ECE-CS 5424 Assignment 4

April 11, 2019

1 ECE-5424 / CS-5824 Advanced Machine Learning

2 Assignment 4: K-means Clustering and Principal Component Analysis

2.1 Submission guideline

- 1. Click the Save button at the top of the Jupyter Notebook.
- 2. Please make sure to have entered your Virginia Tech PID below.
- 3. Select Cell -> All Output -> Clear. This will clear all the outputs from all cells (but will keep the content of ll cells).
- 4. Select Cell -> Run All. This will run all the cells in order.
- 5. Once you've rerun everything, select File -> Download as -> PDF via LaTeX
- 6. Look at the PDF file and make sure all your solutions are there, displayed correctly.
- 7. Zip the all the files along with this notebook (Please don't include the data)
- 8. Submit your zipped file and the PDF INDEPENDENTLY.

2.1.1 Please Write Your VT PID Here: 906208012

2.2 Introduction

In this assignment, you will implement the K-means clustering algorithm and apply it to compress an image. In the second part, you will use principal component analysis to find a low-dimensional representation of face images. We will use the following packages/libraries (as always): - numpy - matplotlib - scipy

All the materials here are modified from Stanford CS 229 and Andrew Ng's Machine Learning Course.

```
plt.rcParams["animation.html"] = "jshtml"
except ValueError:
   plt.rcParams["animation.html"] = "html5"

# will be used to load MATLAB mat datafile format from scipy.io import loadmat
# utility functions

%load_ext autoreload
%autoreload 2
%matplotlib inline
```

2.3 Section 1. K-means Clustering [50 pts]

In this exercise, you will implement K-means algorithm and use it for image compression. You will first start on an example 2D dataset that will help you gain an intuition of how the K-means algorithm works. After that, you wil use the K-means algorithm for image compression by reducing the number of colors that occur in an image to only those that are most common in that image.

2.3.1 1.1 Implementing K-means [35 pts]

The K-means algorithm is a method to automatically cluster similar data examples together. Concretely, you are given a training set $\{x^{(1)}, \cdots, x^{(m)}\}$ (where $x^{(i)} \in \mathbb{R}^n$), and want to group the data into a few cohesive "clusters". The intuition behind K-means is an iterative procedure that starts by guessing the initial centroids, and then refines this guess by repeatedly assigning examples to their closest centroids and then recomputing the centroids based on the assignments.

The K-means algorithm is as follows:

```
centroids = init_kmeans_centroids(X, K)
for i in range(iterations):
    # Cluster assignment step: Assign each data point to the
    # closest centroid. idx[i] corresponds to c(i), the index
    # of the centroid assigned to example i
    idx = find_closest_centroids(X, centroids)

# Move centroid step: Compute means based on centroid
    # assignments
    centroids = compute_centroids(X, idx, K)
```

The inner-loop of the algorithm repeatedly carries out two steps: (1) Assigning each training example $x^{(i)}$ to its closest centroid, and (2) Recomputing the mean of each centroid using the points assigned to it. The K-means algorithm will always converge to some final set of means for the centroids. Note that the converged solution may not always be ideal and depends on the initial setting of the centroids. Therefore, in practice the K-means algorithm is usually run a few times with different random initializations. One way to choose between these different solutions from different random initializations is to choose the one with the lowest cost function value (distortion). You will implement the two phases of the K-means algorithm separately in the next sections.

1.1.1 Finding closest centroids [20 pts]

In the "cluster assignment" phase of the K-means algorithm, the algorithm assigns every training example $x^{(i)}$ to its closest centroid, given the current positions of centroids. Specifically, for every example i we set

$$c^{(i)} := j$$
 that minimizes $||x^{(i)} - \mu_j||^2$,

where $c^{(i)}$ is the index of the centroid that is closest to $x^{(i)}$, and μ_j is the position (value) of the j^{th} centroid. Note that $c^{(i)}$ corresponds to idx[i] in the starter code.

Your task is to complete the code in the function find_closest_centroids in kmeans.py. This function takes the data matrix X and the locations of all centroids inside centroids and should output a one-dimensional array idx that holds the index (a value in $\{1, ..., K\}$, where K is total number of centroids) of the closest centroid to every training example.

