Robert Heeter
ELEC 378
2/13/2023

Problem Set # 4

1. a. $\mathcal{L}(\underline{w}) = \langle \underline{a}, \underline{w} \rangle$ where $\underline{a} \in \mathbb{R}^p$

$$\langle \underline{a}, \underline{w} \rangle = \underline{a}^T \underline{w} = \sum_i a_i w_i$$

$$\nabla \mathcal{L}(\underline{w}) = \left[\frac{\partial L}{\partial w_1}, \frac{\partial L}{\partial w_2}, \dots, \frac{\partial L}{\partial w_p} \right]^T$$

Kronecker delta tensor:

$$\delta_{ik} = \frac{\partial w_i}{\partial w_k} \rightarrow \delta_{ik} = \begin{cases} 0 & \text{for } i \neq k \\ 1 & \text{for } i = k \end{cases}$$

$$\frac{\partial L}{\partial w_k} = \sum_{i=1} a_i \frac{\partial w_i}{\partial w_k} = \sum_{i=1} a_i \delta_{ik} = a_k$$

$$\therefore \nabla \mathcal{L}(\underline{w}) = [a_1, a_2 \dots a_p]^T = \underline{a} \longrightarrow \boxed{\nabla \mathcal{L}(\underline{w}) = \nabla \langle \underline{a}, \underline{w} \rangle = \underline{a}}$$

b. $\mathcal{L}(\underline{w}) = \langle \underline{w}, \underline{w} \rangle$

$$\langle \underline{w}, \underline{w} \rangle = \sum_i w_i w_i = \sum_i w_i^2$$

$$\nabla \mathcal{L}(\underline{w}) = \left[\frac{\partial L}{\partial w_1}, \frac{\partial L}{\partial w_2} \dots \frac{\partial L}{\partial w_p} \right]^T$$

Kronecker delta tensor:

$$\delta_{ik} = \frac{\partial w_i}{\partial w_k} \rightarrow \delta_{ik} = \begin{cases} 0 & \text{for } i \neq k \\ 1 & \text{for } i = k \end{cases}$$

$$\frac{\partial L}{\partial w_k} = \sum_{i=1} \frac{\partial}{\partial w_k}(w_i^2) = \sum_{i=1} \underbrace{2\left(\frac{\partial w_i}{\partial w_k}\right)(w_i)}_{\text{chain rule}} = \sum_{i=1} 2 \delta_{ik} w_i = 2 w_k$$

$$\therefore \nabla \mathcal{L}(\underline{w}) = [2w_1, 2w_2 \dots 2w_k]^T = 2\underline{w} \longrightarrow \boxed{\nabla \mathcal{L}(\underline{w}) = \nabla \langle \underline{w}, \underline{w} \rangle = 2\underline{w}}$$

2. Next page

2. ① Gradient descent :

$$\mathcal{L}(\underline{w}) = \sum_{i=1}^{3} \mathcal{L}_i(\underline{w}) = (2w_1^2 + w_1w_2 - 4w_2^2) + (3w_1^2 + 4w_1w_2 + 5w_2^2) + (-w_1^2 - 4w_1w_2 + 3w_2^2)$$

$$= 4w_1^2 + w_1w_2 + 4w_2^2$$

$$\nabla \mathcal{L}(\underline{w}) = \left[\frac{\partial}{\partial w_1}(4w_1^2 + w_1w_2 + 4w_2^2), \frac{\partial}{\partial w_2}(4w_1^2 + w_1w_2 + 4w_2^2)\right]^T$$

$$\boxed{\nabla \mathcal{L}(\underline{w}) = [8w_1 + w_2, \ w_1 + 8w_2]} \rightarrow GD: \underline{w}^{t+1} = \underline{w}^t - \mu^t \sum_{t=1}^{T} \nabla \mathcal{L}_t(\underline{w})$$

