

K-means 聚类

1.找到数据中每个实例最近的聚类中心的函数。

```
In [1]: import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sb
from scipy.io import loadmat
```

```
In [2]: 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) # **2—平方
            if dist < min_dist:
                min_dist = dist
                idx[i] = j

    return idx
```

```
In [3]: #test
data = loadmat('data/machine-learning-ex7/ex7/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]
```

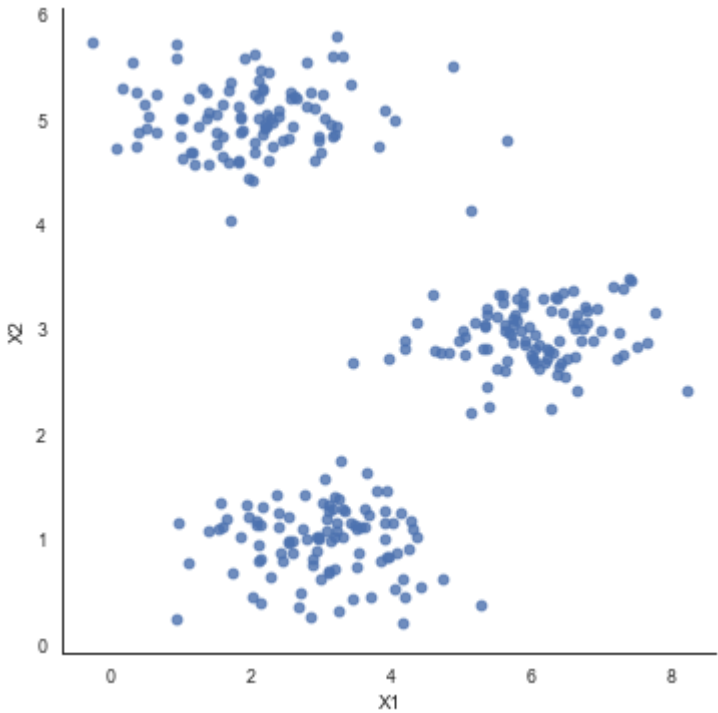
Out[3]: array([0., 2., 1.])

```
In [4]: data2 = pd.DataFrame(data.get('X'), columns=['X1', 'X2'])
data2.head()
```

Out[4]:

	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

```
In [5]: sb.set(context="paper", style="white") #绘图风格
sb.lmplot(x='X1', y='X2', data=data2, fit_reg=False) #sb.lmplot:多图叠加,一个x多个y
plt.show()
```



```
In [6]: 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) #只有条件 (condition), 没有x和y, 则输出满足条件 (即非0) 元素的坐标
        centroids[i,:] = (np.sum(X[indices,:], axis=1) / len(indices[0])).ravel()
        #[i,:]第一维度元素保留到i, 保留第二个维度所有元素,
    return centroids
```

```
In [7]: compute_centroids(X, idx, 3)
```

Out[7]: array([[2.42830111, 3.15792418],
[5.81350331, 2.63365645],
[7.11938687, 3.6166844]])

```
In [8]: #为了运行算法, 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。
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
```

