Assignment3

April 20, 2021

1 IN3050/IN4050 Mandatory Assignment 3, 2021: Unsupervised Learning

Name: Eirik Fredborg

Username: eefrebo

1.0.1 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.

1.1 Principal Component Analysis (PCA)

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

1.1.1 Principle of Maximum Variance: what is PCA supposed to do?

First of all, let us recall the principle/assumption of PCA:

- 1. What is the variance?
- 2. What is the covariance?
- 3. How do we compute the covariance matrix?
- 4. What is the meaning of the principle of maximum variance?
- 5. Why do we need this principle?
- 6. Does the principle always apply?

Variance is a measure of how much the data varies within its own parameter dimension. Covariance is the degree of variation for one parameter dimension with respect to another. We compute the covariance matrix using the realtion:

$$\mathbf{C} = \frac{1}{N} \mathbf{X}^T \mathbf{X}$$

Where \mathbf{X} is a vector containing N datapoints with some number of features. The principle of maximum variance is that when compressing the data into fewer dimensions one projects the data into a dimension that will result in the largest variance.

1.2 Implementation: how is PCA implemented?

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

1.2.1 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.

```
[1]: import numpy as np
  from numpy import newaxis as nax
  import matplotlib.pyplot as plt
  plt.rcParams['font.size'] = 16

import syntheticdata
```

1.2.2 Centering the Data

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

```
[2]: def center_data(A):
    # INPUT:
    # A    [NxM] numpy data matrix (N samples, M features)
#
# OUTPUT:
    # X    [NxM] numpy centered data matrix (N samples, M features)
    return A - np.mean(A,0)[nax]
```

Test your function checking the following assertion on testcase:

```
[3]: 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), answer)
```

1.2.3 Computing Covariance Matrix

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

```
[4]: def compute_covariance_matrix(A):
    # INPUT:
    # A    [NxM] centered numpy data matrix (N samples, M features)
    #
    # OUTPUT:
    # C    [MxM] numpy covariance matrix (M features, M features)
    #
    # Do not apply centering here. We assume that A is centered before this
    →function is called.
    return 1/A.shape[0]*(A.T@A)
```

Test your function checking the following assertion on testcase:

1.2.4 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!

```
[6]: def compute_eigenvalue_eigenvectors(A):
    # INPUT:
    # A [DxD] numpy matrix (not NxD?)
    #
# 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:

```
[7]: 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)
```

1.2.5 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].

```
[8]: 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
                           [DxD] numpy array of eigenvectors
         # sorted_eigvec
        sorted_eigval = np.flip(np.sort(eigval)) # sorting from large to small
        #looping over the sorted eigenvalues and and sorting the eigenvectors by \Box
      → pairing them to their eigenvalues
         sorted_eigvec = np.array(([(eigvec[:,np.where(eigval == val)[0][0]])).
      →tolist() for val in sorted_eigval])).T
        return sorted_eigval, sorted_eigvec
```

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

```
[9]: 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)
```

1.2.6 PCA Algorithm

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

```
[10]: def pca(A,m, test=False):
          # INPUT:
          # A
                  [NxM] numpy data matrix (N samples, M features)
                 integer number denoting the number of learned features (m <= M)
          # OUTPUT:
          # pca_eiqvec
                          [Mxm] numpy matrix containing the eigenvectors (M_{\perp})
       \rightarrow dimensions, m eigenvectors)
                           [Nxm] numpy PCA data matrix (N samples, m features)
          cov = compute_covariance_matrix(A)
          eigval, eigvec = compute_eigenvalue_eigenvectors(cov) # computing eigvals_
       \rightarrow and eigrecs from cov matrix
          sorted_eigval, sorted_eigvec = sort_eigenvalue_eigenvectors(eigval, eigvec)
          if test== True:
              pca_eigvec = np.array((eigvec[:,0], eigvec[:,-1])).T
              pca_eigvec = sorted_eigvec[:,:m]
          P = A@pca_eigvec
          return pca_eigvec, P
```

Test your function checking the following assertion on testcase:

```
np.testing.assert_almost_equal(test_arr_y, 0)
```

```
Traceback (most recent call last)
AssertionError
<ipython-input-11-f161f8f63838> in <module>
     10 test_arr_y = np.sum(np.abs(np.abs(y) - np.abs(answer2)))
---> 12 np.testing.assert_almost_equal(test_arr_y, 0)
~/miniconda3/lib/python3.8/site-packages/numpy/testing/_private/utils.py in_
→assert_almost_equal(actual, desired, decimal, err_msg, verbose)
    593
    594
            if abs(desired - actual) \geq= 1.5 * 10.0**(-decimal):
                raise AssertionError( build err msg())
--> 595
    596
    597
AssertionError:
Arrays are not almost equal to 7 decimals
 ACTUAL: 52.699620491992164
 DESIRED: 0
```

The pca function is given an extra feature to make it work with the test case which happens to have two equal eigenvalues. After some trial and error i just made the function chose the eigenvector that made the test for eigenvectors work. I did however not make it work for the pca matrix.

1.3 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.

1.3.1 Loading the data

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

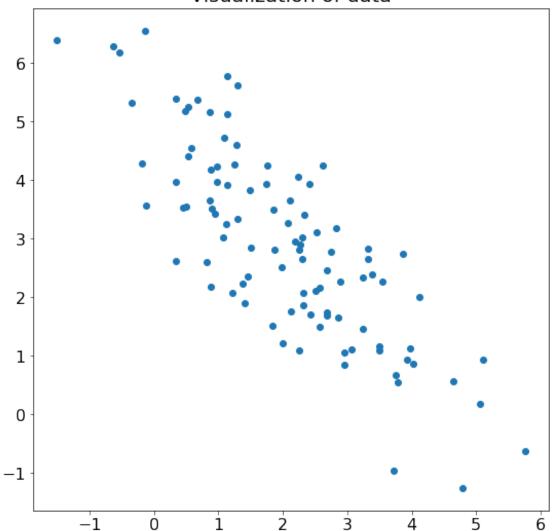
```
[12]: X = syntheticdata.get_synthetic_data1()
```

1.3.2 Visualizing the data

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

```
[13]: plt.figure(figsize=(9,9))
   plt.title('Visualization of data')
   plt.scatter(X[:,0],X[:,1])
   plt.show()
```

Visualization of data

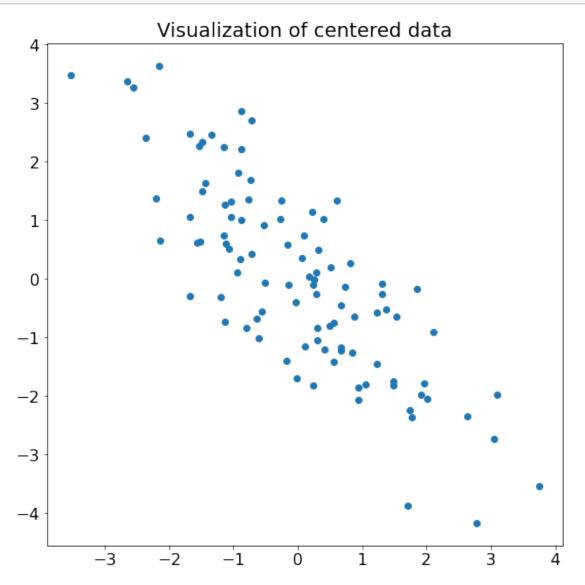


Above we have a simple scatter plot to visualize the data.

1.3.3 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.