Once you have completed the code in find_closest_centroids, the following cell will run your code and you should see the output [0 2 1] corresponding to the centroid assignments for the first 3 examples.

```
In [2]: from kmeans import find_closest_centroids
        # Load an example dataset that we will be using
        data = loadmat(os.path.join('Data', 'ex7data2.mat'))
        X = data['X']
        print("Shape of X", X.shape)
        # Select an initial set of centroids
        K = 3 # 3 Centroids
        initial_centroids = np.array([[3, 3], [6, 2], [8, 5]])
        # Find the closest centroids for the examples using the initial_centroids
        idx = find_closest_centroids(X, initial_centroids)
        print('Closest centroids for the first 3 examples:')
        print(idx[:3])
        print('(the closest centroids should be 0, 2, 1 respectively)')
Shape of X (300, 2)
Closest centroids for the first 3 examples:
[0, 2, 1]
(the closest centroids should be 0, 2, 1 respectively)
```

1.1.2 Computing centroid means [15 pts]

Given assignments of every point to a centroid, the second phase of the algorithm recomputes, for each centroid, the mean of the points that were assigned to it. Specifically, for every centroid k we set

$$\mu_k := \frac{1}{|C_k|} \sum_{i \in C_k} x^{(i)}$$

where C_k is the set of examples that are assigned to centroid k. Concretely, if two examples say $x^{(3)}$ and $x^{(5)}$ are assigned to centroid k = 2, then you should update $\mu_2 = \frac{1}{2} \left(x^{(3)} + x^{(5)} \right)$.

You should now complete the function compute_centroids in kmeans.py. You can implement this function using a loop over the centroids. You can also use a loop over the examples; but if you can use a vectorized implementation that does not use such a loop, your code may run faster.

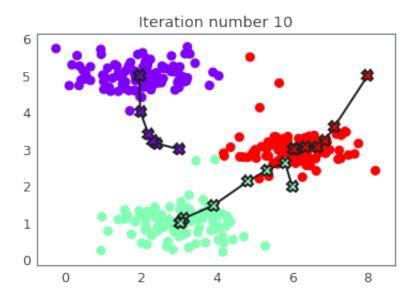
Once you have completed the code, the following cell will run your code and output the centroids after the first step of K-means.

```
In [3]: from kmeans import compute_centroids
        # Compute means based on the closest centroids found in the previous part.
        K = 3 # 3 Centroids
        centroids = compute_centroids(X, idx, K)
        print('Centroids computed after initial finding of closest centroids:')
        print(centroids)
        print('\nThe centroids should be')
        print(' [ 2.428301 3.157924 ]')
                [ 5.813503 2.633656 ]')
        print('
                [ 7.119387 3.616684 ]')
        print('
Centroids computed after initial finding of closest centroids:
[[2.42830111 3.15792418]
 [5.81350331 2.63365645]
 [7.11938687 3.6166844 ]]
The centroids should be
   [ 2.428301 3.157924 ]
   [ 5.813503 2.633656 ]
   [ 7.119387 3.616684 ]
```

2.3.2 1.2 K-means on example dataset [5 pts]

After you have completed the two functions (find_closest_centroids and compute_centroids), you have all the necessary pieces to run the K-means algorithm. The next cell will run the K-means algorithm on a toy 2D dataset to help you understand how K-means works. Your functions are called from inside the run_kmeans function (in utils.py module). We encourage you to take a look at the function to understand how it works. Notice that the code calls the two functions you implemented in a loop.

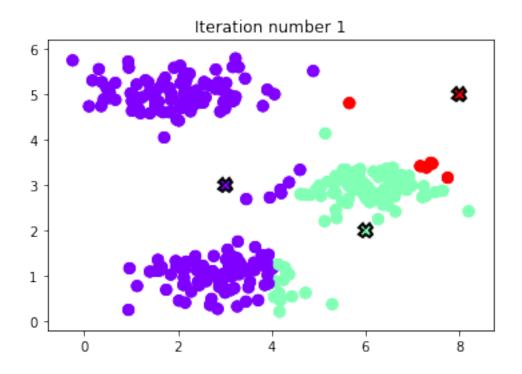
When you run the next step, the K-means code will produce an animation that steps you through the progress of the algorithm at each iteration. At the end, your figure should look as the one displayed below.



```
# Settings for running K-Means
        K = 3
        max_iters = 10
        # For consistency, here we set centroids to specific values
        # but in practice you want to generate them automatically, such as by
        # settings them to be random examples (as can be seen in
        # kMeansInitCentroids).
        initial_centroids = np.array([[3, 3], [6, 2], [8, 5]])
        # Run K-Means algorithm. The 'true' at the end tells our function to plot
        # the progress of K-Means
        from utils import run_kmeans
        centroids, idx, anim = run_kmeans(X, initial_centroids,
                                          find_closest_centroids,
                                          compute_centroids, max_iters, True)
        anim
Index is (utils) 300
Compute_Centroids size (3, 2)
```

```
Index is (utils) 300
Compute_Centroids size (3, 2)
```

