Assignment 3

Part II: K-means Segmentation

Problem 1

Show algebraic equivalence between two non-parametric formulations for K-means (objectives $E(S)$ at the bottom of slide 57, Topic 9):

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

Solution:

Lets apply the property of $(a-b)^2 = a^2 + b^2 - 2ab$

Applying this to $\|f_p - f_q\|^2$ gives us:

$$\|f_p - f_q\|^2 = \langle f_p, f_p \rangle + \langle f_q, f_q \rangle - 2\langle f_p, f_q \rangle$$

Subbing this into the right hand equation, gives us:

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

Breaking it up gives us:

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

Simplyfying a bit further by removing the 2 to give us:

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

The right part of the equation is now in the form we want. Since the left part is a summation over all p and q, we can simplyfy it as follows:

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

Let that be the constant. Therefore const = $\sum_{k=1}^{K} \sum_{p \in S^k} \langle f_p, f_p \rangle$

Subbing it into the above equation gives us:

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

Since we let the right part be the constant, we get:

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

This gives us the outcome we were looking for:

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

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-form 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 $\Lambda = diag(\lambda_1, \ldots, \lambda_n)$ 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: Q is an $n \times n$ matrix (so is Q^T). Λ is a diagonal matrix of size $n \times n$.

Therefore the resulting martix $A = Q \Lambda Q^T$ will also be an $n \times n$ matrix

$$Q \Lambda Q^T = \begin{bmatrix} Q_{11}\Lambda_1 Q_{11} + \ldots + Q_{1n}\Lambda_n Q_{1n} & \ldots & Q_{11}\Lambda_1 Q_{n1} + \ldots + Q_{1n}\Lambda_n Q_{nn} \\ Q_{21}\Lambda_1 Q_{11} + \ldots + Q_{2n}\Lambda_n Q_{1n} & \ldots & Q_{21}\Lambda_1 Q_{n1} + \ldots + Q_{2n}\Lambda_n Q_{nn} \\ & \cdot & \\ & \cdot & \\ & \cdot & \\ Q_{n1}\Lambda_1 Q_{11} + \ldots + Q_{nn}\Lambda_n Q_{1n} & \ldots & Q_{n1}\Lambda_1 Q_{n1} + \ldots + Q_{nn}\Lambda_n Q_{nn} \end{bmatrix}$$

From this we can see that $A_{ij} = Q_{i1}\Lambda_1 Q_{j1} + \ldots + Q_{in}\Lambda_n Q_{jn}$

And since $A_{ij} = \langle \phi_i, \phi_j \rangle$, we can break up the above expression to find ϕ_i and ϕ_j

Therefore, $\phi_i = \begin{bmatrix} Q_{i1} * \sqrt{\Lambda_1} \\ Q_{i2} * \sqrt{\Lambda_2} \\ \cdot \\ \cdot \\ \cdot \\ Q_{in} * \sqrt{\Lambda_n} \end{bmatrix}$ and $\phi_j = \begin{bmatrix} \sqrt{\Lambda_1} * Q_{j1} \\ \sqrt{\Lambda_2} * Q_{j2} \\ \cdot \\ \cdot \\ \cdot \\ \sqrt{\Lambda_n} * Q_{jn} \end{bmatrix}$

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 $m < n$. That is, $\tilde{A} = Q\Lambda_m Q^T$ where $\Lambda_m = diag(\lambda_1, \ldots, \lambda_m, 0, \ldots, 0)$ is a diagonal matrix of the largest m eigen values of A (a la Eckart–Young–Mirsky theorem, Topic 8). Using your solution for problem 2, specify a formula for "Euclidean embedding" $\{\tilde{\phi}_i\}$ such that $\langle \tilde{\phi}_i, \tilde{\phi}_j \rangle = \tilde{A}_{ij}$ and show that $\tilde{\phi}_i \in \mathcal{R}^m$.

