

1. (Correlation coefficient) The entries of a two-dimensional random vector have a correlation coefficient equal to one. What is the variance of the second principal component? Provide both a proof and an intuitive justification.

Let  $X$  and  $Y$  the two components of a random vector. If  $\rho_{X,Y} = \frac{\text{Cov}(X,Y)}{\sigma_X \sigma_Y} = 1$  then  $\text{Cov}(X, Y) = \sigma_X \sigma_Y$ . The covariance matrix is then  $\Sigma = \begin{bmatrix} \sigma_X^2 & \text{Cov}(X, Y) \\ \text{Cov}(X, Y) & \sigma_Y^2 \end{bmatrix} = \begin{bmatrix} \sigma_X^2 & \sigma_X \sigma_Y \\ \sigma_X \sigma_Y & \sigma_Y^2 \end{bmatrix}$ .  $\det(\Sigma - \lambda I) = \lambda(\lambda - (\sigma_X^2 + \sigma_Y^2))$ ,  $\lambda \in \mathbf{R} \Rightarrow$  the eigenvalues are 0 and  $\sigma_X^2 + \sigma_Y^2$ . The sample variance of the second principal component is the smaller eigenvalue 0. We can expect such result since there  $X$  and  $Y$  are positively correlated with a coefficient of one thus the variance of the data is completely expressed by the variance of the first principal component, there is no information on the second principal component.

2. (Not centering) To analyze what happens if we apply PCA without centering, let  $\tilde{x}$  be a  $d$ -dimensional vector with mean  $\mu \in \mathbb{R}^d$  and covariance matrix  $\Sigma_{\tilde{x}}$  equal to the identity matrix. If we compute the eigendecomposition of the matrix  $E(\tilde{x}\tilde{x}^T)$  what is the value of the largest eigenvalue? What is the direction of the corresponding eigenvector?

$$\begin{aligned}
E((\tilde{x} - \mu)(\tilde{x} - \mu)^T) &= E(\tilde{x}\tilde{x}^T - 2\mu^T\tilde{x} + \mu^T\mu) \\
&= E(\tilde{x}\tilde{x}^T) - 2\mu E(\tilde{x}^T) + \mu\mu^T \\
&= E(\tilde{x}\tilde{x}^T) - 2\mu\mu^T + \mu\mu^T \\
&= E(\tilde{x}\tilde{x}^T) - \mu\mu^T \\
\Rightarrow E(\tilde{x}\tilde{x}^T) &= E((\tilde{x} - \mu)(\tilde{x} - \mu)^T) + \mu\mu^T \\
&= \Sigma_{\tilde{x}} + \mu\mu^T
\end{aligned}$$

We have

$$E(\tilde{x}\tilde{x}^T) = \begin{bmatrix} 1 + \mu_1^2 & \mu_1\mu_2 & \dots & \mu_1\mu_d \\ \mu_1\mu_2 & 1 + \mu_2^2 & \dots & \mu_2\mu_d \\ \vdots & \ddots & & \vdots \\ \mu_1\mu_d & \dots & & 1 + \mu_d^2 \end{bmatrix}$$

We note that an eigenvector of this matrix is  $u = [\mu_1 \ \mu_2 \ \dots \ \mu_d]^T$  since  $E(\tilde{x}\tilde{x}^T)u = (1 + \sum_{i=1}^d \mu_i^2)u$ . Let's prove that if  $A$  and  $B = I + A$  matrices share the same number of eigenvalues and eigenvector. If  $\lambda$  and the corresponding eigenvector  $v$ ,  $v \neq 0$ , is an eigenvalue of  $A$  then  $Bv = (I + A)v = (1 + \lambda)v$  thus  $(1 + \lambda)$  is an eigenvalue of  $B$  and  $v$  is also an eigenvector. Now if  $\mu$  is an eigenvalue of  $B$  then  $Av = (A + I)v - Iv = Bv - Iv = (\mu - 1)v$  thus  $(\mu - 1)$  is an

eigenvalue of  $A$  for the same eigenvector  $v$ . Let  $A = \begin{bmatrix} \mu_1^2 & \mu_1\mu_2 & \dots & \mu_1\mu_d \\ \mu_1\mu_2 & \mu_2^2 & \dots & \mu_2\mu_d \\ \vdots & \ddots & & \vdots \\ \mu_1\mu_d & \dots & & \mu_d^2 \end{bmatrix}$ , we know that