Out[4]: <matplotlib.animation.FuncAnimation at 0x7fe26ab8a518>



2.3.3 1.3 Random initialization [5 pts]

The initial assignments of centroids for the example dataset in the previous cell were designed so that you will see the same figure as that shown in the cell above. In practice, a good strategy for initializing the centroids is to select random examples from the training set.

In this part of the exercise, you should complete the function init_kmeans_centroids in kmeans.py with the following code:

```
# Initialize the centroids to be random examples
```

Randomly reorder the indices of examples

```
randidx = np.random.permutation(X.shape[0])
# Take the first K examples as centroids
centroids = X[randidx[:K], :]
```

The code above first randomly permutes the indices of the examples (using permute within the np.random module). Then, it selects the first *K* examples based on the random permutation of the indices. This allows the examples to be selected at random without the risk of selecting the same example twice.

2.3.4 1.4 Image compression with K-means [5 pts]

In this section, you will apply K-means to image compression. We will use the image below as an example.



In a straightfor-

ward 24-bit color representation of an image, each pixel is represented as three 8-bit unsigned integers (ranging from 0 to 255) that specify the red, green and blue intensity values. This encoding is often referred to as the RGB encoding. Our image contains thousands of colors, and in this part of the exercise, you will reduce the number of colors to 16 colors.

By making this reduction, it is possible to represent (compress) the photo in an efficient way. Specifically, you only need to store the RGB values of the 16 selected colors, and for each pixel in the image you now need to only store the index of the color at that location (where only 4 bits are

necessary to represent 16 possibilities).

In this exercise, you will use the K-means algorithm to select the 16 colors that will be used to represent the compressed image. Concretely, you will treat every pixel in the original image as a data example and use the K-means algorithm to find the 16 colors that best group (cluster) the pixels in the 3-dimensional RGB space. Once you have computed the cluster centroids on the image, you will then use the 16 colors to replace the pixels in the original image.

1.4.1 K-means on pixels In python, images can be read in as follows:

```
# Load 500x500 color image (small_clawed_otter.png)
img = mpl.image.imread(os.path.join('Data', 'small_clawed_otter.png'))
# We have already imported matplotlib as mpl at the beginning of this notebook.
```

This creates a three-dimensional matrix A whose first two indices identify a pixel position and whose last index represents red, green, or blue. For example, A[50, 33, 2] gives the blue intensity of the pixel at row 51 and column 34.

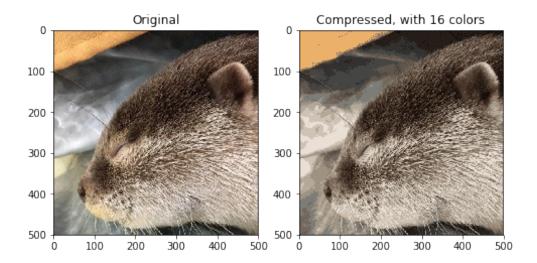
The code in the following cell first loads the image, and then reshapes it to create an m \times 3 matrix of pixel colors (where m = 250000 = 500 \times 500), and calls your K-means function on it.

After finding the top K = 16 colors to represent the image, you can now assign each pixel position to its closest centroid using the find_closest_centroids function. This allows you to represent the original image using the centroid assignments of each pixel. Notice that you have significantly reduced the number of bits that are required to describe the image. The original image required 24 bits for each one of the 128 x 128 pixel locations, resulting in total size of 500 x 500 x 24 = 6,000,000 bits. The new representation requires some overhead storage in form of a dictionary of 16 colors, each of which require 24 bits, but the image itself then only requires 4 bits per pixel location. The final number of bits used is therefore $16 \times 24 + 500 \times 500 \times 4 = 1,000,384$ bits, which corresponds to compressing the original image by about a factor of 6.