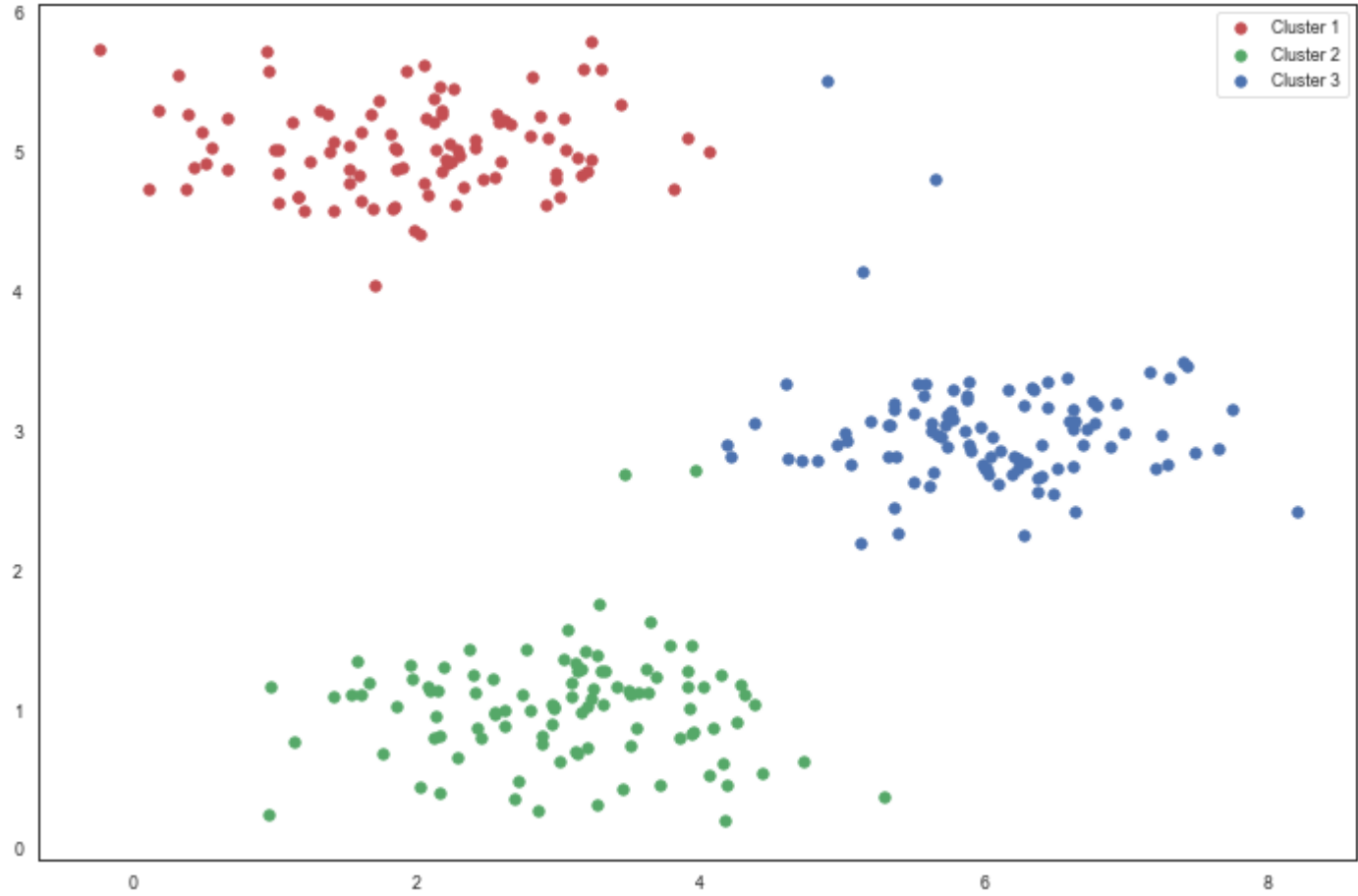
```
In [9]: idx, centroids = run_k_means(X, initial_centroids, 10)
centroids
```

Out[9]: array([[1.95399466, 5.02557006],
[3.04367119, 1.01541041],
[6.03366736, 3.00052511]])

```
In [10]: 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=(12,8))
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()
```



```
In [11]: #初始化聚类中心的过程可以影响算法的收敛，因此，创建一个选择随机样本并将其用作初始聚类中心的函数。
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
```

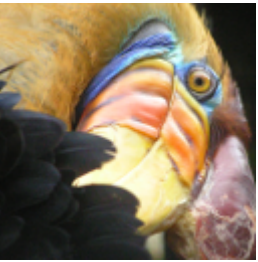
```
In [12]: init_centroids(X, 3)
```

```
Out[12]: array([[1.82975993, 4.59657288],
                [0.10511804, 4.72916344],
                [1.70725482, 4.04231479]])
```

2.将K-means应用于图像压缩。

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。

```
In [13]: from IPython.display import Image
Image(filename='data/machine-learning-ex7/ex7/bird_small.png')
```



```
In [14]: #像素点数值
image_data = loadmat('data/machine-learning-ex7/ex7/bird_small.mat')
image_data
```

```
Out[14]: {'__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)}
```

```
In [15]: A = image_data['A']
A.shape
```

```
Out[15]: (128, 128, 3)
```

```
In [16]: #预处理
# normalize value ranges
```

```
A = A / 255.
# reshape the array
X = np.reshape(A, (A.shape[0] * A.shape[1], A.shape[2])) #在不改变数据内容的情况下，改变一个数组的格式，参数及返回值
X.shape
```