All T gradients used each step/iteration

② Stochastic gradient descent:

$$\nabla \mathcal{L}_1(\underline{w}) = \left[\frac{\partial}{\partial w_1}(2w_1^2 + w_1w_2 + 4w_2^2), \frac{\partial}{\partial w_2}(2w_1^2 + w_1w_2 - 4w_2^2)\right]$$

$$= [4w_1 + w_2, \ w_1 - 8w_2]$$

$$\nabla \mathcal{L}_2(\underline{w}) = \left[\frac{\partial}{\partial w_1}(3w_1^2 + 4w_1w_2 + 5w_2^2), \frac{\partial}{\partial w_2}(3w_1^2 + 4w_1w_2 + 5w_2^2)\right]$$

$$= [6w_1 + 4w_2, \ 4w_1 + 10w_2]$$

$$\nabla \mathcal{L}_3(\underline{w}) = \left[\frac{\partial}{\partial w_1}(-w_1^2 - 4w_1w_2 + 3w_2^2), \frac{\partial}{\partial w_2}(-w_1^2 - 4w_1w_2 + 3w_2^2)\right]$$

$$= [-2w_1 - 4w_2, \ -4w_1 + 6w_2] \rightarrow SGD: \underline{w}^{t+1} = \underline{w}^t - \mu^t \sum_{t=1}^{T'} \nabla \mathcal{L}_t(\underline{w})$$

mini-batch/subset of gradients used each step/iteration until all T gradients have been used (1 epoch)

See attached code for implementation of of both algorithms and plots.

The gradient descent algorithm "descends" much more smoothly than the stochastic gradient descent algorithm. The stochastic gradient descent algorithm is much "rougher"/more "noisy" and overshoots for parameter w_2 due to its randomness in choosing a subset of gradients to use for each iteration. Both descent types choose random initial w_1 and w_2 values, but there is much more variability in the stochastic gradient descent result between runs due to the extra randomness.

3. Next page

3. a. Each RGB coordinate is quantized to 8 bits:

$2^{8\text{ bits}} = 256$ possible color values for each of R, G, and B

binary

∴ total number of possible colors (i.e. combinations of R, G, B values) is 256^3

$= \boxed{16{,}777{,}216 \text{ total possible unique colors}}$ → i.e the maximum number of distinctly colored pixels in any RGB image is 16,777,216 pixels

b. Data matrix: $X = [x_1 \dots x_n]^T$

- Feature vectors represent individual pixels, each with an R, G, and B value:

$\{x_i \in \mathbb{R}^p\}_{i=1}^{n}$ ← $p = 3$ for R, G, and B values (i.e. 3D space for features/RGB)

n = # of total pixels (i.e. number of feature vectors)

c. See code and scatter plot below. From the scatter plot, it is not immediately clear how the feature vectors should be clustered since there are no obvious groupings of colors on the dimensionality-reduced data.

d. See code, images, and plots below.

4. $K = 14$ clusters was chosen since there are 14 unique cancer types in the data set. See code and output below.

Due to the randomness of the initial centroid selection in the data, the output classification error changes slightly between runs. Between 12 and 24 retained principal components give a more robust clustering with a total error (i.e. false positive + false negative) of only 1 or 2 patients.

total error = 1

In the included output, $p = 12$ (i.e. 12 retained PCs) gives the lowest error (more robust clustering) and is the smallest number of PCs to give this error.

