机器学习基础练习 7 - K-means 和PCA

在本次作业中，我们将进行K-means聚类和PCA降维的练习，并使用它们来压缩图像。

- 我们将从一个简单的2D数据集开始，以了解K-means是如何工作的，然后我们将其应用于图像压缩。
- 我们还将对PCA降维进行实验，了解如何使用它来找到人脸图像的低维表示。

1. K-means 聚类

为了可视化方便，我们将实施和应用K-means到一个简单的二维数据集，以获得工作原理的直观理解。K-means是一个迭代的，无监督的聚类算法，将类别相近的样本组合成簇。该算法从猜测每个簇的初始聚类中心开始，然后重复将样本分配给最近的簇，并重新计算该簇的聚类中心。

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sb
from scipy.io import loadmat
```

我们首先要实现的是找到数据中每个实例最接近的聚类中心的函数，已为大家准备好了。

```
def find_closest_centroids(X, centroids):
    m = X.shape[0]
    k = centroids.shape[0]
    idx = np.zeros(m)

    for i in range(m):
        min_dist = 1000000
        for j in range(k):
            dist = np.sum((X[i,:] - centroids[j,:]) ** 2)
            if dist < min_dist:
                min_dist = dist
                idx[i] = j

    return idx
```

让我们来测试这个函数，以确保它的工作正常。 我们将使用练习中提供的测试用例。

```
data = loadmat('data/ex7data2.mat')
X = data['X']
initial_centroids = initial_centroids = np.array([[3, 3], [6, 2], [8, 5]])

idx = find_closest_centroids(X, initial_centroids)
idx[0:3]
```

```
array([0., 2., 1.])
```

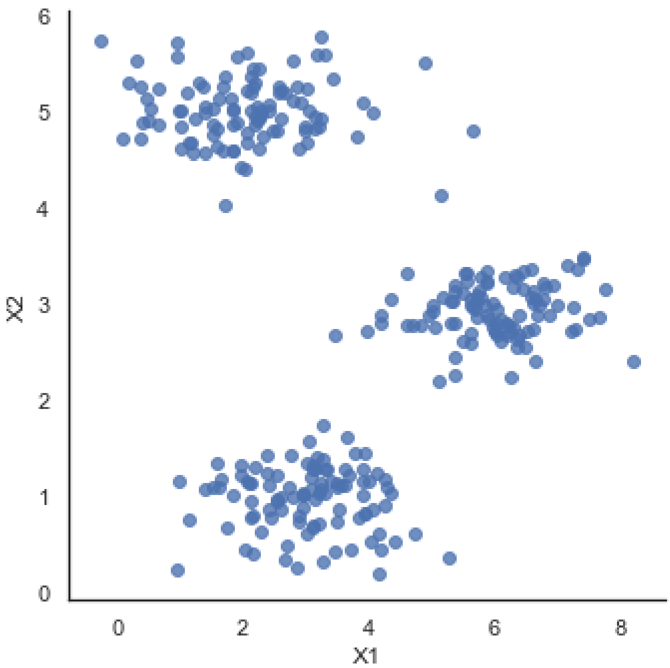
输出与文本中的预期值匹配（记住我们的数组是从0开始索引的，而不是从1开始索引）。
接下来，我们需要一个函数来计算簇的聚类中心。聚类中心只是当前分配给簇的所有样本的平均值。

```
data2 = pd.DataFrame(data.get('X'), columns=['X1', 'X2'])
data2.head()
```

```
.dataframe tbody tr th {
    vertical-align: top;
}

.dataframe thead th {
    text-align: right;
}
```

	X1	X2
0	1.842080	4.607572
1	5.658583	4.799964
2	6.352579	3.290854
3	2.904017	4.612204
4	3.231979	4.939894

```
sb.set(context="notebook", style="white")
sb.lmplot('X1', 'X2', data=data2, fit_reg=False)
plt.show()
```