Out[16]: (16384, 3)

```
In [17]: # 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)

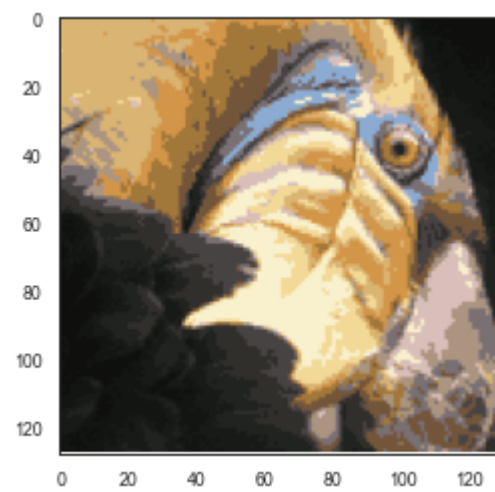
# map each pixel to the centroid value
X_recovered = centroids[idx.astype(int),:] #astype: 转换数组的数据类型。
X_recovered.shape
```

Out[17]: (16384, 3)

```
In [18]: # reshape to the original dimensions
X_recovered = np.reshape(X_recovered, (A.shape[0], A.shape[1], A.shape[2]))
X_recovered.shape
```

Out[18]: (128, 128, 3)

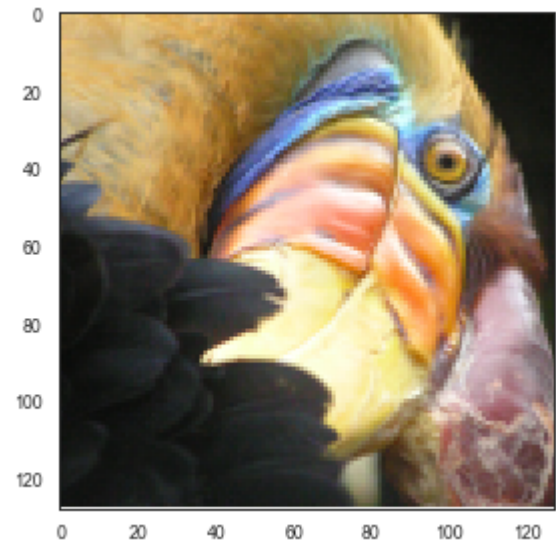
```
In [19]: plt.imshow(X_recovered)
plt.show()
#对图像进行了压缩，但图像的主要特征仍然存在,这就是K-means。
```



下面用scikit-learn实现K-means。

```
In [20]: from skimage import io

# cast to float, you need to do this otherwise the color would be weird after clustering
pic = io.imread('data/machine-learning-ex7/ex7/bird_small.png') / 255.
io.imshow(pic)
plt.show()
```



```
In [21]: data = pic.reshape(128*128, 3)
data.shape
```

Out[21]: (16384, 3)

```
In [22]: from sklearn.cluster import KMeans#导入kmeans库
model = KMeans(n_clusters=16, n_init=100)
model.fit(data)
```

Out[22]: KMeans(n_clusters=16, n_init=100)

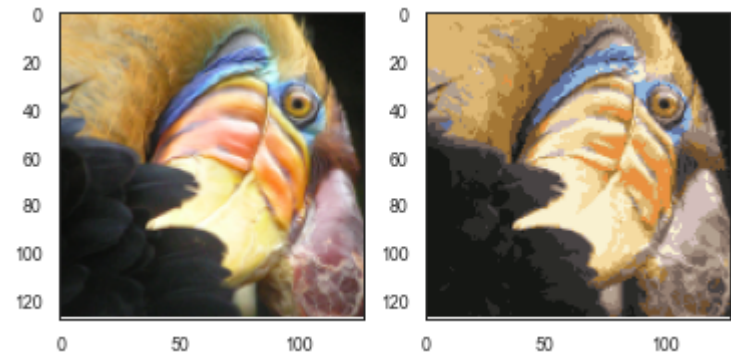
```
In [23]: centroids = model.cluster_centers_ #KMeans.cluster_centers_返回中心的坐标
print(centroids.shape)

C = model.predict(data)
print(C.shape)
print(centroids[C].shape)
```