```
[14]: X = center_data(X)
    plt.figure(figsize=(9,9))
    plt.title('Visualization of centered data')
    plt.scatter(X[:,0],X[:,1])
    plt.show()
```

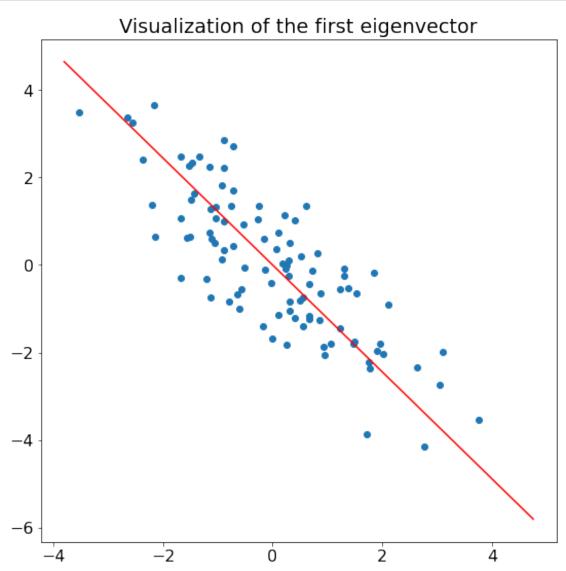


The data is centered and visualized again.

1.3.4 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.

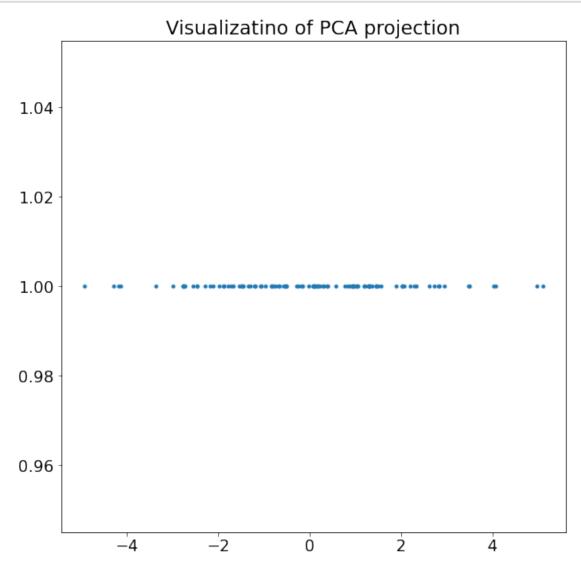


The first eigenvector spanning the dimension which results in the maximal variance is presented above.

1.3.5 Visualize the PCA projection

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

```
[16]: P = pca(X,1)[1]
   plt.figure(figsize=(9,9))
   plt.title('Visualizatino of PCA projection')
   plt.plot(P,np.ones(len(P)), '.')
   plt.show()
```



In the figure above we see the data presented after being projected into the dimension of maximum variance.

1.4 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.

1.4.1 Loading the first set of labels

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

```
[17]: X,y = syntheticdata.get_synthetic_data_with_labels1()
```

1.4.2 Running PCA

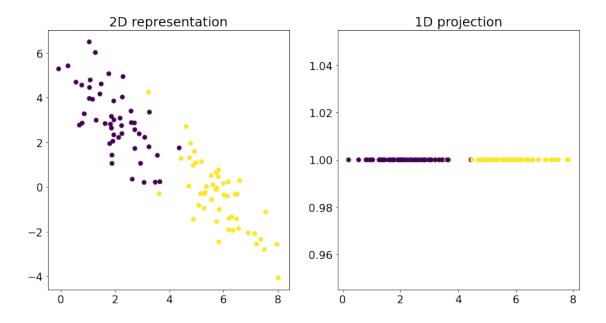
Process the data using the PCA algorithm and project it in one dimension. Plot the labeled data using scatter() before and after running PCA. Comment on the results.

```
[18]: plt.figure(figsize=(14,7))

plt.subplot(121)
plt.title('2D representation')
plt.scatter(X[:,0],X[:,1],c=y[:,0])

