Assignment 3

Part I: Segmentation

Problem 1

Show algebraic equivalence between two non-parametric formulations for K-means (objectives $E(S)$ at the bottom of slide 58, Topic 9):

$$\sum_{k=1}^{K} \frac{\sum_{pq \in S^k} ||f_p - f_q||^2}{2\ |S^k|} \quad = \quad const - \sum_{k=1}^{K} \frac{\sum_{pq \in S^k} \langle f_p, f_q \rangle}{|S^k|}$$

Proof:

$$\begin{aligned}
LHS &= \sum_{k=1}^{K} \frac{\sum_{pq \in S^k} ||f_p - f_q||^2}{2\ |S^k|} \\
&= \sum_{k=1}^{K} \frac{\sum_{pq \in S^k} \langle f_p - f_q, f_p - f_q \rangle}{2\ |S^k|} \\
&= \sum_{k=1}^{K} \frac{\sum_{pq \in S^k} (\langle f_p, f_p \rangle + \langle f_q, f_q \rangle - 2\langle f_p, f_q \rangle)}{2\ |S^k|} \quad \text{(by properties of inner product)} \\
&= \sum_{k=1}^{K} \frac{\sum_{pq \in S^k} (||f_p||^2 + ||f_q||^2 - 2\langle f_p, f_q \rangle)}{2\ |S^k|} \\
&= \sum_{k=1}^{K} \frac{\sum_{pq \in S^k} (||f_p||^2 + ||f_q||^2) - 2\sum_{pq \in S^k} \langle f_p, f_q \rangle}{2\ |S^k|}
\end{aligned}$$

Note that $\sum_{pq \in S^k} (||f_p||^2 + ||f_q||^2)$ is just the sum of the square of norms of all pairs of points (p, q). Each point can form $|S^k|$ points with another point (including itself). So the summation is equivalent to $|S^k| \sum_{p \in S^k} ||f_p||^2$.

Therefore, the above equation becomes \begin{align} LHS &= \sum*{k=1}^K *frac{|S^k|* *sum*{p\in S^k}|f*p|^2 - 2* *sum*{pq\in S^k}\langle f_p, f*q *rangle}{2\;|S^k|} \ &= *sum*{k=1}^K \frac{\sum_{p\in S^k}|f*p|^2}{2} - *frac{2* *sum*{pq\in S^k}\langle f_p, f*q *rangle}{2\;|S^k|} \ &= *frac{\sum*{p\in S}|f*p|^2}{2} - *sum*{k=1}^K \frac{2* \sum_{pq\in S^k}\langle f_p, f*q *rangle}{2\;|S^k|} \ &= *const* - *sum*{k=1}^K \frac{\sum_{pq\in S^k}\langle f_p, f_q \rangle}{\;|S^k|} \ &= RHS \end{align}

Problem 2 (a simple finite-dimensional version of Mercer theorem)

Let A be an $n \times n$ positive semi-definite matrix defining pairwise affinities between n ponts. Find a closed expression for n vectors ϕ_i (a so-called "Euclidean embedding") such that their Euclidean dot products agree with the given affinites, i.e. $\langle \phi_i, \phi_j \rangle = A_{ij}$ for all $1 \leq i, j \leq n$. You can assume known eigen-decomposition $A = Q \Lambda Q^T$ where $\Lambda = diag(\lambda_1, \dots, \lambda_n)$ is a diagonal matrix of (non-negative!) eigen-values and Q is an orthogonal $n \times n$ matrix whose columns Q_i are unit eigen-vectors of A.

