Assignment 2

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Objective: Dimensionality Reduction using PCA

Author: Jason Wong

Conduct a Principal Component Analysis to investigate if you can reduce the dimension of the chemical data set used for assignment #1 without impacting the model's accuracy.

1 Write a Python program(s) to create the following based on the steps specified on slide #23:

(a) Covariance matrix

(b) Eigenvectors and eigenvalues

(c) Projection matrix

(d) Component matrix and coefficients (loadings) of each PC

(e) Explained variance for each PC

(f) Correlation matrix between the data set and PC scores

[1]:
```
import pandas as pd
data = pd.read_csv("https://gist.githubusercontent.com/jaasonw/
 ↪d00e9782bf6de5ec1b1ec305790eeb88/raw/
 ↪b8028c4471f547809581c24c31a8f31940c02268/air.csv")
data
```

[1]:

	T	P	TC	SV	Idx
0	253.15	17.7	0.026827	389.355242	54.102967
1	253.15	17.7	0.026970	388.007160	54.162740
2	253.15	17.7	0.026912	385.677846	54.232917
3	253.15	17.7	0.026815	384.292031	54.304434
4	253.15	17.7	0.026731	392.060606	54.070973
…	…	…	…	…	…
419995	353.15	300.0	0.041824	435.341910	53.755453
419996	353.15	300.0	0.041518	426.840370	54.234870
419997	353.15	300.0	0.041744	428.069807	54.106685
419998	353.15	300.0	0.041607	430.308699	53.970731
419999	353.15	300.0	0.041669	432.137751	54.077029

[420000 rows x 5 columns]

1.1 Step 1: Standardize the dataset

[2]:
```
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler()
scaler.fit(data)
data_std = pd.DataFrame(scaler.transform(data))
data_std.columns = data.columns

# Split test and training data
X_train, X_test, y_train, y_test = train_test_split(data.iloc[:,0:4], data.
 ↪iloc[:,4], test_size=0.40, random_state=42)

data_std
```

[2]:

	T	P	TC	SV	Idx
0	-1.46385	-1.085147	-1.932988	-1.148942	0.518523
1	-1.46385	-1.085147	-1.897869	-1.208770	0.755887
2	-1.46385	-1.085147	-1.912251	-1.312146	1.034562
3	-1.46385	-1.085147	-1.935958	-1.373649	1.318563
4	-1.46385	-1.085147	-1.956603	-1.028877	0.391472
…	…	…	…	…	…
419995	1.46385	1.877493	1.751194	0.891960	-0.861483
419996	1.46385	1.877493	1.675923	0.514659	1.042318
419997	1.46385	1.877493	1.731570	0.569222	0.533287
419998	1.46385	1.877493	1.697805	0.668584	-0.006598
419999	1.46385	1.877493	1.713198	0.749758	0.415521

[420000 rows x 5 columns]

1.2 Step 2: Create the covariance matrix

[3]:
```
data_cov = X_train.cov()
```

1.3 Step 3: Create Eigenpairs

[4]:
```
import numpy as np
from numpy.linalg import svd
from numpy.linalg import eig

# Step 2.5 compute the eigenvectors and eigenvalues of the covariance matrix
e_vals, e_vecs = eig(data_cov)
```

```
# Order by largest eigenvalue
idx = e_vals.argsort()[::-1]
e_vals = e_vals[idx]
e_vecs = e_vecs[:,idx]

np.set_printoptions(precision=3)
print("Eigenvalues:")
print(e_vals)
print("Eigenvectors:")
print(e_vecs)
```

```
Eigenvalues:
[9.123e+03 1.617e+03 9.227e+00 1.095e-06]
Eigenvectors:
[[ 6.121e-03  8.490e-01  5.284e-01  1.058e-04]
 [-9.970e-01  4.564e-02 -6.179e-02  1.442e-05]
 [-1.342e-05  9.258e-05  5.154e-05 -1.000e+00]
 [ 7.657e-02  5.264e-01 -8.468e-01  4.061e-06]]
```

1.4 Step 4: Create component matrix and loadings

[5]:
```
pca_train = np.matmul(X_train, e_vecs)
pca_train.columns = [f"PCA{n + 1}" for n in range(4)]
pca_train
```

[5]:

	PCA1	PCA2	PCA3	PCA4
119749	6.489258	536.569502	-193.885549	-0.000310
58136	19.603115	541.852816	-202.527218	-0.000741
113887	7.093904	540.726131	-200.571825	-0.000661
343026	-164.668356	516.778799	-197.954617	0.001785
92282	5.121129	494.887397	-202.598212	0.000566
…	…	…	…	…
259178	-117.373042	448.503695	-202.352559	0.000404
365838	-269.377421	422.385363	-196.475688	-0.004981
131932	-17.179169	447.303669	-201.585066	0.001501
146867	-16.615990	467.313698	-195.891965	0.001448
121958	-18.637937	421.136930	-197.374597	0.000811

[252000 rows x 4 columns]

[18]:
```
# Use SVD method for test dataset
u, s, vh = np.linalg.svd(X_test, full_matrices=False)
pca_test = pd.DataFrame(np.matmul(u, np.diag(s)))
pca_test.columns = [f"PCA{n + 1}" for n in range(4)]
pca_test
```

[18]:

	PCA1	PCA2	PCA3	PCA4
0	-524.623021	-95.210705	-0.653700	0.000159
1	-505.467915	186.589114	20.008772	0.005382
2	-559.154948	-102.811536	-24.443158	0.000881
3	-522.477307	28.606228	5.022178	-0.000503
4	-577.422137	-35.279988	-21.013187	0.000635
…	…	…	…	…
167995	-502.171399	-90.050022	7.366962	-0.000637
167996	-530.137719	180.846572	13.645256	-0.001000
167997	-506.267760	186.379304	20.606315	0.003982
167998	-506.339266	186.360547	20.659735	0.004636
167999	-487.732211	87.922460	21.354556	0.000774

[168000 rows x 4 columns]

1.5 Step 5: Calculate the explained variances

After detemining the Principal Components, to compute the percentage of information accounted for by each component, we divide the eigenvalue of each component by the sum of eigenvalues.

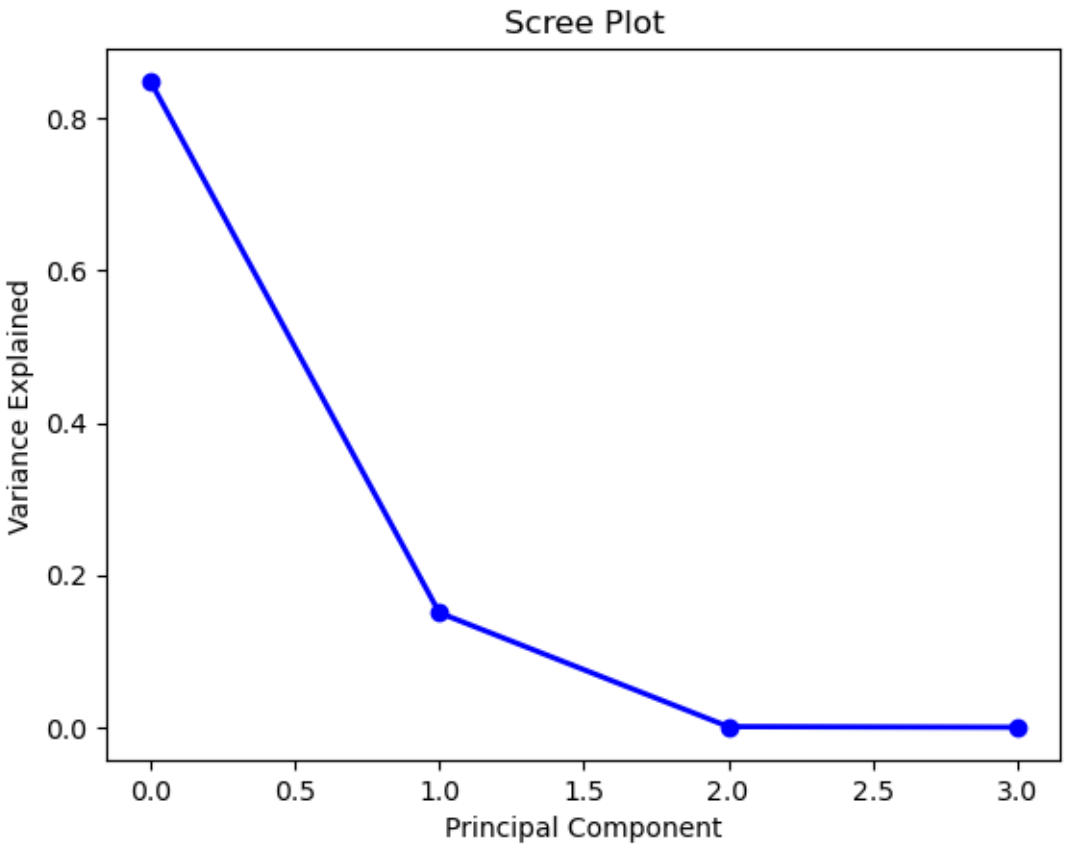
[46]:
```
# explained_variances = [(e_vals[i] , np.sum(x_pca[:,i])) for i, v in␣
↪enumerate(e_vals)]
explained_variances = [e_vals[i] / sum(e_vals) for i, v in enumerate(e_vals)]
explained_variances
```