P = pca(X,1)[1]
plt.subplot(122)
plt.title('1D projection')
plt.scatter(P,np.ones(P.shape[0]),c=y[:,0])

plt.show()
```



On the left we have the raw 2D representation of the data, while on the right the data are projected into one dimension before visualized. The two classes appear to be separated and should be quite simple to classify.

1.4.3 Loading the second set of labels

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

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

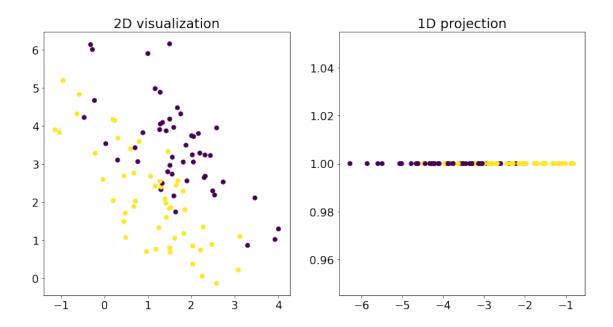
1.4.4 Running PCA

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.

```
plt.figure(figsize=(14,7))

plt.subplot(121)
plt.title('2D visualization')
plt.scatter(X[:,0],X[:,1],c=y[:,0])

plt.subplot(122)
plt.title('1D projection')
P = pca(X,1)[1]
plt.scatter(P,np.ones(P.shape[0]),c=y[:,0])
plt.show()
```



As apposed to the previous data set which could easly be saparated in the projected dimension, this dataset happens to be oriented in such a way that a projection into the dimension resulting in maximum variance will make the classification much harder.

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

The two classes would be much simpler to distinguish if the data were projected into the second eigenvector.

1.5 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.

1.5.1 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].

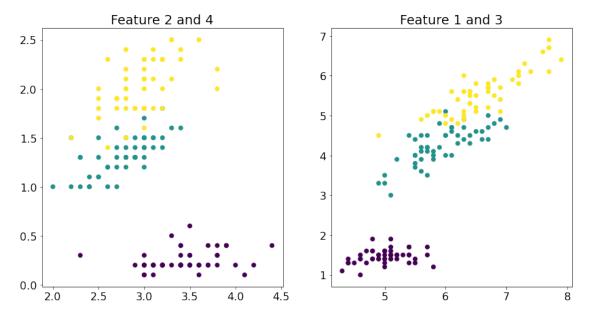
1.5.2 Visualizing the data by selecting features

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.

```
[22]: plt.figure(figsize = (14,7))
  plt.subplot(121)
  plt.title('Feature 2 and 4')
  plt.scatter(X[:,1], X[:,3], c = y[:])

plt.subplot(122)
  plt.title('Feature 1 and 3')
  plt.scatter(X[:,0], X[:,2], c = y[:])

plt.show()
```



Feature 2 and 4 are visialized in the left figure, while feature 1 and 3 are visualized in the right figure. The data appears to be distributed with a regular distanse between the datapoints.

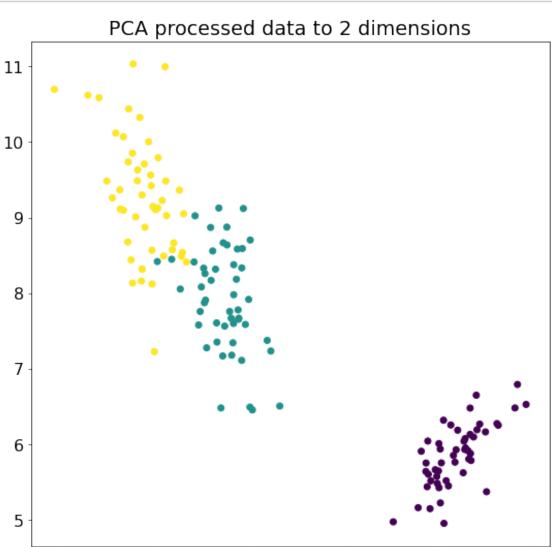
1.5.3 Visualizing the data by PCA

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

```
[23]: P = pca(X,2)[1]

plt.figure(figsize=(9,9))
plt.title('PCA processed data to 2 dimensions')
```

plt.scatter(P[:,1],P[:,0], c=y[:])
plt.show()



The four features are compressed down to two features using the PCA method. The visualization above does not show the same regular distribution as before. The yellow and green feature has some overlap just as before the data were compressed.

Ó

i

Ż

3

1.6 Case study 2: PCA for compression

-1

-2

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).

1.6.1 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:)