Solution:

$$
\begin{aligned}
A &= Q \Lambda Q^T \\
&= [q_1 \ \dots \ q_n] \ diag(\lambda_1, \dots, \lambda_n) \begin{bmatrix} q_1^T \\ \dots \\ q_n^T \end{bmatrix} \\
&= [\lambda_1 q_1 \ \dots \ \lambda_n q_n] \begin{bmatrix} q_1^T \\ \dots \\ q_n^T \end{bmatrix}
\end{aligned}
$$

Let q_{ij} denote the j-th component of the i-th eigenvector q_i. Then, multiplying the two matrices above gives

$$
\begin{aligned}
A_{ij} &= \lambda_1 q_{1i} q_{1j} + \dots + \lambda_n q_{ni} q_{nj} \\
&= \sqrt{\lambda_1} q_{1i} \sqrt{\lambda_1} q_{1j} + \dots \sqrt{\lambda_n} q_{ni} \sqrt{\lambda_n} q_{nj} \\
&= \langle \phi_i, \phi_j \rangle
\end{aligned}
$$

Therefore, \begin{align} \phi_i = \begin{bmatrix} \sqrt{\lambda*1}q*{1i} \ \ldots \ \sqrt{\lambda*n}q*{ni} \end{bmatrix} \end{align}

Hence, ϕ_i is the i-th row of the eigenvector matrix, with each component multiplied by $\sqrt{\lambda_i}$.

Problem 3 (approximate low-dimenstional Euclidean embedding)

Assume that $\tilde{A}$ is a low-rank approximation of matrix A in problem 2 of given rank $m

Comment: basic K-means (Lloyd's algorithm) over such points $\{\tilde{\phi}_i\}$ can be used as an approximate algorithm for kernel clusterng (e.g. for average association criteria). This approach is an example of "spectral clustering", which uses eigen decomposition of the affinity matrix A.

Solution:

The last $n - m$ eigenvalues are 0. Hence, we can write the matrix $\tilde{A}$ as

$$\tilde{A} = [q_1 \ \dots \ q_m] \ diag(\lambda_1, \dots, \lambda_m) \begin{bmatrix} q_1^T \\ \dots \\ q_m^T \end{bmatrix}$$

Following our work in the previous problem, we get

$$\tilde{\phi}_i = \begin{bmatrix} \sqrt{\lambda_1} q_{1i} \\ \dots \\ \sqrt{\lambda_m} q_{mi} \end{bmatrix}$$

Since $\tilde{\phi}_i$ has m components, it is trivial to see that the $\tilde{\phi}_i$ belongs to $\mathcal{R}^m$.

Problem 4 (K-means).

Subproblem 4.1

Implement K-means algorithm for clustering pixel features. Most of the work is already done for you, but you do get a chance to play with numpy and to evaluate empirical properties of K-means.

The provided code below only computes random pixel segments. You need to write code producing correct clusters and correct "means". To achive this you only need to complete implementation of functions *compute_means* **and** *compute_labels* **inside "MyKmenasApp" corresponding to the two iterative steps in Lloyd's algorithm (as in "compute_k_means_clusters").**

Your implementation of the main two steps of K-means algorithm should use RGBXY features. Relative contribution of "squared errors" from XY features must be set by parameter "weightXY" (or self.w inside MyKmeansApp), so that the squared error between RGBXY feture $F_p = [R_p, G_p, B_p, X_p, Y_p]$ at any pixel p and any given cluster mean $m = [R_m, G_m, B_m, X_m, Y_m]$ is

$$||F_p - m||^2 = (R_p - R_m)^2 + (G_p - G_m)^2 + (B_p - B_m)^2 + w \cdot (X_p - X_m)^2 + w \cdot (Y_p - Y_m)^2.$$

Fully implemented "KmeansPresenter" visulaizes the segmentation results (cluster labels mask) where each cluster is highlighted either by some random color (press r-key) or by the "mean" segment color (press m-key). All keys that "KmeansPresenter" responds to are as follows:

1. press 'i'-key for each (i)teration of K-means
2. press 'c'-key to run K-means to (c)onvergence (when energy improvement is less than given threshold)
3. press 'v'-key to run K-means to convergence with (v)isualization of each iteration
4. press 'r'-key to start over from (r)andom means
5. press 's'-key to change to a random (s)olid color-palette for displaying clusters
6. press 't'-key to change to a random (t)ransparent palette for displaying clusters
7. press 'm'-key to change to the (m)ean-color palette for displaying clusters

In [1]:
```
%matplotlib notebook
# loading standard modules
import numpy as np
import math
import matplotlib.pyplot as plt
from skimage import img_as_ubyte
from skimage.color import rgb2grey

# loading custom module (requires file asg1.py in the same directory as
 the notebook file)
from asg1_error_handling import Figure, KmeansPresenter
```