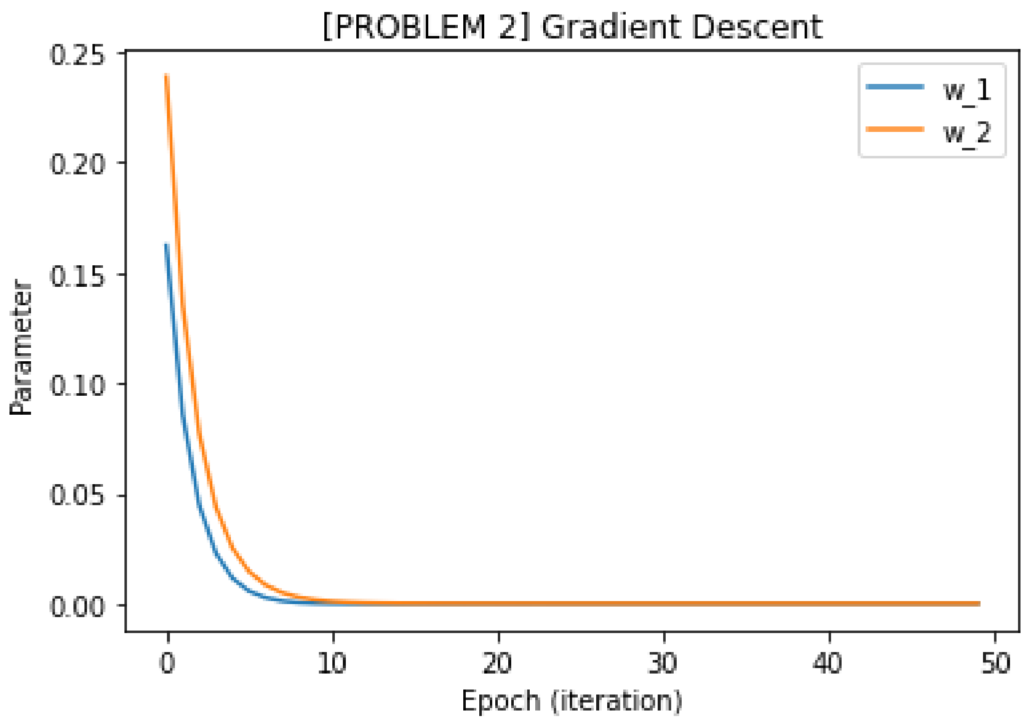
ELEC378-HW4

February 13, 2023

[1]:
```
# ROBERT HEETER
# ELEC 378 Machine Learning
# 13 February 2023

# PROBLEM SET 4
```

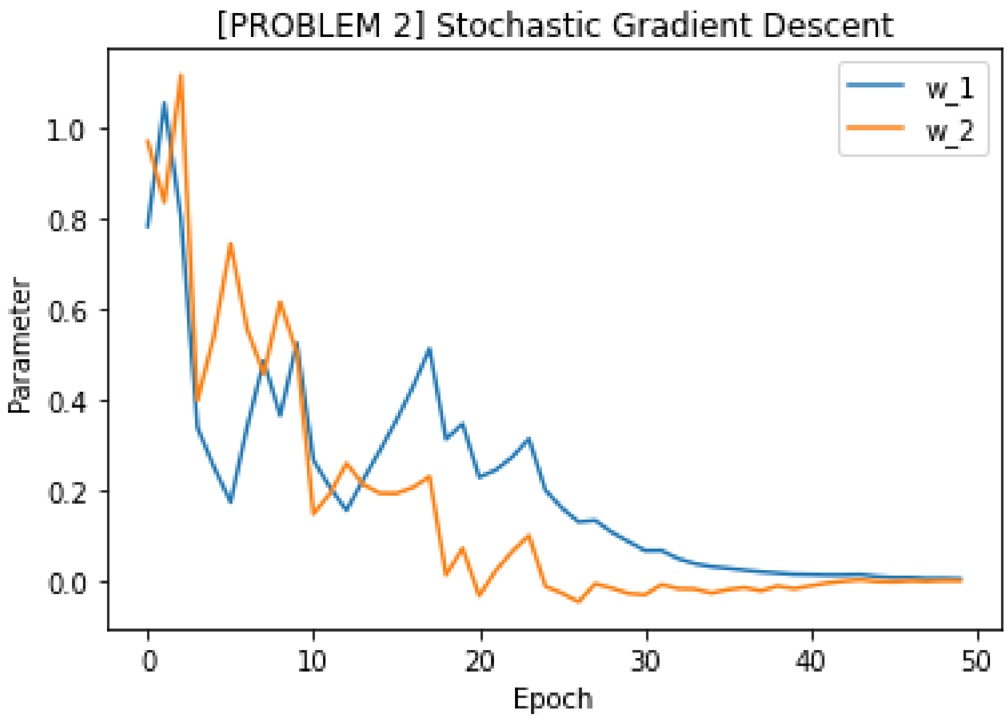
[2]:
```
import numpy as np
import matplotlib.pyplot as plt
```

