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3d95019 on Dec 10, 2018

1 contributor

5689 lines (5688 sloc) 329 KB

Problem 0: Gene Expression Analysis with Principal Component Analysis

This problem was inspired by a Kaggle problem (https://www.kaggle.com/crawford/principle-component-analysis-gene-expression). This problem is an application of the material in Notebook 15, but based on a slightly different description and procedure.

You will carry out a PCA on gene expression data from patients with two different types of leukemia. And then you will implement kmeans clustering method on both the original gene set and the gene set reconstructed from PCA, comparing the classification accuracy bewteen two gene sets. Based on the final results, you can draw your own conclusion whether PCA is effective for this application of distinguishing leukemia patients.

Description of data set

This dataset comes from a proof-of-concept study published in 1999 by Golub, et al. It showed how new cases of cancer could be classified by gene expression monitoring (via DNA microarray) and thereby provided a general approach for identifying new cancer classes and assigning tumors to known classes. These data were used to classify patients with acute myeloid leukemia (AML) and acute lymphoblastic leukemia (ALL).

> **Reference.** T.R. Golub, D.K. Slonim, P. Tamayo, C. Huard, M. Gaasenbeek, J.P. Mesirov, H. Coller, M. Loh, J.R. Downing, M.A. Caligiuri, C.D. Bloomfield, and E.S. Lander. "Molecular Classification of Cancer: Class Discovery and Class Prediction by Gene Expression (https://www.ncbi.nlm.nih.gov/pubmed/10521349)." *Science* 286:531-537, 1999.

In [2]:
```
import os
import pandas as pd
import numpy as np
import scipy as sp
from IPython.display import display, Image
```

In [3]:
```
DATA_PATH = "../resource/asnlib/publicdata/"

# Input train dataset
with open(DATA_PATH + "data_set_ALL_AML_train.csv") as fp:
    trainfile = set(fp.read().splitlines())

# Input test dataset
with open(DATA_PATH + "data_set_ALL_AML_independent.csv") as fp:
    testfile = set(fp.read().splitlines())

# Input y label dataset
with open(DATA_PATH + "actual.csv") as fp:
    labels = set(fp.read().splitlines())

assert len(trainfile)==7131 ,  "The train file is corrupted!"
assert len(testfile)==7131, "The test file is corrupted!"
assert len(labels)==74, "The label file is corrupted!"

# Loading the files into a pandas dataframe for you
X_train = pd.read_csv(DATA_PATH + "data_set_ALL_AML_train.csv")
X_test = pd.read_csv(DATA_PATH + "data_set_ALL_AML_independent.csv")
y = pd.read_csv(DATA_PATH + "actual.csv")

print("X_train has {} rows and {} columns: ========>".format(X_train.shape[0], X_train.shape[1]))
display(X_train.head())
print('\n')
print("X_test has {} rows and {} columns: ========>".format(X_test.shape[0], X_test.shape[1]))
display(X_test.head())
print('\n')
print("y has {} rows and {} columns: ========>".format(y.shape[0], y.shape[1]))
display(y.head())
```

```
X_train has 7129 rows and 78 columns: ========>
```

	Gene Description	Gene Accession Number	1	call	2	call.1	3	call.2	4	call.3	...	29	call.33	30	call.34	31	call.3

0	AFFX-BioB-5_at (endogenous control)	AFFX-BioB-5_at	-214	A	-139	A	-76	A	-135	A	...	15	A	-318	A	-32	A
1	AFFX-BioB-M_at (endogenous control)	AFFX-BioB-M_at	-153	A	-73	A	-49	A	-114	A	...	-114	A	-192	A	-49	A
2	AFFX-BioB-3_at (endogenous control)	AFFX-BioB-3_at	-58	A	-1	A	-307	A	265	A	...	2	A	-95	A	49	A
3	AFFX-BioC-5_at (endogenous control)	AFFX-BioC-5_at	88	A	283	A	309	A	12	A	...	193	A	312	A	230	P
4	AFFX-BioC-3_at (endogenous control)	AFFX-BioC-3_at	-295	A	-264	A	-376	A	-419	A	...	-51	A	-139	A	-367	A

5 rows × 78 columns

```
X_test has 7129 rows and 70 columns: ========>
```

	Gene Description	Gene Accession Number	39	call	40	call.1	42	call.2	47	call.3	...	65	call.29	66	call.30	63	call.
0	AFFX-BioB-5_at (endogenous control)	AFFX-BioB-5_at	-342	A	-87	A	22	A	-243	A	...	-62	A	-58	A	-161	A
1	AFFX-BioB-M_at (endogenous control)	AFFX-BioB-M_at	-200	A	-248	A	-153	A	-218	A	...	-198	A	-217	A	-215	A
2	AFFX-BioB-3_at (endogenous control)	AFFX-BioB-3_at	41	A	262	A	17	A	-163	A	...	-5	A	63	A	-46	A
3	AFFX-BioC-5_at (endogenous control)	AFFX-BioC-5_at	328	A	295	A	276	A	182	A	...	141	A	95	A	146	A
4	AFFX-BioC-3_at (endogenous control)	AFFX-BioC-3_at	-224	A	-226	A	-211	A	-289	A	...	-256	A	-191	A	-172	A

5 rows × 70 columns

```
y has 72 rows and 2 columns: ========>
```

	patient	cancer
0	1	ALL
1	2	ALL
2	3	ALL

3	4	ALL
4	5	ALL

Data Cleaning

Exercise 0 (`clean_data`: 2.5 points).

First you need to do some data cleaning using pandas.

As you can seen from the previous cell, there are 3 data frames: `X_train`, `X_test` and `y`.

The `X_train` data frame has 7129 rows and 78 columns. Each row is a gene. The first two columns `'Gene Description'` and `"Gene Accession Number"` encode some basic information for each gene. We will be interested primarily in so-called genes corresponding to mRNA expression values (https://www.biosyn.com/tew/The-role-of-mRNA-in-Gene-Expression.aspx), and we'll explain below how to find those. The rest of the columns hold patient information. The columns whose names consist only of an integer (such as "1", "2", "3") store patient ids. The vaules in these columns are the gene expression values. The columns with "call" in the name are the columns to measure the quality of the detection call. In this problem, you will ignore "call" columns.

`X_test` has similar format as `X_train`. The row labels are the same but `X_test` has fewer patients than `X_train`.

Lastly, the data frame y contains 2 columns. The first is `'patient'`, which holds patient ids intended to correspond to the patient ids in the `X_train` and `X_test` data sets. The second is `'cancer'`, which indicates the cancer type for each patient. There are only two types: "ALL" (acute lymphoblastic leukemia) and "AML" (acute myeloid leukemia).

Your task. To clean the training and testing data sets, create a function `clean_data(X_train, X_test)`, which should return a new cleaned data frame `X`. The original data frames (`X_train`, `X_test`) shouldn't be changed. The cleaning process has 5 sequential steps:

- Step 1: Delete all the columns containing "call" in the column name.
- Step 2: Only keep the rows (or genes) whose `"Gene Description"` column contain the substring `"mRNA"`.
- Step 3: Delete the `"Gene Description"` column, and only keep the columns with patient ids and the `"Gene Accession Number"` column. Then, transpose the data frame, so now each column represents a gene and each row represents a patient. Use the `"Gene Accession Number"` as the new column name for each gene. Use the `'patient_id'` as the new row name for each patient. **Note: `X_test` has different patient_ids with `X_train`.**
- Step 4: Concatenate new `X_train` and `X_test data` frames into one data frame, with `X_train` above `X_test`. Then sort this combined data frame by its index in **numerical order**.
- Step 5: Convert the data type to numeric type. This last step is designed to make the later PCA and Kmeans calculations easier.

There are 2 test cells to give you some partial credits.

In [4]:
```
def clean_data(X_train, X_test, y):
    # copy frames
    train = X_train.copy()
    test = X_test.copy()

    # take out call columns
    subset_train = [col for col in train.columns if 'call' not in col]
    subset_test = [col for col in test.columns if 'call' not in col]

    train = train[subset_train]
    test = test[subset_test]

    # filter rows by mRNA
    train = train[train['Gene Description'].str.contains("mRNA")]
    test = test[test['Gene Description'].str.contains("mRNA")]

    # delete gene description
    train = train.drop('Gene Description', axis=1)
    test = test.drop('Gene Description', axis=1)

    # transpose the data
    train = train.transpose().reset_index()
    train.columns = train.iloc[0]
    train = train.iloc[1:, :]

    test = test.transpose().reset_index()
```

```
    test.columns = test.iloc[0]
    test = test.iloc[1:, :]

    # concatenate train and test
    X = pd.concat([train, test], axis=0)

    # change type to numeric all columns
    X = X.apply(pd.to_numeric)

    # set index
    X = X.set_index('Gene Accession Number').sort_index()




    return X
```

In [5]:
```
# `clean_data_0`: Test cell (0.5 points)
# This test cell is to give you some partial credits

# Your solution for clean_data
X = clean_data(X_train, X_test, y)
assert X_train.shape == (7129, 78), "You shouldn't modify on X_train!"
assert X_test.shape == (7129, 70), "You shouldn't modify on X_test!"
assert X.shape == (72, 2037), "The shape of your X is wrong!"
print ("\n(Passed.)")
```

```
(Passed.)
```

In [6]:
```
# `clean_data_1`: Test cell (2 points)

# functions from notebook to compare tibbles
def canonicalize_tibble(X):
    var_names = sorted(X.columns)
    Y = X[var_names].copy()
    Y.sort_values(by=var_names, inplace=True)
    Y.reset_index(drop=True, inplace=True)
    return Y

def tibbles_are_equivalent(A, B):
    A_hat = canonicalize_tibble(A)
    B_hat = canonicalize_tibble(B)
    equal = (A_hat == B_hat)
    return equal.all().all()

# Loading the files into a pandas dataframe for you
X_solution = pd.read_csv(DATA_PATH + "X_solution.csv", index_col="Gene Accession Number")

# Compare your solution with teacher's solution
print("=== Last few rows of your solution ===")
display(X.tail())

print ("=== Last few rows of the instructor's solution ===")
display(X_solution.tail())

# Check it
assert tibbles_are_equivalent(canonicalize_tibble(X), canonicalize_tibble(X_solution)), \
"Please check your solution, which is different from the instructor's solution"
print ("\n(Passed.)")
```

```
=== Last few rows of your solution ===
```

	AB000115_at	AB000460_at	AB000464_at	AB000466_at	AB000467_at	AB000584_at	AC000099_at	AC
Gene Accession Number								
68	101	1910	548	-819	-296	-154	138	16
69	1421	1813	348	-532	-716	-365	150	10
70	215	1249	371	-628	-745	80	125	57
71	174	1300	620	-538	-976	-133	110	52
72	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

72	154	1541	882	-466	-558	81	77	10

5 rows × 2037 columns

```
=== Last few rows of the instructor's solution ===
```

	AB000115_at	AB000460_at	AB000464_at	AB000466_at	AB000467_at	AB000584_at	AC000099_at	AC
Gene Accession Number								
68	101	1910	548	-819	-296	-154	138	16
69	1421	1813	348	-532	-716	-365	150	10
70	215	1249	371	-628	-745	80	125	57
71	174	1300	620	-538	-976	-133	110	52
72	154	1541	882	-466	-558	81	77	10

5 rows × 2037 columns

```
(Passed.)
```

Principal Components Analysis

Principal Components Analysis (PCA) is a simple yet popular and useful linear transformation technique that is used in numerous applications, such as the analysis of gene expression data. In this section, you will reimplement PCA from Notebook 15 but with a couple variations in the basic steps.

Introduction

The main goal of a PCA analysis is to identify patterns in data; PCA aims to detect the correlation between variables. If a strong correlation between variables exists, it's likely the dimensionality can be reduced. Put differently, PCA finds the directions of maximum variance in high-dimensional data and projects the data points onto a smaller dimensional subspace while attempting to preserve most of the "information" of the data, as measured by the magnitude of the projections of the original data onto the subspace.

PCA and Dimensionality Reduction

Often, the desired goal is to reduce the dimensions of a d-dimensional dataset by projecting it onto a k-dimensional subspace (where $k<d$). An important question is how large k should be.

We will compute the eigenvectors (the principal components) of the dataset and collect them into a projection matrix. Each of those eigenvectors is associated with an eigenvalue, which can be interpreted as the "length" or "magnitude" of the corresponding eigenvector. If some eigenvalues have a significantly larger magnitude than others, then the reduction of the dataset via PCA onto a smaller dimensional subspace by dropping the "less informative" eigenpairs is reasonable.

A Summary of the PCA Approach

In the exercises below, you will implement the following procedure.

1. Standardize the data.
2. Obtain the Eigenvectors and Eigenvalues from the covariance matrix.
3. Sort eigenvalues in descending order and choose the k eigenvectors that correspond to the k largest eigenvalues, where k is the number of dimensions of the new feature subspace ($k \leq d$).
4. Construct the projection matrix W from the selected k eigenvectors.
5. Transform the original dataset X via W to obtain a k-dimensional feature subspace Y.