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: From Q2, we calculated ϕ_i. But now we are given Λ_m, where the last $n-m$ elements are zero. Taking that into account, we get:

$$\phi_i = \begin{bmatrix} Q_{i1} * \sqrt{\Lambda_1} \\ Q_{i2} * \sqrt{\Lambda_2} \\ . \\ . \\ . \\ Q_{im} * \sqrt{\Lambda_m} \\ 0 \\ . \\ . \\ . \\ 0 \end{bmatrix} \text{ and } \phi_j = \begin{bmatrix} \sqrt{\Lambda_1} * Q_{j1} \\ \sqrt{\Lambda_2} * Q_{j2} \\ . \\ . \\ . \\ \sqrt{\Lambda_m} * Q_{jm} \\ 0 \\ . \\ . \\ . \\ 0 \end{bmatrix}$$

Removing the $n-m$ zeros we get:

$$\tilde{\phi}_i = \begin{bmatrix} Q_{i1} * \sqrt{\Lambda_1} \\ Q_{i2} * \sqrt{\Lambda_2} \\ . \\ . \\ . \\ Q_{im} * \sqrt{\Lambda_m} \end{bmatrix} \text{ and } \tilde{\phi}_j = \begin{bmatrix} \sqrt{\Lambda_1} * Q_{j1} \\ \sqrt{\Lambda_2} * Q_{j2} \\ . \\ . \\ . \\ \sqrt{\Lambda_m} * Q_{jm} \end{bmatrix}$$

Which gives us $\langle \tilde{\phi}_i, \tilde{\phi}_j \rangle = \tilde{A}_{ij} = Q_{i1}\Lambda_1 Q_{j1} + \ldots + Q_{im}\Lambda_m Q_{jm} = Q\Lambda_m Q^T$

And by definition of $\tilde{\phi}_i$, we have that $\tilde{\phi}_i \in \mathcal{R}^m$

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)
        self.kCoord = []
        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 (double) matrix of size Kx5
        self.init_means()

        self.no_label = num_clusters  # special label value indicating pixels 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_label, dtype=np.int)

        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 each row)
        random_pixels = np.array([np.random.choice(poolX,self.k),np.random.choice(poolY,self.k)]).T
        self.kCoord = random_pixels
        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
 (feature component) at pixels in each cluster
    # represented by labels in given mask "self.labels" storing indec
es 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
        non_empty_clusters = 0
        k = self.k
        im = self.im

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


        means = np.full((k, 5), np.inf, dtype = float)

        for i in range (k):
            location = np.argwhere(labels == i)
            if len(location != 0):

                rgb = np.mean(np.array([im[p[0], p[1], :3] for p in l
ocation]), axis = 0)

                xy = np.mean(location, axis = 0)
                means[i, :3] = rgb
                means[i, 3:] = xy
                non_empty_clusters += 1
        self.means = means
        return non_empty_clusters









    # The segmentation mask is used by KmeanPresenter to paint segmen
ts in distinct colors
    # NOTE: valid region labels are in [0,K), but the color map in Km
eansPresenter
    #       accepts labels in range [0,K] where pixels with no_label=
K are 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
 save 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)
        k = self.k
        w = self.w
        im = self.im
        means = self.means
        opt_labels = np.full(shape, fill_value=self.no_label, dtype=n
p.int) # 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
use this array to store and update
                                                      # the (squared)
distance 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_labe
ls" array of labels in range [0,K) where
        # each pixel's label is an index 'i' such that self.mean[i] i
s the closest to R,G,B,X,Y values of this pixel.
        # Your code should also update min_dist so that it contains t
he optimal squared errors
        # update the labels based on opt_labels computed above

        distance = np.zeros((k, shape[0], shape[1]))
        x, y = np.mgrid[0 : shape[0], 0 : shape[1]]

        for i in range(k):
            distance[i] = ((im[:, :, :3] - means[i, :3]) ** 2).sum(ax
is = 2) + w * ((x - means[i, 3]) ** 2 + (y - means[i, 4]) ** 2)

        opt_labels = np.argmin(distance, axis = 0)
        min_dist = np.amin(distance, axis = 0)

        self.labels = opt_labels

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




    # The function below is called by "on_key_down" in KmeansPresente
r".
```

```
    # 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},
 SSE/p = {:_>7.1f},   improve/p = {:_>7.3f}    '.format(
                         self.iteration,       num_clusters,
energy_per_pixel,    improve_per_pixel),
                         bbox={'facecolor':'white', 'edgecolor':'non
e'})

        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 [4]:
```
img = plt.imread('images/rose.bmp')
app = MyKmeansApp(img, num_clusters=80, weightXY=2.0)
app.run()
```