$\sum_{i=1}^d \lambda_i = \text{tr}(A) = \sum_{i=1}^d \mu_i^2$  where  $\lambda_i, i = 1, \dots, d$  are the eigenvalues of  $A$  thus  $(\sum_{i=1}^d \mu_i^2)$  is the only eigenvalue  $A$ .

Setting  $E(\tilde{x}\tilde{x}^T) = B = I + A$ , we can conclude that the largest eigenvalue of  $E(\tilde{x}\tilde{x}^T)$  is  $1 + \|\mu\|_2^2$  with eigenvector  $u = [\mu_1 \ \mu_2 \ \dots \ \mu_d]^T$ .

3. (Financial data) In this exercise you will use the code in the findata folder. For the data loading code to work properly, make sure you have the pandas Python package installed on your system.

Throughout, we will be using the data obtained by calling `load_data` in `findata_tools.py`. This will give you the names, and closing prices for a set of 18 stocks over a period of 433 days ordered chronologically. For a fixed stock (such as msft), let  $P_1, \dots, P_{433}$  denote its sequence of closing prices ordered in time. For that stock, define the daily returns series  $R_i := P_{i+1} - P_i$  for  $i = 1, \dots, 432$ . Throughout we think of the daily stock returns as features, and each day (but the last) as a separate datapoint in  $\mathbb{R}^{18}$ . That is, we have 432 datapoints each having 18 features.

- (a) Looking at the first two principal directions of the centered data, give the two stocks with the largest coefficients (in absolute value) in each direction. Give a hypothesis why these two stocks have the largest coefficients, and confirm your hypothesis using the data. The file `findata_tools.py` has `pretty_print` functions that can help you output your results. You are not required to include the principal directions in your submission.

The two stocks corresponding to the two principal directions of the centered data with the largest coefficients (in absolute value) in each direction are: "amzn" and "goog". It can be explained by computing the absolute return for each stock over the period of 433 days:

```

aapl      amzn      msft      goog      xom      apc \
454.14342 3423.779352 208.844523 2799.940424 258.501684 388.899131
cvx      c      gs      jpm      aet      jnj \
381.849154 247.140956 901.311051 277.9143 505.556593 275.823333
dgx      spy      xlf      sso      sds      uso
257.409551 424.583189 64.368439 277.841774 276.939997 77.16

```

Figure 1: Stocks returns over a period of 433 days (output of `pretty_print`).

In term of return goog and amzn stocks returned about 4 and 3 times more than the next stock after amzn and goog stocks with the highest return: gs, 53 and 43 times more than the last stock in term of return among the 18 stocks: xlf.

amzn/gs	amzn/xlf	goog/gs	goog/xlf
3.8	53.2	3.1	43.5

So most of the variance in the data will be explained by these two stocks: goog and amzn.

- (b) Standardize the centered data so that each stock (feature) has variance 1 and compute the first 2 principal directions. This is equivalent to computing the principal directions of the correlation matrix (the previous part used the covariance matrix). Using the information in the comments of `generate_findata.py` as a guide to the stocks, give an English interpretation of the first 2 principal directions computed here. You are not required to include the principal directions in your submission.

We can think of each of the entries of the principal directions as a weighting on the corresponding stock.

- SPY - A security that roughly tracks the S&P 500, a weighted average of the stock prices of 500 top US companies. We have only 18 stocks and excluding the ETF

(Exchange traded products), we are left with 13 stocks. We can notice that among these 13 stocks, SPY entry in the principal directions, has the same than the other 13 entries for the same principal direction. For a given day, computing a weighted average using the absolute values of entries in the first principal direction and the prices of these 13 stocks, we obtain a weighted average price in the range of the SPY price reported for the same day. It is less true using the entries of the second principal direction.