Finally, you can view the effects of the compression by reconstructing the image based only on the centroid assignments. Specifically, you can replace each pixel location with the mean of the centroid assigned to it. The figure below shows the reconstruction we obtained.

Even though the resulting image retains most of the characteristics of the original, we also see some compression artifacts.

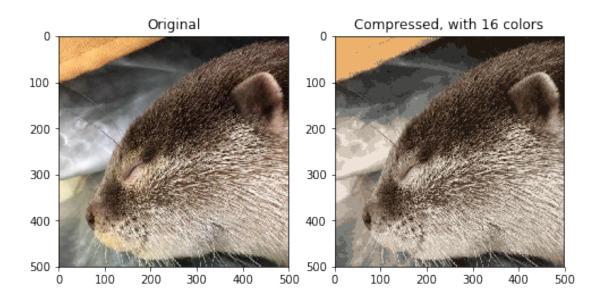
Run the following cell to compute the centroids and the centroid allocation of each pixel in the image.



```
X = A.reshape(-1, 3)
print('Shape of X', X.shape)
# When using K-Means, it is important to randomly initialize centroids
# You should complete the code in kMeansInitCentroids above before proceeding
from kmeans import init_kmeans_centroids
initial_centroids = init_kmeans_centroids(X, K)
print('Shape of initial centroids', initial_centroids.shape)
# Run K-Means
centroids, idx = run_kmeans(X, initial_centroids,
                                 find_closest_centroids,
                                 compute_centroids,
                                 max_iters)
# We can now recover the image from the indices (idx) by mapping each pixel
# (specified by its index in idx) to the centroid value
# Reshape the recovered image into proper dimensions
print('Final centroids',centroids.shape)
print('Size of indices',len(idx))
X_recovered = centroids[idx, :].reshape(A.shape)
fig, ax = plt.subplots(1, 2, figsize=(8, 4))
ax[0].imshow(A)
ax[0].set_title('Original')
ax[0].grid(False)
# Display compressed image, rescale back by 255
# and convert it back to uint8 image
ax[1].imshow(X_recovered)
ax[1].set_title('Compressed, with %d colors' % K)
```

ax[1].grid(False)

Shape of X (250000, 3) Shape of initial centroids (16, 3) Index is (utils) 250000 Compute_Centroids size (16, 3) Final centroids (16, 3) Size of indices 250000



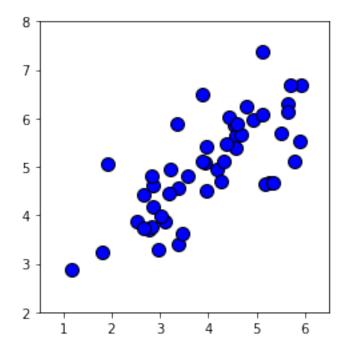
2.4 Section 2. Principal Component Analysis [50 pts]

In this exercise, you will use principal component analysis (PCA) to perform dimensionality reduction. You will first experiment with an example 2D dataset to get intuition on how PCA works, and then use it on a bigger dataset of 5000 face image dataset.

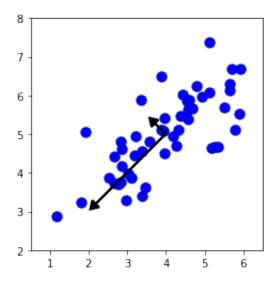
2.4.1 2.1 Example Dataset

To help you understand how PCA works, you will first start with a 2D dataset which has one direction of large variation and one of smaller variation. The cell below will plot the training data, also shown in here:

In this part of the exercise, you will visualize what happens when you use PCA to reduce the data from 2D to 1D. In practice, you might want to reduce data from 256 to 50 dimensions, say; but using lower dimensional data in this example allows us to visualize the algorithms better.



2.2 Implementing PCA [20 pts] In this part of the exercise, you will implement PCA. PCA consists of two computational steps:



- 1. Compute the covariance matrix of the data.
- 2. Use SVD (in python we use numpy's implementation np.linalg.svd) to compute the eigenvectors $U_1, U_2, ..., U_n$. These will correspond to the principal components of variation in the data.

First, you should compute the covariance matrix of the data, which is given by:

$$\Sigma = \frac{1}{m} X^T X$$

where *X* is the data matrix with examples in rows, and *m* is the number of examples. Note that Σ is a $n \times n$ matrix and not the summation operator.