```
def compute_centroids(X, idx, k):
    m, n = X.shape
    centroids = np.zeros((k, n))

    for i in range(k):
        indices = np.where(idx == i)
        centroids[i,:] = (np.sum(X[indices,:], axis=1) / len(indices[0])).ravel()

    return centroids
```

```
compute_centroids(X, idx, 3)
```

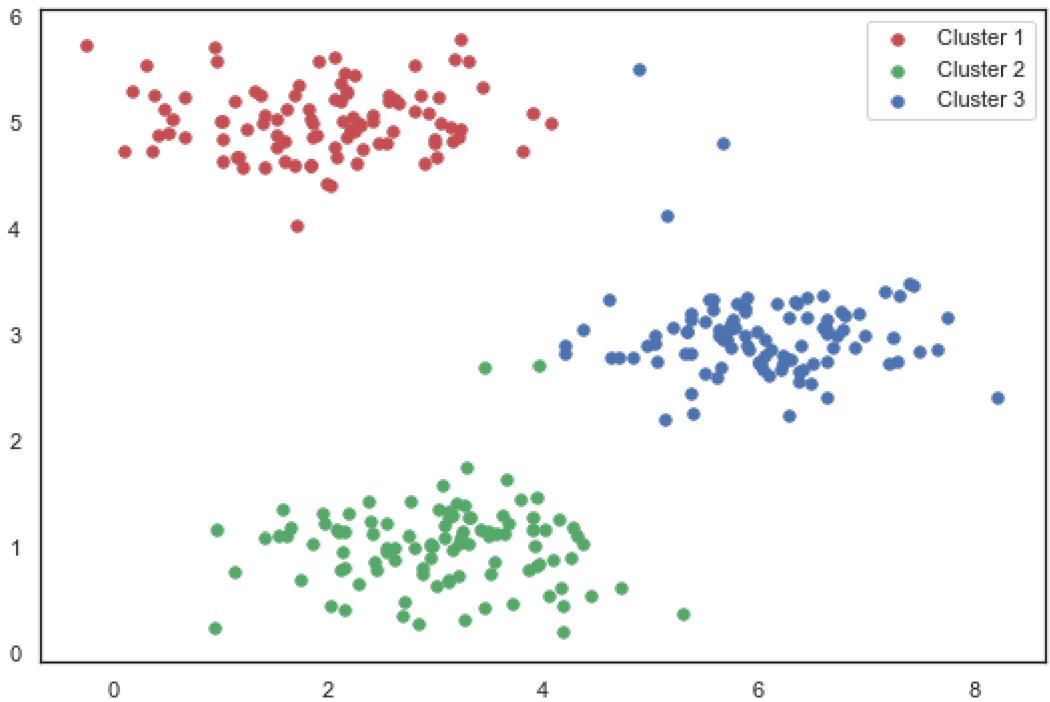
```
array([[2.42830111, 3.15792418],
       [5.81350331, 2.63365645],
       [7.11938687, 3.6166844 ]])
```

此输出也符合练习中的预期值。
下一部分涉及实际运行该算法的一些迭代次数和可视化结果。
这个步骤是由于并不复杂，我将从头开始构建它。 为了运行算法，我们只需要在将样本分配给最近的簇并重新计算簇的聚类中心。

```python
def run_k_means(X, initial_centroids, max_iters):
    m, n = X.shape
    k = initial_centroids.shape[0]
    idx = np.zeros(m)
    centroids = initial_centroids

    for i in range(max_iters):
        idx= find_closest_centroids(X, centroids)
        centroids= compute_centroids(X, idx, k)

    return idx, centroids
```

```python
idx, centroids = run_k_means(X, initial_centroids, 10)
```

```python
cluster1 = X[np.where(idx == 0)[0],:]
cluster2 = X[np.where(idx == 1)[0],:]
cluster3 = X[np.where(idx == 2)[0],:]

fig, ax = plt.subplots(figsize=(9,6))
ax.scatter(cluster1[:,0], cluster1[:,1], s=30, color='r', label='Cluster 1')
ax.scatter(cluster2[:,0], cluster2[:,1], s=30, color='g', label='Cluster 2')
ax.scatter(cluster3[:,0], cluster3[:,1], s=30, color='b', label='Cluster 3')
ax.legend()
plt.show()
```



我们跳过的一个步骤是初始化聚类中心的过程，这会影响算法的收敛效果。
接下来，让我们实现这个选择随机样本并将其用作初始聚类中心的函数。