[3]:
```
# PROBLEM 2

# GD (Gradient Descent)
T = 50 # number of epochs
w = np.empty((T, 2))
w[0] = np.random.rand(1,2) # start with random w

grad_L = lambda x: np.array([[8*x[0]+x[1],x[0]+8*x[1]]])
mu = 0.05

for t in range(1,T):
    w[t] = w[t-1] - mu*grad_L(w[t-1])

fig,ax = plt.subplots(1,1)
ax.plot(w[:,0])
ax.plot(w[:,1])
ax.set_xlabel('Epoch (iteration)')
ax.set_ylabel('Parameter')
ax.legend(('w_1','w_2'))
plt.title('[PROBLEM 2] Gradient Descent')
plt.show()
```



[4]:
```
# SGD (Stochastic Gradient Descent)
T = 50 # number of epochs
w = np.empty((T, 2))
w[0] = np.random.rand(1,2) # start with random w

grad_L1 = lambda x: np.array([[4*x[0]+x[1], x[0]-8*x[1]]])
grad_L2 = lambda x: np.array([[6*x[0]+4*x[1], 4*x[0]+10*x[1]]])
grad_L3 = lambda x: np.array([[-2*x[0]-4*x[1], -4*x[0]+6*x[1]]])
grads = [grad_L1, grad_L2, grad_L3]

mu = 0.05

for t in range(1,T):
    i = np.random.choice(3)  # randomly select one of the gradients
    w[t] = w[t-1] - mu*grads[i](w[t-1])

fig, ax = plt.subplots(1,1)
ax.plot(w[:,0])
ax.plot(w[:,1])
ax.set_xlabel('Epoch')
ax.set_ylabel('Parameter')
ax.legend(('w_1','w_2'))
plt.title('[PROBLEM 2] Stochastic Gradient Descent')
```

```
plt.show()
```



