IN3050 assignment 3

April 21, 2023

1 IN3050/IN4050 Mandatory Assignment 3: Unsupervised Learning

Name: Evan Matel Username: evanjm

1.0.1 Rules

Before begin the exercise, review the rules atthis website: you https://www.uio.no/english/studies/examinations/compulsory-activities/mn-ifi-mandatory.html , in particular the paragraph on cooperation. This is an individual assignment. not allowed to deliver together or copy/share source-code/answers with others. Read also the "Routines for handling suspicion of cheating and attempted cheating at the University of Oslo" https://www.uio.no/english/about/regulations/studies-examinations/routinescheating.html By submitting this assignment, you confirm that you are familiar with the rules and the consequences of breaking them.

1.0.2 Delivery

Deadline: Friday, April 21, 2023, 23:59

Your submission should be delivered in Devilry. You may redeliver in Devilry before the deadline, but include all files in the last delivery, as only the last delivery will be read. You are recommended to upload preliminary versions hours (or days) before the final deadline.

1.0.3 What to deliver?

You are recommended to solve the exercise in a Jupyter notebook, but you might solve it in a Python program if you prefer.

If you choose Jupyter, you should deliver the notebook. You should answer all questions and explain what you are doing in Markdown. Still, the code should be properly commented. The notebook should contain results of your runs. In addition, you should make a pdf of your solution which shows the results of the runs.

If you prefer not to use notebooks, you should deliver the code, your run results, and a pdf-report where you answer all the questions and explain your work.

Your report/notebook should contain your name and username.

Deliver one single zipped folder (.zip, .tgz or .tar.gz) which contains your complete solution.

Important: if you weren't able to finish the assignment, use the PDF report/Markdown to elaborate on what you've tried and what problems you encountered. Students who have made an effort and attempted all parts of the assignment will get a second chance even if they fail initially. This exercise will be graded PASS/FAIL.

1.0.4 Goals of the exercise

This exercise has three parts. The first part is focused on Principal Component Analysis (PCA). You will go through some basic theory, and implent PCA from scratch to do compression and visualization of data.

The second part focuses on clustering using K-means. You will use scikit-learn to run K-means clustering, and use PCA to visualize the results.

The last part ties supervised and unsupervised learning together in an effort to evaluate the output of K-means using a logistic regression for multi-class classification approach.

The master students will also have to do one extra part about tuning PCA to balance compression with information lost.

1.0.5 Tools

You may freely use code from the weekly exercises and the published solutions. In the first part about PCA you may **NOT** use ML libraries like scikit-learn. In the K-means part and beyond we encurage the use of scikit-learn to iterate quickly on the problems.

1.0.6 Beware

This is a new assignment. There might occur typos or ambiguities. If anything is unclear, do not hesitate to ask. Also, if you think some assumptions are missing, make your own and explain them!

2 Principal Component Analysis (PCA)

In this section, you will work with the PCA algorithm in order to understand its definition and explore its uses.

2.1 Implementation: how is PCA implemented?

Here we implement the basic steps of PCA and we assemble them.

2.1.1 Importing libraries

We start importing the *numpy* library for performing matrix computations, the *pyplot* library for plotting data, and the *syntheticdata* module to import synthetic data.

```
[59]: import numpy as np import matplotlib.pyplot as plt import syntheticdata
```

2.1.2 Centering the Data

Implement a function with the following signature to center the data as explained in Marsland.

```
[60]: def center_data(A):
    N, M = np.shape(A)
    means = np.zeros((N, M))
    for i in range(M):
        means[:, i] = np.mean(A[:, i])
    Y = A - means

# INPUT:
# A [NxM] numpy data matrix (N samples, M features)
#
# OUTPUT:
# X [NxM] numpy centered data matrix (N samples, M features)
return Y, means
```

Test your function checking the following assertion on testcase:

```
[61]: testcase = np.array([[3.,11.,4.3],[4.,5.,4.3],[5.,17.,4.5],[4,13.,4.4]])
answer = np.array([[-1.,-0.5,-0.075],[0.,-6.5,-0.075],[1.,5.5,0.125],[0.,1.5,0.

-025]])
np.testing.assert_array_almost_equal(center_data(testcase)[0], answer)
```

2.1.3 Computing Covariance Matrix

Implement a function with the following signature to compute the covariance matrix as explained in *Marsland*.

Test your function checking the following assertion on *testcase*:

2.1.4 Computing eigenvalues and eigenvectors

Use the linear algebra package of numpy and its function np.linalg.eig() to compute eigenvalues and eigenvectors. Notice that we take the real part of the eigenvectors and eigenvalues. The covriance matrix *should* be a symmetric matrix, but the actual implementation in compute_covariance_matrix() can lead to small round off errors that lead to tiny imaginary additions to the eigenvalues and eigenvectors. These are purely numerical artifacts that we can safely remove.