```python
def init_centroids(X, k):
    m, n = X.shape
    centroids = np.zeros((k, n))
    idx = np.random.randint(0, m, k)

    for i in range(k):
        centroids[i,:]= X[idx[i],:]

    return centroids
```

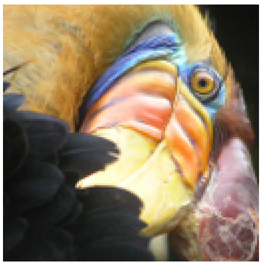
```python
init_centroids(X, 3)
```

```
array([[3.02836363, 1.35635189],
       [1.95538864, 1.32156857],
       [3.32648885, 1.28019066]])
```

我们的下一个任务是将K-means应用于图像压缩。
在下面的练习中，我们可以使用聚类来找到最具代表性的少数颜色，并使用聚类分配将原始的24位颜色映射到较低维的颜色空间。

下面是我们要压缩的图像。

```python
from IPython.display import Image
Image(filename='data/bird_small.png')
```



The raw pixel data has been pre-loaded for us so let's pull it in.

```python
image_data = loadmat('data/bird_small.mat')
image_data
```

```
{'__header__': b'MATLAB 5.0 MAT-file, Platform: GLNXA64, Created on: Tue Jun  5 04:06:24 2012',
 '__version__': '1.0',
 '__globals__': [],
 'A': array([[[219, 180, 103],
         [230, 185, 116],
         [226, 186, 110],
```

```
        ...,
        [ 14,  15,  13],
        [ 13,  15,  12],
        [ 12,  14,  12]],

       [[230, 193, 119],
        [224, 192, 120],
        [226, 192, 124],
        ...,
        [ 16,  16,  13],
        [ 14,  15,  10],
        [ 11,  14,   9]],

       [[228, 191, 123],
        [228, 191, 121],
        [220, 185, 118],
        ...,
        [ 14,  16,  13],
        [ 13,  13,  11],
        [ 11,  15,  10]],

       ...,

       [[ 15,  18,  16],
        [ 18,  21,  18],
        [ 18,  19,  16],
        ...,
        [ 81,  45,  45],
        [ 70,  43,  35],
        [ 72,  51,  43]],

       [[ 16,  17,  17],
        [ 17,  18,  19],
        [ 20,  19,  20],
        ...,
        [ 80,  38,  40],
        [ 68,  39,  40],
        [ 59,  43,  42]],

       [[ 15,  19,  19],
        [ 20,  20,  18],
        [ 18,  19,  17],
        ...,
        [ 65,  43,  39],
        [ 58,  37,  38],
        [ 52,  39,  34]]], dtype=uint8)}
```

```
A = image_data['A']
A.shape
```

```
(128, 128, 3)
```

现在我们需要对数据应用一些预处理，并将其提供给K-means算法。

```
# normalize value ranges
A = A / 255.

# reshape the array
X = np.reshape(A, (A.shape[0] * A.shape[1], A.shape[2]))
X.shape
```

```
(16384, 3)
```

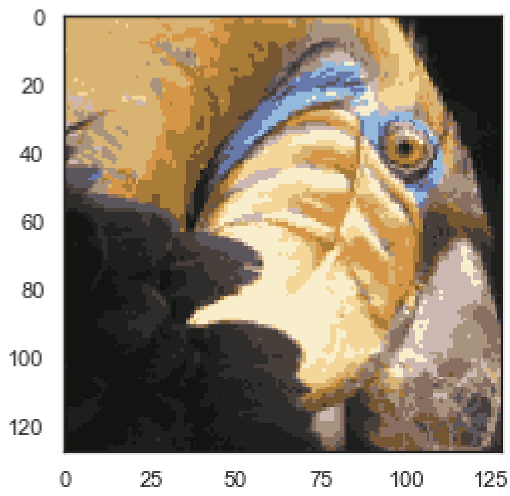
```
# randomly initialize the centroids
initial_centroids = init_centroids(X, 16)

# run the algorithm
idx, centroids = run_k_means(X, initial_centroids, 10)

# get the closest centroids one last time
idx = find_closest_centroids(X, centroids)

# map each pixel to the centroid value
X_recovered = centroids[idx.astype(int),:]
X_recovered.shape
```

```
(16384, 3)
```

```
# reshape to the original dimensions
X_recovered = np.reshape(X_recovered, (A.shape[0], A.shape[1], A.shape[2]))
X_recovered.shape
```