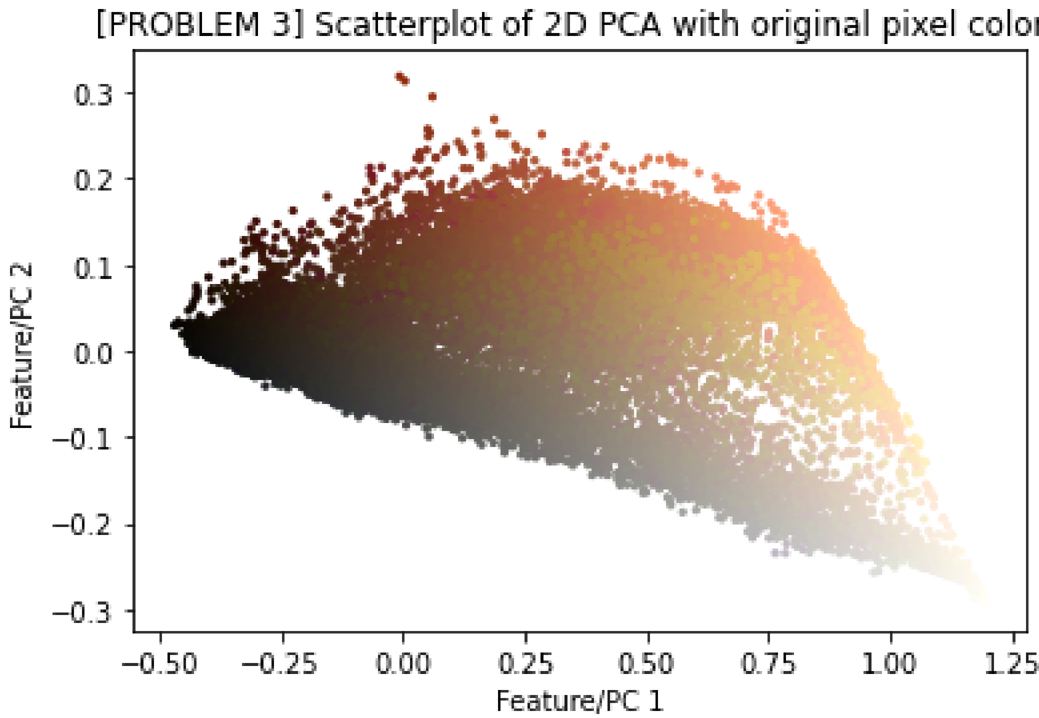
[5]:
```
# PROBLEM 3

import numpy as np

import scipy.io as sc
from scipy import signal, linalg

import matplotlib.image as im
import matplotlib.pyplot as plt

import time
from sklearn.decomposition import PCA

# read in original image and show image and shape
image = im.imread('objection.png')
print(image.shape)
plt.imshow(image)
plt.title('Original Image')
plt.show()
```

```
(248, 208, 3)
```

[6]:
```
# form the nxp data matrix, n = # of pixels, p = 3 (R,G,B color values)
X = image.reshape(-1,3)
print(np.shape(X))
```

```
(51584, 3)
```

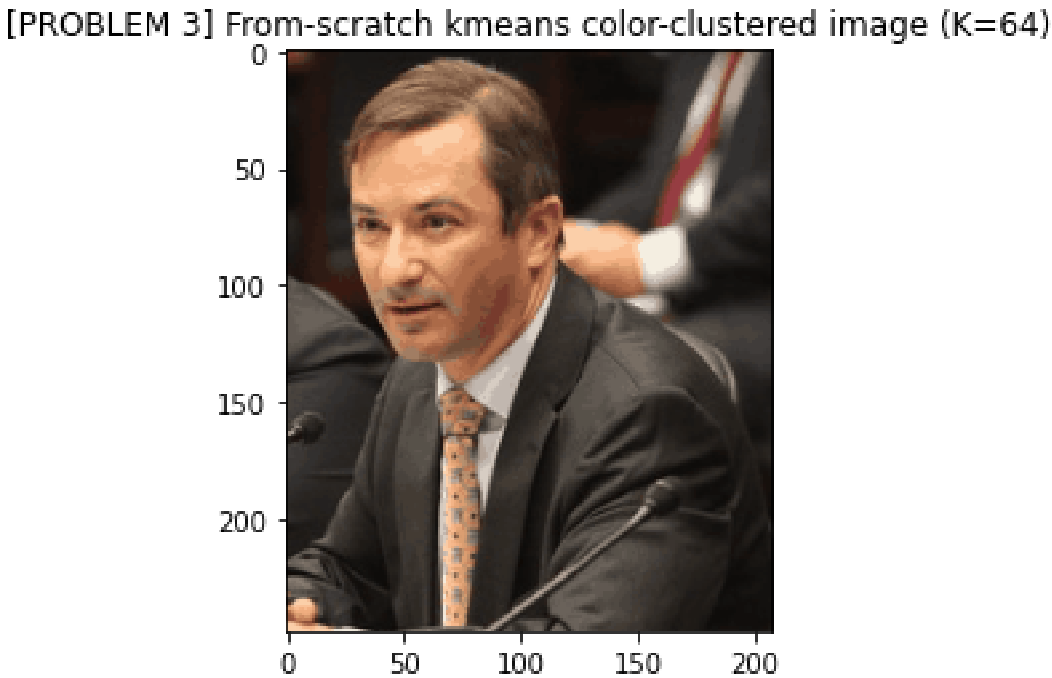
[7]:
```
# run and plot PCA on flattened array
pca = PCA(n_components=2)
pca.fit(X)

# project pixels into 2D space
pixels_transformed = pca.fit_transform(X)

# plot pixels in 2D space with original colors
plt.scatter(pixels_transformed[:, 0],pixels_transformed[:,1],c=X,s=5)
plt.xlabel('Feature/PC 1')
plt.ylabel('Feature/PC 2')
plt.title('[PROBLEM 3] Scatterplot of 2D PCA with original pixel colors')
plt.show()
```