Note: If you decide to NOT use np.linalg.eig() you must make sure that the eigenvalues you compute are of unit length!

```
[64]: def compute_eigenvalue_eigenvectors(A):
    # INPUT:
    # A [DxD] numpy matrix
    #
    # OUTPUT:
    # eigval [D] numpy vector of eigenvalues
    # eigvec [DxD] numpy array of eigenvectors
    eigval, eigvec = np.linalg.eig(A)

# Numerical roundoff can lead to (tiny) imaginary parts. We correct that
    →here.
    eigval = eigval.real
    eigvec = eigvec.real
    return eigval, eigvec
```

Test your function checking the following assertion on testcase:

```
[65]: testcase = np.array([[2,0,0],[0,5,0],[0,0,3]])
    answer1 = np.array([2.,5.,3.])
    answer2 = np.array([[1.,0.,0.],[0.,1.,0.],[0.,0.,1.]])
    x,y = compute_eigenvalue_eigenvectors(testcase)
```

```
np.testing.assert_array_almost_equal(x, answer1)
np.testing.assert_array_almost_equal(y, answer2)
```

2.1.5 Sorting eigenvalues and eigenvectors

Implement a function with the following signature to sort eigenvalues and eigenvectors as explained in *Marsland*.

Remember that eigenvalue eigval[i] corresponds to eigenvector eigvec[:,i].

```
[66]: def sort_eigenvalue_eigenvectors(eigval, eigvec):
    # INPUT:
    # eigval    [D] numpy vector of eigenvalues
    # eigvec    [DxD] numpy array of eigenvectors
#
    # OUTPUT:
    # sorted_eigval    [D] numpy vector of eigenvalues
# sorted_eigvec    [DxD] numpy array of eigenvectors
indices = np.argsort(eigval)
indices = indices[::-1]

sorted_eigval = eigval[indices]
sorted_eigvec = eigvec[:,indices]
return sorted_eigval, sorted_eigvec
```

Test your function checking the following assertion on testcase:

```
[67]: testcase = np.array([[2,0,0],[0,5,0],[0,0,3]])
    answer1 = np.array([5.,3.,2.])
    answer2 = np.array([[0.,0.,1.],[1.,0.,0.],[0.,1.,0.]]))
    x,y = compute_eigenvalue_eigenvectors(testcase)
    x,y = sort_eigenvalue_eigenvectors(x,y)
    np.testing.assert_array_almost_equal(x, answer1)
    np.testing.assert_array_almost_equal(y, answer2)
```

2.1.6 PCA Algorithm

Implement a function with the following signature to compute PCA as explained in *Marsland* using the functions implemented above.

```
[68]: def pca(A,m=None):
    # INPUT:
    # A    [NxM] numpy data matrix (N samples, M features)
    # m    integer number denoting the number of learned features (m <= M)
    #
    # OUTPUT:
    # pca_eigvec    [Mxm] numpy matrix containing the eigenvectors (M
    →dimensions, m eigenvectors)
```

Test your function checking the following assertion on testcase:

2.2 Understanding: how does PCA work?

We now use the PCA algorithm you implemented on a toy data set in order to understand its inner workings.

2.2.1 Loading the data

The module *synthetic data* provides a small synthetic dataset of dimension [100x2] (100 samples, 2 features).

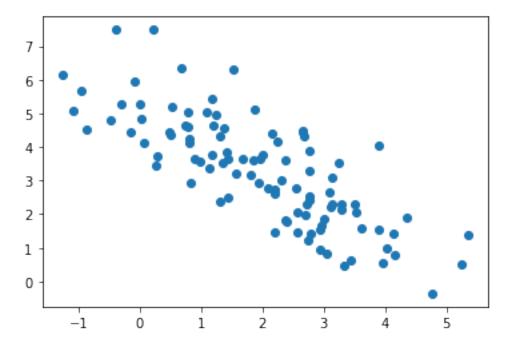
```
[70]: X = syntheticdata.get_synthetic_data1()
```

2.2.2 Visualizing the data

Visualize the synthetic data using the function scatter() from the matplotlib library.

```
[71]: plt.scatter(X[:,0],X[:,1])
```

[71]: <matplotlib.collections.PathCollection at 0x19be6979a30>

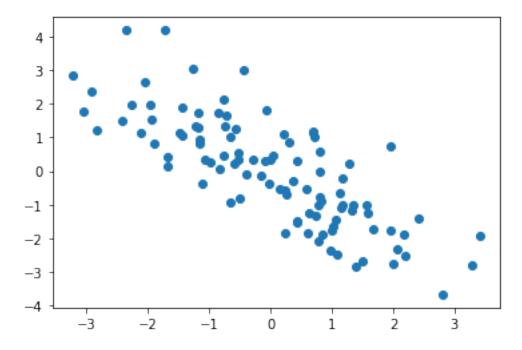


2.2.3 Visualize the centered data

Notice that the data visualized above is not centered on the origin (0,0). Use the function defined above to center the data, and the replot it.

```
[72]: Y, _ = center_data(X)
plt.scatter(Y[:,0],Y[:,1])
```