[46]:
```
[0.8486981115390654,
 0.15044352221652765,
 0.0008583661425364786,
 1.018705347956594e-10]
```

Create a scree plot to display the variances

[20]:
```
import matplotlib.pyplot as plt

plt.plot(range(0,len(e_vals)), explained_variances, 'o-', linewidth=2,␣
↪color='blue')
plt.title('Scree Plot')
plt.xlabel('Principal Component')
plt.ylabel('Variance Explained')
plt.show()
```



2 Determine if a feature or features can be removed from the data set based on the following criteria:

(a) Explained variance >80%

(b) Kaiser criteria

(c) Correlation r>0.5 from the correlation matrix

Which feature(s) meet all the above criteria?

Which features can be removed from the data set? Justify your decision. Are those features removed the same features removed by LASSO regression? If they are different, explain possible reasons.

[21]:
```
# Determine the eiganvalues satisfying the kaiser criterion

kaiser = [k for k in e_vals if k >= np.mean(e_vals)]
kaiser = pd.DataFrame(kaiser)
kaiser
```

[21]:
```
                0
0  9123.220264
```

Based on the above criteria, we should remove PCA2 - PCA4

2.1 Compare with LASSO feature selection

[39]:
```
from sklearn.model_selection import GridSearchCV
from sklearn.pipeline import Pipeline
from sklearn.linear_model import Lasso

pipeline = Pipeline([ ('scaler',StandardScaler()), ('model',Lasso()) ])
search = GridSearchCV(pipeline,
                      {'model__alpha':np.arange(0.01,10,0.01)},
                      cv = 5, scoring="neg_mean_squared_error",
                      # verbose=3
                     )
search.fit(X_train,y_train)
search.best_params_
```

[39]:
```
{'model__alpha': 0.01}
```

[40]:
```
coefficients = search.best_estimator_.named_steps['model'].coef_
importance = np.abs(coefficients)
importance
```

[40]:
```
array([0.405, 0.126, 0.   , 0.442])
```

[41]:
```
np.array(data_std.iloc[:,0:4].columns)[importance > 0]
```

[41]:
```
array(['T', 'P', 'SV'], dtype=object)
```

LASSO regression would tell us to remove TC. PCA would tell us that the first principal component accounts for 84% of the data but since PCA projects our dataset into an arbitrary PCA dimension, it is not possible to determine what features are represented by each principal component

3 Compare the models created by the Least Square method with the new data set with only selected features by PCA and the original data set in terms of training and testing errors. Is there any difference in accuracy?

[35]:
```
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import KFold, cross_val_score, train_test_split
from sklearn.metrics import mean_squared_error

# k fold cross validation
```

```
cv = KFold(n_splits=10, shuffle=True, random_state=42)

# Perform a linear regression on the original dataset
original_data_reg = LinearRegression().fit(X_train, y_train)
original_data_score_train = -1 * cross_val_score(original_data_reg, X_train,␣
 ↪y_train, cv=cv, scoring='neg_root_mean_squared_error').mean()
original_data_score_test = mean_squared_error(y_test, original_data_reg.
 ↪predict(X_test), squared=False)
```

[66]:
```
# Perform a linear regression on the PCA dataset, using only PC1

pca_reg = LinearRegression().fit(np.array(pca_train["PCA1"]).reshape(-1, 1),␣
 ↪y_train)
pca_score_train = -1 * cross_val_score(pca_reg, np.array(pca_train["PCA1"]).
 ↪reshape(-1, 1), y_train, cv=cv, scoring='neg_root_mean_squared_error').mean()
pca_score_test = mean_squared_error(y_test, pca_reg.predict(np.
 ↪array(pca_test["PCA1"]).reshape(-1, 1)), squared=False)
```

[67]:
```
pd.DataFrame([
    ["Linear Regression", original_data_score_train, original_data_score_test],
    ["PCA", pca_score_train, pca_score_test],
],  columns=['', 'RMSE (Training)', 'RMSE (Test)']).set_index("")
```

[67]:

	RMSE (Training)	RMSE (Test)
Linear Regression	0.136458	0.136112
PCA	0.251969	0.251628

Compared to the least squares method, PCA performs slightly worse in this case.