[8]:
```
# implement k-means
import numpy as np
import pandas as pd
from scipy.spatial import distance
import matplotlib.pyplot as plt
from sklearn.preprocessing import StandardScaler

def kmeans(X, k=3, max_iterations=100):
    '''
    Parameter:
    X: multidimensional data (ndarray)
    k: number of clusters (int)
    max_iterations: number of repetitions before clusters are established (int)

    Steps:
    1. Convert data to numpy array if necessary
    2. Pick indices of k random points without replacement
    3. Find class (P) of each data point using Euclidean distance.
    4. Stop when max_iteration is reached or P matrix doesn't change.

    Return:
    P: an np.array containing class of each data point
    centroids: an np.array containing the centroid of each class
```

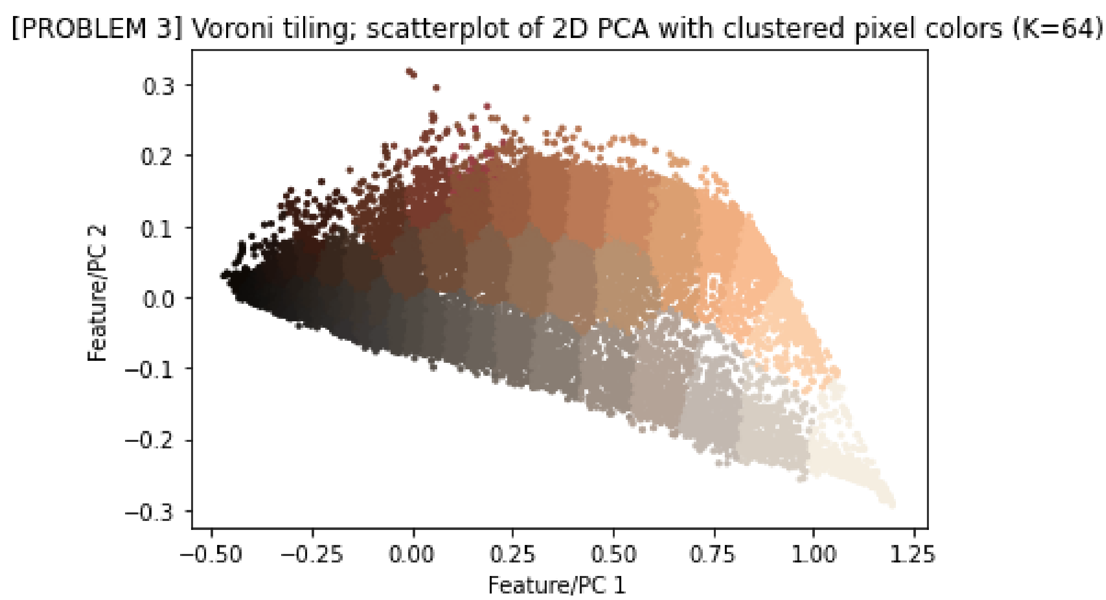
```
    '''

    # choose k random data points to serve as the initial centroids
    centroid_indices = np.random.default_rng().choice(len(X),k,replace=False)
    centroids = X[centroid_indices,:]

    # assign a cluster label to each data point based on closest centroid
    P = distance.cdist(X,centroids,'euclidean').argmin(axis=1)

    for iteration in range(max_iterations):
        # move centroids to the average of their cluster points
        # X[?,?].mean(axis=0) calculates the mean value, along each dimension,␣
↪of all elements of X belonging to the class i.
        # np.vstack then stacks these mean values of each class, returning a␣
↪(k,N) array,
        # where each of the k rows is a class containing N columns (dimensions).
        # Thus, "centroids" is a (k,N) array contining the N-dimensional␣
↪coordinates of each of the k centroids.
        centroids = np.vstack([X[np.where(P==i)[0],:].mean(axis=0) for i in np.
↪unique(P)])

        # re-assign clusters based on new centroids
        tmp = distance.cdist(X,centroids,'euclidean').argmin(axis=1)

        if np.array_equal(P,tmp): break # exit if P stops changing
        P = tmp

    return P,centroids # return arrays of classes and their centroids
```

[9]:
```
# run kmeans on pixels (from-scratch implementation)
K = 2**6

labels,centroids = kmeans(X,k=K,max_iterations=100)

# replace each pixel with its nearest centroid, then plot the resulting image
color_quantized_data_matrix = np.take(centroids,labels,axis=0)
plt.imshow(color_quantized_data_matrix.reshape(image.shape))
plt.title('[PROBLEM 3] From-scratch kmeans color-clustered image (K=64)')
plt.show()
```

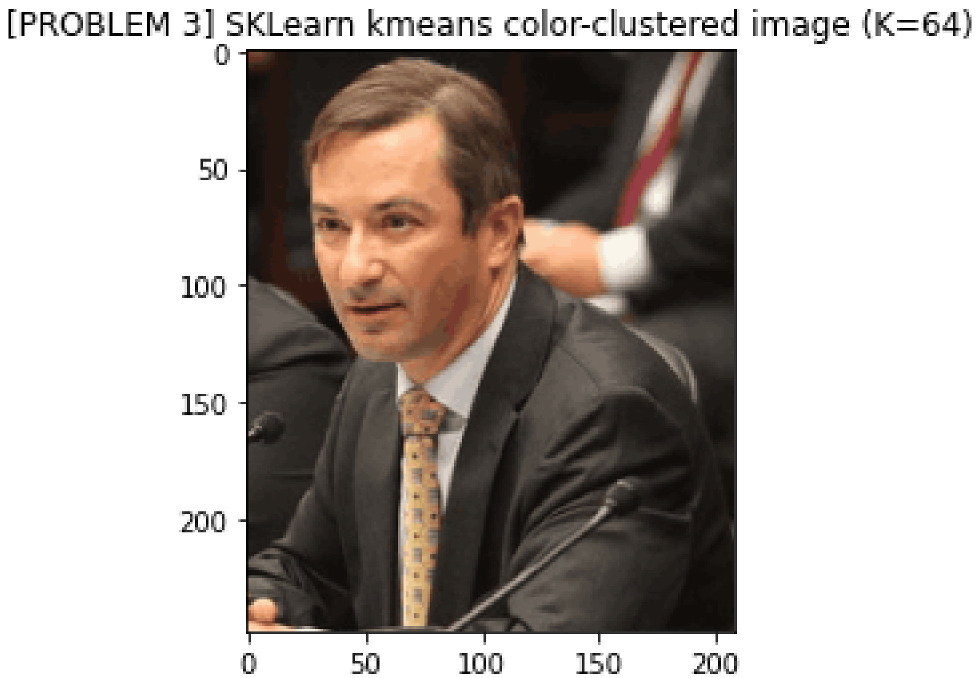


[10]:

```
# show previous PCA plot with new color quantization scheme (Voronoi tiling)
# plot pixels in 2D space, with each pixel having its quantized color

plt.scatter(pixels_transformed[:, 0],pixels_transformed[:,␣
↪1],c=color_quantized_data_matrix,s=5)
plt.xlabel('Feature/PC 1')
plt.ylabel('Feature/PC 2')
plt.title('[PROBLEM 3] Voroni tiling; scatterplot of 2D PCA with clustered␣
↪pixel colors (K=64)')
plt.show()
```