In [2]:
```
class MyKmeansApp:

    def __init__(self, img, num_clusters=2, weightXY=1.0):
        self.k = num_clusters
        self.w = weightXY
        self.iteration = 0   # iteration counter
        self.energy = np.infty  # energy - "sum of squared errors" (SSE)

        num_rows = self.num_rows = img.shape[0]
        num_cols = self.num_cols = img.shape[1]

        self.im = img

        self.means = np.zeros((self.k,5),'d') # creates a zero-valued (d
ouble) matrix of size Kx5
        self.init_means()

        self.no_label = num_clusters  # special label value indicating p
ixels not in any cluster (e.g. not yet)

        # mask "labels" where pixels of each "region" will have a unique
 index-label (like 0,1,2,3,..,K-1)
        # the default mask value is "no-label" (K) implying pixels that
 do not belong to any region (yet)
        self.labels = np.full((num_rows, num_cols), fill_value=self.no_l
abel, dtype=np.int)

        x, y = np.indices((num_rows, num_cols))
        self.rgbxy = np.zeros((num_rows, num_cols, 5), dtype=np.int)
        self.rgbxy[:,:,:3] = img
        self.rgbxy[:,:,3] = x
        self.rgbxy[:,:,4] = y

        self.fig = Figure()
        self.pres = KmeansPresenter(img, self)
        self.pres.connect_figure(self.fig)

    def run(self):
        self.fig.show()

    def init_means(self):
        self.iteration = 0           # resets iteration counter
        self.energy = np.infty       # and the energy

        poolX = range(self.num_cols)
        poolY = range(self.num_rows)

        # generate K random pixels (Kx2 array with X,Y coordinates in ea
ch row)
        random_pixels = np.array([np.random.choice(poolX,self.k),np.rand
om.choice(poolY,self.k)]).T

        for label in range(self.k):
            self.means[label,:3] = self.im[random_pixels[label,1],random
_pixels[label,0],:3]
            self.means[label,3] = random_pixels[label,0]
```

```
            self.means[label,4] = random_pixels[label,1]

    # This function compute average values for R, G, B, X, Y channel (fe
ature component) at pixels in each cluster
    # represented by labels in given mask "self.labels" storing indeces
 in range [0,K). The averages should be
    # saved in (Kx5) matrix "self.means". The return value should be the
 number of non-empty clusters.
    def compute_means(self):
        labels = self.labels
        num_clusters = np.zeros((self.k, 1), dtype=np.int)

        # Your code below should compute average values for R,G,B,X,Y fe
atures in each segment
        # and save them in (Kx5) matrix "self.means". For empty clusters
 set the corresponding mean values
        # to infinity (np.infty). Report the correct number of non-empty
 clusters by the return value.

        for k in range(self.k):
            i, j = np.where(labels == k)
            num_clusters[k] = i.shape[0]
            if num_clusters[k] == 0:
                self.means[k,:] = np.infty
            else:
                k_label_pts = self.im[i, j]
                r = k_label_pts[:,0]
                g = k_label_pts[:,1]
                b = k_label_pts[:,2]
                self.means[k,:] = np.array([r.mean(), g.mean(), b.mean
(), i.mean(), j.mean()]).astype(np.int)

        return np.sum(num_clusters > 0)

    # The segmentation mask is used by KmeanPresenter to paint segments
 in distinct colors
    # NOTE: valid region labels are in [0,K), but the color map in Kmean
sPresenter
    #       accepts labels in range [0,K] where pixels with no_label=K a
re not painted/colored.
    def get_region_mask(self):
        return self.labels

    # This function computes optimal (cluster) index/label in range 0,
1,...,K-1 for pixel x,y based on
    # given current cluster means (self.means). The functions should sav
e these labels in "self.labels".
    # The return value should be the corresponding optimal SSE.
    def compute_labels(self):
        shape = (self.num_rows,self.num_cols)
        opt_labels = np.full(shape, fill_value=self.no_label, dtype=np.i
nt) # HINT: you can use this array to store and update

    # currently the best label for each pixel.

        min_dist = np.full(shape, fill_value=np.inf)  # HINT: you can us
e this array to store and update
```

```
                                                        # the (squared) di
stance from each pixel to its current "opt_label".
                                                        # use 'self.w' as
 a relative weight of sq. errors for X and Y components

        # Replace the code below by your code that computes "opt_labels"
 array of labels in range [0,K) where
        # each pixel's label is an index 'i' such that self.mean[i] is t
he closest to R,G,B,X,Y values of this pixel.
        # Your code should also update min_dist so that it contains the
 optmail squared errors

        distances = np.full((self.num_rows, self.num_cols, self.k), fill
_value=np.inf)

        for k in range(self.k):
            distances[:,:,k] = (((self.rgbxy - self.means[k])**2) * [1,
1, 1, self.w, self.w]).sum(axis=2)

        min_dist[:,:] = distances.min(axis=2)
        opt_labels[:,:] = distances.argmin(axis=2)

        # update the labels based on opt_labels computed above
        self.labels = opt_labels

        # returns the optimal SSE (corresponding to optimal clusters/cla
bels for given means)
        return min_dist.sum()

    # The function below is called by "on_key_down" in KmeansPresenter".
    # It's goal is to run an iteration of K-means procedure
    # updating the means and the (segment) labels
    def compute_k_means_clusters(self):
        self.iteration += 1

        # the main two steps of K-means algorithm
        energy = self.compute_labels()
        num_clusters = self.compute_means()

        # computing improvement and printing some information
        num_pixels = self.num_rows*self.num_cols
        improve_per_pixel = (self.energy - energy)/num_pixels
        energy_per_pixel = energy/num_pixels
        self.energy = energy

        self.fig.ax.text(0, -8,   # text location
                         'iteration = {:_>2d},  clusters = {:_>2d},  SS
E/p = {:_>7.1f},   improve/p = {:_>7.3f}    '.format(
                          self.iteration,       num_clusters,        ene
rgy_per_pixel,    improve_per_pixel),
                          bbox={'facecolor':'white', 'edgecolor':'none'
})

        return improve_per_pixel
```