1 - Standardizing

Whether to standardize the data prior to a PCA on the covariance matrix depends on the measurement scales of the original features. Since one interpretation of PCA is that it yields a feature subspace that maximizes the variance along the subspace's axes, it makes sense to standardize the data, especially, if it was measured on different scales. Let us continue with the transformation of the data so that it has unit scale (mean=0 and variance=1), which is a requirement for the optimal performance of many machine learning algorithms.

Recall the following concepts from basic statistics:

Standardization (z-score). Let

$$\mu = \frac{1}{n}\sum_{i=0}^{n-1}(x_i)$$

be the mean of a collection of values $x_0, x_1, \ldots, x_{n-1}$. Let

$$\sigma = \sqrt{\frac{1}{(n-1)}\sum_{i=0}^{n-1}(x_i - \mu)^2}$$

be the (**unbiased**) standard deviation of those values. Then *standardizing the data* (or *calculating the z-scores*) means computing for each item x_i the value

$$z_i = \frac{x_i - \mu}{\sigma}.$$

Exercise 1 (`Standardize`: 1 point)

Given the data matrix `X`, return a new matrix `X_std` of the same size in which each `X_std[i, j]` element is the standardized value (z-score) with respect to the elements in the same column, `X[:, j]`. Use the definition of z-score as it appears above; in particular, be sure to compute the **unbiased** standard deviation.

In [7]:
```
X_std = (X - X.mean()) / X.std()
```

In [8]:
```
# `Standardization`: Test cell (1 point)
import math
sum_tol = 1e-4

print(X_std)
print(X_std.shape)

# Check it
assert X_std.shape==(72,2037), "Expected 72 rows and 2037 columns."

sum_X_std = sorted(X_std.sum(axis=1))

# Compare your solution with teacher's solution
print("=== First 2 elements and Last 2 elements of your solution ===")
print(sum_X_std[:2])
print(sum_X_std[70:])

# Check it
sum_tests = [(0,-867.0718922111674),(1,-776.1804067699011),
             (70,1078.304154730164),(71,1663.9557654929808)]

print ("=== First 2 elements and Last 2 elements of instructor's solution ===")
result_array = np.array([sum_tests[0][1],sum_tests[1][1],
                         sum_tests[2][1],sum_tests[3][1]])
print(result_array[:2])
print(result_array[2:])

# Test elements close
for i,j in sum_tests:
    assert math.isclose(sum_X_std[i],j,abs_tol=sum_tol), ("Row "+str(i)+" should sum to "+str(j)+" b
ut yours had "+str(sum_X_std[i]))

print ("\n(Passed.)")
```

```
0                     AB000115_at  AB000460_at  AB000464_at  AB000466_at  \
Gene Accession Number
1                       -0.040869    -0.314559     0.128975     0.012511
2                       -0.123946     0.388869     0.007705     0.208954
3                        0.165485     0.307157     4.543723    -1.954322
4                       -0.477695     0.539857     1.899002    -0.167163
5                       -0.265981    -0.383836    -1.112108     1.090555
6                       -0.603650    -0.835024    -0.007776    -1.051160
7                       -0.343699    -0.071201    -0.887630    -1.468004
8                       -0.000670     1.930725     0.828213    -2.155557
9                       -0.263301     0.520317     1.914484     0.182602
10                      -0.491094    -0.739102    -1.308205     0.949212
11                      -0.354419     0.520317    -0.121306     0.788703
12                      -0.298140    -0.685812    -0.319982     0.632985
13                      -0.496454     0.767227     0.544390     0.889320
```

```
14                        -0.351739   -0.092517   -0.224515   -0.191120
15                        -0.327619   -0.096070   -0.528980    0.426959
16                        -0.397297   -0.163571   -0.219354    0.422168
17                        -0.303500    2.394348    0.967545   -0.435477
18                        -0.265981   -0.952262    0.221863    1.203151
19                        -0.190944   -0.550811    0.139296    0.151459
20                         5.085805    1.559471    1.302973    0.115524
21                        -0.282061   -0.744431   -1.403673    1.021081
22                        -0.528613    0.028273   -0.012937    0.652150
23                        -0.265981   -0.710681    0.384416    0.803077
24                        -0.016749    0.792096    1.171382    0.951607
25                         3.384060   -0.746207   -0.701854    1.152842
26                        -0.499134   -0.612983    0.118654    1.188777
27                        -0.316900    0.889794    0.959804   -1.901617
28                        -0.220423    0.623345    0.118654    0.220933
29                        -0.517893   -1.506478   -0.965036   -0.229450
30                        -0.153425   -0.101399    0.232184   -0.370794
...                             ...         ...         ...         ...
43                        -0.394617   -1.669900   -0.771520   -0.217472
44                        -0.207023   -1.236475   -1.075985    1.210338
45                         0.773825   -0.390941   -0.954715    1.303768
46                        -0.453575   -1.845757   -1.246280    0.750372
47                         2.279936   -0.490416   -0.441253    1.073786
48                        -0.450895    0.706832   -0.415450   -0.351629
49                         0.082407    1.852566   -0.007776   -2.493344
50                        -0.303500    0.273407    0.159937   -1.707569
51                        -0.461615   -0.367849   -0.012937   -0.778055
52                        -0.528613   -1.971877   -1.447536    0.407794
53                        -0.617050    1.193547    0.864336   -1.118238
54                        -0.118586   -0.072978    0.405058    0.942025
55                        -0.568812   -0.872327   -1.047603    0.014906
56                        -0.442856    0.300052   -0.376747    0.014906
57                        -0.442856   -0.609430   -0.707015    0.362276
58                         1.508121    0.218341    0.425700   -0.516929
59                        -0.346379   -1.051737   -1.478499   -0.054568
60                        -0.282061   -0.572127   -0.237416    0.589863
61                        -0.619730    0.873807    1.981569    0.110732
62                         0.216403    0.035379   -0.030998    0.168228
63                         0.101167    1.477760    0.639857   -1.254791
64                        -0.164145    3.101328    0.567611   -2.014213
65                        -0.512533   -0.758642   -0.201293    0.939629
66                        -0.509853   -1.410556   -0.655410    1.040246
67                         0.548712   -0.566798   -0.407710    1.179194
68                        -0.523253    0.152617   -0.528980    0.192185
69                         3.014232   -0.019688   -1.045023    0.879738
70                        -0.217743   -1.021539   -0.985678    0.649755
71                        -0.327619   -0.930946   -0.343204    0.865364
72                        -0.381218   -0.502850    0.332812    1.037851

0                       AB000467_at  AB000584_at  AC000099_at  \
Gene Accession Number
1                          0.309300     0.301688     1.373514
2                          0.105404    -0.266264     0.005068
3                          0.396255     0.288541    -0.006335
4                         -0.521274    -0.105870    -0.291428
5                          1.442718     0.412123    -0.405466
6                          0.285312    -0.176864    -0.371254
7                         -0.263407     0.722393     1.293688
8                         -0.533268     0.404235    -0.895825
9                          0.147383     0.341129    -1.226533
10                         0.351278    -0.739557     0.335776
11                         0.771063     0.112371     0.506832
12                         0.935978     0.217547    -0.690558
13                         0.270320    -1.899126    -0.200199
14                         0.852021     0.401605    -0.679155
15                         1.211837     0.146553    -0.747577
16                         0.507198    -0.253117     0.039279
17                        -0.155462    -0.660675     0.529639
18                         0.348280    -0.387217    -0.314236
19                         0.759069    -0.466099    -0.348447
20                         0.465220    -1.325915     0.506832
21                         1.343769    -0.174235    -1.237937
22                         0.891001     0.722393    -1.523030
23                        -0.296390     0.464711     0.073491
```

```
24                        1.106890    0.375311    0.062087
25                        1.151867    0.648770   -1.044074
26                        0.855020   -1.007757   -0.736173
27                       -3.405794   -0.129535    2.411253
28                       -0.857102    0.033488   -0.086161
29                        1.241821    0.404235    0.062087
30                       -0.371351   -0.124276   -2.059005
...                            ...         ...         ...
43                       -1.138957    0.646140   -0.519503
44                        0.591155    0.638252   -0.223006
45                       -0.410331   -0.410881   -0.165987
46                       -0.569250    0.409494   -0.302832
47                        1.097895   -0.358293   -1.135303
48                       -1.162945   -0.734298    0.700695
49                       -1.975528   -0.500281    2.377042
50                       -1.040008    0.398976   -0.861614
51                       -2.584216   -0.153199    0.985788
52                        0.063426   -0.297817    0.427006
53                       -0.056513    0.333241    1.396322
54                        0.660120   -0.460840    1.875278
55                        0.813041   -0.955169   -0.006335
56                       -0.905077   -0.679081   -0.895825
57                        1.451714   -0.673822   -0.553714
58                       -0.344365   -0.489764    0.552447
59                        0.864015    0.383200   -0.211602
60                        0.318295   -0.166346   -0.610732
61                       -0.758153   -2.785236    1.955104
62                       -1.567737   -0.103241   -0.873018
63                       -1.558742    0.527817   -0.508099
64                       -1.477784   -1.988525    1.236670
65                        0.462221   -0.132164   -0.451080
66                        0.870012    0.798646   -1.887949
67                        1.667603    0.572517   -0.382658
68                        1.316783   -0.034876    0.153317
69                        0.057429   -0.589681    0.290161
70                       -0.029527    0.580405    0.005068
71                       -0.722171    0.020341   -0.165987
72                        0.531186    0.583034   -0.542310

0                     AC002045_xpt1_at  AF000177_at  AF000234_at  \
Gene Accession Number
1                            -0.816627    -1.226950     0.299295
2                             0.418136     1.390500     0.724143
3                            -0.569675     0.225882    -0.428454
4                             0.081382     0.137653    -0.113752
5                             0.070157     0.990530     0.110474
6                            -0.075770    -1.691621     0.271759
7                            -1.018679     0.378811    -0.959514
8                             0.328335    -2.203347    -1.856416
9                            -0.064544     1.266980     0.492050
10                           -0.782952    -0.132915     0.743812
11                            1.450846     2.196321     0.208818
12                           -0.592125    -0.991674     0.295361
13                           -0.311497     1.396382     0.649401
14                           -0.457424    -0.115269    -0.235699
15                           -0.985004     0.514095    -0.027209
16                           -1.007454    -0.379955     0.098672
17                            2.214154     0.472922     1.215866
18                           -1.748312    -0.009395     0.464514
19                           -0.861528    -1.091666    -1.946893
20                            2.247830     1.590485    -1.797409
21                           -0.906428     0.596442     0.106540
22                            0.193633    -0.556412    -0.625143
23                            1.955977    -0.662287    -0.212096
24                            1.439621     2.066919    -0.003606
25                            0.272209    -0.174088    -1.038190
26                           -0.390073    -0.385837    -0.302573
27                            0.025257     0.961120     0.311096
28                           -1.029905     0.114125     0.444845
29                           -0.266597     0.255291    -0.180626
30                            0.182408    -1.085784     2.041959
...                                ...          ...          ...
43                           -0.906428    -0.515239    -2.053105
44                           -1.321758     0.067070     0.189149
45                            4.212225    -0.974028    -0.121619
```

```
46                           -0.794177   -0.174088    0.570726
47                            1.316145   -0.338782   -0.334043
48                            1.282470    1.984573   -0.920177
49                            0.934491    1.396382   -0.349779
50                            0.440586   -0.768161    0.924766
51                            0.260984   -0.715224    0.031798
52                           -0.906428    0.249409    1.282740
53                            1.114093    1.919872   -0.440255
54                           -0.457424    0.278819    0.735945
55                           -0.154345   -0.074096    0.586461
56                            0.496711    0.037661    0.173414
57                           -0.614575   -1.103430    0.082937
58                            0.092607   -1.891606   -1.077528
59                           -0.491099   -1.297533    0.342567
60                            0.260984   -1.079902    1.377151
61                            0.799790    1.049349    1.927880
62                           -0.154345   -1.091666    1.219799
63                            0.317110    0.537623    0.763481
64                            1.316145    1.219924    2.140304
65                           -1.086030   -0.568176    0.869693
66                           -0.558450    1.537548   -0.503196
67                           -1.086030    0.031779   -0.046878
68                            0.260984    0.902301    1.027044
69                           -0.457424    1.166987   -0.695951
70                           -0.962554   -1.044611    0.338633
71                           -1.018679   -0.456420   -0.133421
72                           -0.378848    0.667025   -0.168825

0                         ...       L41268_f_at  X99479_f_at  S80905_f_at  \
Gene Accession Number     ...
1                         ...          0.840699     0.519659     1.224299
2                         ...         -0.522051    -1.189719    -0.794959
3                         ...          0.640829     0.866740     1.557072
4                         ...          1.198042     2.033803     0.145207
5                         ...         -0.818827     0.003374    -0.452493
6                         ...          0.065446     1.213822     0.600752
7                         ...          1.179872     2.580457     1.657228
8                         ...          0.216862     2.090204     3.195095
9                         ...          1.089022     1.482810     0.074129
10                        ...         -0.213161     0.393841     0.303517
11                        ...         -0.497824    -0.504233    -0.436339
12                        ...          0.683225     0.215962     0.096745
13                        ...         -0.691638    -0.300322     0.148438
14                        ...         -1.024754    -0.894700    -0.255414
15                        ...         -0.413031    -0.122443     0.061206
16                        ...          0.168409     0.016390     0.313209
17                        ...          2.669812     0.779970     0.368133
18                        ...         -0.273728     0.090145     0.555520
19                        ...          0.319826     0.419873    -0.132643
20                        ...         -0.764317    -0.339369    -1.922513
21                        ...         -0.328238    -0.543279     0.003051
22                        ...         -0.116254    -1.367599     0.710599
23                        ...          1.440309     0.723569     0.393980
24                        ...         -0.727978    -1.068241     0.423057
25                        ...          2.142882     0.454581    -0.323261
26                        ...          0.059389    -0.009641     0.410134
27                        ...          0.331939     2.996955     1.227529
28                        ...          0.713509    -0.998824     1.172606
29                        ...         -1.188284     0.025067    -1.347429
30                        ...         -0.370634    -1.640925    -0.704497
...                       ...               ...          ...          ...
43                        ...         -1.430551    -1.645264    -2.684985
44                        ...         -1.194341     0.051098    -0.358800
45                        ...         -1.539571    -0.161489    -1.017886
46                        ...         -0.782487    -1.029194    -0.584957
47                        ...         -0.667411    -0.426139    -0.397569
48                        ...         -0.188934     0.359133     0.671830
49                        ...          2.475998    -0.070380     1.734767
50                        ...          0.222919    -1.024855    -0.232798
51                        ...         -0.001178     1.235515     0.681522
52                        ...         -1.121661    -0.469524    -1.046963
53                        ...          1.331289    -0.630050     0.765523
54                        ...         -0.522051    -0.356723    -0.009872
55                        ...         -0.564448    -1.168027     0.109668
```

```
56                          ...          0.247146     0.202946    -0.051872
57                          ...         -0.679524    -0.348046     0.190438
58                          ...         -1.648591     1.278900     0.374595
59                          ...         -0.019348    -2.031392    -0.985577
60                          ...         -0.049631    -0.890361    -1.305428
61                          ...         -0.285841    -0.204875    -0.572033
62                          ...         -0.449371     1.014250    -0.210182
63                          ...          0.126012    -0.178844     0.949680
64                          ...          2.857568     2.090204     0.859217
65                          ...          0.356166     0.159561     0.923833
66                          ...         -1.206454    -0.365400    -1.014655
67                          ...         -0.503881     0.424211    -0.681881
68                          ...         -0.079914    -0.317676    -1.127733
69                          ...         -0.564448    -0.053026     0.138745
70                          ...          0.053332     0.393841    -0.462186
71                          ...         -0.849111     0.124853    -0.362031
72                          ...         -0.158651    -1.020517    -0.517110

0                      Z34822_f_at  U87593_f_at  L34355_at  U48730_at  \
Gene Accession Number
1                        -1.211632    -1.298968   0.190798   0.102543
2                         0.249596    -1.595965  -1.211514  -0.067427
3                        -0.481018    -0.224123  -0.084471   1.483553
4                        -1.560582     0.285015  -0.635008   0.686816
5                         1.481826     0.058732  -0.126021  -0.205528
6                        -1.058966     0.299158  -1.040120  -0.641078
7                        -1.604201    -1.313111   2.881160  -1.544045
8                        -1.309774     0.440585   0.736142   1.207351
9                        -0.306543    -1.171684  -0.624620   1.919102
10                        0.783926    -0.690832  -0.380514  -1.416568
11                       -0.197496    -0.704975   0.273898   0.102543
12                       -0.622779    -1.016114  -1.445233  -1.352829
13                        1.318256    -0.308979   0.097311   0.399991
14                       -0.033926     0.921437  -0.437645   0.973641
15                        0.805735     0.850723  -0.105246  -0.587962
16                        0.380452     0.709296   0.554361  -1.023511
17                        1.241923    -0.436263  -2.104839   0.697439
18                        1.634492    -0.125124   1.234742   0.113166
19                        0.445881     0.681011  -0.079277   1.515422
20                        1.045638     1.628572   0.632267   0.527469
21                        0.773021     0.610297   0.569942  -0.768555
22                       -0.044830     0.200159  -0.749270  -0.184282
23                       -0.622779    -0.902973  -1.066089  -0.492354
24                       -0.939015    -0.818116   0.092117   0.006935
25                        0.914782     0.101160   0.891954  -0.396745
26                        0.227787     1.939712   1.026992   0.155659
27                        0.500404    -1.892962  -1.201127  -0.587962
28                        0.042407    -0.096838  -1.138802  -0.024935
29                        0.783926    -0.719117  -0.323383  -0.024935
30                       -0.306543    -1.723250  -1.647789   0.527469
...                            ...          ...        ...        ...
43                       -0.960824     0.553726  -1.175158   1.759754
44                        0.107835     1.628572   0.975054   0.049427
45                        0.151454    -0.238265  -1.003764  -1.469683
46                       -0.023021     0.709296   0.071342  -0.768555
47                        1.579968    -0.238265  -0.977795  -0.014312
48                        0.980210    -0.252408   0.808854   0.612454
49                        0.816640    -0.902973   1.323035  -1.055381
50                       -1.636915    -0.323122  -1.003764  -0.439238
51                       -0.491923    -0.096838  -0.967408  -0.311760
52                       -0.699112    -0.620118   0.003823  -2.478883
53                       -1.037157    -0.676689  -1.502364   0.315006
54                        0.642165     0.285015   0.933504  -0.609208
55                        0.838449     0.200159   0.845211  -0.938526
56                        0.424071    -0.676689   1.650242   0.325629
57                        0.991115    -0.139266   0.808854  -0.449861
58                        0.107835     1.996282  -0.255864   1.515422
59                        0.064216    -0.323122   0.268704   0.208774
60                        1.492731    -1.171684   0.092117  -0.194905
61                        0.140549     1.260862   0.279092   1.770378
62                       -0.208401     1.543716  -0.505164  -1.002265
63                       -1.615105    -0.535262   0.014211  -0.481730
64                       -0.917205     2.858987   2.039773  -0.970395
65                        1.023829    -1.086828  -0.744077  -0.885410
```

```
66                          1.154685     0.228444  -1.055702  -1.193481
67                          1.241923     0.610297  -0.001371   0.038804
68                          0.576737     2.081139  -0.531133   0.410614
69                          1.187399     0.454727   0.382967   2.482129
70                          0.773021     0.751724   1.078929  -0.471107
71                          0.849354     1.402289  -0.505164   0.410614
72                          0.783926    -0.393835   0.408936   0.325629

0                       U58516_at  U73738_at  Z78285_f_at
Gene Accession Number
1                       -0.514763  -1.295717    -0.159994
2                        0.551561  -0.277449     0.412253
3                        1.735638   0.511994    -0.259515
4                        0.545019   2.628618    -1.503531
5                       -0.063374   0.786583     0.138569
6                        1.807598  -0.735098    -0.558079
7                        0.492684  -1.902101    -0.284396
8                       -0.128793  -0.849510     1.258183
9                        1.019304   0.203081    -0.209755
10                       1.038929   0.431906     0.934739
11                      -0.086271   0.500553    -0.782002
12                      -1.453520   0.820907    -1.229847
13                      -0.279256   0.168758     0.486894
14                      -0.746999   0.729377     0.213210
15                       0.175404   0.363258     0.312732
16                      -0.122251  -0.163037    -0.309276
17                       1.787973   1.587468    -1.304488
18                      -0.311965  -0.517715     0.437133
19                      -0.887649  -0.414744     0.163450
20                       1.150141  -1.124099     0.362492
21                      -0.240005  -0.002860     0.213210
22                      -0.871294   0.786583     0.088809
23                       1.274436   1.736204     1.656268
24                       0.185216   0.283170    -1.578172
25                      -0.904004   0.225964    -0.259515
26                       0.031483   1.015407     0.287851
27                       0.482871   0.649289     1.009380
28                       0.283344  -0.128714    -0.383917
29                      -0.576910   0.752260     0.710816
30                       0.224468   0.855230    -0.010712
...                           ...        ...          ...
43                      -1.888554  -0.826627    -1.254728
44                       0.070734  -1.490218    -1.926496
45                      -1.777342  -1.982190    -3.966681
46                      -0.246546   0.134434    -0.782002
47                      -1.280161   0.203081    -1.055685
48                      -0.083000   0.717936     0.287851
49                       2.572996  -1.272835    -0.831762
50                       0.070734   0.042905     0.934739
51                      -0.154960   0.523435     0.661056
52                      -1.437165   0.008581    -0.309276
53                      -0.648871  -0.471950    -1.005925
54                      -1.388101   0.294611     1.258183
55                       0.276803  -0.117272     1.357704
56                       0.103443  -0.563480     1.208423
57                      -0.779708   0.489112    -0.060473
58                      -0.851669  -3.011898    -1.005925
59                       0.829590   0.740818     2.701241
60                      -1.093718  -1.352923    -0.458558
61                       0.986595  -1.078334    -0.259515
62                      -0.308694   1.644674    -0.732241
63                      -0.096084  -0.174478     1.158662
64                       1.545924  -1.249952    -1.055685
65                      -0.446073  -0.254567     0.884979
66                      -1.214742   0.546318    -0.458558
67                      -0.560556   0.489112     0.462013
68                      -0.419906   0.283170     0.735697
69                      -0.168044  -0.254567     0.014168
70                      -1.146052   0.534877     1.755789
71                       0.299699  -0.300332     0.462013
72                       0.093630   0.168758     0.710816

[72 rows x 2037 columns]
(72, 2037)
=== First 2 elements and Last 2 elements of your solution ===
```

```
=== First 2 elements and Last 2 elements of your solution ===
[-867.0718922111693, -776.1804067698997]
[1078.3041547301668, 1663.955765492982]
=== First 2 elements and Last 2 elements of instructor's solution ===
[-867.07189221 -776.18040677]
[1078.30415473 1663.95576549]

(Passed.)
```