K-means

iteration = 57, clusters = 41, SSE/p = _2435.7, improve/p = __0.482

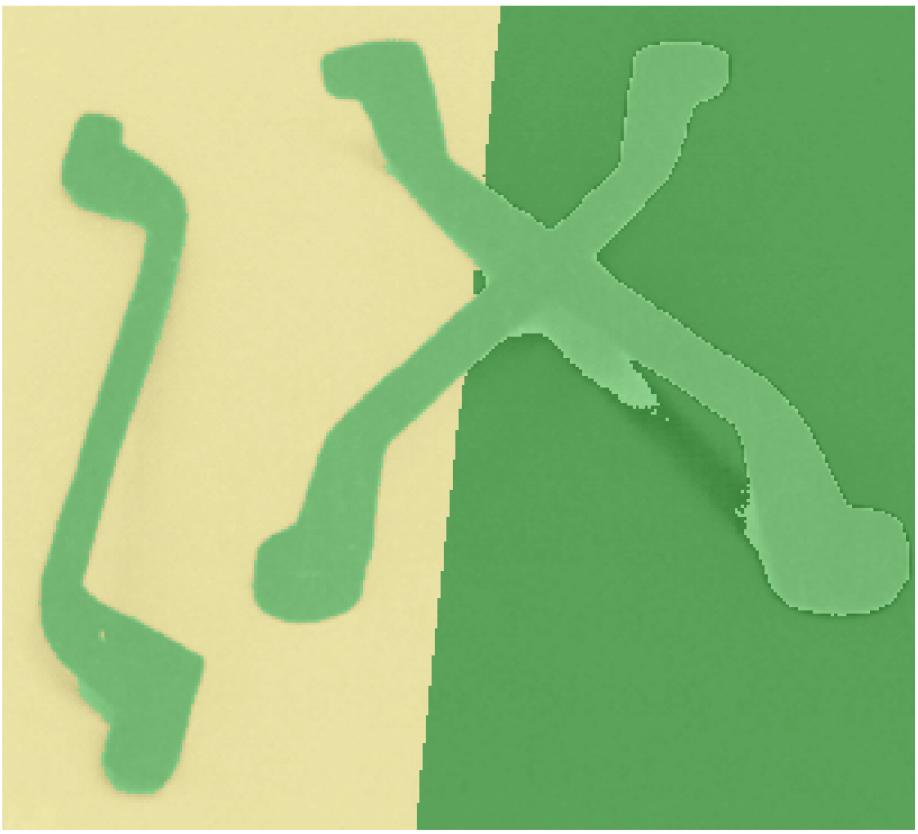
Subprobelm 4.3

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.

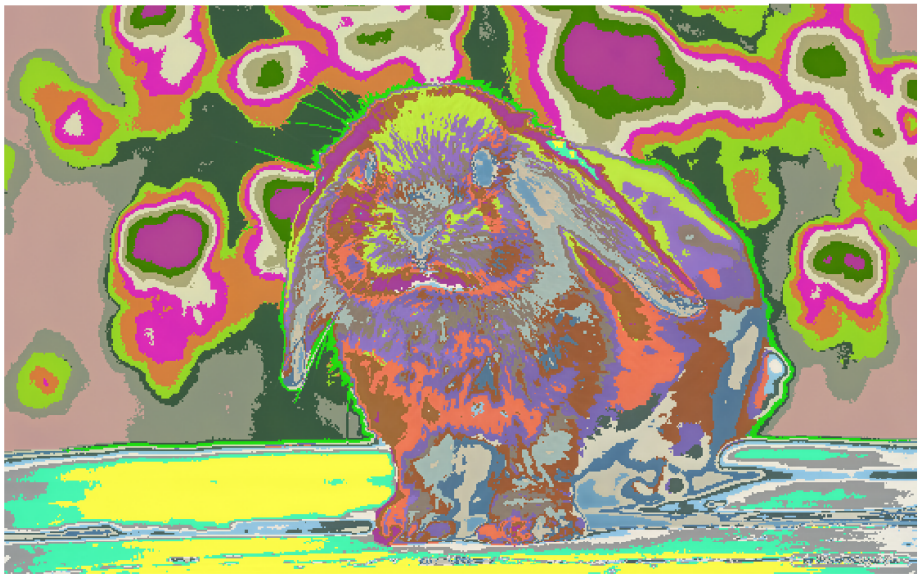
In [3]:
```
img = plt.imread('images/tools.bmp')
app = MyKmeansApp(img, num_clusters=3, weightXY=1.0)
app.run()
```

K-means

iteration = 18, clusters = _3, SSE/p = _9882.9, improve/p = __0.000



In [4]:
```
img = plt.imread('images/bunny.bmp')
app = MyKmeansApp(img, num_clusters=30, weightXY=0.0)
app.run()
```



In [ ]:
```

```