```
[24]: X,y,h,w = syntheticdata.get_lfw_data()
```

1.6.2 Inspecting the data

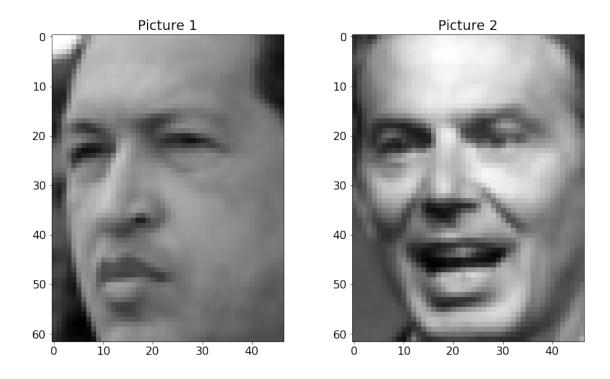
Choose one datapoint to visualize (first coordinate of the matrix X) and use the function imshow() to plot and inspect some of the pictures.

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.

```
[25]: plt.figure(figsize = (14,8))
   plt.subplot(121)
   plt.title('Picture 1')
   plt.imshow(X[0,:].reshape((h, w)), cmap=plt.cm.gray)

   plt.subplot(122)
   plt.title('Picture 2')
   plt.imshow(X[1,:].reshape((h, w)), cmap=plt.cm.gray)

   plt.show()
```



The two first pixels are presented above and we can they contain the picture of faces.

1.6.3 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.

1.6.4 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).

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

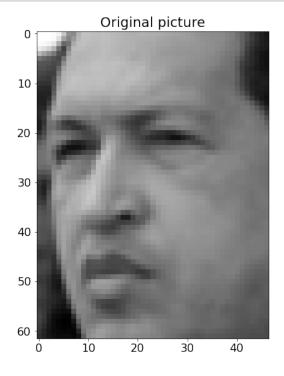
1.6.5 Inspecting the reconstructed data

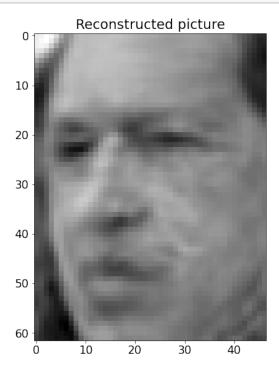
Use the function imshow to plot and compare original and reconstructed pictures. Comment on the results.

```
[28]: plt.figure(figsize = (14,8))
  plt.subplot(121)
  plt.title('Original picture')
  plt.imshow(X[0,:].reshape((h, w)), cmap=plt.cm.gray)

plt.subplot(122)
  plt.title('Reconstructed picture')
  plt.imshow(Xhat[0,:].reshape((h, w)), cmap=plt.cm.gray)

plt.show()
```





We see that the reconstructed picture loses some information, especially in the area were neighbouring pixels are similar. The compression-decompression also seem to smoothe away some of the

contrast.

1.6.6 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.

```
[29]: m_arr = np.array((100,200,500,1000))
    plt.figure(figsize = (14,14))
    plt.subplot(221)

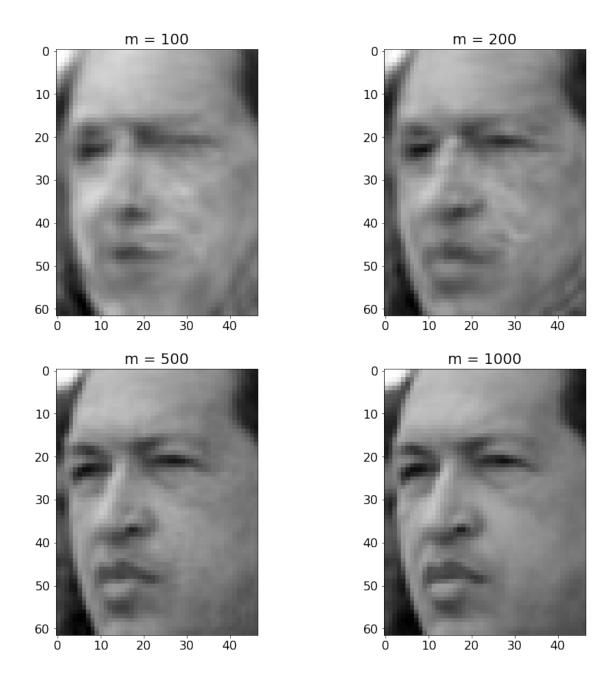
plt.title(f'm = {m_arr[0]}')
    plt.imshow(encode_decode_pca(X,m_arr[0])[0,:].reshape((h, w)), cmap=plt.cm.gray)