PD0	aapl	amzn	msft	goog	xom	apc	cvx	\
	-0.184648	-0.168095	-0.227645	-0.197887	-0.208861	-0.194808	-0.223865	
	c	gs	jpm	aet	jnj	dgx	spy	\
	-0.280147	-0.260443	-0.27294	-0.188555	-0.150783	-0.196612	-0.336632	
	xlf	sso	sds	uso				
	-0.198364	-0.334826	0.327259	-0.159213				
PD1	aapl	amzn	msft	goog	xom	apc	cvx	\
	0.285821	0.3302	0.302005	0.389346	-0.293444	-0.329116	-0.308272	
	c	gs	jpm	aet	jnj	dgx	spy	\
	-0.133288	-0.137664	-0.155599	0.071286	0.108239	0.165412	0.084872	
	xlf	sso	sds	uso				
	-0.124933	0.091568	-0.056002	-0.370943				

Figure 2: First two Principal Directions.

Weights for the first 13 stock prices using PD0								
aapl	amzn	msft	goog	xom	apc	cvx	\	
-0.184648	-0.168095	-0.227645	-0.197887	-0.208861	-0.194808	-0.223865		
c	gs	jpm	aet	jnj	dgx			
-0.280147	-0.260443	-0.27294	-0.188555	-0.150783	-0.196612			
Absolute values of weights for the first 13 stock prices using PD0								
aapl	amzn	msft	goog	xom	apc	cvx	\	
0.184648	0.168095	0.227645	0.197887	0.208861	0.194808	0.223865		
c	gs	jpm	aet	jnj	dgx			
0.280147	0.260443	0.27294	0.188555	0.150783	0.196612			
Day0 prices								
aapl	amzn	msft	goog	xom	apc			
101.790649	636.98999	52.433533	741.849027	72.740799	48.801582			
cvx	c	gs	jpm	aet	jnj	dgx		
82.577927	50.149045	172.800156	61.10005	107.291946	95.626782	68.369864		
Day0, computed SPY weighted average prices:163.92740408192924								
Day0 SPY price								
SPY weight:-0.3366318246190488								
spy								
194.027725								

Figure 3: Weighted average of the 13 stock prices and SPY price using PD0.

- XLF - A security that tracks a weighted average of top US financial companies. Among the 18 stocks, there are only 3 financial stocks: c, gs and jpm. Entry for xlf has the same sign as the entries for these three stocks in the first two principal directions. To some extent the weighted average price of these 3 stocks is somewhat close to XLF price.

Weights for the 3 financial stock prices using PD0				
c	gs	jpm		
-0.280147	-0.260443	-0.27294		
Absolute values of weights for the 3 financial stock prices using PD0				
c	gs	jpm		
0.280147	0.260443	0.27294		
Day100 prices				
c	gs	jpm		
45.329781	155.994034	62.998978		
Day100, computed XLF weighted average prices:86.68575537909774				
Day100 XLF price				
XLF weight:-0.19836417024240857				
Day100 XLF price				
xlf				
14.347868				

Figure 4: Weighted average of the 3 financial stock prices and XLF price using PD0.

- SSO - ProShares levered ETF that roughly corresponds to twice the daily performance of the S&P 500. We have similar entries for SSO and SPY which indicate a strong correlation between these two stocks

	SSO	SPY
First PD	-0.3348	-0.3366
Second PD	0.09156	0.0848

We can also pick two random days (200 and 201) and compare the returns for spy vs. xlf, you can see the return for xlf tracks the return of spy:

```

aapl  amzn  msft  goog  xom  apc  cvx  \
-0.343941  0.039978 -0.126941  6.23999  0.385491  0.956391  0.461364
c  gs  jpm  aet  jnj  dgx  spy  \
0.483455  1.856705  0.639229 -0.366638 -0.798614 -0.71032  0.558686
xlf  sso  sds  uso
0.167292  0.33892 -0.240006  0.21