2 - Eigendecomposition - Computing Eigenvectors and Eigenvalues

The eigenvectors and eigenvalues of a covariance (or correlation) matrix represent the "core" computation of a PCA. The eigenvectors are known as the *principal components*, and they determine the axes of the new feature space. The eigenvalues measure the variance of the data along the new feature axes.

Covariance Matrix

One method to calculate PCA is to perform the eigendecomposition on the covariance matrix Σ, which is a $d \times d$ matrix where each element σ_{ij} is the covariance between two features i and j. The covariance between two features is calculated as follows:

$$\sigma_{jk} = \frac{1}{n-1}\sum_{i=1}^{N}\left(x_{ij} - \bar{x}_j\right)\left(x_{ik} - \bar{x}_k\right)$$

We can summarize the calculation of the covariance matrix via the following matrix equation:

$$\Sigma = \frac{1}{n-1}\left(\left(\mathbf{X} - \mathbf{\bar{x}}\right)^T \left(\mathbf{X} - \mathbf{\bar{x}}\right)\right)$$

where $\mathbf{\bar{x}}$ is the mean vector $\mathbf{\bar{x}} = \sum\limits_{k=0}^{n-1} x_{i}$.

The mean vector is a d-dimensional vector where each value in this vector represents the sample mean of a feature column in the dataset.

Exercise 2 (Calculate Σ : 1 point)

Because our data has been standardized, `X_std` is approximately equal to $\mathbf{X} - \mathbf{\bar{x}}$. Calculate a covariance matrix, `cov_mat`, using the equation for Σ above.