[72]: <matplotlib.collections.PathCollection at 0x19b802ada30>



2.2.4 Visualize the first eigenvector

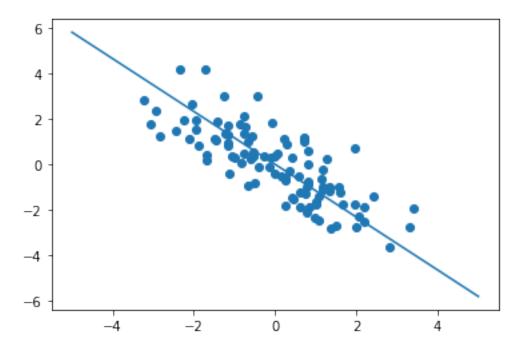
Visualize the vector defined by the first eigenvector. To do this you need: - Use the PCA() function to recover the eigenvectors - Plot the centered data as done above - The first eigenvector is a 2D vector (x0,y0). This defines a vector with origin in (0,0) and head in (x0,y0). Use the function plot() from matplotlib to plot a line over the first eigenvector.

```
[73]: pca_eigvec, _ = pca(Y)
first_eigvec = pca_eigvec[0]

plt.scatter(Y[:,0],Y[:,1])

x = np.linspace(-5, 5, 1000)
y = first_eigvec[1]/first_eigvec[0] * x
plt.plot(x,y)
```

[73]: [<matplotlib.lines.Line2D at 0x19b814d5400>]

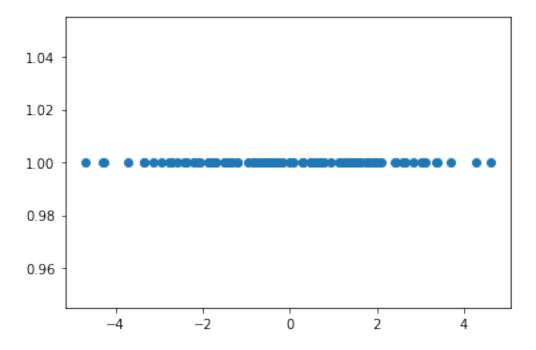


2.2.5 Visualize the PCA projection

Finally, use the PCA() algorithm to project on a single dimension and visualize the result using again the scatter() function.

```
[74]: _,P = pca(Y, 1)
plt.scatter(P,np.ones(P.shape[0]))
```

[74]: <matplotlib.collections.PathCollection at 0x19b801f9a00>



2.3 Evaluation: when are the results of PCA sensible?

So far we have used PCA on synthetic data. Let us now imagine we are using PCA as a preprocessing step before a classification task. This is a common setup with high-dimensional data. We explore when the use of PCA is sensible.

2.3.1 Loading the first set of labels

The function $get_synthetic_data_with_labels1()$ from the module syntethicdata provides a first labeled dataset.

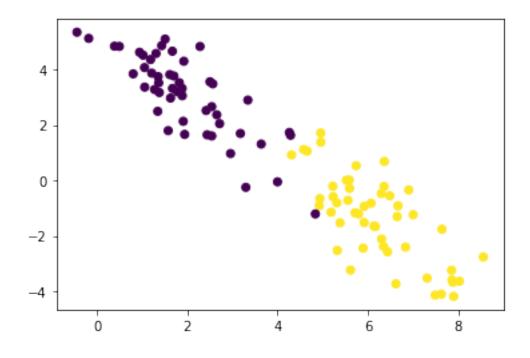
2.3.2 Running PCA

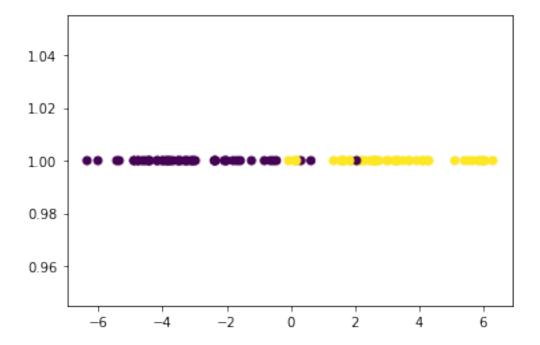
Process the data using the PCA algorithm and project it in one dimension. Plot the labeled data using *scatter()* before and after running PCA. Comment on the results.

```
[76]: plt.scatter(X[:,0], X[:,1], c=y[:,0])

plt.figure()
Y, _ = center_data(X)
_,P = pca(Y, 1)
plt.scatter(P,np.ones(P.shape[0]),c=y[:,0])
```

[76]: <matplotlib.collections.PathCollection at 0x19b80fa8d00>





Comment: The values are all grouped quite nicely so collapsing it onto one dimension makes it easier to understand the data.