Subproblem 4.2

Use K-means to generate 3-4 representative results (you can use your own images) with color quantization and superpixels. Experiment with different values of parameter K (in the range 2-80). Compare representative values of optimal SSE for smaller and larger K and explain the observed differences. Add more cells (code and/or text) as necessary.

In [3]:
```
img = plt.imread('images/rose.bmp')
clusters = [2, 10, 40, 80]
apps = []
for c in clusters:
    app = MyKmeansApp(img, num_clusters=c, weightXY=2.0)
    app.run()
    apps.append(app)
```

K-means

K-means

iteration = 23, clusters = _6, SSE/p = 12945.1, improve/p = _-0.175

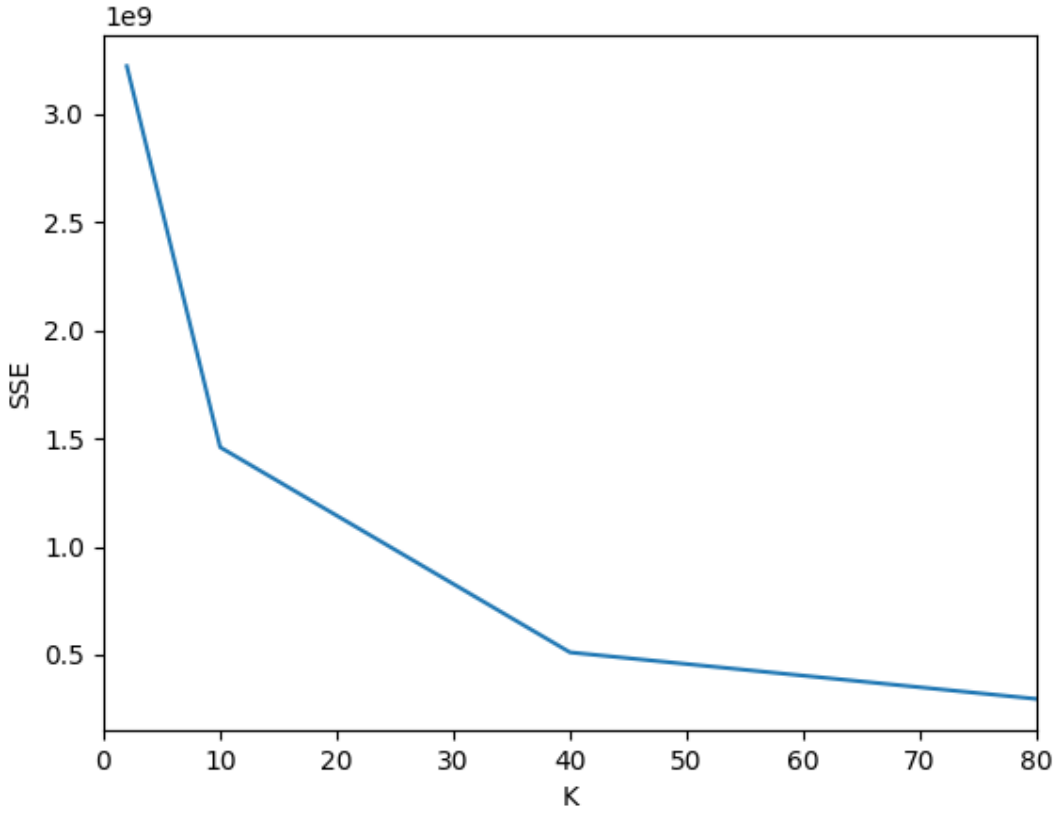
K-means

iteration = 76, clusters = 21, SSE/p = _4535.8, improve/p = __0.000

K-means

iteration = 72, clusters = 37, SSE/p = _2628.0, improve/p = _-0.019

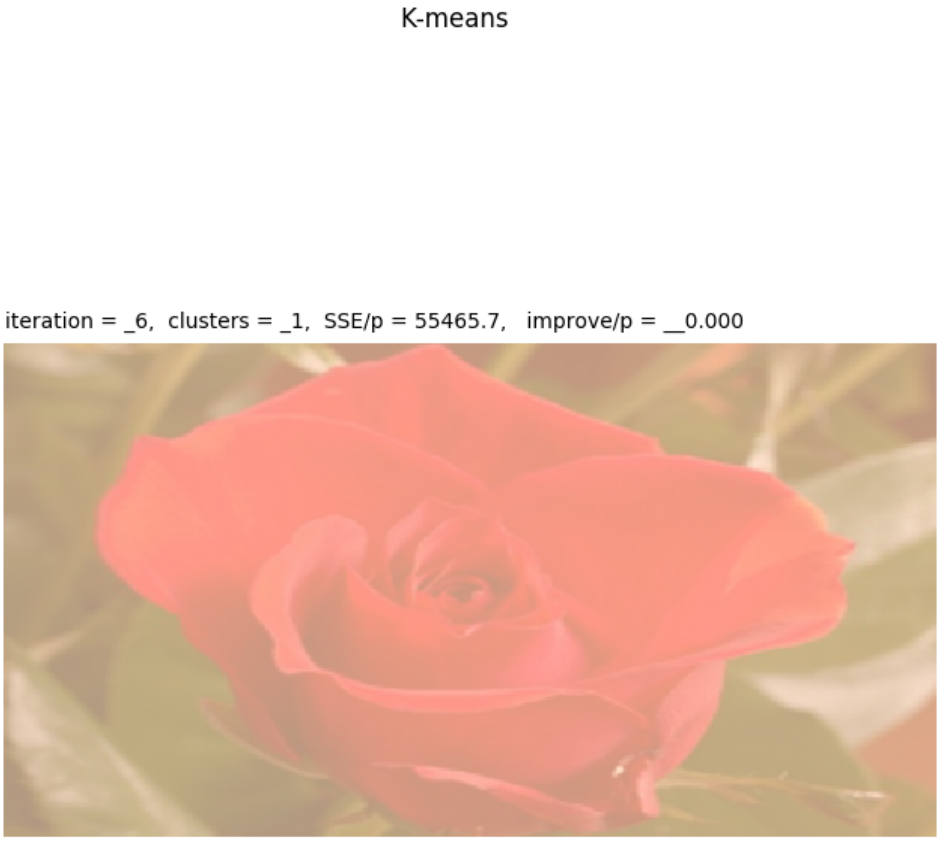
In [4]:
```
# Plot SSE vs k
plt.figure()
sse = [app.energy for app in apps]
plt.plot(clusters, sse)
plt.xlabel('K')
plt.ylabel('SSE')
plt.xlim(0, 80);
```