```
(128, 128, 3)
```

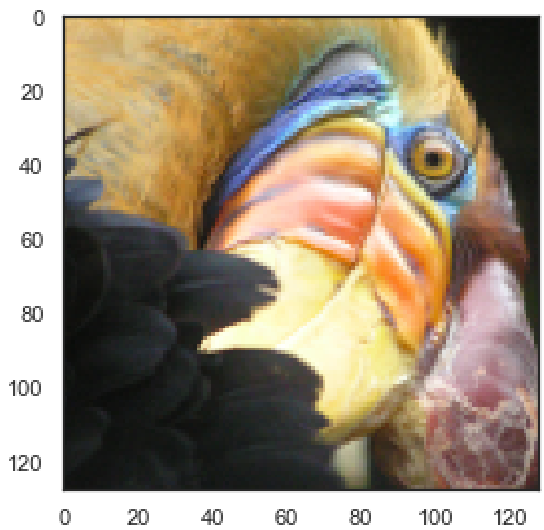
```
plt.imshow(X_recovered)
plt.show()
```



您可以看到我们对图像进行了压缩，但图像的主要特征仍然存在。这就是K-means。

下面我们来用scikit-learn来实现K-means。

```
from skimage import io

# cast to float, you need to do this otherwise the color would be weird after clustring
pic = io.imread('data/bird_small.png') / 255.
io.imshow(pic)
plt.show()
```




```
pic.shape
```

```
(128, 128, 3)
```

```
# serialize data
data = pic.reshape(128*128, 3)
```

```
data.shape
```

```
(16384, 3)
```

```
from sklearn.cluster import KMeans #导入K-Means库

model = KMeans(n_clusters=16, n_init=100, n_jobs=-1)
```

```
model.fit(data)
```

```
KMeans(algorithm='auto', copy_x=True, init='k-means++', max_iter=300,
    n_clusters=16, n_init=100, n_jobs=-1, precompute_distances='auto',
    random_state=None, tol=0.0001, verbose=0)
```

```
centroids = model.cluster_centers_
print(centroids.shape)

C = model.predict(data)
print(C.shape)
```

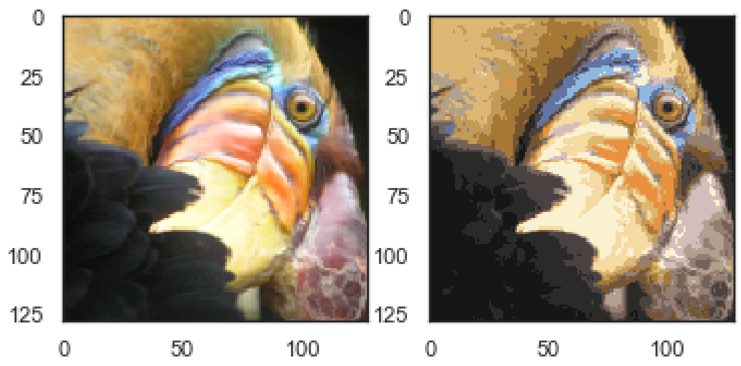
```
(16, 3)
(16384,)
```