In [9]:
```
shp = X_std.shape

cov_mat = (1/(shp[0]-1)) * (X_std.T.dot(X_std))
```

In [10]:
```
# `Covariance Matrix`: Test cell (1 point)
import math
sum_tol = 1e-4

print('Covariance matrix \n%s' %cov_mat)
print(cov_mat.shape)
print()

# Check it
assert cov_mat.shape==(2037,2037), "Expected 2037 rows and 2037 columns."

sum_cov_mat = sorted(cov_mat.sum(axis=1))

# Compare your solution with teacher's solution
print("=== First 2 elements and Last 2 elements of your solution ===")
print(sum_cov_mat[:2])
print(sum_cov_mat[2035:])

# Check it
sum_tests = [(0,-231.7563891769041),(1,-230.18940653827477),
             (2035,367.64881498520253),(2036,382.36014302238704)]

print ("=== First 2 elements and Last 2 elements of instructor's solution ===")
result_array = np.array([sum_tests[0][1],sum_tests[1][1],
                         sum_tests[2][1],sum_tests[3][1]])
print(result_array[:2])
print(result_array[2:])

# Test elements close
for i,j in sum_tests:
    assert math.isclose(sum_cov_mat[i],j,abs_tol=sum_tol), ("Row "+str(i)+" should sum to "+str(j)+"
but yours had "+str(sum_cov_mat[i]))
```

```
print ("\n(Passed.)")
```

```
Covariance matrix
0                AB000115_at  AB000460_at  AB000464_at  AB000466_at  \
0
AB000115_at         1.000000     0.180767     0.111231     0.091335
AB000460_at         0.180767     1.000000     0.512389    -0.479128
AB000464_at         0.111231     0.512389     1.000000    -0.357822
AB000466_at         0.091335    -0.479128    -0.357822     1.000000
AB000467_at         0.000147    -0.410275    -0.283896     0.533504
AB000584_at        -0.079254    -0.208673    -0.224306    -0.202898
AC000099_at         0.016718     0.347152     0.177972    -0.303668
AC002045_xpt1_at    0.255875     0.436467     0.237483    -0.146870
AF000177_at         0.047427     0.304363     0.131856     0.075939
AF000234_at        -0.339367     0.065910     0.011985     0.233296
AF000430_at        -0.012278     0.161882     0.042581    -0.119979
AF000560_at         0.027021     0.341690     0.247177    -0.115441
AF000562_at         0.288256     0.487626     0.321538    -0.493626
AF000959_at         0.058534    -0.347406    -0.320606     0.466966
AF001294_at        -0.116184    -0.050234    -0.048478    -0.130137
AF001620_at        -0.124428    -0.214841    -0.176513    -0.001045
AF002020_at         0.090252     0.317229     0.106549    -0.191656
AF002224_at        -0.102310     0.422236     0.261937    -0.293676
AF002700_at         0.068435     0.472464     0.539728    -0.592050
AF003743_at        -0.234240     0.068718     0.041461    -0.361446
AF005037_at         0.276962     0.044093    -0.028171     0.256450
AF005043_at         0.131553     0.109544     0.124150     0.006056
AF005361_at         0.087775     0.153851     0.083158    -0.194027
AF005775_at        -0.084434     0.264045     0.346285    -0.353295
AF005887_at         0.226263     0.151574     0.204022    -0.009392
AF006041_at         0.172067     0.388712     0.418025    -0.162292
AF006084_at         0.059930     0.202888     0.142273    -0.200733
AF006087_at         0.178393     0.330466     0.430780    -0.143523
AF006609_at         0.123226    -0.357986    -0.174061     0.460452
AF007111_at         0.174211     0.163708     0.285266    -0.138748
...                      ...          ...          ...          ...
U04241_at           0.145404     0.303664     0.403816    -0.165051
U14187_at          -0.074435     0.487993     0.426257    -0.672411
U20499_at           0.013383     0.429833     0.237794    -0.158122
U35234_at          -0.060829     0.312536     0.292640    -0.337102
U46744_at          -0.041710    -0.457347    -0.197677     0.429441
U47677_at          -0.020497     0.485124     0.394479    -0.518565
U69611_at           0.116621     0.271357     0.271888    -0.010669
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K03204_f_at         0.047370    -0.441841    -0.427227     0.489253
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X99479_f_at         0.063834     0.269551     0.266692    -0.389960
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U87593_f_at         0.230136     0.025104     0.000081     0.178791
L34355_at           0.062910     0.058895    -0.103606    -0.104108
U48730_at           0.186339     0.159613     0.413335    -0.055533
U58516_at          -0.061551     0.441568     0.355457    -0.381255
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AF000234_at         -0.050811   -0.486124   -0.047808        -0.009267
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U04241_at            0.054412    0.053868    0.001732         0.273614
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U20499_at           -0.138096   -0.161266    0.054543         0.162354
U35234_at           -0.194056    0.133888    0.015216         0.073379
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U88898_r_at         -0.354575    0.106247    0.303299         0.096859
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D38498_f_at         -0.113185    0.066923   -0.032903         0.258378
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K03204_f_at          0.434450    0.124324   -0.309602        -0.270781
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S80905_f_at         -0.276682   -0.208359    0.212108         0.013320
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AB000464_at          0.131856     0.011985     ...          0.308143
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Z34822_f_at          0.291114   0.147831   ...       -0.229147
U87593_f_at         -0.085535  -0.002988   ...       -0.188742
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U48730_at            0.067306  -0.242572   ...       -0.023951
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Z78285_f_at         -0.070139   0.033015   ...        0.017629

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J00117_f_at	-0.156413	-0.266168	0.290394	0.212558
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K03189_f_at        -0.141586  -0.020606   0.301248   0.094669     0.059546
K03204_f_at        -0.096267  -0.180471  -0.296111   0.227487     0.094564
M20030_f_at        -0.267072  -0.126752  -0.054092  -0.012353    -0.226822
M92269_f_at        -0.182671  -0.009035  -0.268524   0.147802    -0.112382
U65918_f_at        -0.055300   0.003557  -0.062591  -0.134542     0.030761
L41268_f_at         0.216760  -0.023951   0.552196   0.084410     0.017629
X99479_f_at         0.134943  -0.036218   0.140160  -0.008581    -0.078793
S80905_f_at         0.270038   0.057961   0.357574  -0.104453     0.050260
Z34822_f_at        -0.049727   0.046102  -0.182314   0.054876     0.112440
U87593_f_at         0.213200   0.226185  -0.072885  -0.070572    -0.118157
L34355_at           1.000000   0.034759   0.198122  -0.237092     0.129265
U48730_at           0.034759   1.000000   0.146673   0.005488     0.027303
U58516_at           0.198122   0.146673   1.000000   0.135409     0.179205
U73738_at          -0.237092   0.005488   0.135409   1.000000     0.245856
Z78285_f_at         0.129265   0.027303   0.179205   0.245856     1.000000

[2037 rows x 2037 columns]
(2037, 2037)

=== First 2 elements and Last 2 elements of your solution ===
[-231.7563891769041, -230.18940653827477]
[367.64881498520253, 382.36014302238704]
=== First 2 elements and Last 2 elements of instructor's solution ===
[-231.75638918 -230.18940654]
[367.64881499 382.36014302]

(Passed.)
```

Exercise 3 (`Eigendecomposition on the covariance matrix`: 1 point)

Eigenvectors and eigenvalues are numbers and vectors associated to square matrices, and together they provide the eigendecomposition of a matrix which analyzes the structure of this matrix. Even though the eigendecomposition does not exist for all square matrices, it has a particularly simple expression for a class of matrices often used in multivariate analysis such as correlation, covariance, or cross-product matrices. The eigendecomposition of this type of matrices is important in statistics because it is used to find the maximum (or minimum) of functions involving these matrices. For example, principal component analysis is obtained from the eigen-decomposition of a covariance matrix and gives the least square estimate of the original data matrix.

Calculate `eig_vals` (eigenvalues) and `eig_vecs` (eigenvectors) for `cov_mat` (the covariance matrix).

> Hint: Because this is a symmetrical array, we need to use https://docs.scipy.org/doc/numpy-1.15.0/reference/generated/numpy.linalg.eigh.html (https://docs.scipy.org/doc/numpy-1.15.0/reference/generated/numpy.linalg.eigh.html) for real numbers rather than np.linalg.eig (which may find solutions using complex numbers).

In [11]:
```python
eig_vals, eig_vecs = np.linalg.eigh(cov_mat)
```

In [12]:
```python
# `Eigendecomposition`: Test cell (1 point)
import math
sum_tol = 1e-4

print('Eigenvectors \n%s' %eig_vecs)
print(eig_vecs.shape)
print('\nEigenvalues \n%s' %eig_vals)
print(eig_vals.shape)
print()

# Check it
assert eig_vecs.shape==(2037,2037), "eig_vecs: Expected 2037 rows and 2037 columns."
assert eig_vals.shape==(2037,), "eig_vals: Expected 2037 values."
```

```
sum_evec = sorted(eig_vecs.sum(axis=1))
sum_eval = sorted(eig_vals)

print("=== Sum of largest 4 elements of your eig_vals solution ===")
print("Sum:",sum_eval[-4:]," = ",sum(sum_eval[-4:]))
print("=== Sum of largest 4 elements of instructor's eig_vals solution ===")
print("Sum: [79.29171678892715, 88.80223529674713, 206.78777407920407, 309.13985245025475]  =  684.0
215786151332")

assert math.isclose(sum(sum_eval[-4:]),684.0215786151332,abs_tol=sum_tol), ("Your sum is "+str(sum(s
um_eval[-4:]))+" but should be ~"+str(684.0215786151332))

print ("\n(Passed.)")
```

```
Eigenvectors
[[ 0.00000000e+00  0.00000000e+00  0.00000000e+00 ... -3.89372903e-03
   2.16511781e-02 -9.40331438e-03]
 [ 4.14564304e-01 -4.51291745e-01 -7.76758784e-02 ...  1.80149457e-02
   6.99866944e-03 -4.60275107e-02]
 [ 6.39314831e-01  3.06520336e-02 -1.56907802e-01 ... -6.01557472e-03
  -2.26319433e-04 -3.74154131e-02]
 ...
 [ 2.56915799e-02  1.99882009e-03 -7.62556039e-03 ... -2.22951710e-03
   3.08951885e-03 -3.37014924e-02]
 [ 3.11888921e-03  7.24722671e-03  2.18952398e-02 ... -2.75004907e-02
   1.14262773e-02  4.69653264e-03]
 [ 7.70675950e-03  4.88618868e-03  9.53699458e-03 ... -1.83383834e-02
  -7.82591261e-04  5.03114201e-04]]
(2037, 2037)

Eigenvalues
[-8.36950640e-14 -5.16462854e-14 -3.12658162e-14 ...  8.88022353e+01
  2.06787774e+02  3.09139852e+02]
(2037,)

=== Sum of largest 4 elements of your eig_vals solution ===
Sum: [79.29171678892715, 88.80223529674716, 206.78777407920393, 309.1398524502548]  =  684.021578615
133
=== Sum of largest 4 elements of instructor's eig_vals solution ===
Sum: [79.29171678892715, 88.80223529674713, 206.78777407920407, 309.13985245025475]  =  684.02157861
51332

(Passed.)
```

3 - Selecting Principal Components

The typical goal of a PCA is to reduce the dimensionality of the original feature space by projecting it onto a smaller subspace, where the eigenvectors will form the axes. However, the eigenvectors only define the directions of the new axis, since they have all the same unit length 1, which can confirmed by the following two lines of code:

In [13]:
```
# Just execute this code
for ev in eig_vecs:
    np.testing.assert_array_almost_equal(1.0, np.linalg.norm(ev))
print('Everything ok!')
```

```
Everything ok!
```

In order to decide which eigenvector(s) can be dropped without losing too much information for the construction of lower-dimensional subspace, we need to inspect the corresponding eigenvalues. The eigenvectors with the lowest eigenvalues explain the least variance about the distribution of the data; those are the ones can be dropped.

In order to do so, the common approach is to rank the eigenvalues from highest to lowest and to choose the top k eigenvectors.