plt.subplot(222)
    plt.title(f'm = {m_arr[1]}')
    plt.imshow(encode_decode_pca(X,m_arr[1])[0,:].reshape((h, w)), cmap=plt.cm.gray)

plt.subplot(223)
    plt.title(f'm = {m_arr[2]}')
    plt.imshow(encode_decode_pca(X,m_arr[2])[0,:].reshape((h, w)), cmap=plt.cm.gray)

plt.subplot(224)
    plt.title(f'm = {m_arr[3]}')
    plt.title(f'm = {m_arr[3]}')
    plt.imshow(encode_decode_pca(X,m_arr[3])[0,:].reshape((h, w)), cmap=plt.cm.gray)

plt.show()
```



When comparing the figures above to the original uncompressed image, it appears that m=1000 has not appearant loss of information. The case of m=500 might have some slight loss in the smooth areas. This indicate that to compress down to m=1000 features might be effective.

2 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.

2.0.1 Importing scikit-learn library

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

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

2.0.2 Loading the data

We will use once again the *iris* data set. 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].

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

2.0.3 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.

```
[32]: P = pca(X, m = 2)[1]
```

2.0.4 Running k-means

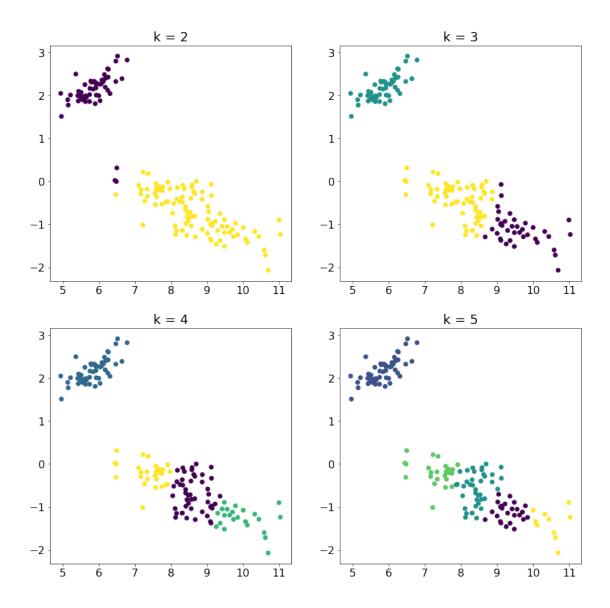
We will now consider the *iris* data set as an unlabeled set, and perform clustering to this unlabeled set. We can compare the results of the clustering to the labeled calsses.

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 $k = \{2, 3, 4, 5\}$.

2.0.5 Qualitative assessment

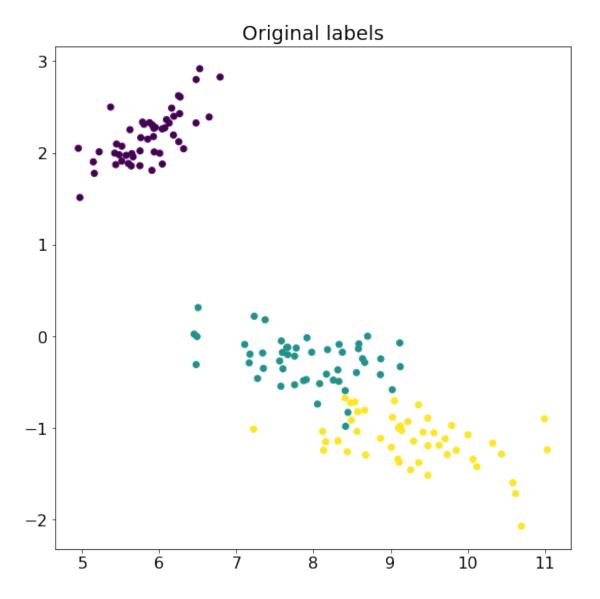
Plot the results of running the k-means algorithm, compare with the true labels, and comment.