```
centroids[C].shape
```

```
(16384, 3)
```

```
compressed_pic = centroids[C].reshape((128,128,3))
```

```
fig, ax = plt.subplots(1, 2)
ax[0].imshow(pic)
ax[1].imshow(compressed_pic)
plt.show()
```



2. Principal component analysis（主成分分析）

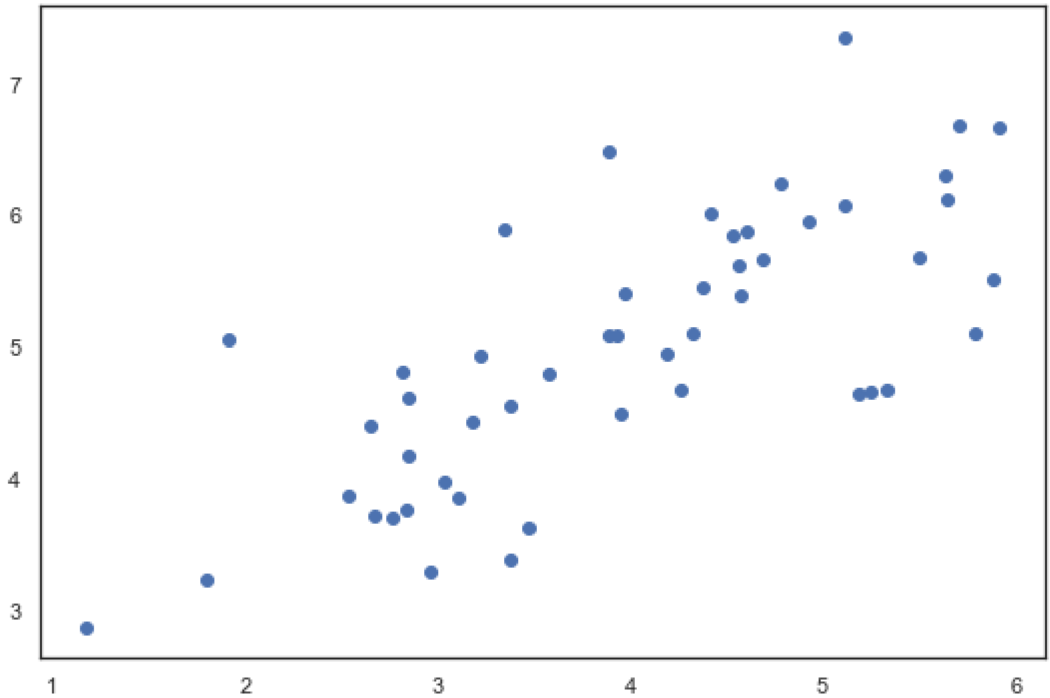
PCA是在数据集中找到"主成分"或最大方差方向的线性变换。 它可以用于降维。
在本练习中，我们将实现PCA应用于一个简单的二维数据集，以了解它是如何工作的。
我们从首先加载和可视化数据集开始。

```
data = loadmat('data/ex7data1.mat')
data
```

```
{'__header__': b'MATLAB 5.0 MAT-file, Platform: PCWIN64, Created on: Mon Nov 14 22:41:44
2011',
 '__version__': '1.0',
 '__globals__': [],
 'X': array([[3.38156267, 3.38911268],
        [4.52787538, 5.8541781 ],
        [2.65568187, 4.41199472],
        [2.76523467, 3.71541365],
        [2.84656011, 4.17550645],
        [3.89067196, 6.48838087],
        [3.47580524, 3.63284876],
        [5.91129845, 6.68076853],
        [3.92889397, 5.09844661],
        [4.56183537, 5.62329929],
        [4.57407171, 5.39765069],
        [4.37173356, 5.46116549],
        [4.19169388, 4.95469359],
        [5.24408518, 4.66148767],
        [2.8358402 , 3.76801716],
        [5.63526969, 6.31211438],
        [4.68632968, 5.6652411 ],
        [2.85051337, 4.62645627],
        [5.1101573 , 7.36319662],
        [5.18256377, 4.64650909],
        [5.70732809, 6.68103995],
        [3.57968458, 4.80278074],
        [5.63937773, 6.12043594],
        [4.26346851, 4.68942896],
        [2.53651693, 3.88449078],
        [3.22382902, 4.94255585],
        [4.92948801, 5.95501971],
        [5.79295774, 5.10839305],
        [2.81684824, 4.81895769],
        [3.88882414, 5.10036564],
```

```
       [3.34323419, 5.89301345],
       [5.87973414, 5.52141664],
       [3.10391912, 3.85710242],
       [5.33150572, 4.68074235],
       [3.37542687, 4.56537852],
       [4.77667888, 6.25435039],
       [2.6757463 , 3.73096988],
       [5.50027665, 5.67948113],
       [1.79709714, 3.24753885],
       [4.3225147 , 5.11110472],
       [4.42100445, 6.02563978],
       [3.17929886, 4.43686032],
       [3.03354125, 3.97879278],
       [4.6093482 , 5.879792  ],
       [2.96378859, 3.30024835],
       [3.97176248, 5.40773735],
       [1.18023321, 2.87869409],
       [1.91895045, 5.07107848],
       [3.95524687, 4.5053271 ],
       [5.11795499, 6.08507386]])}
```