Subprobelm 4.3

Evaluate sensitivity of K-means to local minima (you can use your own images). Show 2-3 different solutions for different random initial means and display the corresponding values of the K-means energy. Add more cells (code and/or text) as necessary.

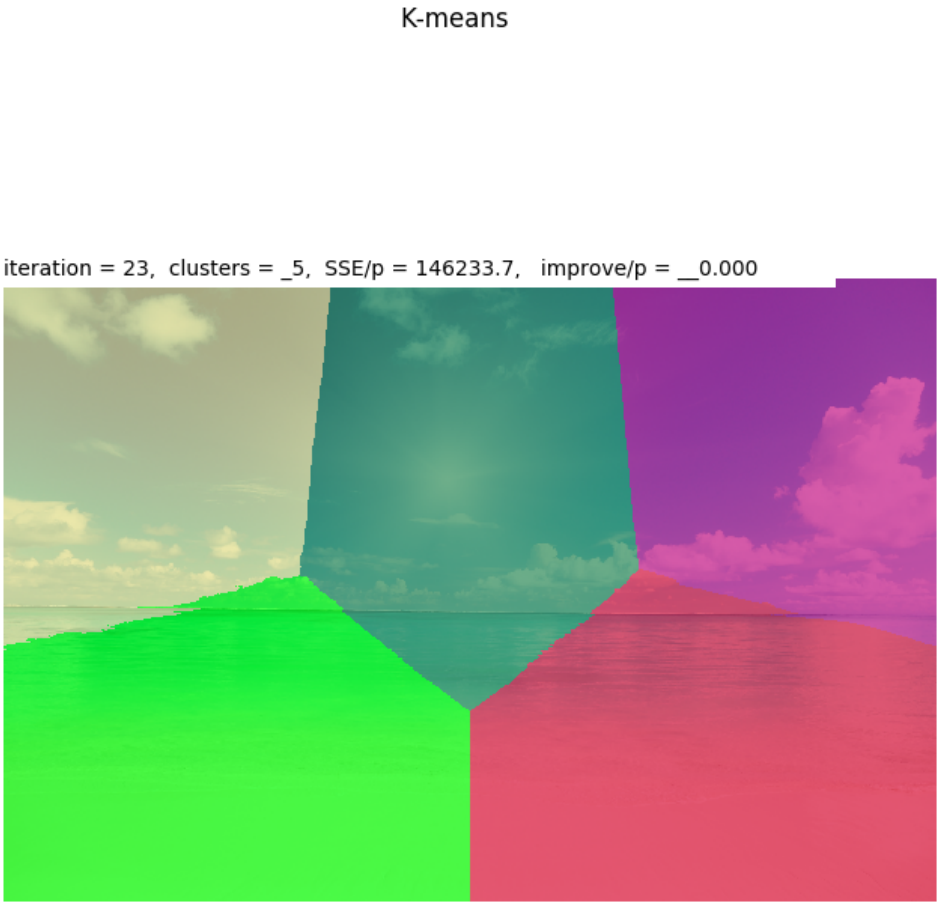
In [29]:
```
img = plt.imread('images/rose.bmp')
app = MyKmeansApp(img, num_clusters=2, weightXY=2.0)
app.run()
```



In [30]:
```
print "The k-means energy is %f" % app.energy
```

```
The k-means energy is 6252534221.000000
```

In [31]:
```
img = plt.imread('images/beach.jpg')
app = MyKmeansApp(img, num_clusters=10, weightXY=2.0)
app.run()
```



In [32]:
```
print "The k-means energy is %f" % app.energy
```

```
The k-means energy is 292534607718.000000
```