```
[33]: k_arr = np.array((2,3,4,5))
plt.figure(figsize=(14,14))
for i,k in enumerate(k_arr):
    KM = KMeans(n_clusters=k)
    yhat = KM.fit_predict(P)
    plt.subplot(2,2,i+1)
    plt.title(f'k = {k}')
    plt.scatter(P[:,0], P[:,1], c = yhat[:])
```



The results of the K-means clustering for k = [2, 3, 4, 5] clusters are presented above.

```
[34]: plt.figure(figsize=(9,9))
   plt.title('Original labels')
   plt.scatter(P[:,0], P[:,1], c = y[:])
   plt.show()
```



The dataset with its original labels is presented above. When comparing to the results of the K-means clustering it is obvious that the case og k=3 is most similar to the original labeling. This being the only case where the number of clusters is the same it is not that surprising. This being the case makes it hard for me to understand the point of this comparison.

3 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 outputed 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.

```
[35]: from sklearn.linear_model import LogisticRegression from sklearn import metrics
```

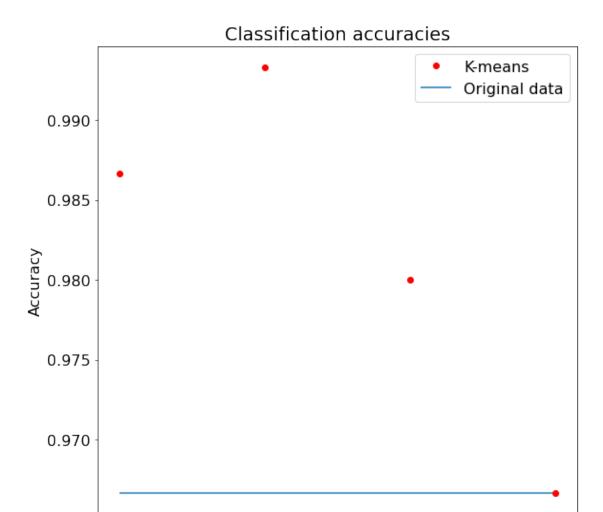
```
[36]: X,y = syntheticdata.get_iris_data()
P = pca(X, m = 2)[1]
```

The accuracy of the training set using the true labels as targets is: 0.9666666666666667

```
[38]: accuracies = np.zeros(len(k_arr))

for i, k in enumerate(k_arr):
    KM = KMeans(n_clusters=k)
    yhat = KM.fit_predict(P)
    clf = LogisticRegression(random_state=0, max_iter = 1e3).fit(P, yhat)
    accuracies[i] = metrics.accuracy_score(yhat, clf.predict(P))
```

```
[39]: plt.figure(figsize=(9,9))
   plt.title('Classification accuracies')
   plt.hlines(acc, 2,5, label='Original data')
   plt.plot(k_arr,accuracies, 'ro', label='K-means')
   plt.ylabel('Accuracy')
   plt.xlabel('Number of clusters')
   plt.legend()
   plt.show()
```



I was very confused when solving this problem. I'm not sure at all if I've solved it correctly, but this was the only way I could find to solve it and actually get presentable results. As far as I can tell the accuracy function does not measure the accuracy with respect to the "true" labels for various k. This not being the case I don's see what the point of this problem is, which again leads me to belive I have misunderstood the problem.

3.5

Number of clusters

4.5

5.0

4.0

3.0

2.5

2.0