[11]:
```
# run sklearn implementation for comparison
# SKLearn implementation of kmeans
from sklearn.cluster import KMeans

K = 2**6

kmeans = KMeans(n_clusters=K,random_state=0,algorithm="lloyd",n_init='auto').
↪fit(X)

# replace each pixel with its nearest centroid, then plot the resulting image
labels = kmeans.predict(X)
kmeans_flat = kmeans.cluster_centers_[labels]

plt.figure(0)
plt.title('[PROBLEM 3] SKLearn kmeans color-clustered image (K=64)')
plt.imshow(kmeans_flat.reshape(image.shape))
plt.show()
```



[12]:
```
# PROBLEM 4

import scipy.io as sc
import numpy as np
import matplotlib.pyplot as plt

from scipy import stats
from sklearn.decomposition import PCA
from sklearn.cluster import KMeans

cancer = sc.loadmat('cancer.mat')
X = np.array(cancer['X'])
Y = ([y[0][:] for y in np.concatenate(cancer['Y'][:])])
```

[13]:
```
# use PCA to reduce the dimensionality of X
false_negative = []
false_positive = []
error = []
p_range = np.arange(2,64,1)

for p in p_range:
    pca = PCA(n_components=p)
    pca.fit(X)
    patients_transformed = pca.fit_transform(X)
```

```
    K = 14 # 14 clusters for 14 different cancers
    kmeans = KMeans(n_clusters=K, random_state=0,␣
↪algorithm="lloyd",n_init='auto').fit(patients_transformed)
    labels = kmeans.labels_

    # the indices of patients who have melanoma
    i_melanoma = np.char.startswith(Y,'MELANOMA')

    # the k-means prediction of melanoma patients
    melanoma_labels = labels[i_melanoma]

    # clusters for melanoma patients
    major_label, major_label_count = stats.mode(melanoma_labels,keepdims=True)

    # false negative: melanoma patients not included in cluster
    fn = np.sum(i_melanoma) - major_label_count[0]

    # false positive: non-melanoma patients included in cluster
    fp = len([y for i,y in enumerate(Y) if labels[i]==major_label[0] and y[0:8]␣
↪not in ['MELANOMA']])

    false_negative.append(fn)
    false_positive.append(fp)

    # error: sum of false positives and false negatives
    error.append(false_negative[-1] + false_positive[-1])

print('[PROBLEM 4]')
print('number of PCs retained:\n', list(p_range), '\n')
print('number of melanoma patients not included in cluster (false negative):
↪\n', false_negative, '\n')
print('number of non-melanoma patients included in cluster (false positive):
↪\n', false_positive, '\n')
print('total error:\n', error, '\n')
```

```
[PROBLEM 4]
number of PCs retained:
 [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22,
23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42,
43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62,
63]

number of melanoma patients not included in cluster (false negative):
 [3, 2, 2, 2, 1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2, 1, 1, 2, 2, 1, 2, 1, 1,
1, 1, 2, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 4,
2, 3, 3, 2, 2, 3, 2, 2, 2]
```

```
number of non-melanoma patients included in cluster (false positive):
 [0, 0, 0, 0, 2, 2, 2, 2, 2, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1,
2, 2, 0, 2, 2, 0, 0, 0, 0]

total error:
 [3, 2, 2, 2, 3, 3, 3, 3, 3, 3, 1, 1, 2, 2, 2, 2, 2, 2, 1, 1, 2, 2, 1, 2, 1, 1,
1, 1, 2, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 5,
4, 5, 3, 4, 4, 3, 2, 2, 2]
```

```
[ ]:
```