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

```
In [24]: compressed_pic = centroids[C].reshape((128,128,3))
```

```
In [25]: fig, ax = plt.subplots(1, 2)
ax[0].imshow(pic)
ax[1].imshow(compressed_pic)
plt.show()
```



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。

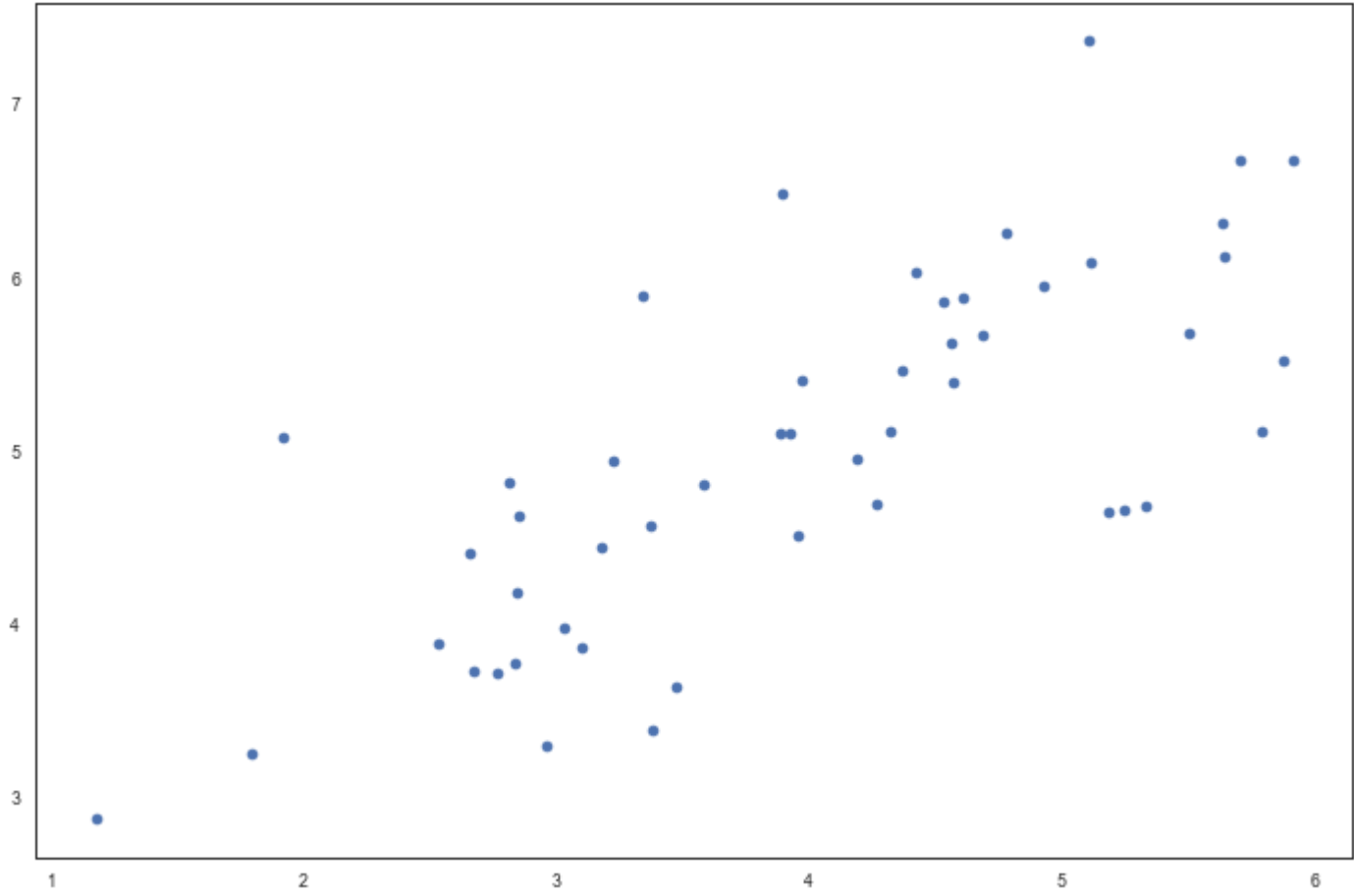
首先实现PCA并将其应用于一个简单的二维数据集，以了解它是如何工作的。从加载和可视化数据集开始。

```
In [26]: data = loadmat('data/machine-learning-ex7/ex7/ex7data1.mat')
data

Out[26]: {'__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]]])
```

```
In [27]: X = data['X']

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