After computing the covariance matrix, you can run SVD on it to compute the principal components. In python and numpy, you can run SVD with the following command: U, S, V = np.linalg.svd(Sigma), where U will contain the principal components and S will contain a diagonal matrix.

Your task here is to complete the fuction pca in pca.py.

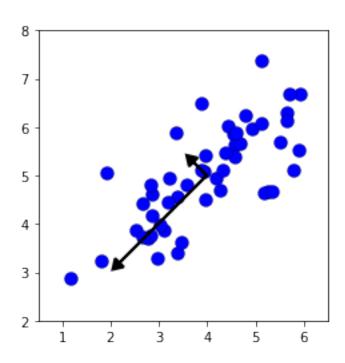
Before using PCA, it is important to first normalize the data by subtracting the mean value of each feature from the dataset, and scaling each dimension so that they are in the same range.

In the next cell, this normalization will be performed for you using the feature_normalize function in utils.py. After normalizing the data, you can run PCA to compute the principal components. Your task is to complete the code in the function pca to compute the principal components of the dataset.

Once you have completed the function pca, the following cell will run PCA on the example dataset and plot the corresponding principal components found similar to the figure below.

The following cell will also output the top principal component (eigenvector) found, and you should expect to see an output of about [-0.707 -0.707]. (It is possible that numpy may instead output the negative of this, since U_1 and $-U_1$ are equally valid choices for the first principal component.)

```
from pca import pca
        X_norm, mu, sigma = feature_normalize(X)
        # Run PCA
        U, S = pca(X_norm)
        # Draw the eigenvectors centered at mean of data. These lines show the
        # directions of maximum variations in the dataset.
        fig, ax = plt.subplots()
        ax.plot(X[:, 0], X[:, 1], 'bo', ms=10, mec='k', mew=0.25)
        for i in range(2):
            ax.arrow(mu[0], mu[1], 1.5 * S[i]*U[0, i], 1.5 * S[i]*U[1, i],
                     head_width=0.25, head_length=0.2, fc='k', ec='k', lw=2, zorder=1000)
        ax.axis([0.5, 6.5, 2, 8])
        ax.set_aspect('equal')
        ax.grid(False)
        print('Top\ eigenvector:\ U[:,\ 0] = [\{:.6f\}\ \{:.6f\}]'.format(U[0,\ 0],\ U[1,\ 0]))
        print(' (you should expect to see [-0.707107 -0.707107])')
Shape of covariance matrix (2, 2)
Top eigenvector: U[:, 0] = [-0.707107 -0.707107]
 (you should expect to see [-0.707107 -0.707107])
```



2.4.2 2.3 Dimensionality Reduction with PCA [20 pts]

After computing the principal components, you can use them to reduce the feature dimension of your dataset by projecting each example onto a lower dimensional space, $x^{(i)} \to z^{(i)}$ (e.g., projecting the data from 2D to 1D). In this part of the exercise, you will use the eigenvectors returned by PCA and project the example dataset into a 1-dimensional space. In practice, if you were using a learning algorithm such as linear regression or perhaps neural networks, you could now use the projected data instead of the original data. By using the projected data, you can train your model faster as there are less dimensions in the input.

2.3.1 Projecting the data onto the principal components [10 pts] You should now complete the function project_data in pca.py. Specifically, you are given a dataset X, the principal components U, and the desired number of dimensions to reduce to K. You should project each example in X onto the top K components in U. Note that the top K components in U are given by the first K columns of U, that is Ureduce = U[:, :K].

Once you have completed the code in project_data, the following cell will project the first example onto the first dimension and you should see a value of about 1.481 (or possibly -1.481, if you got $-U_1$ instead of U_1).

2.3.2 Reconstructing an approximation of the data [10 pts]

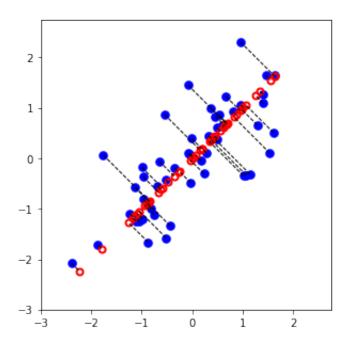
After projecting the data onto the lower dimensional space, you can approximately recover the data by projecting them back onto the original high dimensional space. Your task is to complete the function recover_data to project each example in Z back onto the original space and return the recovered approximation in X_rec.