In [14]:
```
# Just execute this code

# Make a list of (eigenvalue, eigenvector) tuples
eig_pairs = [(np.abs(eig_vals[i]), eig_vecs[:,i]) for i in range(len(eig_vals))]

# Sort the (eigenvalue, eigenvector) tuples from high to low
from operator import itemgetter
eig_pairs.sort(key=itemgetter(0))
eig_pairs.reverse()
```

```python
# Visually confirm that the list is correctly sorted by decreasing eigenvalues
print('Eigenvalues in descending order:')
for i in eig_pairs:
    print(i[0],i[1][:3],"...")
```

```
Eigenvalues in descending order:
309.1398524502548 [-0.00940331 -0.04602751 -0.03741541] ...
206.78777407920393 [ 0.02165118  0.00699867 -0.00022632] ...
88.80223529674716 [-0.00389373  0.01801495 -0.00601557] ...
79.29171678892715 [ 0.00413807  0.00536075 -0.02178184] ...
72.32038783424807 [-0.01130794 -0.00758037  0.01329661] ...
64.98589767573822 [ 0.04330808  0.00695083 -0.00510095] ...
53.27510403805331 [-0.00461638 -0.00421056  0.02328184] ...
47.03826295799616 [ 0.01509312  0.00643272 -0.00835753] ...
46.68386257221233 [-0.0395275  -0.00094225  0.00677754] ...
43.19746764171434 [ 0.00121415 -0.00550408 -0.00810675] ...
38.018674199339294 [-1.44967951e-02 -1.38311689e-02  7.53299615e-05] ...
37.40044831341172 [ 0.05326305 -0.00392827  0.01227851] ...
32.227225531018576 [-0.02891464  0.03273987 -0.01618008] ...
31.69484347185741 [0.01295107 0.0121705  0.00785119] ...
30.54480538036044 [-0.02785237 -0.0101514  -0.02938086] ...
28.74419035074769 [0.03581549 0.00310617 0.0072434 ] ...
28.229322679244397 [ 0.011019   -0.00194013  0.02689362] ...
27.055066867125568 [ 0.00268174 -0.00405748 -0.02443632] ...
26.794336802143683 [-0.04454361 -0.00470399  0.01307476] ...
24.826092697998774 [ 0.03157332 -0.0102343  -0.0125896 ] ...
24.38972239940303 [-0.0234215   0.00877492 -0.02896011] ...
23.282471505247702 [ 0.00259238 -0.00699433 -0.03063196] ...
22.431396867171447 [-0.01435207 -0.01799972  0.00013352] ...
21.91411267358193 [ 0.00784165 -0.01947797  0.03109255] ...
21.579886767337275 [-0.02061956 -0.00498461  0.02236555] ...
20.271989660677466 [ 0.01422608 -0.00313653  0.01556449] ...
20.112091113402712 [-0.03349987 -0.02553559 -0.00787266] ...
19.91823701435004 [0.00406091 0.03800974 0.00788857] ...
19.282258383699574 [-0.00654357  0.00644978  0.02995043] ...
18.729301677535826 [ 0.01204211  0.02466533 -0.03265038] ...
18.53739894277718 [-0.03818033  0.01951485  0.00484068] ...
17.941090535405532 [0.0180284  0.00603258 0.0155944 ] ...
17.693924877869968 [-0.00878146 -0.03233239 -0.02372184] ...
17.40177518394987 [ 0.01730679 -0.00641119 -0.02640065] ...
16.776290544857705 [-0.00058842 -0.0274371  -0.00144992] ...
16.641014204822827 [-0.02086838 -0.01072554 -0.00932384] ...
16.363759760570552 [0.01432505 0.00981731 0.03209059] ...
16.219756015604926 [-0.00844485  0.00846905  0.0170797 ] ...
15.288868544044146 [-0.03596865 -0.00130367  0.00861582] ...
15.171112322434007 [ 0.02944072  0.01801711 -0.03480339] ...
14.77319652201963 [-0.01239264  0.01017732  0.002319  ] ...
14.605412541859787 [0.00365589 0.01690664 0.00376159] ...
14.425079695825524 [ 0.00080557 -0.01482641 -0.03322735] ...
13.96021015206042 [ 0.03548255 -0.01939997 -0.00481506] ...
13.712008229070065 [-0.01615139  0.0199413  -0.00049292] ...
13.477615324285528 [-0.03082974  0.01989446  0.00779503] ...
13.351215043400755 [ 0.05099679 -0.02058693  0.01824376] ...
12.977653373537438 [-0.01740989 -0.03009461 -0.00973062] ...
12.653008959167984 [0.02361471 0.00622066 0.0146297 ] ...
12.52980027533535 [ 0.0110303  -0.02065669 -0.07108731] ...
12.345651778502027 [ 0.02261959 -0.01403367  0.01962421] ...
12.175701110811112 [-0.03283627  0.01332145 -0.00807284] ...
12.023270040645132 [-0.00140567 -0.01394994  0.00977486] ...
11.780817624316349 [0.00738004 0.00380559 0.00134318] ...
11.301824564921416 [ 0.03003231 -0.01441418  0.00096987] ...
11.138273370240489 [-0.00656066  0.00447325  0.01086849] ...
10.893288390829806 [ 0.05199464 -0.00484624  0.01509186] ...
10.595420389030975 [-0.01834748  0.00928046 -0.05232662] ...
10.340758170245582 [-0.00451353  0.00010954  0.04362273] ...
9.91316845879726 [ 0.00306159  0.00688152 -0.0115128 ] ...
9.798660076693372 [-0.02788893  0.02508534  0.00374153] ...
9.325084385288248 [ 0.04060005  0.00552453 -0.0079482 ] ...
9.198100449770873 [-0.02147463 -0.00699834  0.01647814] ...
9.094162056045157 [ 0.02813947  0.0370849  -0.04977496] ...
8.666774450563738 [-0.04148095 -0.058375   -0.01982537] ...
8.015878619866879 [ 0.01723951 -0.02083772 -0.03393754] ...
7.8578714564407095 [-0.01715558  0.00032114  0.01204905] ...
```

```
7.544644146180695 [ 0.05423668  0.00059419 -0.0094683 ] ...
7.4270500107867115 [-0.00821358 -0.02046449 -0.00993851] ...
7.358424843618922 [0.00981052 0.00193035 0.03025039] ...
6.7359488667554475 [-0.00122949 -0.00802203  0.00395823] ...
8.692070152852271e-14 [-5.40708492e-06  4.65230938e-01 -6.00737466e-01] ...
8.369506396309864e-14 [0.         0.4145643  0.63931483] ...
5.270801485529291e-14 [ 0.         -0.35464099  0.00996109] ...
5.164628538253764e-14 [ 0.         -0.45129175  0.03065203] ...
3.324090674113694e-14 [ 0.         -0.0237716  -0.06242898] ...
3.1265816212502105e-14 [ 0.         -0.07767588 -0.1569078 ] ...
2.766743806983917e-14 [ 0.         -0.03424749  0.051927  ] ...
2.6020759039280917e-14 [ 0.         -0.09175257 -0.09819577] ...
2.4283609169651636e-14 [ 0.         -0.10390888 -0.06780208] ...
2.1903713832706735e-14 [0.         0.03720737 0.04063815] ...
2.184892367182356e-14 [ 0.         -0.13410382  0.09912459] ...
2.0879707331291238e-14 [0.         0.03569061 0.04118694] ...
2.0664210428685283e-14 [ 0.         -0.05051354 -0.02082876] ...
1.9876133817859667e-14 [ 0.         -0.05224299 -0.02229772] ...
1.9080549482733654e-14 [ 0.          0.10725688 -0.03358487] ...
1.855482338900306e-14 [ 0.          0.02579382 -0.0187158 ] ...
1.7167499399238497e-14 [0.         0.02932689 0.04133634] ...
1.611563792243987e-14 [0.         0.11367815 0.06226649] ...
1.5903021569899298e-14 [ 0.         -0.01254775  0.02830642] ...
1.5807353015068664e-14 [ 0.         -0.03399416 -0.0036632 ] ...
1.558066806905968e-14 [ 0.          0.06892514 -0.03025418] ...
1.5371013155519925e-14 [ 0.          0.00453673 -0.01670066] ...
1.4663217997845206e-14 [ 0.          0.02204091 -0.01232007] ...
1.41940792459975e-14 [ 0.          0.00213997 -0.00425087] ...
1.3846131353426815e-14 [ 0.         -0.03460572  0.05777932] ...
1.3842835148177001e-14 [0.         0.00098312 0.03621674] ...
1.374975484633392e-14 [ 0.          0.00095994 -0.02137062] ...
1.3743927932942563e-14 [0.         0.31097017 0.18607179] ...
1.3661252342367983e-14 [ 0.         -0.03102429 -0.00184548] ...
1.276483906578506e-14 [ 0.         -0.00882455  0.02017075] ...
1.2741512788543458e-14 [0.         0.00903233 0.00895457] ...
1.2705989161654052e-14 [ 0.         -0.00412965 -0.00703494] ...
1.2664555351889873e-14 [ 0.          0.00674353 -0.00303412] ...
1.2396551147167308e-14 [0.         0.04234905 0.04551033] ...
1.1843920695064647e-14 [ 0.         -0.00334078 -0.0072295 ] ...
1.1659495478461996e-14 [ 0.         -0.04049377 -0.05408645] ...
1.1519511332444357e-14 [0.         0.00498116 0.00782506] ...
1.141313084246064e-14 [ 0.         -0.02244564  0.02055653] ...
1.1404553136059232e-14 [ 0.         -0.01072925 -0.01227889] ...
1.1048916578141162e-14 [ 0.          0.03569848 -0.01278483] ...
1.0991690195188579e-14 [0.00000000e+00 6.46295290e-05 1.08417016e-02] ...
1.0927506640998616e-14 [0.         0.00517669 0.00741679] ...
1.075976959087093e-14 [ 0.          0.01687609 -0.00433591] ...
1.0584411282572843e-14 [0.         0.00136404 0.01209929] ...
1.0173051426818283e-14 [ 0.         -0.00621509 -0.00609918] ...
1.0152566178855088e-14 [-1.34856609e-18 -2.12716457e-01  2.59838209e-01] ...
1.0016457858980137e-14 [ 0.         -0.00257865 -0.00112228] ...
9.914770885227183e-15 [ 0.          0.00814212 -0.00364771] ...
9.91016311588123e-15 [ 0.         -0.00268352  0.00655478] ...
9.901295658200829e-15 [ 0.         -0.01014073 -0.00925011] ...
9.586073706496421e-15 [ 0.         -0.01348035  0.0073079 ] ...
9.562378677827477e-15 [ 0.         -0.00935109 -0.00608779] ...
9.349571447400818e-15 [ 0.         -0.0451751  -0.01730456] ...
9.323798039361429e-15 [ 0.         -0.00954994 -0.00683433] ...
9.310445486866869e-15 [ 0.          0.00240979 -0.00724813] ...
9.122838449922559e-15 [ 0.          0.00485976 -0.01130345] ...
9.034473843872724e-15 [ 0.          0.01301999 -0.00356097] ...
8.849698923616049e-15 [0.         0.0162611  0.00993388] ...
8.783023795680838e-15 [ 0.         -0.0165565   0.01071599] ...
8.629291406711141e-15 [ 0.         -0.00451166  0.00152223] ...
8.499732614384957e-15 [0.         0.00111535 0.00213328] ...
8.330383051687717e-15 [ 0.         -0.01300431  0.00452114] ...
8.155798141365082e-15 [ 0.         -0.00392925 -0.01646509] ...
8.155602517676418e-15 [ 0.         -0.00091967 -0.01195739] ...
8.142960865074877e-15 [ 0.         -0.00270922  0.00224228] ...
8.134937316576827e-15 [ 0.         -0.00076602  0.00279021] ...
8.06658523204094e-15 [ 0.         -0.00824571  0.00715385] ...
8.040775237621143e-15 [ 0.         -0.00361048 -0.00143462] ...
7.995212272000537e-15 [ 0.         -0.00495092  0.01495272] ...
7.978664594256719e-15 [ 0.         -0.00929958  0.00327723] ...
7.81819002145393e-15 [ 0.         -0.00210879 -0.00424495]
```

```
7.818190021455595e-15 [ 0.          0.00210879  0.00424495] ...
7.798524962409226e-15 [ 0.         -0.00319044 -0.00756253] ...
7.749373684048583e-15 [0.         0.02716624 0.02392072] ...
7.736055941692227e-15 [ 0.          0.00832445 -0.00832296] ...
7.708277436619962e-15 [ 0.         -0.0041065   0.00163806] ...
7.674665024957604e-15 [ 0.         -0.00094179  0.00046423] ...
7.652880435490656e-15 [ 0.          0.00670326 -0.0026089 ] ...
7.57098161108492e-15 [ 0.         -0.00342689  0.0063886 ] ...
7.549531871160163e-15 [ 0.         -0.00049196 -0.00313359] ...
7.536427330643245e-15 [ 0.          0.00088446 -0.00221026] ...
7.471339866825151e-15 [ 0.         -0.00799134 -0.00300921] ...
7.455225411677183e-15 [ 0.         -0.00291458 -0.00389054] ...
7.451642499421915e-15 [ 0.         -0.02088238 -0.00391026] ...
7.374727769915024e-15 [ 0.          0.00460948 -0.00459834] ...
7.36793751740666e-15 [0.         0.0114488  0.00649757] ...
7.344137128911574e-15 [ 0.          0.00582617 -0.00369472] ...
7.284581483141254e-15 [ 0.          0.00166501 -0.00144252] ...
7.282604273781125e-15 [0.         0.01348545 0.00040316] ...
7.278713662247332e-15 [ 0.         -0.00114192  0.00309725] ...
7.232297570156531e-15 [ 0.         -0.00523894 -0.00085161] ...
7.231433637029461e-15 [ 0.         -0.00375053  0.00093923] ...
7.185079001212406e-15 [ 0.         -0.00755208  0.01055926] ...
7.169329913152956e-15 [ 0.         -0.00063922  0.00260232] ...
7.154389608311672e-15 [ 0.          0.00901587 -0.00171661] ...
7.131258684508638e-15 [ 0.         -0.00242225 -0.00437655] ...
7.0923423836691995e-15 [ 0.         -0.00187537 -0.00080297] ...
7.087587391711087e-15 [ 0.         -0.00188926 -0.0027635 ] ...
7.052304243419272e-15 [0.         0.00265075 0.00618546] ...
6.990600330276112e-15 [0.         0.00054786 0.00192831] ...
6.9614809944231915e-15 [ 0.         -0.00728948  0.00023687] ...
6.946376681480763e-15 [ 0.         -0.00166298 -0.00053959] ...
6.93289821243116e-15 [0.         0.00406794 0.00271378] ...
6.9165454116601775e-15 [ 0.          0.00309156 -0.00292211] ...
6.907587051473671e-15 [ 0.         -0.0023046  -0.00015016] ...
6.898105741416708e-15 [ 0.00000000e+00  5.38927517e-05 -3.80763475e-04] ...
6.89096198072962e-15 [ 0.          0.00359968 -0.00270596] ...
6.883489137610051e-15 [ 0.         -0.00071326 -0.00158131] ...
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4.300939843798679e-17 [ 0.          -0.00387776  0.00190484] ...
4.1016653727401283e-17 [ 0.           0.00265089 -0.00092477] ...
4.099568527894899e-17 [ 0.          -0.00342318 -0.00045437] ...
4.084719038335027e-17 [0.         0.00284014 0.00098929] ...
4.0382187404914826e-17 [ 0.           0.00297174 -0.00248909] ...
4.0198474301142777e-17 [ 0.          -0.00049013 -0.00173407] ...
3.9663246093114863e-17 [ 0.           0.00284854 -0.00163418] ...
3.8359391751866616e-17 [ 0.          -0.00450429  0.00104076] ...
3.760602107738797e-17 [ 0.           0.00048247 -0.00035722] ...
3.754149797980946e-17 [ 0.          -0.00417738  0.00439573] ...
3.704011102580294e-17 [0.         0.00370597 0.0017926 ] ...
3.6968553119983043e-17 [0.         0.00254732 0.00023903] ...
3.578091684875791e-17 [ 0.00000000e+00 -8.92889797e-05 -1.45773352e-03] ...
3.5675259448267544e-17 [ 0.          -0.00047308 -0.00196858] ...
3.5219305251689693e-17 [ 0.          -0.00278034 -0.00254799] ...
3.497525969271446e-17 [ 0.          -0.00016718 -0.00140228] ...
3.4531464494588033e-17 [0.         0.00132638 0.00098446] ...
3.425319645756201e-17 [ 0.          -0.0022223   0.00053063] ...
3.36883970463678e-17 [ 0.          0.00095573 -0.00039087] ...
3.288655589605923e-17 [ 0.          -0.0012254   0.00069656] ...
3.273595366542285e-17 [ 0.          -0.00527439  0.00172599] ...
3.185082719555059e-17 [ 0.          -0.00200899  0.00171731] ...
3.1639362944317165e-17 [ 0.           0.00151302 -0.0016734 ] ...
3.158185861052894e-17 [0.         0.00222465 0.00302913] ...
3.1181553778006947e-17 [ 0.          -0.00253874 -0.00253984] ...
3.097345694084463e-17 [ 0.           0.00056269 -0.00096003] ...
3.033789672010677e-17 [ 0.          -0.00198265 -0.00145447] ...
2.885845741575808e-17 [ 0.           0.00073068 -0.00310999] ...
2.872798875616874e-17 [ 0.           0.0008944  -0.00102645] ...
2.863473721222028e-17 [ 0.          -0.0004976  -0.00196811] ...
2.7576298535530873e-17 [ 0.          -0.00147103  0.00129005] ...
2.7450245769410646e-17 [ 0.          -0.00244557 -0.00241237] ...
2.71969955455047e-17 [ 0.          -0.00027953  0.00264736] ...
2.6759980958542855e-17 [ 0.00000000e+00 -2.49403204e-03  1.93231424e-05] ...
2.6264255530860755e-17 [0.         0.00017765 0.00191913] ...
2.5576917353115617e-17 [ 0.          -0.00114057 -0.00023962] ...
2.55441745436393e-17 [ 0.          -0.00039829  0.00080525] ...
2.5233467887207427e-17 [ 0.          -0.00222584 -0.00015967] ...
```

```
2.4645310156538003e-17 [0.00000000e+00 2.92755071e-03 4.16529112e-05] ...
2.324878308241479e-17 [ 0.00000000e+00 -8.11383033e-05  1.10597965e-03] ...
2.291261387190945e-17 [ 0.          0.00013681 -0.00145267] ...
2.2905001481430157e-17 [ 0.          -0.00150167  0.00086273] ...
2.174461640808453e-17 [ 0.         -0.00319048 -0.00113715] ...
2.1644576228476603e-17 [ 0.          0.0025789 -0.0040433] ...
2.1508861262971196e-17 [ 0.          -0.00094432  0.00098968] ...
2.0894060067220744e-17 [ 0.           0.0024071  -0.00062068] ...
2.0743091974760518e-17 [0.         0.00217766 0.00114748] ...
2.0741920156623157e-17 [ 0.          -0.00102161 -0.00226106] ...
1.7977160593587933e-17 [ 0.          -0.00249341 -0.00094637] ...
1.782077790113499e-17 [ 0.          0.0001123  -0.00199794] ...
1.663111330211248e-17 [0.         0.00128047 0.00143009] ...
1.4782805348847016e-17 [ 0.          -0.00161951 -0.00172602] ...
1.3399946506390561e-17 [ 0.          -0.00140043 -0.00096001] ...
1.3285438313751181e-17 [ 0.          -0.00080126 -0.00188925] ...
1.2170552156017458e-17 [ 0.          -0.00102877  0.00165056] ...
1.2129984553888638e-17 [ 0.          -0.00071572  0.00102183] ...
1.2060223881292059e-17 [ 0.          -0.00274578  0.00280552] ...
1.1087837391795143e-17 [ 0.00000000e+00 -3.57434264e-05 -2.81760914e-04] ...
1.0491542074368344e-17 [ 0.          -0.00221421  0.00336969] ...
9.284375022333829e-18 [0.         0.00069773 0.00358426] ...
9.054798469724684e-18 [ 0.         -0.001526   -0.00018068] ...
8.328088897073241e-18 [ 0.         -0.00422196 -0.00020201] ...
7.324026871069282e-18 [0.         0.00106897 0.00116971] ...
6.073734914936397e-18 [ 0.         -0.00233112 -0.00207291] ...
5.8478126814878635e-18 [ 0.          -0.00163739 -0.00154904] ...
5.776645438360462e-18 [ 0.          0.00453295 -0.00189378] ...
5.1587237279686785e-18 [ 0.           0.0008643  -0.00028181] ...
4.4685093658288375e-18 [ 0.          -0.00031268  0.00081986] ...
4.302423926151831e-18 [ 0.         -0.00182534 -0.00194801] ...
4.276162750073896e-18 [ 0.          0.00069708 -0.00112924] ...
4.259538440746396e-18 [ 0.          0.00611227 -0.00117964] ...
4.207706743132084e-18 [ 0.         -0.00016824 -0.00046177] ...
3.3240447986289017e-18 [ 0.           0.00172092 -0.00056916] ...
1.983327243389598e-18 [0.         0.00091581 0.00210229] ...
1.129406547373301e-18 [0.         0.00066236 0.0021643 ] ...
2.4836004888526862e-19 [ 0.           0.00333417 -0.0023029 ] ...
```

Exercise 4 (`Compute dimensionality reduction`: 2 points)

After sorting the eigenpairs, the next question is "how many principal components should we choose for our new feature subspace?" A useful measure is the so-called "explained variance," which can be calculated from the eigenvalues. The explained variance tells us how much information (variance) can be attributed to each of the principal components.

You'll use a **75%** goal for the explained variance to choose the top k components. That is, select the minimum number of the k-largest eigenvalues such that

$$explained\_variance = \sum_{i=0}^{k-1} \left(\frac{eigenvalue_i}{\sum_{j=0}^{N-1} \left(eigenvalue_j \right)} \right) \geq 75\%,$$

where k is the number of the top-k components to choose and the covariance matrix is $N \times N$. Store the value of k in a variable named `k_use` and store the explained variance from the above equation in a variable named `explained_variance`.

> Hint: See [np.cumsum (https://het.as.utexas.edu/HET/Software/Numpy/reference/generated/numpy.cumsum.html)](https://het.as.utexas.edu/HET/Software/Numpy/reference/generated/numpy.cumsum.html) function as used in Notebook 15.

In [16]:
```
eig_total = sum(eig_vals)

explained_variance = 0
k_use = 0

for k, i in enumerate(eig_pairs):
    if explained_variance <= .75:
        ev = i[0] / eig_total
        explained_variance = explained_variance + ev
        k_use = k
```

In [17]:
```
# `select_components`: Test cell (2 points)
```

```
import math
sum_tol = 1e-4

print("Number of Components for",str(100*explained_variance),"% of variance:",k_use)

# Check it
assert k_use==29, ("Your calculated k_use is "+str(k_use)+" but should be 29.")

# Check it
assert math.isclose(explained_variance,0.7505984465835792,abs_tol=sum_tol), ("Your explained varianc
e is "+str(explained_variance)+" but should be ~"+str(0.7505984465835792))

print ("\n(Passed.)")
```

```
Number of Components for 75.0598446583579 % of variance: 29

(Passed.)
```

4 - Construct the projection matrix W from the selected k eigenvectors.

It's about time to get to the really interesting part: The construction of the projection matrix that will be used to transform the gene expression data onto the new feature subspace. The "projection matrix" is nothing more than a matrix whose columns are our top k eigenvectors.

The code cell below computes the $d \times k$ projection matrix W.

In [18]:
```
num_features = X.shape[1]

p = np.array(eig_pairs[0][1].reshape(num_features,1))

for i in range(1,k_use):
    p = np.append(p, eig_pairs[i][1].reshape(num_features,1), 0)

p=p.reshape(num_features,k_use)

matrix_w = np.hstack(np.vsplit(p,1))

print('Matrix W:\n', matrix_w)
print(matrix_w.shape)
```

```
Matrix W:
 [[-0.00940331 -0.04602751 -0.03741541 ... -0.01512247 -0.02157882
   0.02455123]
 [-0.01303358 -0.00035806 -0.00681776 ...  0.00824519 -0.03727329
   0.02460511]
 [-0.0002826  -0.00933614 -0.04544453 ... -0.02125062 -0.01634545
   0.00613641]
 ...
 [ 0.01198928  0.01553509  0.00416808 ... -0.01282362 -0.04878263
  -0.0058803 ]
 [ 0.01483216 -0.00776181 -0.01263376 ... -0.03376636 -0.0237215
  -0.03499303]
 [-0.01606375  0.0044885   0.00433831 ... -0.01457857  0.00349194
  -0.00887598]]
(2037, 29)
```

5 - Projection Onto the New Feature Space

In this last step we will use the 2037Unknown characterUnknown character$k$-dimensional projection matrix W to transform our samples onto the new subspace via the equation

$Y = X$Unknown characterUnknown character$W$, where Y is a 72Unknown characterUnknown character$k$ matrix of our transformed samples.

In [19]:
```
Y_calc = X_std.dot(matrix_w)

print(Y_calc)
print(Y_calc.shape)
```

```
                              0         1         2         3         4  \
Gene Accession Number
1                     -1.004462 -1.957466 -0.337312 -0.493736 -1.007024
```

```
1                      [illegible] [illegible] [illegible] [illegible] [illegible]
2                       1.300662 -0.336089 -0.189284 -0.519404  0.629756
3                       1.597998 -0.631023 -3.327653  0.248270  1.245970
4                       0.559081  0.026557 -2.099599 -0.202852 -0.484994
5                       0.215966  1.302240  0.251360  0.126948 -1.645542
6                      -0.522915  0.156602 -0.348410  0.183875  0.595347
7                       0.264036 -0.347724 -0.461893 -1.185948  0.263115
8                      -1.198207 -0.179004 -2.086847  0.232710  1.697997
9                       1.840883 -0.864249 -1.389545 -0.247218  0.938665
10                     -0.178288  0.077262  0.259325 -0.032251 -1.158089
11                      1.286581  0.931675 -0.134079  0.261472 -0.224650
12                      1.034661 -0.854450  0.697616 -0.473488  0.376891
13                     -0.366239  1.266195  0.986444 -0.258811 -0.891528
14                      0.713104  0.263953  0.273471  0.865154  0.160540
15                      0.583070  1.493531  0.093997  0.369370 -0.928442
16                     -1.552079  0.506524  0.290568 -0.314728  0.108410
17                     -0.129137 -2.000556 -2.666367 -0.369712  2.323272
18                      0.345054  0.798473 -0.131610  0.223827  0.232245
19                     -0.911530  0.509468  0.923029  0.008589 -0.284760
20                      0.424320 -0.422791 -1.425154  1.903535 -2.141096
21                      0.502344  1.775447  2.554967  0.853595  2.507997
22                      0.244316 -0.431205 -0.506282 -0.437036  1.832890
23                     -0.006966 -0.477454 -0.257451  1.589248  0.926328
24                     -1.103131  1.349438 -1.910452  0.459560  0.037373
25                      0.675519 -0.837144 -0.790198 -0.638150  0.542563
26                     -0.034191  0.069387 -0.042949  0.237499 -1.313381
27                      0.236308 -0.506311  1.066103 -0.194358  0.199385
28                      0.597160 -2.340092 -1.571054 -0.449601  0.915946
29                      0.052052  0.693597  1.375229  1.323221 -0.513982
30                      1.475021  0.504420 -0.234184  0.921531  0.044251
...                          ...       ...       ...       ...       ...
43                     -0.104803 -0.530256  0.937554 -0.385225 -0.736914
44                     -1.033092 -0.307790 -0.073320 -0.934457 -2.909691
45                     -1.584777 -0.259580  0.257146 -1.033022 -2.993147
46                     -0.891245  0.208522  0.799434 -0.187411 -1.557005
47                     -1.894539  1.744854  0.050252  0.269730  1.695063
48                      0.110098  1.402479  1.360290 -0.001459 -1.326399
49                      0.158462  1.254418 -0.573560  0.592850  1.159538
50                      0.812179 -0.944945 -0.527570 -0.561262  0.547053
51                      0.290052 -1.027427 -0.811783 -0.997828  0.119855
52                      0.563737  1.225235  1.126321 -2.734590 -0.766335
53                      0.001437  2.098505 -1.244650  1.951634  2.392087
54                      0.734882 -0.650586 -1.524432  0.704767  1.516575
55                      0.129601  0.927557  0.651195 -0.085262  0.074497
56                     -0.685804 -1.153700  0.040549  1.480233  0.864604
57                     -0.715267 -0.163808  0.891033 -0.851402 -0.178139
58                     -0.363461  0.497161  1.166109  0.621242  2.017756
59                     -0.586063  1.132066  2.308568 -1.669201 -2.437639
60                      0.023484 -0.068198  0.771134 -1.246263 -1.336934
61                      0.081620 -1.627392 -0.805539 -0.185495  0.215059
62                      1.105655  1.038919  0.841747 -1.041299 -0.698548
63                     -0.318425 -0.868063  1.036646 -1.629651 -1.127831
64                     -0.281806  2.406220  1.348647  0.859300  2.129943
65                     -0.910617 -0.830603  1.327544 -1.288443  0.059427
66                     -0.433058  1.085297  1.258056 -0.179450 -0.352293
67                      0.392455 -0.517746  1.069716  0.399494  1.448667
68                      0.553454 -0.269186 -0.550122  1.077119 -0.962482
69                     -0.456658  0.515377  1.117230  0.417036 -1.307770
70                     -1.159890  0.825323  0.314105  0.983542  0.377588
71                     -0.033370  0.004776  1.255178  0.028499 -0.461596
72                      0.334265  0.745362 -0.027819  0.036304 -0.029544

                               5         6         7         8         9   \
Gene Accession Number
1                      -0.506043 -0.634038  0.246102 -0.488286  0.051722
2                       0.180967 -0.362605  1.250817  0.784950 -1.193309
3                      -0.587709 -0.032919  0.677621  0.600055 -1.401751
4                       0.695418 -0.746734  0.972923 -0.341210  0.095433
5                      -0.079150 -0.690229 -1.097525  0.312186 -0.777963
6                      -1.153003  0.492845 -0.724996  0.266253 -0.123491
7                      -0.473249  0.703087  0.863287 -0.619431 -0.201561
8                       0.003184 -1.147565  1.081684 -1.400065  1.037792
9                      -0.147761  0.775766  2.790081  1.381426  1.187355
10                     -0.965086  1.185459 -0.050588  0.094789  0.365321
11                     -0.153125 -1.310473  0.442536 -0.850394  0.406587
```

```
12                    -0.510442 -0.566456 -0.070441 -0.757219  0.390715
13                    -0.132545  0.287048 -1.964564 -0.143967 -0.144127
14                     0.641782  0.338845 -0.170473  0.756540  0.942262
15                     0.478819  1.502539 -1.350608  1.111059 -0.601982
16                     0.459440 -0.769087 -1.353143 -1.751882 -1.084433
17                     2.589493 -1.173996  1.177361  2.081090 -0.005633
18                     0.190358  1.278195 -0.489585  0.169980 -0.931758
19                    -1.075098 -0.711808 -0.626323 -0.196372 -0.991460
20                     0.729387 -0.285667 -0.700527  3.157098  1.344127
21                     0.568495  1.080507  0.307757  0.524616  0.440518
22                    -0.279734 -0.406652 -0.485071  0.004665  0.145759
23                    -1.322985  0.784128 -0.752223 -0.491592 -1.301170
24                     0.353268  1.038841 -0.943078  1.157086 -0.669301
25                     0.880341 -1.145557 -0.241536 -0.667708  0.093181
26                    -0.055981  0.133825 -0.395071 -1.099748 -0.502728
27                     0.268885  0.078534  0.396007  1.170881 -1.136886
28                    -0.213095 -1.195057 -0.073722 -1.664117 -0.745768
29                     0.440125 -0.432312 -0.493440 -0.194189 -1.330185
30                     0.323992  0.048246  1.699609  1.759009 -0.079954
...                         ...       ...       ...       ...       ...
43                    -0.203527 -0.375941 -1.066247 -0.758347  1.283236
44                    -1.428425  0.311097  0.319647 -1.036829  0.092546
45                    -0.279056 -0.187656  0.488393 -0.184301 -0.350646
46                    -0.575836  0.594869 -0.918057 -0.723967  0.260617
47                     0.269517  0.761875 -1.896538 -0.258090  0.380593
48                    -0.317005 -1.583361 -0.431708  0.542669  0.839801
49                     1.495770 -0.795905  0.066432  0.758664 -0.859441
50                    -0.152356  1.001487 -0.812937  0.613037  0.202821
51                    -0.874759 -1.912687 -0.436837  0.682097 -0.696255
52                    -1.157940  0.283197  0.471966  0.223708  0.014623
53                     1.129301  0.191226 -0.096079 -0.485229  0.529735
54                    -0.577529  0.768355 -0.686315  0.854073 -1.012326
55                     0.771874  1.590315 -0.983700  0.699318 -0.640991
56                     1.005190  0.039562 -0.025501 -2.164161  0.670443
57                    -1.407602  0.562127  0.365160 -0.076976  0.265650
58                    -1.013699  0.608343  2.163738  0.616869  1.228200
59                    -2.390353  0.340920 -0.570566 -0.388661  0.224969
60                    -0.271028  0.679134  0.865913 -0.420736 -0.583735
61                    -0.311714  0.377871 -0.326508 -1.012640 -0.503011
62                     0.276457  0.236079  0.456192  0.617647  0.453623
63                     0.794844 -0.445411  0.621734  0.406362  0.518852
64                    -0.682309 -0.537390  2.492889  0.297244  2.420932
65                    -0.440645  0.472441 -0.167876 -0.257186 -0.451325
66                    -0.667082  0.115806 -0.795022  0.203295 -0.989058
67                    -0.070054 -0.334556  0.126392  0.160071  0.792167
68                     1.031708  0.356890 -0.679089  0.953188  0.153103
69                     0.885325 -1.000835 -1.103862  0.736470  1.482496
70                    -1.480572  0.773331 -0.919135 -0.235350 -0.390693
71                     0.817978  0.617932 -1.111881 -0.197007  0.259462
72                     0.228593  0.512057 -0.486299 -0.648940  0.951069

                        ...        19        20        21        22  \
Gene Accession Number   ...
1                       ...  1.271867  0.892972  0.738229  0.201555
2                       ...  0.527481 -0.279214  0.180374 -1.270660
3                       ...  1.034717  1.053575  0.713612  0.407903
4                       ...  1.688559  1.806838  0.249254 -0.969826
5                       ...  0.822556  0.821910 -0.471095  0.252530
6                       ...  0.357286  0.496512  2.321672 -0.559146
7                       ...  0.474549  2.040679  1.008387  0.397754
8                       ... -0.170008 -1.392150  0.116634 -1.224606
9                       ...  0.867626  0.249075  2.974708  0.377823
10                      ...  1.370415 -0.719725  0.344096  0.062723
11                      ...  1.034671  0.028274  1.887052 -0.948475
12                      ... -0.023697  0.653513  0.078475  0.063964
13                      ...  0.048212 -0.471050 -0.631795  0.017215
14                      ... -1.348787  0.813835  0.304115 -1.225851
15                      ...  0.577744  0.874646  0.054649 -0.815735
16                      ... -1.075961  1.081794 -0.676304  0.045587
17                      ... -0.346756 -0.668879 -0.297889 -0.441347
18                      ... -0.278001  0.170998 -0.377204  0.095443
19                      ... -1.099127 -0.314497 -0.547775 -0.246879
20                      ... -1.804003 -0.350041 -0.762321 -0.302155
21                      ...  0.096814 -0.490876  1.804397  0.242042
```

```
22                         ...    -0.187522  0.827856 -1.094579 -0.709138
23                         ...    -0.232334 -0.460612  1.039498 -0.094055
24                         ...    -0.992816 -0.848788  0.157519 -0.266168
25                         ...     0.113657 -0.209315 -0.917136  0.218935
26                         ...    -1.439808 -0.436483  0.509001  0.193837
27                         ...     0.981219  1.402751 -0.869820  1.790796
28                         ...     1.573858  0.729207 -0.552584  0.411880
29                         ...    -0.962808 -0.276223 -1.889448 -0.280752
30                         ...     0.841076 -1.173221 -1.242445 -1.390004
...                        ...          ...       ...       ...       ...
43                         ...    -1.321103 -0.586974 -1.983389  0.008859
44                         ...    -1.861941  0.943166 -0.332652  1.071974
45                         ...    -1.013526  1.056117 -1.425942  1.181527
46                         ...    -0.616230  1.136830 -0.224663 -0.325930
47                         ...    -0.067504  1.005388 -0.747037  0.473670
48                         ...     0.995147  0.170717 -1.833882 -0.509445
49                         ...     1.308860  1.738575  1.652159  0.222640
50                         ...     1.163367  0.550345  0.643575 -0.531018
51                         ...    -0.487833 -0.745913  0.330685 -0.992236
52                         ...    -0.966277 -0.291589 -0.132194 -1.046641
53                         ...     1.843232 -1.650656  1.267084  0.368951
54                         ...     0.513697 -0.120476  0.126329  2.227418
55                         ...    -0.069123  0.062984  0.309360  0.289498
56                         ...    -0.523955 -1.122022  0.938412  1.704210
57                         ...     0.116131 -0.690446  0.120828  0.784127
58                         ...    -1.224788 -0.952567  1.220094 -0.084874
59                         ...    -0.254347  0.106430 -0.256548 -0.303441
60                         ...     0.175272 -0.527039 -0.600148  0.295999
61                         ...    -1.018521 -1.844931 -1.047678  1.012592
62                         ...     0.679109  0.114952 -0.922081 -0.543901
63                         ...     1.372621  0.649705  1.563698  1.283995
64                         ...     0.358051 -0.939355 -2.592821  0.068446
65                         ...     0.227948  0.155109  0.766035  1.232681
66                         ...     0.095082  0.492221 -0.403173  0.310951
67                         ...    -0.903206 -0.325050  0.934770 -0.596152
68                         ...     0.145545  1.673773 -0.912730  1.657996
69                         ...     0.549506  1.574230 -0.844054 -0.333110
70                         ...    -0.574588  1.183369  0.558358 -0.539866
71                         ...    -0.869713  0.263565 -0.137930  0.169070
72                         ...    -0.474353 -0.040890 -0.289676 -0.246421

                             23        24        25        26        27  \
Gene Accession Number
1                      1.406962 -0.697746  0.016360  0.117838 -0.985163
2                      1.295463  1.172132  0.371002  0.149475  0.250651
3                      0.436850  1.510640 -1.059470 -1.182527 -0.220100
4                      0.620942 -0.352228 -1.549038 -1.366858  0.904220
5                      0.494216 -1.057692  0.775819 -1.215971  1.053585
6                      0.147943  1.640444 -0.284291  0.722333  0.597153
7                      1.455363  0.506197 -1.201146  1.317928 -0.415517
8                      1.391951 -1.101414  0.986718  0.552963  0.058704
9                     -0.053394  0.458407  0.649265  0.382515 -0.602817
10                    -0.895622  0.148276  0.035384 -0.636566  0.354172
11                     0.179786  0.270348  0.532680  0.073933 -1.650151
12                    -0.826392 -0.264056 -0.290681 -0.184538 -0.915561
13                    -0.325363 -1.034059  0.631924 -0.402141  0.598721
14                     0.555968  1.653543  1.152990  0.305834  1.698203
15                     1.440792 -0.253965  0.995661 -1.953078  0.107930
16                    -0.416916 -1.420200 -0.757583 -0.374193 -0.083847
17                    -1.370442  1.924605  0.742064  1.805865  3.175742
18                    -0.676826 -1.056615 -1.378618 -0.313420  0.124468
19                     1.212184 -0.459535  0.691410 -0.016304 -0.716776
20                     3.192369  0.694001  1.624135  1.483533  2.992505
21                    -0.958800 -3.675036  0.986748 -0.979611  1.512309
22                     0.726710 -0.122885 -0.178975 -0.125602 -2.044247
23                    -1.341102  0.561466 -0.526369 -0.346670 -0.011999
24                     0.107703 -0.321856  0.857858 -0.605456  1.114741
25                     0.562041 -1.397564  0.215081 -0.230993 -0.750609
26                    -0.289996 -1.688999  0.336442  0.146485 -0.042135
27                    -0.598651 -0.460682 -0.746400 -0.990758  1.614676
28                     1.488295  0.353115  0.054469  0.186334  0.177617
29                     0.038672 -1.246138  0.330623 -0.628737 -0.469152
30                     0.479189  0.392818  1.303398 -1.785973  0.214267
...                         ...       ...       ...       ...       ...
```

```
43                  -1.829327  0.236117 -1.028464 -0.719961  1.202055
44                  -1.045521  0.237028 -0.942537 -0.698889  0.150711
45                  -0.733172  0.310391 -1.120794 -1.158137 -0.277088
46                  -0.804330  0.597585  0.595048  0.198066 -1.822172
47                  -0.817973 -0.301871  1.384305  0.381680  0.210766
48                   0.259311 -0.700534  1.051778  0.642228  1.009035
49                   1.672240  0.297304 -2.917643 -0.568382  1.633619
50                   2.307278 -0.699318 -1.811299  0.274770 -0.163509
51                   1.837552  0.650945  1.269013  0.190992  0.095658
52                  -0.663213 -2.000075 -0.088616 -0.603876 -1.562467
53                   0.014641  1.026662  1.536357  0.721811 -0.888338
54                   2.048713  1.424647  0.350675  0.002744  1.368896
55                  -2.134497 -1.044421 -0.650175 -0.799932 -0.710620
56                   0.681219  0.353084  0.200867  0.993882  0.065348
57                  -0.886851  0.003705 -1.177101  0.000771 -0.957834
58                  -0.807315  2.117579 -0.491919 -0.632893 -0.613360
59                   0.448566 -0.842890 -0.978688 -0.116163 -0.405151
60                  -0.750727  0.634083 -1.136646 -0.734592 -1.042560
61                  -0.702942 -0.304720 -1.314770 -0.650442 -0.117048
62                  -0.285041  0.840923 -0.584402  0.872241  0.174587
63                  -1.320298  0.040687 -0.291162  0.127049 -0.276188
64                  -1.006923  3.321401  1.876961  0.461164  3.129681
65                  -0.714069 -1.682073 -0.261474  0.289083 -2.181826
66                  -0.456520 -0.733929  0.788365  0.260320  0.061266
67                  -0.545093 -0.238024  0.359279 -0.112489 -0.099663
68                   0.305222 -0.769575  0.455346 -0.348108  0.963122
69                  -0.220060  0.585273  0.819528 -0.271452 -0.434605
70                  -0.570976 -1.584229 -0.511809 -0.937662 -0.362068
71                  -0.114966 -0.953099  0.164387  1.043360 -1.461917
72                  -0.658796 -1.512535  0.375587 -0.015232 -0.542871

                           28
Gene Accession Number
1                   -1.498116
2                   -0.013001
3                    1.041528
4                    0.084141
5                    0.722660
6                    1.699341
7                    0.958816
8                    0.743702
9                    1.907221
10                   1.179394
11                  -0.789266
12                   0.346436
13                  -1.694999
14                   0.278227
15                  -0.341521
16                   0.299314
17                  -0.652435
18                  -0.475253
19                  -0.391590
20                   1.069341
21                  -2.595472
22                  -1.573680
23                   1.244393
24                  -0.479634
25                   0.513026
26                  -0.398738
27                   0.787902
28                  -0.523427
29                  -0.323727
30                   0.194078
...                       ...
43                  -0.090814
44                   0.184589
45                   1.053914
46                  -0.483733
47                  -1.058809
48                  -1.113791
49                   1.554615
50                  -0.979536
51                  -0.588185
52                   0.479234
53                   1.305074
```

```
54                    -1.097523
55                     0.622776
56                     0.938718
57                    -0.256402
58                    -0.220902
59                     0.371222
60                    -1.053139
61                     0.562342
62                    -0.222034
63                     0.620973
64                     0.853033
65                    -0.160444
66                    -0.244728
67                    -1.236755
68                     0.233936
69                    -1.113619
70                     1.266286
71                    -0.287502
72                    -1.946075

[72 rows x 29 columns]
(72, 29)
```

Shortcut - PCA in scikit-learn

For educational purposes, we went a long way to apply the PCA to the Gene Expression dataset. But luckily, there is already implementation in scikit-learn.

In [20]:
```
from sklearn.decomposition import PCA as sklearnPCA
sklearn_pca = sklearnPCA(n_components=k_use)
Y_sklearn = sklearn_pca.fit_transform(X_std)

print(Y_sklearn)
print(Y_sklearn.shape)
```

```
[[ 15.37761032   3.22022452   0.96875489 ...   0.27815135   7.49733916
    0.5367048 ]
 [  3.55628996   7.87850935 -11.50161375 ...   7.79210781  -5.9569517
   -2.44920953]
 [ 33.50974262   2.34889207  -5.9811807  ...  -2.27917817   7.01825224
   14.09741499]
 ...
 [-24.60252152  -7.28972663   0.701094   ...  -3.08214559   2.97111965
    1.01832411]
 [-11.59790658   2.60313947  -4.21848613 ...  -1.29541514   2.17737695
   -4.44590187]
 [ -1.96149321   9.01805144  -1.34471463 ...  -0.93251268   0.88258935
   -8.19226909]]
(72, 29)
```

Note: Any differences between `Y_calc` & `Y_sklearn` may be ignored and are due to the way the data was standardized for the PCA algorithm exercises.

Kmeans Clustering

Exercise 5 (`Kmeans_accuracy`: 2.5 points)

Create a function `kmeans_accuracy(X_std, initial_index, y_labels)`, which using kmeans clustering to cluster the dataset X into K clusters. `K = len(initial_index)`. The output should be the accuarcy of clustering comparing to the `y_labels`. To make it easier, we will tell you to write this function in 2 steps. To give you some partial credits, we split the test into 2 cells. One is to check your accuracy on standardized original data set `X_std`, which has 1.5 points. The other is to check the accuracy on PCA reconstrcuted data set `Y_calc`, which has 1 point.

- **Step 1**: Performing kmeans clustering on standardized data. Given the `initial_index` as a list of pre-selected patient_id, generate the intial_centers from X_std, and perform kmeans clustering, return the clustering labels for all the patients.
- **Step 2**: Comparing the accuracy between your clustering labels and the `y_labels` (i.e. `y['cancer']`). **Note**: The clustering label 0 may or may not be associated with patient type "ALL", you need to figure out which cluster label is associated with which patient type.

Hint: You can use functions from Notebook 14, which are included in the cell below.

Notes:

1. You need to use the specified index to generate the initial centroids, instead of just using cluster number K. The inital_index is given in the test cell.
2. You can use any functions in notebook 14 (all needed functions are provided in the cell below) **OR** create your own functions, **OR** using the vq module from scipy.cluster package (You can use either kmeans or kmeans2 functions from scipy.cluster.vq).

In [23]:
```
## function from notebook 14
def compute_d2(X, centers):
    """Computing the distance matrix S."""
    m = len(X)
    k = len(centers)
    S = np.empty((m, k))
    for i in range(m):
        d_i = np.linalg.norm(X[i, :] - centers, ord=2, axis=1)
        S[i, :] = d_i**2
    return S

def assign_cluster_labels(S):
    return np.argmin(S, axis=1)

def update_centers(X, y):
    # X[:m, :d] == m points, each of dimension d
    # y[:m] == cluster labels
    m, d = X.shape
    k = max(y) + 1
    assert m == len(y)
    assert (min(y) >= 0)

    centers = np.empty((k, d))
    for j in range(k):
        # Compute the new center of cluster j,
        # i.e., centers[j, :d].
        centers[j, :d] = np.mean(X[y == j, :], axis=0)
    return centers

def WCSS(S):
    return np.sum(np.amin(S, axis=1))

def has_converged(old_centers, centers):
    return set([tuple(x) for x in old_centers]) == set([tuple(x) for x in centers])

def kmeans(X, starting_centers, max_steps=np.inf):
    centers = starting_centers
    converged = False
    labels = np.zeros(len(X))
    i = 1
    while (not converged) and (i <= max_steps):
        old_centers = centers
        S = compute_d2(X, centers)
        labels = assign_cluster_labels(S)
        centers = update_centers(X, labels)
        converged = has_converged(old_centers, centers)
        #print ("iteration", i, "WCSS = ", WCSS (S))
        i += 1
    return labels



def mark_matches(a, b, exact=False):
    """
    Given two Numpy arrays of {0, 1} labels, returns a new boolean
    array indicating at which locations the input arrays have the
    same label (i.e., the corresponding entry is True).

    This function can consider "inexact" matches. That is, if `exact`
    is False, then the function will assume the {0, 1} labels may be
    regarded as the same up to a swapping of the labels. This feature
    allows
```

```
      a == [0, 0, 1, 1, 0, 1, 1]
      b == [1, 1, 0, 0, 1, 0, 0]

    to be regarded as equal. (That is, use `exact=False` when you
    only care about "relative" labeling.)
    """
    assert a.shape == b.shape
    a_int = a.astype(dtype=int)
    b_int = b.astype(dtype=int)
    all_axes = tuple(range(len(a.shape)))
    assert ((a_int == 0) | (a_int == 1)).all()
    assert ((b_int == 0) | (b_int == 1)).all()

    exact_matches = (a_int == b_int)
    if exact:
        return exact_matches

    assert exact == False
    num_exact_matches = np.sum(exact_matches)
    if (2*num_exact_matches) >= np.prod (a.shape):
        return exact_matches
    return exact_matches == False # Invert

def count_matches(a, b, exact=False):
    """
    Given two sets of {0, 1} labels, returns the number of mismatches.

    This function can consider "inexact" matches. That is, if `exact`
    is False, then the function will assume the {0, 1} labels may be
    regarded as similar up to a swapping of the labels. This feature
    allows

      a == [0, 0, 1, 1, 0, 1, 1]
      b == [1, 1, 0, 0, 1, 0, 0]

    to be regarded as equal. (That is, use `exact=False` when you
    only care about "relative" labeling.)
    """
    matches = mark_matches(a, b, exact=exact)
    return np.sum(matches)
```

In [41]:

```
from scipy.cluster import vq

def kmeans_accuracy(X, initial_index, y_labels):

    X = X.copy()

    first = np.asarray(X[X.index == initial_index[0]])
    second = np.asarray(X[X.index == initial_index[1]])
    my_array = np.column_stack((first[0], second[0])).T

    centers_vq, distortion_vq = vq.kmeans(X, k_or_guess=my_array)
    clustering_vq, _ = vq.vq(X, centers_vq)
    clustering = pd.DataFrame(clustering_vq)
    clustering['labels'] = y_labels
    clustering['labels'] = np.where(clustering.labels == 'ALL', 1, 0)
    clustering.columns = ['kmeans', 'labels']
    n_matches_vq = count_matches(clustering['labels'], clustering['kmeans'], exact=True)


    return n_matches_vq / len(clustering)


initial_index = [30, 50]

# Note: this is not the solution for exercise 1. We made them different intendedly.
Y_std = (Y_calc/np.std(Y_calc, axis=0))

kmeans_accuracy(Y_std, initial_index, y['cancer'])
```

Out[41]: 0.6666666666666666

In [42]:

```
# `kmeans_accuracy_test0`: Test cell 0 (1.5 points)
# initial index
```

```
initial_index = [30, 50]

%timeit acc_original = kmeans_accuracy(X_std, initial_index, y['cancer'])
acc_original = kmeans_accuracy(X_std, initial_index, y['cancer'])

sum_tol = 1e-4
assert (acc_original - 0.6944444444444444) <= sum_tol, "Your clustering accuracy on original data se
t is wrong!"

print ("\n(Passed.)")
```

```
6.55 ms ± 98.2 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)

(Passed.)
```

In [43]:

```
# `kmeans_accuracy_test1`: Test cell 1 (1 points)
# initial index
initial_index = [30, 50]

# Note: this is not the solution for exercise 1. We made them different intendedly.
Y_std = (Y_calc/np.std(Y_calc, axis=0))

%timeit acc_pca = kmeans_accuracy(Y_std, initial_index, y['cancer'])
acc_pca = kmeans_accuracy(Y_std, initial_index, y['cancer'])

sum_tol = 1e-4
assert (acc_pca - 0.625) <= sum_tol, "Your clustering accuracy on pca data set is wrong!"

print ("\n(Passed.)")
```

```
3.75 ms ± 6.34 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
---------------------------------------------------------------------------
AssertionError                            Traceback (most recent call last)
<ipython-input-43-09d3eb7316c7> in <module>()
     10 
     11 sum_tol = 1e-4
---> 12 assert (acc_pca - 0.625) <= sum_tol, "Your clustering accuracy on pca data set is wrong!"
     13 
     14 print ("\n(Passed.)")

AssertionError: Your clustering accuracy on pca data set is wrong!
```

Congratulations! Now you have implemented kmeans_accuracy on both original and PCA reconstructed gene expression data set. Do you have a conclusion which method is better? It's hard to tell on this small data set. But imaging you have more genes and more patients, then performing PCA will be faster and with similar accuracy.

Visualizing the results of PCA

> The remaining code cells below are optional. There is no code to write, so you can just run the cells to verify that they complete and submit the notebook. Later, when you come back to this material, you may wish to study or use the cells below as examples of different visualization techniques.

The analysis reveals that k_use principle components are needed to account for 75% of the variance. PC 1-3 add up to about ~30% and