2.3.3 Loading the second set of labels

The function $get_synthetic_data_with_labels2()$ from the module syntethicdata provides a second labeled dataset.

```
[77]: X,y = syntheticdata.get_synthetic_data_with_labels2()
```

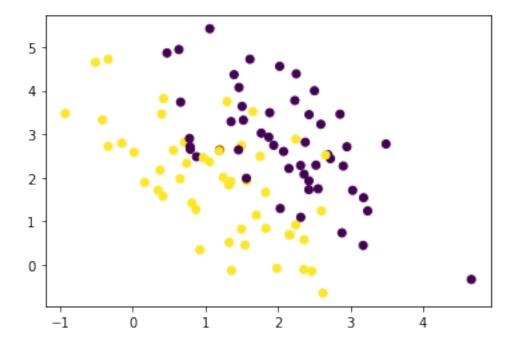
2.3.4 Running PCA

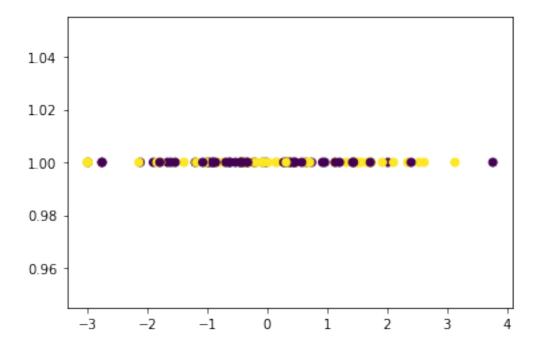
As before, process the data using the PCA algorithm and project it in one dimension. Plot the labeled data using *scatter()* before and after running PCA. Comment on the results.

```
[78]: plt.scatter(X[:,0], X[:,1], c=y[:,0])

plt.figure()
Y, _ = center_data(X)
_,P = pca(Y, 1)
plt.scatter(P,np.ones(P.shape[0]),c=y[:,0])
```

[78]: <matplotlib.collections.PathCollection at 0x19b825086a0>





Comment: In this example, with this data, this method doesn't work particularly well, the data is too indistiguishable.

How would the result change if you were to consider the second eigenvector? Or if you were to consider both eigenvectors?

Answer: Enter your answer here.

2.4 Case study 1: PCA for visualization

We now consider the *iris* dataset, a simple collection of data (N=150) describing iris flowers with four (M=4) features. The features are: Sepal Length, Sepal Width, Petal Length and Petal Width. Each sample has a label, identifying each flower as one of 3 possible types of iris: Setosa, Versicolour, and Virginica.

Visualizing a 4-dimensional dataset is impossible; therefore we will use PCA to project our data in 2 dimensions and visualize it.

2.4.1 Loading the data

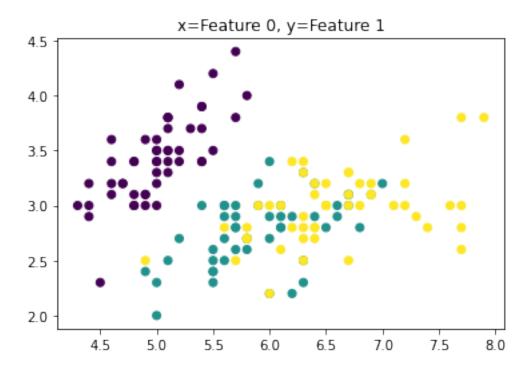
The function $get_iris_data()$ from the module syntethicdata returns the iris dataset. It returns a data matrix of dimension [150x4] and a label vector of dimension [150].

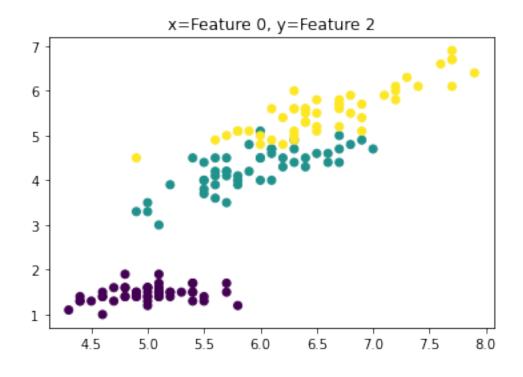
2.4.2 Visualizing the data by selecting features

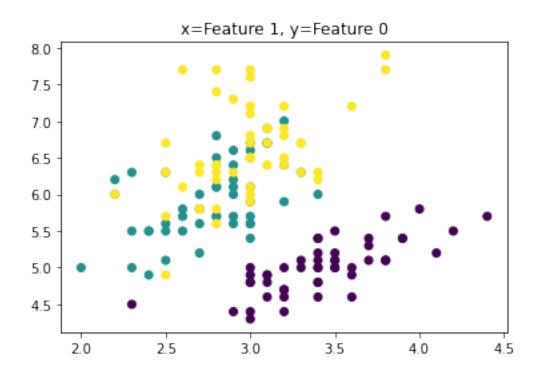
Try to visualize the data (using label information) by randomly selecting two out of the four features of the data. You may try different pairs of features.

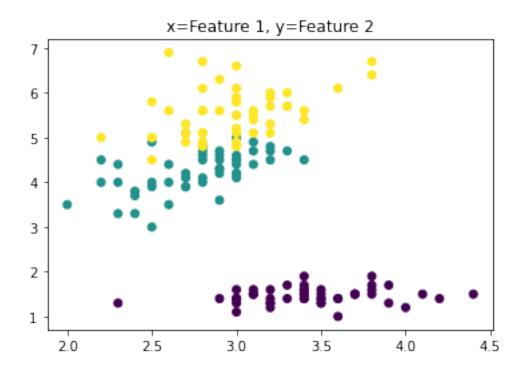
```
[80]: for i in range(3):
    for j in range(3):
        if i == j:
            continue

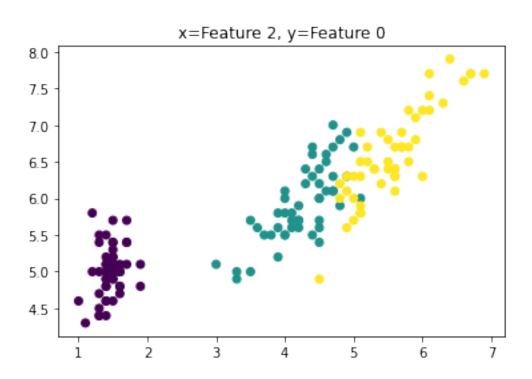
        plt.scatter(X[:,i], X[:,j], c=y)
        plt.title(f'x=Feature {i}, y=Feature {j}')
        plt.figure()
```

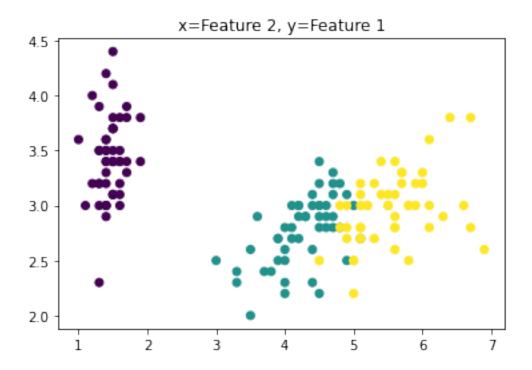












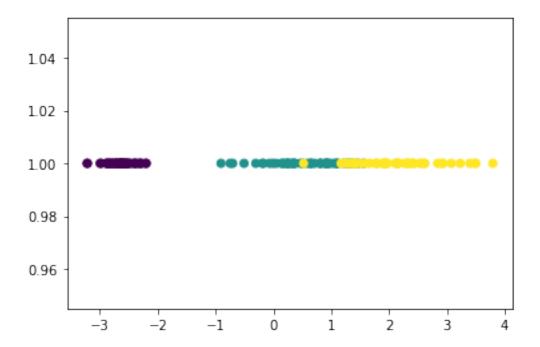
<Figure size 432x288 with 0 Axes>

2.4.3 Visualizing the data by PCA

Process the data using PCA and visualize it (using label information). Compare with the previous visualization and comment on the results.

```
[81]: Y, _ = center_data(X)
_,P = pca(Y, 1)
plt.scatter(P,np.ones(P.shape[0]),c=y)
```

[81]: <matplotlib.collections.PathCollection at 0x19be677e820>



Comment: Enter your comment here.

2.5 Case study 2: PCA for compression

We now consider the faces in the wild (lfw) dataset, a collection of pictures (N=1280) of people. Each pixel in the image is a feature (M=2914).

2.5.1 Loading the data

The function $get_lfw_data()$ from the module syntethicdata returns the lfw dataset. It returns a data matrix of dimension [1280x2914] and a label vector of dimension [1280]. It also returns two parameters, h and w, reporting the height and the width of the images (these parameters are necessary to plot the data samples as images). Beware, it might take some time to download the data. Be patient:)

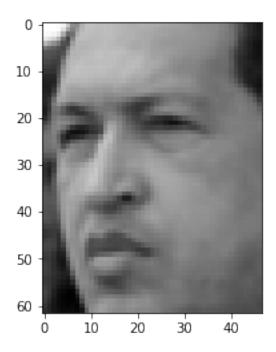
2.5.2 Inspecting the data

Choose one datapoint to visualize (first coordinate of the matrix X) and use the function $\operatorname{imshow}()$ to plot and inspect some of the pictures.

Notice that imshow receives as a first argument an image to be plot; the image must be provided as a rectangular matrix, therefore we reshape a sample from the matrix X to have height h and width w. The parameter cmap specifies the color coding; in our case we will visualize the image in black-and-white with different gradations of grey.

```
[83]: plt.imshow(X[0,:].reshape((h, w)), cmap=plt.cm.gray)
```

[83]: <matplotlib.image.AxesImage at 0x19b802df1f0>



2.5.3 Implementing a compression-decompression function

Implement a function that first uses PCA to project samples in low-dimensions, and the reconstruct the original image.

Hint: Most of the code is the same as the previous PCA() function you implemented. You may want to refer to *Marsland* to check out how reconstruction is performed.

```
[84]: def encode_decode_pca(A,m):
    # INPUT:
    # A    [NxM] numpy data matrix (N samples, M features)
    # m    integer number denoting the number of learned features (m <= M)
    #
    # OUTPUT:
    # Ahat [NxM] numpy PCA reconstructed data matrix (N samples, M features)

Y, mean = center_data(A)
    C = compute_covariance_matrix(Y)
    eigval, eigvec = compute_eigenvalue_eigenvectors(C)
    sorted_eigval, sorted_eigvec = sort_eigenvalue_eigenvectors(eigval, eigvec)

if m:</pre>
```

```
pca_eigvec = sorted_eigvec[:, :m] # reducing the matrix by m axis
else:
    pca_eigvec = sorted_eigvec

P = np.transpose(pca_eigvec) @ np.transpose(Y)

Ahat = np.transpose(P) @ np.transpose(pca_eigvec) + mean # reversing the
→projection of the eigenvalues and adding the mean back
return Ahat
```

2.5.4 Compressing and decompressing the data

Use the implemented function to encode and decode the data by projecting on a lower dimensional space of dimension 200 (m=200).

```
[85]: Xhat = encode_decode_pca(X,200)
```

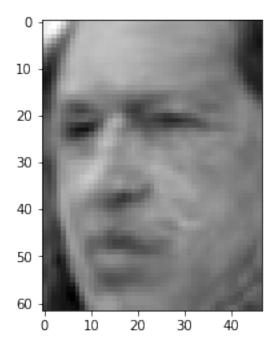
2.5.5 Inspecting the reconstructed data

Use the function *imshow* to plot and compare original and reconstructed pictures. Comment on the results.

```
[86]: print(Xhat.shape)
plt.imshow(Xhat[0,:].reshape((h, w)), cmap=plt.cm.gray)

(1288, 2914)
```

[86]: <matplotlib.image.AxesImage at 0x19b82619250>



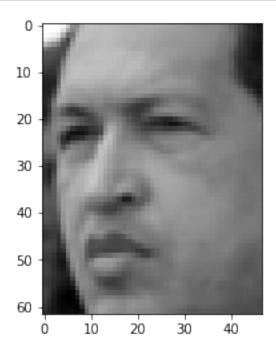
Comment: The man in the image is slightly disfigured.

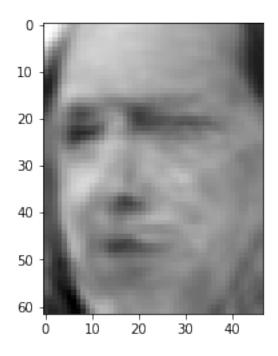
2.5.6 Evaluating different compressions

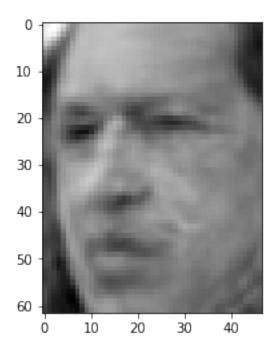
Use the previous setup to generate compressed images using different values of low dimensions in the PCA algorithm (e.g.: 100, 200, 500, 1000). Plot and comment on the results.

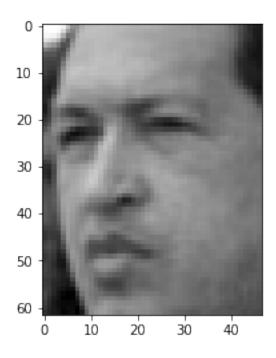
```
[87]: plt.imshow(X[0,:].reshape((h, w)), cmap=plt.cm.gray)

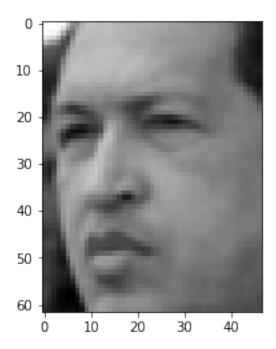
m_list = [100, 200, 500, 1000]
for i in m_list:
    plt.figure()
    Xhat = encode_decode_pca(X, i)
    plt.imshow(Xhat[0,:].reshape((h, w)), cmap=plt.cm.gray)
```











Comment: It's obvious that the fewer dimensions, the more data that is lost, and therefor the image becomes more disfigured.

3 K-Means Clustering (Bachelor and master students)

In this section you will use the k-means clustering algorithm to perform unsupervised clustering. Then you will perform a qualitative assessment of the results.

3.0.1 Importing scikit-learn library

We start importing the module *cluster.KMeans* from the standard machine learning library *scikit-learn*.

```
[]: from sklearn.cluster import KMeans
```

3.0.2 Loading the data

We will use once again the *iris* data set. The function $get_iris_data()$ from the module syntethic data returns the *iris* dataset. It returns a data matrix of dimension [150x4] and a label vector of dimension [150].

```
[93]: X,y = syntheticdata.get_iris_data()
```

3.0.3 Projecting the data using PCA

To allow for visualization, we project our data in two dimensions as we did previously. This step is not necessary, and we may want to try to use k-means later without the PCA pre-processing. However, we use PCA, as this will allow for an easy visualization.

```
[94]: _,P = pca(X)
```

3.0.4 Running k-means

We will now consider the *iris* data set as an unlabeled set, and perform clustering to this unlabeled set. We can compare the results of the clustering to the lableled calsses.

Use the class *KMeans* to fit and predict the output of the *k-means* algorithm on the projected data. Run the algorithm using the following values of $k = \{2, 3, 4, 5\}$.

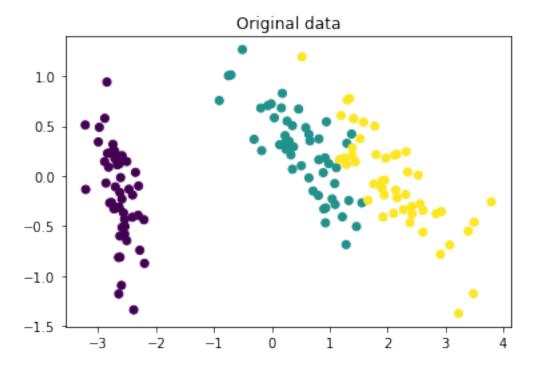
```
[]: k_list = [2, 3, 4, 5]
  yhat_list = []
  for i in k_list:
      KM = KMeans(i)
      yhat = KM.fit_predict(P)
      yhat_list.append(yhat)
```

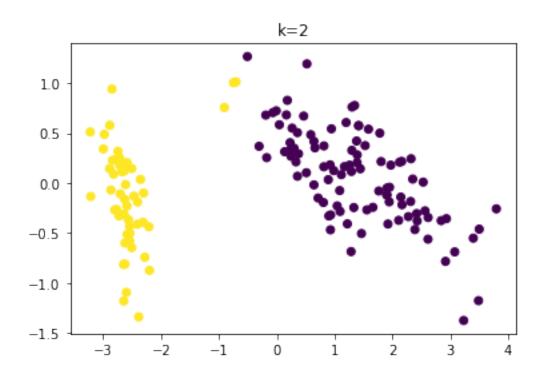
3.0.5 Qualitative assessment

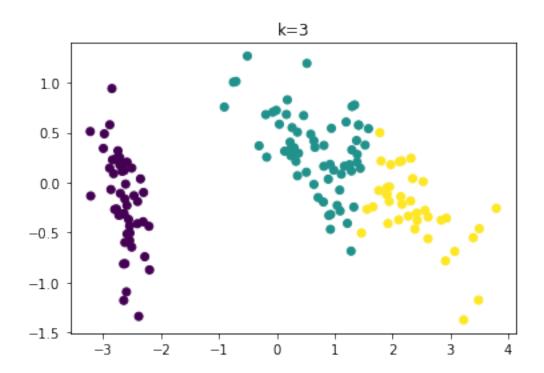
Plot the results of running the k-means algorithm, compare with the true labels, and comment.

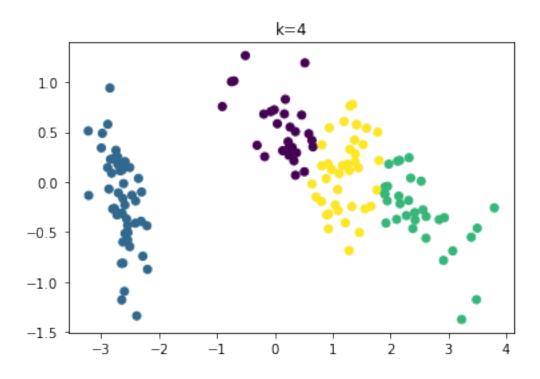
```
[104]: plt.figure()
   plt.scatter(P[:,0],P[:,1],c=y)
   plt.title('Original data')
```

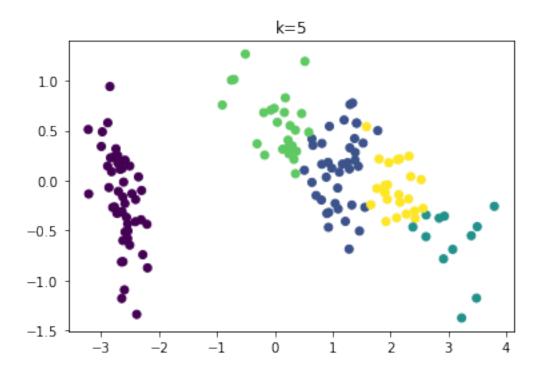
```
for i in range(len(k_list)):
   plt.figure()
   plt.scatter(P[:,0],P[:,1],c=yhat_list[i])
   plt.title(f'k={k_list[i]}')
```











Comment: I'm assuming that the group on the left and the group on the right that is turned into more and more different groups are two families of irises. All the 4 groups on the right must be

4 Quantitative Assessment of K-Means (Bachelor and master students)

We used k-means for clustering and we assessed the results qualitatively by visualizing them. However, we often want to be able to measure in a quantitative way how good the clustering was. To do this, we will use a classification task to evaluate numerically the goodness of the representation learned via k-means.

Reload the *iris* dataset. Import a standard LogisticRegression classifier from the module sklearn.linear_model. Use the k-means representations learned previously (yhat2,...,yhat5) and the true label to train the classifier. Evaluate your model on the training data (we do not have a test set, so this procedure will assess the model fit instead of generalization) using the accuracy_score() function from the *sklearn.metrics* module. Plot a graph showing how the accuracy score varies when changing the value of k. Comment on the results.

- Train a Logistic regression model using the first two dimensions of the PCA of the iris data set as input, and the true classes as targets.
- Report the model fit/accuracy on the training set.
- For each value of K:
 - One-Hot-Encode the classes output by the K-means algorithm.
 - Train a Logistic regression model on the K-means classes as input vs the real classes as targets.
 - Calculate model fit/accuracy vs. value of K.
- Plot your results in a graph and comment on the K-means fit.

```
[103]: from sklearn.linear model import LogisticRegression
       from sklearn import metrics
       from sklearn import preprocessing
       import matplotlib.pyplot as plt
       _{,P} = pca(X, 2)
       log_cl = LogisticRegression()
       log_cl.fit(P, y)
       pca_score = metrics.accuracy_score(log_cl.predict(P), y)
       print(f'Accuracy of PCA is {pca_score*100:.2f}%.')
       acc_list = []
       for i in range(len(k list)):
           OHE = preprocessing.OneHotEncoder()
           yhat OHE = OHE.fit transform(yhat list[i].reshape(-1, 1))
           K_means_class = LogisticRegression()
           K means class.fit(yhat OHE, y)
           score = metrics.accuracy_score(K_means_class.predict(yhat_OHE), y)
           acc_list.append(score)
           print(f'Accuracy with {k_list[i]}-clusters is {score*100:.2f}%.')
```

```
plt.plot(k_list, acc_list)
plt.ylabel('Accuracy')
plt.xlabel('k-clusters')
plt.show()
```

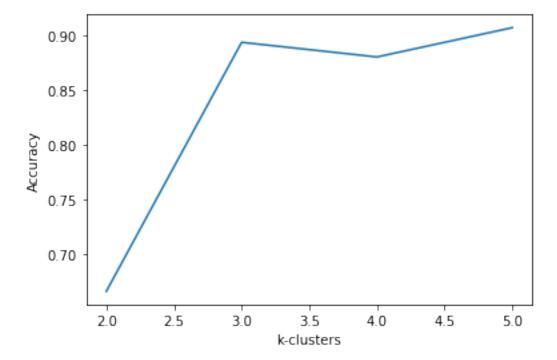
```
Accuracy of PCA is 96.67%.

Accuracy with 2-clusters is 66.67%.

Accuracy with 3-clusters is 89.33%.

Accuracy with 4-clusters is 88.00%.

Accuracy with 5-clusters is 90.67%.
```



Comment: In general the trend is positive, which i would expect; the more categories, the more accurate the machine can be, but why there is a slight drop at 4 is beyond me.

5 Conclusions

In this notebook we studied **unsupervised learning** considering two important and representative algorithms: **PCA** and **k-means**.

First, we implemented the PCA algorithm step by step; we then run the algorithm on synthetic data in order to see its working and evaluate when it may make sense to use it and when not. We then considered two typical uses of PCA: for **visualization** on the *iris* dataset, and for **compression-decompression** on the *lfw* dateset.

We then moved to consider the k-means algorithm. In this case we used the implementation provided by *scikit-learn* and we applied it to another prototypical unsupervised learning problem: **clustering**; we used *k-means* to process the *iris* dataset and we evaluated the results visually.

In the final part, we considered two additional questions that may arise when using the above algorithms. For PCA, we considered the problem of **selection of hyper-parameters**, that is, how we can select the hyper-parameter of ou algorithm in a reasonable fashion. For k-means, we considered the problem of the **quantitative evaluation** of our results, that is, how can we measure the performance or usefulness of our algorithms.