Once you have completed the code in recover_data, the following cell will recover an approximation of the first example and you should see a value of about [-1.047 -1.047]. The code will then plot the data in this reduced dimension space. This will show you what the data looks like when using only the corresponding eigenvectors to reconstruct it. An example of what you should get for PCA projection is shown in this figure:

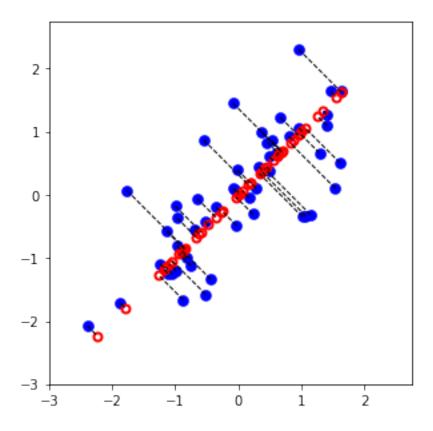
In the figure above, the original data points are indicated with the blue circles, while the projected data points are indicated with the red circles. The projection effectively only retains the information in the direction given by U_1 . The dotted lines show the distance from the data points in original space to the projected space. Those dotted lines represent the error measure due to PCA projection.

```
In [9]: from pca import recover_data

X_rec = recover_data(Z, U, K)
```



```
print('Approximation of the first example: [{:.6f}]'.format(X_rec[0, 0], X_rec[0,
        print('
                      (this value should be about [-1.047419 -1.047419])')
        # Plot the normalized dataset (returned from featureNormalize)
        fig, ax = plt.subplots(figsize=(5, 5))
        ax.plot(X_norm[:, 0], X_norm[:, 1], 'bo', ms=8, mec='b', mew=0.5)
        ax.set_aspect('equal')
        ax.grid(False)
        plt.axis([-3, 2.75, -3, 2.75])
        # Draw lines connecting the projected points to the original points
       ax.plot(X_rec[:, 0], X_rec[:, 1], 'ro', mec='r', mew=2, mfc='none')
        for xnorm, xrec in zip(X_norm, X_rec):
            ax.plot([xnorm[0], xrec[0]], [xnorm[1], xrec[1]], '--k', lw=1)
Shape of Z (50, 1)
Shape of U (2, 2)
Shape of Ureduce (2, 1)
Approximation of the first example: [-1.047419 -1.047419]
       (this value should be about [-1.047419 -1.047419])
```



2.4.3 2.4 Face Image Dataset [10 pts]

In this part of the exercise, you will run PCA on face images to see how it can be used in practice for dimension reduction. The dataset ex7faces.mat contains a dataset X of face images, each 32×32 in grayscale. This dataset was based on a cropped version of the labeled faces in the wild dataset. Each row of X corresponds to one face image (a row vector of length 1024).

The next cell will load and visualize the first 100 of these face images similar to what is shown in this figure:

```
In [10]: # Load Face dataset
    data = loadmat(os.path.join('Data', 'ex7faces.mat'))
    X = data['X']

# Display the first 100 faces in the dataset
    from utils import display_data
    display_data(X[:100, :], figsize=(8, 8))
```



Faces



2.4.1 PCA on Faces To run PCA on the face dataset, we first normalize the dataset by subtracting the mean of each feature from the data matrix X. After running PCA, you will obtain the principal components of the dataset. Notice that each principal component in V (each column) is a vector of length V (where for the face dataset, V = 1024). It turns out that we can visualize these principal components by reshaping each of them into a 32 \times 32 matrix that corresponds to the pixels in the original dataset.

The following cell will first normalize the dataset for you and then run your PCA code. Then, the first 36 principal components (conveniently called eigenfaces) that describe the largest variations are displayed. If you want, you can also change the code to display more principal components to see how they capture more and more details.

```
In [11]: # normalize X by subtracting the mean value from each feature
    X_norm, mu, sigma = feature_normalize(X)
```

```
# Run PCA
U, S = pca(X_norm)

# Visualize the top 36 eigenvectors found
display_data(U[:, :36].T, figsize=(8, 8))
```

Shape of covariance matrix (1024, 1024)



2.4.2 Dimensionality Reduction Now that you have computed the principal components for the face dataset, you can use it to reduce the dimension of the face dataset. This allows you to use your learning algorithm with a smaller input size (e.g., 100 dimensions) instead of the original 1024 dimensions. This can help speed up your learning algorithm.

