with adjusted R^2, model with 4 features is the best.