```
In [28]: #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。
def pca(X):
    #均值归一化
    X = (X - X.mean()) / X.std()

    #计算协方差矩阵
    X = np.matrix(X)
    cov = (X.T * X) / X.shape[0]

    """
    奇异值分解SVD，U叫做左奇异值，S叫做奇异值，V叫做右奇异值。
    其中s是对矩阵a的奇异值分解。s除了对角元素不为0，其他元素都为0，并且对角元素从大到小排列。
    s中有n个奇异值，一般排在后面的比较接近0，所以仅保留比较大的r个奇异值。
    """

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

    return U, S, V
```

```
In [29]: U, S, V = pca(X)
U, S, V
```

```
Out[29]: (matrix([[ -0.79241747, -0.60997914],
 [ -0.60997914,  0.79241747]]),
 array([1.43584536, 0.56415464]),
 matrix([[ -0.79241747, -0.60997914],
 [ -0.60997914,  0.79241747]]))
```

```
In [30]: #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，我们将实现一个计算投影并且仅选择顶部K个分量的函数，有效地减少了维数。
def project_data(X, U, k):
    U_reduced = U[:, :k]
    return np.dot(X, U_reduced)
```

```
In [31]: Z = project_data(X, U, 1)
Z
```

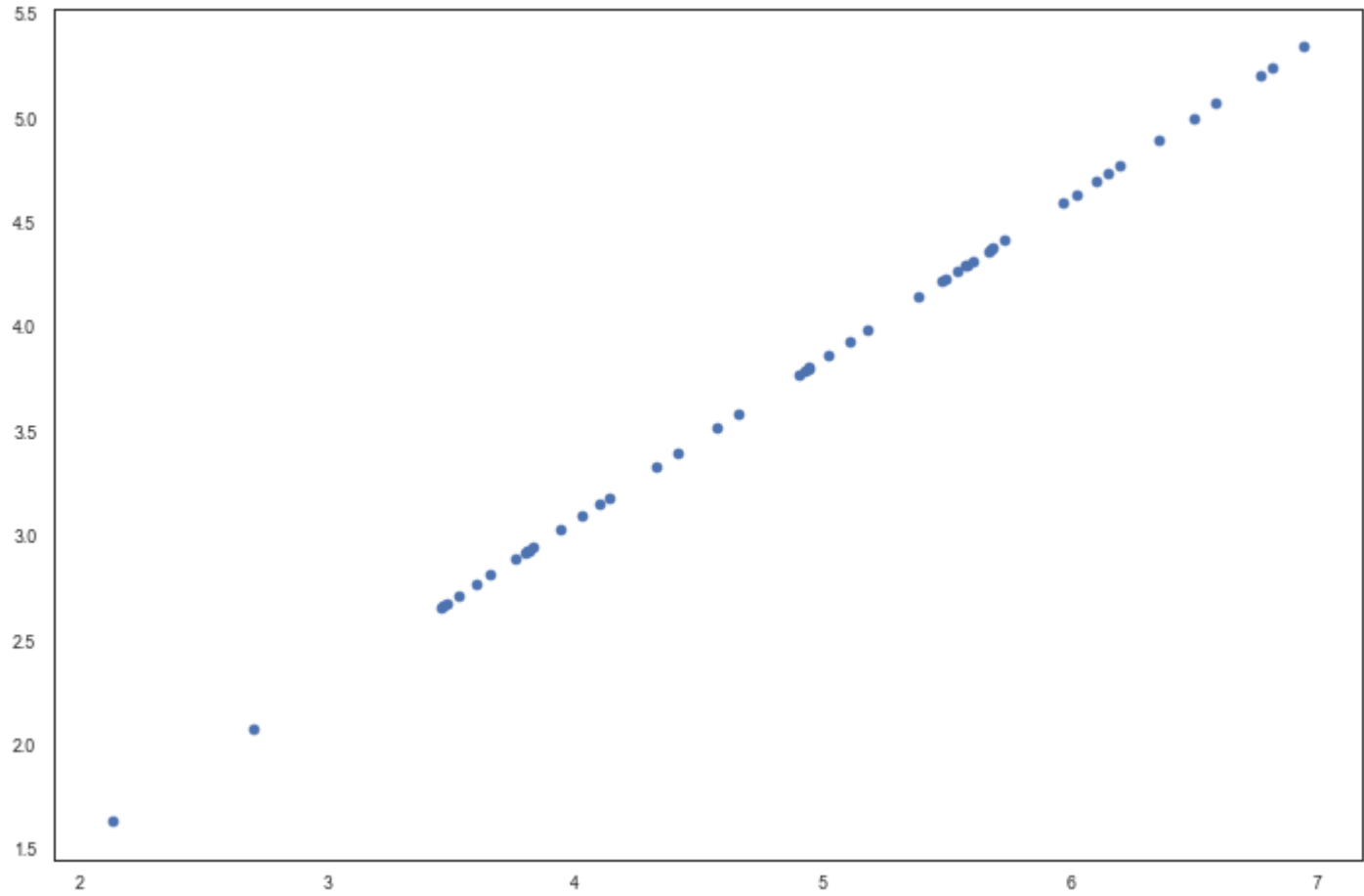
```
Out[31]: matrix([[ -4.74689738],
                [ -7.15889408],
                [ -4.79563345],
                [ -4.45754509],
                [ -4.80263579],
                [ -7.04081342],
                [ -4.97025076],
                [ -8.75934561],
                [ -6.2232703 ],
                [ -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]])
```

```
In [32]: #也可以通过反向转换步骤来恢复原始数据。
def recover_data(Z, U, k):
    U_reduced = U[:, :k]
    return np.dot(Z, U_reduced.T)
```

```
In [33]: X_recovered = recover_data(Z, U, 1)
X_recovered
```

```
Out[33]: 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]])
```

```
In [34]: fig, ax = plt.subplots(figsize=(12,8))
ax.scatter(list(X_recovered[:, 0]), list(X_recovered[:, 1]))
plt.show()
#第一主成分的投影轴基本上是数据集中的对角线，当将数据减少到一维时，失去了该对角线周围的变化，所以在再现中，一切都沿着该对角线。
```



将PCA应用于脸部图像。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”。

```
In [35]: faces = loadmat('data/machine-learning-ex7/ex7/ex7faces.mat')
X = faces['X']
X.shape
```

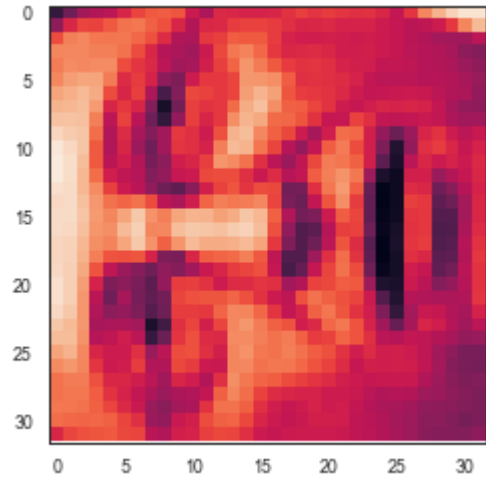
Out[35]: (5000, 1024)

```
In [36]: def plot_n_image(X, n): #plot first n images, n has to be a square number

    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([]))
```

```
In [37]: face = np.reshape(X[3,:], (32, 32))
plt.imshow(face)
plt.show()
```



```
In [38]: #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)
Z
```

Out[38]: matrix([[526.09608833, 734.37008142, 194.48322788, ..., -19.27422565,
-3.22314155, 20.93551538],
[304.5906028 , 493.0633805 , -162.10424193, ..., -20.94839919,
17.86358442, -8.14045979],
[-389.99893833, 600.20010851, -293.91694459, ..., -27.86998851,
48.74829475, 17.98452065],
...,
[487.55926046, 430.86037345, 490.71749378, ..., -31.76395627,
23.77770829, 51.74592358],
[1358.99575656, 402.85437502, -136.10305216, ..., -10.45305753,
-2.76084233, 2.96467067],
[372.01599145, 360.59923883, 105.10564415, ..., -48.29644614,
-8.75071522, -30.24094867]])

```
In [39]: #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[3,:], (32, 32))
plt.imshow(face)
plt.show()
```