```
X = data['X']

fig, ax = plt.subplots(figsize=(9,6))
ax.scatter(X[:, 0], X[:, 1])
plt.show()
```



PCA的算法相当简单。 在确保数据被归一化之后，输出仅仅是原始数据的协方差矩阵的奇异值分解。
请实现PCA算法。

```
def pca(X):
    # normalize the features 归一化
    X = (X - X.mean()) / X.std()

    # compute the covariance matrix
    X = np.matrix(X)
    cov = (X.T * X) / X.shape[0]

    # perform SVD
    U, S, V = np.linalg.svd(cov)

    return U, S, V
```

```
U, S, V = pca(X)
U, S, V
```

```
(matrix([[-0.79241747, -0.60997914],
         [-0.60997914,  0.79241747]]),
 array([1.43584536, 0.56415464]),
 matrix([[-0.79241747, -0.60997914],
         [-0.60997914,  0.79241747]]))
```

现在我们有主成分（矩阵U），我们可以用这些来将原始数据投影到一个较低维的空间中。
对于这个任务，我们将实现一个投影函数，仅选择顶部k个分量，从而有效地减少了维数。

```
def project_data(X, U, k):
    U_reduced = U[:,:k]
    return np.dot(X, U_reduced)
```

```
Z = project_data(X, U, 1)
Z
```

```
matrix([[-4.74689738],
        [-7.15889408],
        [-4.79563345],
        [-4.45754509],
        [-4.80263579],
        [-7.04081342],
        [-4.97025076],
        [-8.75934561],
        [-6.2232703 ],
        [-7.04497331],
        [-6.91702866],
        [-6.79543508],
        [-6.3438312 ],
        [-6.99891495],
        [-4.54558119],
        [-8.31574426],
```

```
        [-7.16920841],
        [-5.08083842],
        [-8.54077427],
        [-6.94102769],
        [-8.5978815 ],
        [-5.76620067],
        [-8.2020797 ],
        [-6.23890078],
        [-4.37943868],
        [-5.56947441],
        [-7.53865023],
        [-7.70645413],
        [-5.17158343],
        [-6.19268884],
        [-6.24385246],
        [-8.02715303],
        [-4.81235176],
        [-7.07993347],
        [-5.45953289],
        [-7.60014707],
        [-4.39612191],
        [-7.82288033],
        [-3.40498213],
        [-6.54290343],
        [-7.17879573],
        [-5.22572421],
        [-4.83081168],
        [-7.23907851],
        [-4.36164051],
        [-6.44590096],
        [-2.69118076],
        [-4.61386195],
        [-5.88236227],
        [-7.76732508]])
```

我们也可以通过反向转换步骤来恢复原始数据，请实现这个函数。

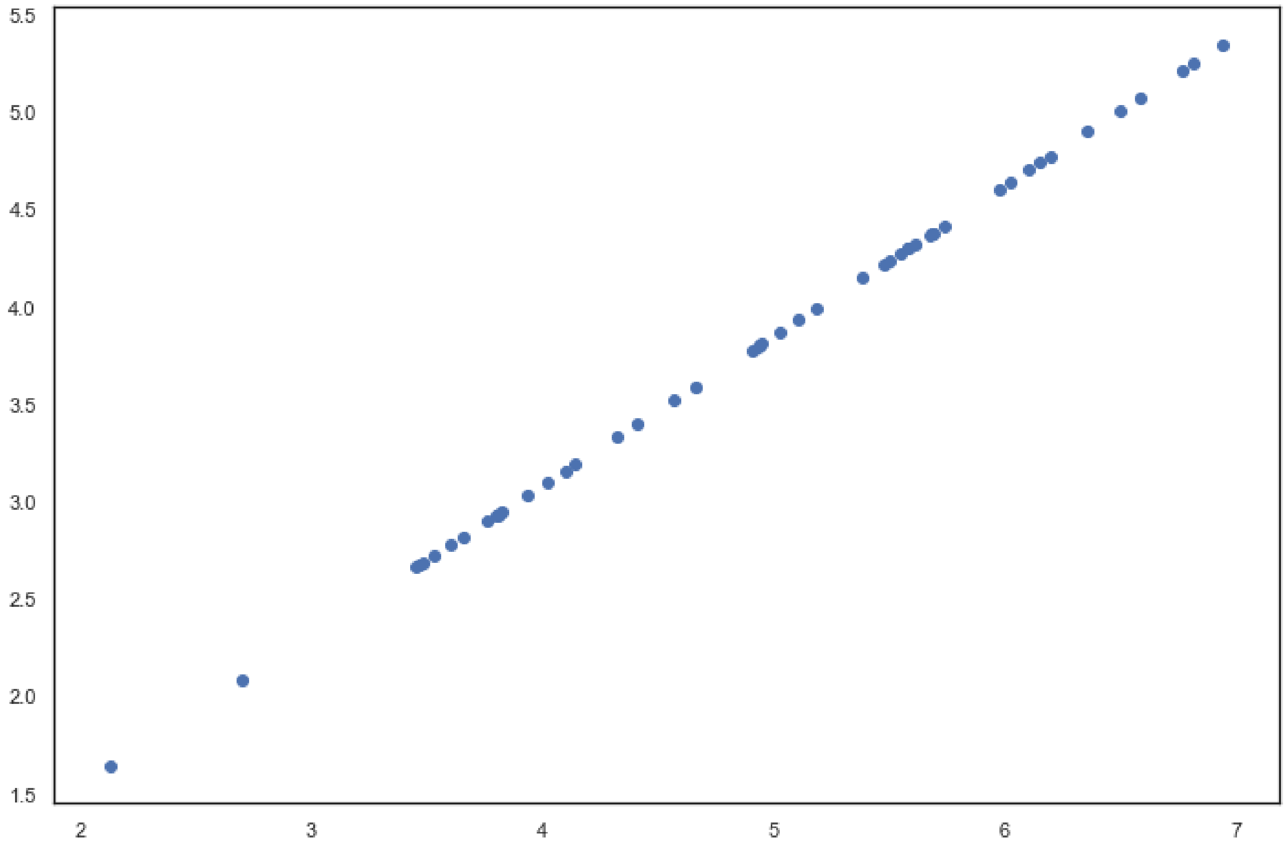
```
def recover_data(Z, U, k):
    U_reduced = U[:,:k]

    return Z @ U_reduced.T
```

```
X_recovered = recover_data(Z, U, 1)
X_recovered
```

```
matrix([[3.76152442, 2.89550838],
        [5.67283275, 4.36677606],
        [3.80014373, 2.92523637],
        [3.53223661, 2.71900952],
        [3.80569251, 2.92950765],
        [5.57926356, 4.29474931],
        [3.93851354, 3.03174929],
```

```
       [6.94105849, 5.3430181 ],
       [4.93142811, 3.79606507],
       [5.58255993, 4.29728676],
       [5.48117436, 4.21924319],
       [5.38482148, 4.14507365],
       [5.02696267, 3.8696047 ],
       [5.54606249, 4.26919213],
       [3.60199795, 2.77270971],
       [6.58954104, 5.07243054],
       [5.681006  , 4.37306758],
       [4.02614513, 3.09920545],
       [6.76785875, 5.20969415],
       [5.50019161, 4.2338821 ],
       [6.81311151, 5.24452836],
       [4.56923815, 3.51726213],
       [6.49947125, 5.00309752],
       [4.94381398, 3.80559934],
       [3.47034372, 2.67136624],
       [4.41334883, 3.39726321],
       [5.97375815, 4.59841938],
       [6.10672889, 4.70077626],
       [4.09805306, 3.15455801],
       [4.90719483, 3.77741101],
       [4.94773778, 3.80861976],
       [6.36085631, 4.8963959 ],
       [3.81339161, 2.93543419],
       [5.61026298, 4.31861173],
       [4.32622924, 3.33020118],
       [6.02248932, 4.63593118],
       [3.48356381, 2.68154267],
       [6.19898705, 4.77179382],
       [2.69816733, 2.07696807],
       [5.18471099, 3.99103461],
       [5.68860316, 4.37891565],
       [4.14095516, 3.18758276],
       [3.82801958, 2.94669436],
       [5.73637229, 4.41568689],
       [3.45624014, 2.66050973],
       [5.10784454, 3.93186513],
       [2.13253865, 1.64156413],
       [3.65610482, 2.81435955],
       [4.66128664, 3.58811828],
       [6.1549641 , 4.73790627]])
```

```
fig, ax = plt.subplots(figsize=(12,8))
ax.scatter(list(X_recovered[:, 0]), list(X_recovered[:, 1]))
plt.show()
```



我们看到，第一主成分的投影轴基本上是数据集中的对角线。当我们将数据减少到仅有一个维度时，我们失去了该对角线周围的变化，所以在我们的恢复数据中，一切都沿着该对角线。

我们在此练习中的最后一个任务是将PCA应用于人脸图像。通过使用相同的降维技术，我们可以使用比原始图像少得多的数据来捕获图像的“本质”。

```
faces = loadmat('data/ex7faces.mat')
X = faces['X']
X.shape
```

```
(5000, 1024)
```

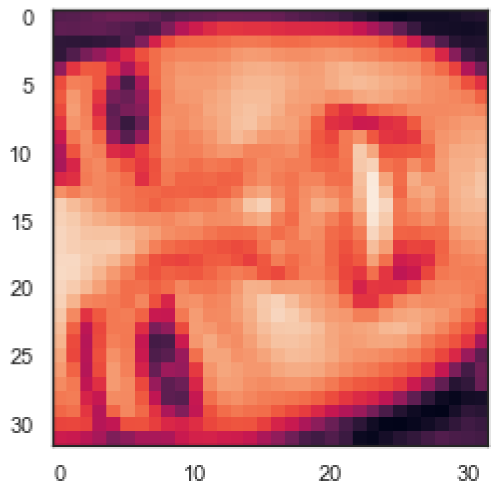
```
def plot_n_image(X, n):
    """ plot first n images
    n has to be a square number
    """
    pic_size = int(np.sqrt(X.shape[1]))
    grid_size = int(np.sqrt(n))

    first_n_images = X[:n, :]

    fig, ax_array = plt.subplots(nrows=grid_size, ncols=grid_size,
                                 sharey=True, sharex=True, figsize=(8, 8))

    for r in range(grid_size):
        for c in range(grid_size):
```

```
            ax_array[r, c].imshow(first_n_images[grid_size * r + c].reshape((pic_size, pic_size)))
            plt.xticks(np.array([]))
            plt.yticks(np.array([]))
```

上述函数用来显示前n张人脸图像，你可以使用这个函数查看一下都有哪些人脸图像，选择一个你喜欢的进行接下来的练习，:)
有条件的同学可以尝试替换成自己的大头照进行下面的测试。

```
face = np.reshape(X[30,:], (32, 32))
```

```
plt.imshow(face)
plt.show()
```

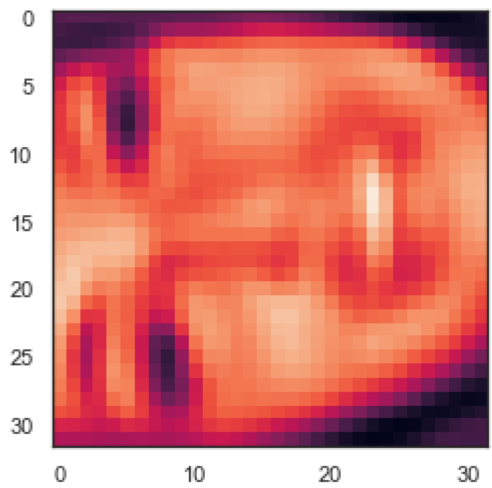


看起来很糟糕，马赛克效果比较明显吧。这些是只有32 x 32灰度的图像。
我们的下一步是在面数据集上运行PCA，并取得前100个主要特征。

```
U, S, V = pca(X)
Z = project_data(X, U, 100)
```

现在我们可以尝试恢复原来的结构并再次渲染。

```
X_recovered = recover_data(Z, U, 100)
face = np.reshape(X_recovered[30,:], (32, 32))
plt.imshow(face)
plt.show()
```



请注意，我们失去了一些细节，尽管没有像您预期的维度数量减少10倍，但总得显示效果还不错。