```

Figure 5: Returns for day 200

```

aapl  amzn  msft  goog  xom  apc  cvx  \
-0.05896 -7.369995 -0.273407 -4.530029  0.038551 -0.169361 -0.384475
c  gs  jpm  aet  jnj  dgx  spy  xlf  \
0.098664  0.0 -0.088517 -0.128807  0.272697  1.568627 -0.39206  0.0
sso  sds  uso
-0.199363  0.200005 -0.23

```

Figure 6: Returns for day 201

- SDS - ProShares inverse levered ETF that roughly corresponds to twice the negative daily performance of the S&P 500. The entries for SDS and SPY are roughly opposite confirming the opposite trend of SDS compared to SPY.

	SDS	SPY
First PD	0.3272	-0.3366
Second PD	-0.0560	0.0848

- USO - Exchange traded product that tracks the price of oil in the US Taking the mean of the entries related to oil company (xom, apc, cvx) from the principal directions and comparing to the entry for USO, they are close, confirming the correlation between uso and (xom, apc, cvx):

	USO	Mean(XOM, APC, CVX)
First PD	-0.1592	-0.2091
Second PD	-0.3709	-0.3102

- (c) Assume the stock returns each day are drawn independently from a multivariate distribution  $\tilde{x}$  where  $\tilde{x}[i]$  corresponds to the  $i$ th stock. Assume further that you hold a portfolio with 200 shares of each of appl, amzn, msft, and goog, and 100 shares of each of the remaining 14 stocks in the dataset. Using the sample covariance matrix as an estimator for the true covariance of  $\tilde{x}$ , approximate the standard deviation of your 1 day portfolio returns  $\tilde{y}$  (this is a measure of the risk of your portfolio). Here  $\tilde{y}$  is given by

$$\tilde{y} := \sum_{i=1}^{18} \alpha[i] \tilde{x}[i],$$

where  $\alpha[i]$  is the number of shares you hold of stock  $i$ .

Using the sample covariance matrix and taking the root square of  $[\text{shares}^T \times \text{covariance} \times \text{shares}]$ , we find that for such portfolio the standard deviation of 1 day is: 4309.94952.

- (d) Assume further that  $\tilde{x}$  from the previous part has a multivariate Gaussian distribution. Compute the probability of losing 1000 or more dollars in a single day. That is, compute

$$\Pr(\tilde{y} \leq -1000).$$

For each day of the 432 days, we compute the daily return  $\tilde{y} := \sum_{i=1}^{18} \alpha[i] \tilde{x}[i]$  and count the number of times over the 432 days:  $\Pr(\tilde{y} \leq -1000)$ , then divide the result by the number of days (432), we obtain: 0.3425.

Note: The assumptions made in the previous parts are often invalid and can lead to inaccurate risk calculations in real financial situations.

4. The following questions refer to the code in the folder `faces`. The Olivetti faces dataset used in `faces` contains images of faces of people associated with a unique numeric id to identify the person.

- (a) Complete the `compute_nearest_neighbors()` function in `nearest_neighbors.py` that finds the image in the training data that is closest to a given test image. Include the generated images in your submitted homework.

The data set consists in 400 rows of a ravelled face image of original size 64 x 64 pixels. Each row represent a datapoint in  $\mathbb{R}^{4096}$ . A label is associated to each face image which correspond to the Subject IDs. In the `nearest_neighbors` function we compute the distance between a test image and a set of reference image (`train_matrix`).

```
def compute_nearest_neighbors(train_matrix, testImage):
    distances = np.sqrt(
        np.sum((train_matrix - testImage) ** 2,
               axis=1))
    idx_of_closest_point_in_train_matrix =
        np.argsort(distances)
    return idx_of_closest_point_in_train_matrix[0]
```

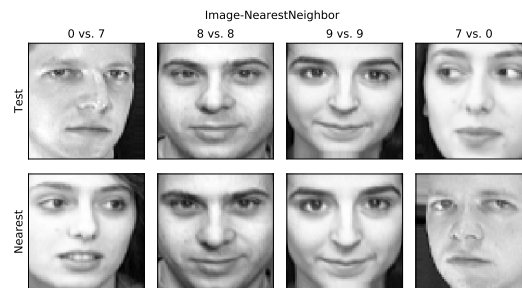


Figure 7: Test images and image found by Nearest Neighbors.

Create a new file in which you must write code to complete the following tasks:

- (b) Generate a plot of  $k$  vs.  $\sigma_k^2$ , where  $\sigma_k^2$  is the variance with the  $k$ th principal component of the data (e.g.,  $\sigma_1^2$  is the largest variance). Include the plot in your submitted homework document. You can limit the x axis to a reasonable number.

We use PCA decomposition from `sklearn` which gives us the singular values ordered which correspond to the variance with each principal component, we select  $k$  of them and plot them for each principal component:

```
faces = fetch_olivetti_faces().data
n_samples, n_features = faces.shape
faces_centered = faces - faces.mean(axis=0)
cov = np.cov(faces_centered, rowvar=False)
eigvals, _ = np.linalg.eigh(cov)
```

```

k = 40
truncated_eigvals = eigvals[:, :-1][:k]
fig, ax = plt.subplots(figsize=(10, 6))
k_range = range(1, k+1)
label_str = "variance for largest {}
principal components".format(k)
ax.plot(k_range, truncated_eigvals, "-", color="red",
label=label_str)
ax.set_xlabel("principal component")
ax.set_ylabel("Variance")
ax.set_title(r"Explained Variance of the $k^{\text{th}}$ component")
ax.legend()
plt.show();
fig.savefig("pb_4_b.pdf", bbox_inches='tight');

```

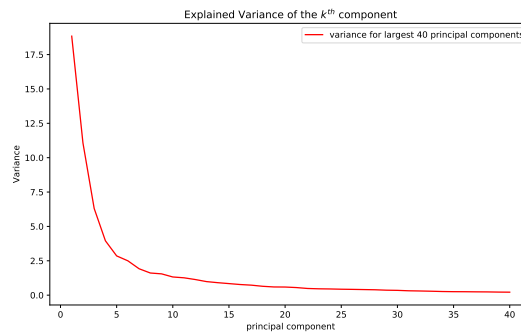


Figure 8: Variance with principal components

- (c) Plot (using `plot_image_grid()` in `plot_tools.py`) the vectors corresponding to the top 10 principal directions of the data. Your principal direction vectors should be elements of  $\mathbb{R}^{4096}$  (i.e., they should represent images). Include the plot in your submitted homework document.

We compute the sample covariance matrix of the data  $\Sigma_{\mathcal{X}}$ , the principal directions are the eigenvectors of the eigendecomposition of  $\Sigma_{\mathcal{X}}$ :

```

faces = fetch_olivetti_faces().data
n_samples, n_features = faces.shape
faces_centered = faces - faces.mean(axis=0)
cov = np.cov(faces_centered, rowvar=False)
_, principal_directions = np.linalg.eigh(cov)
k = 10
top_pd = principal_directions[:, ::-1][:, :k].T
title = "Top {} principal directions vectors".format(k)
plot_tools.plot_image_grid(top_pd, title)

```



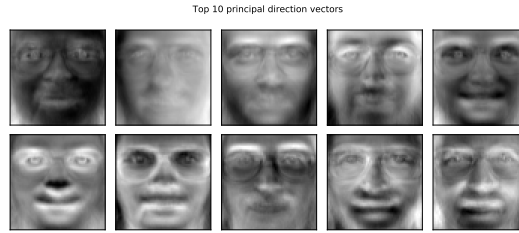


Figure 9: Top 10 principal direction vectors

- (d) Use the variance of principal directions plot to determine a relatively small number  $k$  of principal components that explains the training data reasonably well. Project the training data and the test data onto the first  $k$  principal components, and run nearest neighbors for each test image in this lower dimensional space. Include your choice for  $k$ , and the plots of your nearest neighbor results in your submitted homework document. You should use the code from `nearest_neighbors.py` to generate your image plots. Based on the variance plot, most of the variance of the data is captured by the 40 first principal components. Using the first 40 principal components, we project the training and test data set onto these principal components before finding the nearest neighbors.

```
def compute_nearest_neighbors(train_matrix, testImage):
    distances = np.sqrt(
        np.sum((train_matrix - testImage) ** 2,
               axis=1))
    idx_of_closest_point_in_train_matrix =
        np.argsort(distances)
    return idx_of_closest_point_in_train_matrix[0]

test_idx = [1, 87, 94, 78]

faces = fetch_olivetti_faces()
targets = faces.target
faces = faces.images.reshape((len(faces.images), -1))

train_idx = np.array(list(set(list(range(faces.shape[0]))
- set(test_idx))))

train_set = faces[train_idx]
y_train = targets[train_idx]
test_set = faces[np.array(test_idx)]
y_test = targets[np.array(test_idx)]

k = 40
model = PCA(n_components=k)
# Do PCA and compute principal directions.
model.fit(faces);
```

```

top_principal_components = model.components_

# Projection of training and test data
projected_train_set =
    train_set.dot(top_principal_components.T)
projected_test_set =
    test_set.dot(top_principal_components.T)

imgs = list()
est_labels = list()
for i in range(projected_test_set.shape[0]):
    test_image = projected_test_set[i, :]
    # Nearest neighbors in smaller dimension space
    nnIdx = compute_nearest_neighbors(projected_train_set,
    test_image)
    imgs.extend([test_set[i,:], train_set[nnIdx, :]])
    est_labels.append(y_train[nnIdx])

row_titles = ['Test', 'Nearest']
col_titles =
    ['%d vs. %d' % (i, j) for i, j in zip(y_test, est_labels)]
plot_tools.plot_image_grid(imgs,
                            "PC-Image-NearestNeighbor",
                            (64, 64), len(projected_test_set),
                            n_row=2, bycol=True, row_titles=row_titles,
                            col_titles=col_titles)

```

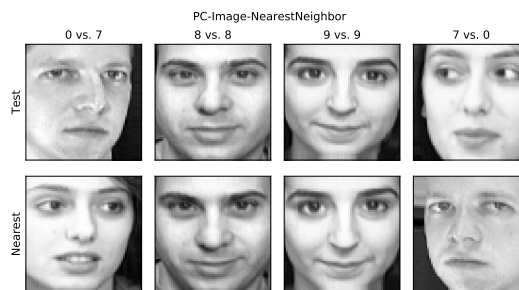


Figure 10: Nearest neighbors using top 10 principal component vectors

- (e) Give a potential reason why the principal component-based nearest-neighbor approach used in the previous part could be more accurate than using the full training set.

Using the top 40 principal directions, we keep most of the variance of the data along these directions and by projecting into the span of these vectors, we can expect to have capture most of the significant characteristics of the data in a space of smaller dimensions ( $\mathbb{R}^{40}$ )

vs.  $\mathbb{R}^{4096}$ ). So performing nearest neighbors in the space with smaller dimension could be more or as accurate than doing it in the original space.

- (f) Use `sklearn.cluster.KMeans` to perform KMeans on the entire dataset (both train and test set) with  $k = 40$ . Use `plot_image_grid()` to create a picture of all the  $k$  cluster centers.

```
rng = RandomState(0)
center = True
n_components = 40

faces = fetch_olivetti_faces().data
faces_centered = faces - faces.mean(axis=0)
estimator = KMeans(n_clusters=n_components, random_state=rng)
estimator.fit(faces)
kmeans_components = estimator.cluster_centers_
plot_tools.plot_image_grid(kmeans_components,
    "KMEANS_clusters", (64, 64), 10, n_row=4, bycol=True)
```



Figure 11: 40 KMeans clusters

Some notes to keep in mind:

- i. The function `np.linalg.eig` might return complex eigenvectors.
- ii. The data points in the training and test data are given as rows.
- iii. Include all new code (or functions) you have filled in your final PDF.