The next cell will project the face dataset onto only the first 100 principal components. Concretely, each face image is now described by a vector $z^{(i)} \in \mathbb{R}^{100}$. To understand what is lost in the dimension reduction, you can recover the data using only the projected dataset.

In the next cell, an approximate recovery of the data is performed and the original and projected face images are displayed similar to what is shown here:

```
    <img src="Figures/faces_original.png" width="300">
    <id><img src="Figures/faces_reconstructed.png" width="300">
```

From the reconstruction, you can observe that the general structure and appearance of the face are kept while the fine details are lost. This is a remarkable reduction (more than 10x) in the dataset size that can help speed up your learning algorithm significantly. For example, if you were training a neural network to perform person recognition (given a face image, predict the identity of the person), you can use the dimension reduced input of only a 100 dimensions instead of the original pixels.

Original faces



Recovered faces



2.4.4 2.5 Optional (ungraded) exercise: PCA for visualization

In the earlier K-means image compression exercise, you used the K-means algorithm in the 3-dimensional RGB space. We reduced each pixel of the RGB image to be represented by 16 clusters. In the next cell, we have provided code to visualize the final pixel assignments in this 3D space. Each data point is colored according to the cluster it has been assigned to. You can drag your mouse on the figure to rotate and inspect this data in 3 dimensions.

```
X = A.reshape(-1, 3)
         # perform the K-means clustering again here
         K = 16
         max_iters = 10
         initial_centroids = init_kmeans_centroids(X, K)
         centroids, idx = run_kmeans(X, initial_centroids,
                                          find_closest_centroids,
                                          compute_centroids, max_iters)
         # Sample 1000 random indexes (since working with all the data is
         # too expensive. If you have a fast computer, you may increase this.
         sel = np.random.choice(X.shape[0], size=1000)
         print('Shape of sel', sel.shape)
         fig = plt.figure(figsize=(6, 6))
         ax = fig.add_subplot(111, projection='3d')
         #print('X[sel,0]',X[sel,0])
         print('idx[sel]',len(idx))
         print('sel',sel.shape)
         idx=np.array([idx])
         print(len(X[sel,0]))
         print(len(idx[0,sel]))
         ax.scatter(X[sel, 0], X[sel, 1], X[sel, 2], cmap='rainbow', c=idx[0,sel], s=8**2)
         ax.set_title('Pixel dataset plotted in 3D.\nColor shows centroid memberships')
         pass
Index is (utils) 250000
Compute_Centroids size (16, 3)
Index is (utils) 250000
```

A = mpl.image.imread(os.path.join('Data', 'small_clawed_otter.png'))

```
Compute_Centroids size (16, 3)
Index is (utils) 250000
Compute_Centroids size (16, 3)
Shape of sel (1000,)

<IPython.core.display.Javascript object>

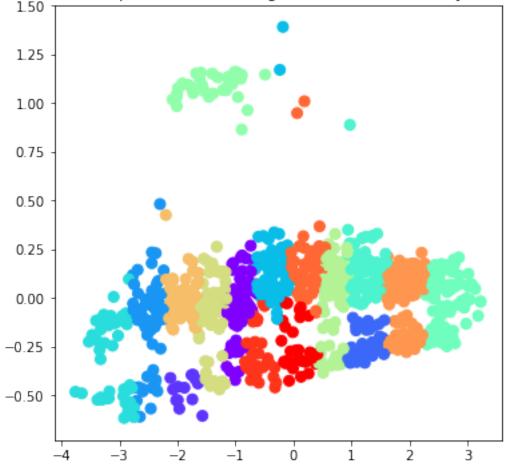
IPython.core.display.HTML object>

idx[sel] 250000
sel (1000,)
1000
1000
```

It turns out that visualizing datasets in 3 dimensions or greater can be cumbersome. Therefore, it is often desirable to only display the data in 2D even at the cost of losing some information. In practice, PCA is often used to reduce the dimensionality of data for visualization purposes.

In the next cell,we will apply your implementation of PCA to the 3-dimensional data to reduce it to 2 dimensions and visualize the result in a 2D scatter plot. The PCA projection can be thought of as a rotation that selects the view that maximizes the spread of the data, which often corresponds to the "best" view.





In []: