> Note: This report was made on `Hackmd.io` and restricted by the `.pdf` format, the `.gif` animation would not display. Please view it on https://hackmd.io/@swchiu/BJwOjuc3U, thanks.

Kernel K-means

Kernel k-means is an approach to k-means algorithm, but mapping the data into higher degree dimentions.
And the mapping-function called `Kernel`.

K-means algorithm is that after comparing the data similarity, we cluster the more similarity datas to the same group.
`K` means that there are k number of group to cluster.

For the regular K-means, we use the following formula to compare and cluster data.

$arg\ min_{(C_1,\mu_1)...(C_k,\mu_k)} \sum_{i=1}^{k} \sum_{x_j \in C_i} ||x_j - \mu_i||^2$

How about kernel k-means?

we transfrom the data to the higher degree, and do the same k-means algorithm on it.

$arg\ min_{(C_1,\mu_1^\phi)...(C_k,\mu_k^\phi)} \sum_{i=1}^{k} \sum_{\phi(x_j) \in C_i} ||\phi(x_j) - \mu_i^\phi||^2$

$$
\begin{aligned}
||\phi(x_j) - \mu_i^\phi||^2 &= \phi^T(x_j)\phi(x_j) - 2\phi^T(x_j)\frac{1}{|C_k|}\sum_{x_n \in c_k}\phi(x_n) + \frac{1}{|C_k|^2}\sum_{x_p \in C_k}\sum_{x_q \in C_k}\phi^T(x_p)\phi(x_q) \\
&= K(x_j, x_j) - \frac{2}{|C_k|}\sum_{x_n \in c_k} K(x_j, x_n) + \frac{1}{|C_k|^2}\sum_{x_p \in C_k}\sum_{x_q \in C_k} K(x_p, x_q)
\end{aligned}
$$

Instead of update μ_k in the k-means algorithm, update only C_k in the kernel k-means algorithm.

The Work

- kernel function: $e^{-\gamma_1||S(x)-S(x')||^2} \times e^{-\gamma_2||C(x)-C(x')||^2}$
- Input data: Two 100*100 images

Step 1

Prepare image data for precompute gram matrix (`kernel`)

```
def img_formater(img):
    n = img.shape[0]*img.shape[1]
    spatial_data = []
    color_data = []
    for i in range(img.shape[0]):
        for j in range(img.shape[1]):
            spatial_data.append([i, j])
            color_data.append(img[i][j])
    return np.array(spatial_data), np.array(color_data, dtype=int)

img = imageio.imread(img_path)
spatial_data, color_data = img_formater(img)
```

Step 2

Compute gram matrix

> At the first, I implement this part by for-loop which is a trivial way.
> But I found that it is too time-consuming! Because there are 10^4 data points for our input data, and we need to calculate a $10^4 \times 10^4$ gram matrix.
> So I replace my for-loop implementation into matrix-computation for efficient.

$$euclidean^2 = ||u-v||^2 = (u-v)^T(u-v) = ||u||^2 - 2u^Tv + ||v||^2$$

Above formula is suitable for vector which is stroed in $d \times 1$ matrix.
But in this work, the vectors are stored in $1 \times d$ matrix, so I applied the following formula revised.

$$euclidean^2 = ||u-v||^2 = (u-v)(u-v)^T = ||u||^2 - 2uv^T + ||v||^2$$

And for the performance, I take all vectors into one matrix D which is $n \times d$ for calculate gram matrix G which is $n \times n$, let E as the euclidean matrix

$$D = \begin{bmatrix} V_1 \\ V_2 \\ \dots \\ V_{n-1} \\ V_n \end{bmatrix}_{n \times d}, V_i = \begin{bmatrix} v_{i1} & v_{i2} & \dots & v_{id} \end{bmatrix}_{1 \times d}$$

$$E = \begin{bmatrix} ||V_1, V_1||^2 & ||V_1, V_2||^2 & \dots & ||V_1, V_n||^2 \\ ||V_2, V_1||^2 & ||V_2, V_2||^2 & \dots & ||V_2, V_n||^2 \\ \vdots & \vdots & \dots & \vdots \\ ||V_n, V_1||^2 & ||V_n, V_2||^2 & \dots & ||V_n, V_n||^2 \end{bmatrix}$$

$$= \begin{bmatrix} ||V_1||^2 - 2V_1V_1^T + ||V_1||^2 & \dots & ||V_1||^2 - 2V_1V_n^T + ||V_n||^2 \\ \vdots & \dots & \vdots \\ ||V_n||^2 - 2V_nV_1^T + ||V_1||^2 & \dots & ||V_n||^2 - 2V_nV_n^T + ||V_n||^2 \end{bmatrix}$$

$$= \begin{bmatrix} ||V_1||^2 & \dots & ||V_1||^2 \\ ||V_2||^2 & \dots & ||V_2||^2 \\ \vdots & \dots & \vdots \\ ||V_n||^2 & \dots & ||V_n||^2 \end{bmatrix} - 2DD^T + \begin{bmatrix} ||V_1||^2 & \dots & ||V_1||^2 \\ ||V_2||^2 & \dots & ||V_2||^2 \\ \vdots & \dots & \vdots \\ ||V_n||^2 & \dots & ||V_n||^2 \end{bmatrix}^T$$

$$= D^2 \begin{bmatrix} 1 & 1 & \dots & 1 \\ \vdots & \vdots & \dots & \vdots \\ 1 & 1 & \dots & 1 \end{bmatrix}_{d \times n} - 2DD^T + \begin{bmatrix} 1 & 1 & \dots & 1 \\ \vdots & \vdots & \dots & \vdots \\ 1 & 1 & \dots & 1 \end{bmatrix}_{n \times d} (D^T)^2$$

So we could calculate G as $G = e^E$ without for-loop.

```
#Origianl trvial implementation
def rbf_img(u, v, g=0.0001):
    s_dis = scipy.spatial.distance.euclidean(u[0], v[0])
    c_dis = scipy.spatial.distance.euclidean(u[1], v[1])
    return math.exp(-1*g*s_dis**2 - g*c_dis**2)

def gram_matrix(data, path, kernel=rbf_img):
    gram = np.ones((len(data), len(data)))
    for i in range(len(data)):
        for j in range(i, len(data)):
            gram[i][j] = kernel(data[i], data[j])
            gram[j][i] = gram[i][j]
    return gram

#-----------------------------------------------------------------------#

#New implementation using matrix computation
def euclidean(self, u, v):
    #This method is defined in kmeans.euclidean
    return np.matmul(u**2, np.ones((u.shape[1],v.shape[0]))) \
        -2*np.matmul(u, v.T) \
```

```
        +np.matmul(np.ones((u.shape[0], v.shape[1])), (v.T)**2)

def rbf(u, v, g=10**-4):
    return np.exp(-1*g*kmeans.euclidean(kmeans, u, v))

gram = rbf(spatial_data, spatial_data) \
    * rbf(color_data, color_data)
```

Step 3

Run Kernel K-means, recall the formula:

$$Let\ s_{jk} = ||\phi(x_j) - \mu_k^{\phi}||^2 = K(x_j, x_j) - \frac{2}{|C_k|}\sum_{x_n \in c_k} K(x_j, x_n) + \frac{1}{|C_k|^2}\sum_{x_p \in C_k}\sum_{x_q \in C_k} K(x_p, x_q)$$

we compare for the $||\phi(x_j) - \mu_k^{\phi}||^2$ for measuring the distance between the k^{th} cluster and the j^{th} mapped data point at every vector x_j on cluster C_k, and for the every C_k, the first terms are the same, so we could ignore it directly. I still use matrix computaion on this part, and I would explain the procedure of my derivation as below.

For each x_j, we have k values of corresponding to the k^{th} cluster (denoted by s_{jk}), and we would go throgh all datas, which means that we have $n \times k$ values in totally and it is suitable for matrix computation!
Let $S_{n\times k}$ is the distance matrix as mentioned (which is `dis` in the code segment).

$$\begin{aligned} s_{jk} &= \frac{2}{|C_k|}\sum_{x_n \in c_k} K(x_j, x_n) + \frac{1}{|C_k|^2}\sum_{x_p \in C_k}\sum_{x_q \in C_k} K(x_p, x_q) \\ &= \frac{2}{|C_k|}[\,K(x_j, x_1) \quad \dots \quad K(x_j, x_n)\,]\,C_k + \frac{1}{|C_k|^2}{C_k}^T G C_k \end{aligned}$$

s_{jk} is the j^{th} row k^{th} col element of $S_{n\times k}$, means the distance between the j^{th} mapped data point and the k^{th} cluster.

I want to do a matrix computation instead of n times computation at each data point. So I need expand the above euation to from 1×1 to $n \times k$.

$$\begin{aligned} S_{n\times k} = &\frac{2}{|C|}\begin{bmatrix} K(x_1,x_1) & K(x_1,x_2) & \dots & K(x_1,x_n) \\ K(x_2,x_1) & K(x_2,x_2) & \dots & K(x_2,x_n) \\ \vdots & \vdots & \dots & \vdots \\ K(x_n,x_1) & K(x_n,x_2) & \dots & K(x_n,x_n) \end{bmatrix}_{n\times n} C_{n\times k} \\ &+ \frac{1}{|C|^2}\begin{bmatrix} 1 & 1 & \dots & 1 \\ \vdots & \vdots & \dots & \vdots \\ 1 & 1 & \dots & 1 \end{bmatrix}_{n\times k} {C_{n\times k}}^T G_{n\times n} C_{n\times k} \end{aligned}$$

$$S_{n\times k} = \frac{2}{|C|}G_{n\times n}C_{n\times k} + \frac{1}{|C|^2}\begin{bmatrix} 1 & \dots & 1 \\ \vdots & \dots & \vdots \\ 1 & \dots & 1 \end{bmatrix}_{n\times k} {C_{n\times k}}^T G_{n\times n} C_{n\times k}$$

For the second term, we only need the diagonal elements, so in the `python` code, I multiply use a diagonal identity matrix `np.eye()`.

And there are many varies of initialization method, e.g. `k-means++` which decide the initial cluster by maxmizing their distance. I would compare `k-means++` and the traditional way at Result part.

```
def __get_init(self, method):
        if method == 'kmeans++':
            return self.__kmeanspp
        elif method == 'default':
            return self.__traditional
        else:
            print('ERROR: \'{}\' is not a pre-defined initialize
method'.format(method))
            return exit(0)

def __kmeanspp(self):
    n, d = self.data.shape
    centers = np.array([self.data[np.random.randint(n), :d]])
    for i in range(self.k-1):
        dist = self.euclidean(self.data, centers)
        dist = np.min(dist, axis=1)
        next_center = np.argmax(dist, axis=0)
        centers = np.vstack((centers, self.data[next_center, :]))
    return centers

def __traditional(self):
    return np.array(self.data[np.random.choice(self.data.shape[0],
size=self.k, replace=False), :])

def __kernel_trick(self, gram, ck):
    c_count = np.sum(ck, axis=0)
    dist = -2*np.matmul(gram, ck)/c_count + \
        np.matmul(np.ones(ck.shape), (np.matmul(ck.T, np.matmul(gram,
ck)))*np.eye(ck.shape[1]))/(c_count**2)
    return dist

def run(self):
    #initial cluster
    centers = self.init()
    dist = self.euclidean(self.data, centers)
    ck = np.zeros((self.data.shape[0], self.k))
    ck[np.arange(dist.shape[0]), np.argmin(dist, axis=1)] = 1

    record = []
    record.append(ck)
    record_iter = 0
    for i in range(self.max_iter):
```

```
        #E-step
        if self.is_kernel:
            dist = self.__kernel_trick(self.data, ck)
        else:
            dist = self.euclidean(self.data, centers)

        #M-step
        update_ck = np.zeros(dist.shape)
        update_ck[np.arange(dist.shape[0]),np.argmin(dist, axis=1)] = 1
        delta_ck = np.count_nonzero(np.abs(update_ck - ck))
        update_centers = np.matmul(update_ck.T, self.data)/np.sum(update_ck,
axis=0, keepdims=True).T

        record.append(update_ck)
        if delta_ck == 0:
            self.converge -= 1
            if self.converge == 0:
                record_iter = i+1
                if self.keep_log == False:
                    break

        ck = update_ck
        centers = update_centers
    return record, record_iter
```

Step 4

Visualization

```
k_visual = colors.to_rgba_array(['tab:blue', \
                        'tab:orange', \
                        'tab:green', \
                        'tab:red', \
                        'tab:purple', \
                        'tab:brown'])
def visualizer(record, save_path, figsize=(100,100,4)):
    gif = []
    for i in range(len(record)):
        c_id = np.argmax(record[i], axis=1)
        img = np.zeros(figsize, dtype=np.uint8)
        for j in range(c_id.shape[0]):
            m, n = (int(j/100), int(j%100))
            img[m][n] = 255*k_visual[c_id[j]]
        gif.append(img)
    imageio.mimsave(save_path, gif)

def merge_gifs(gifs, max_fram, id, method):
    gif = []
    for i in range(len(gifs)):
```

```
        gif.append(imageio.get_reader('output/'+gifs[i]))

    new_gif = imageio.get_writer('output/image'+str(id)+'_'+method+'.gif')

    if max_fram + 5 < 100:
        max_fram += 5
    for frame_number in range(max_fram):
        img = []
        for i in range(len(gif)):
            img.append(gif[i].get_next_data())
        new_image = np.hstack(img)
        new_gif.append_data(new_image)
    for i in range(len(gif)):
        gif[i].close()
    new_gif.close()
```

Screen Shot

```
processing image1...
running kernel k-means (k = 2, default).........[complete at [14] iterations]
visualizing.........[complete]
running kernel k-means (k = 2, kmeans++).........[complete at [10] iterations]
visualizing.........[complete]
faster.....................[kmeans++]
running kernel k-means (k = 3, default).........[complete at [16] iterations]
visualizing.........[complete]
running kernel k-means (k = 3, kmeans++).........[complete at [11] iterations]
visualizing.........[complete]
faster.....................[kmeans++]
running kernel k-means (k = 4, default).........[complete at [41] iterations]
visualizing.........[complete]
running kernel k-means (k = 4, kmeans++).........[complete at [37] iterations]
visualizing.........[complete]
faster.....................[kmeans++]
running kernel k-means (k = 5, default).........[complete at [45] iterations]
visualizing.........[complete]
running kernel k-means (k = 5, kmeans++).........[complete at [62] iterations]
visualizing.........[complete]
faster.....................[tradition]
running kernel k-means (k = 6, default).........[complete at [67] iterations]
visualizing.........[complete]
running kernel k-means (k = 6, kmeans++).........[complete at [37] iterations]
visualizing.........[complete]
faster.....................[kmeans++]
processing image2...
running kernel k-means (k = 2, default).........[complete at [17] iterations]
visualizing.........[complete]
running kernel k-means (k = 2, kmeans++).........[complete at [19] iterations]
visualizing.........[complete]
faster.....................[tradition]
running kernel k-means (k = 3, default).........[complete at [42] iterations]
visualizing.........[complete]
running kernel k-means (k = 3, kmeans++).........[complete at [23] iterations]
visualizing.........[complete]
faster.....................[kmeans++]
running kernel k-means (k = 4, default).........[complete at [56] iterations]
visualizing.........[complete]
running kernel k-means (k = 4, kmeans++).........[complete at [23] iterations]
visualizing.........[complete]
faster.....................[kmeans++]
running kernel k-means (k = 5, default).........[complete at [48] iterations]
visualizing.........[complete]
running kernel k-means (k = 5, kmeans++).........[complete at [27] iterations]
visualizing.........[complete]
faster.....................[kmeans++]
running kernel k-means (k = 6, default).........[complete at [33] iterations]
visualizing.........[complete]
running kernel k-means (k = 6, kmeans++).........[complete at [38] iterations]
visualizing.........[complete]
faster.....................[tradition]
```

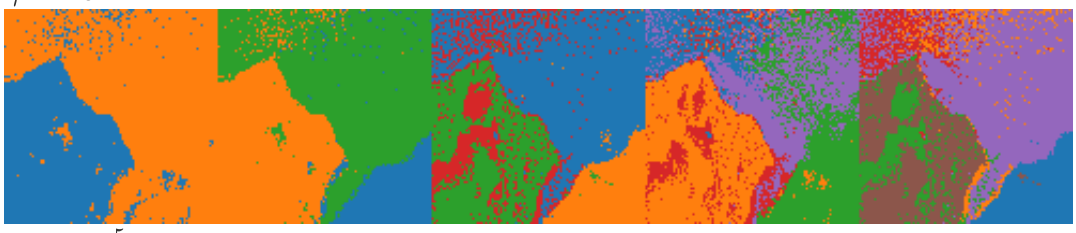
Result and The Discussion

- image1 (k=2, 3, 4, 5, 6)

  Original image:

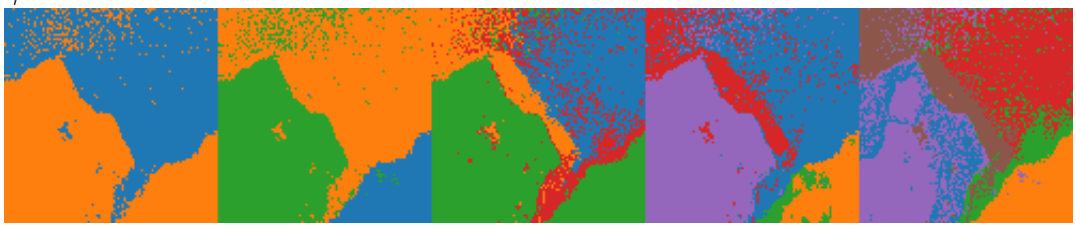
  $\gamma = 10^{-6}$:

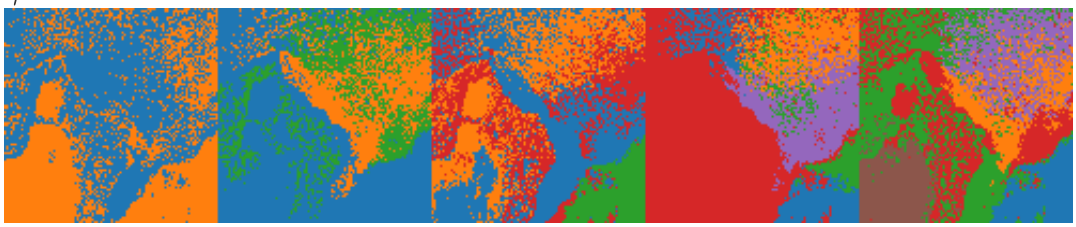
  $\gamma = 10^{-5}$:

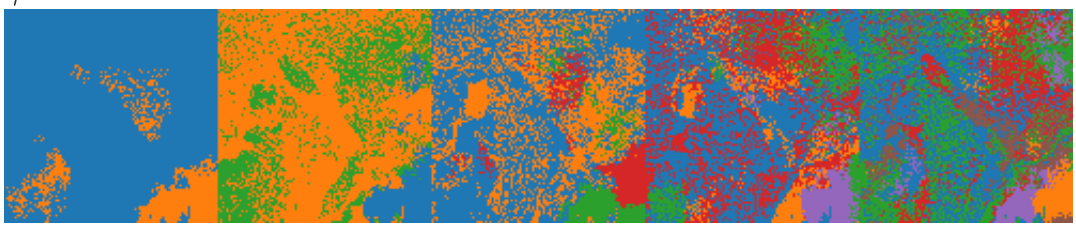
  $\gamma = 10^{-4}$:

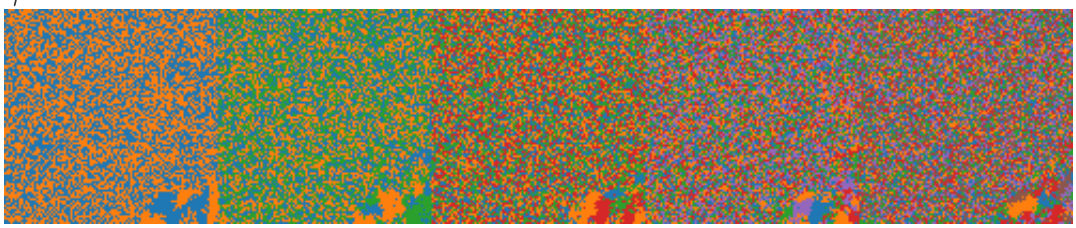
  $\gamma = 10^{-3}$:

  $\gamma = 10^{-2}$:

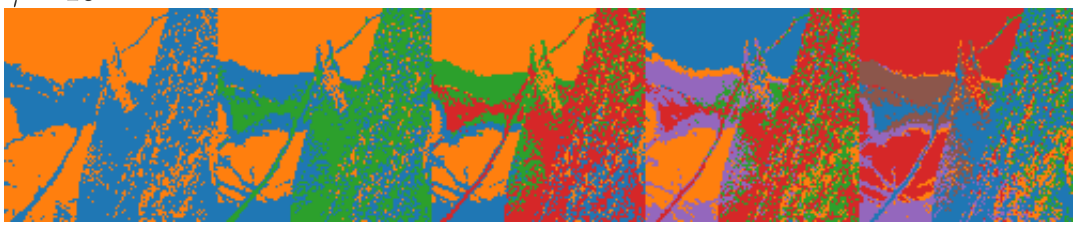
  

  $\gamma = 10^{-1}$:

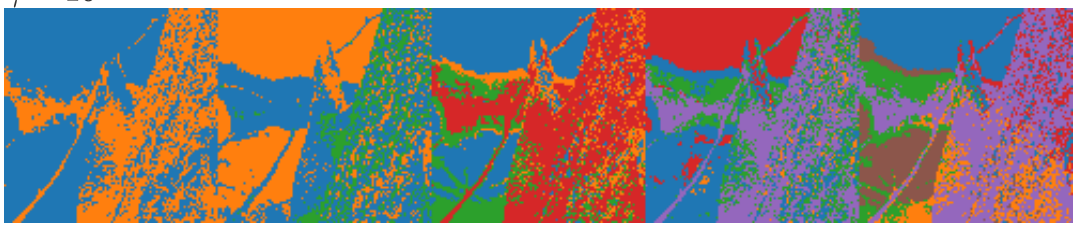
  

- image2 (k=2, 3, 4, 5, 6)

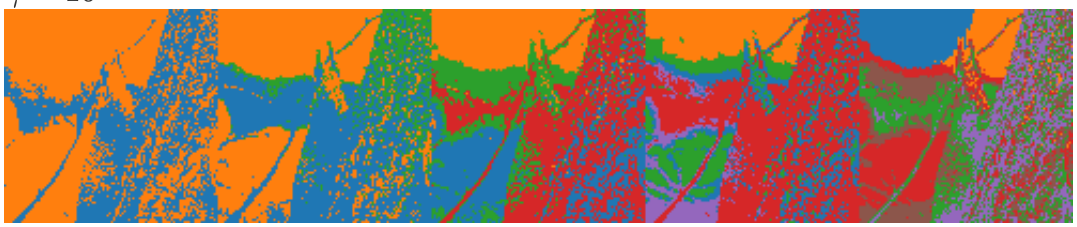
$\gamma = 10^{-6}$:



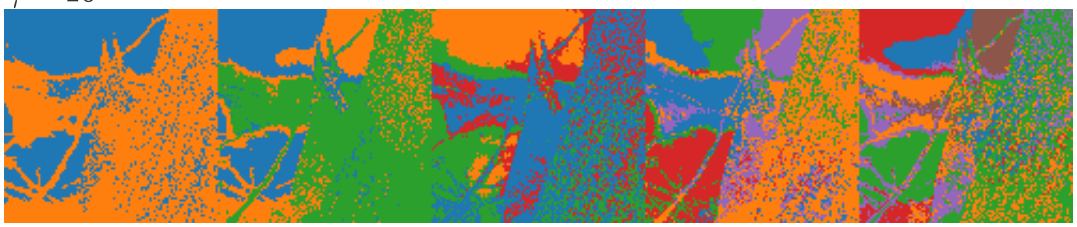
$\gamma = 10^{-5}$:



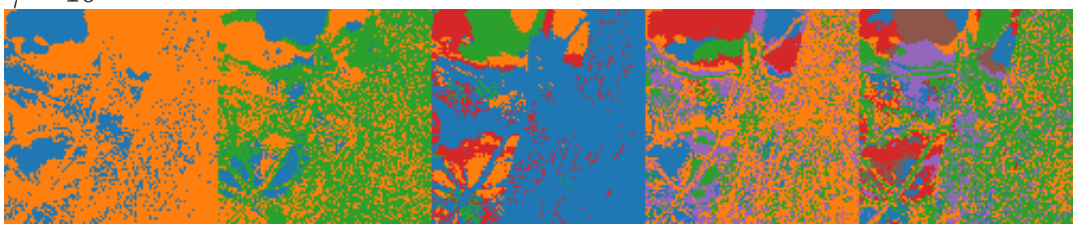
$\gamma = 10^{-4}$:



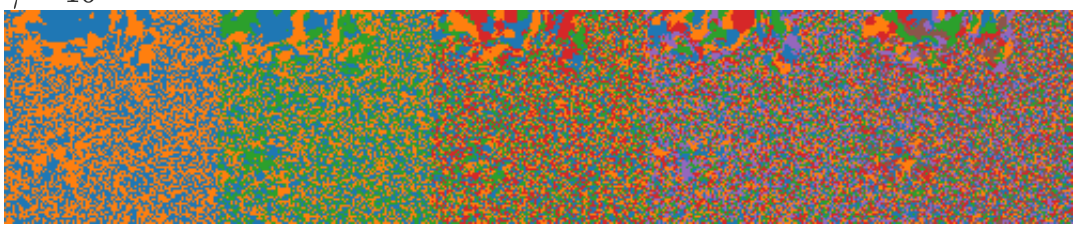
$\gamma = 10^{-3}$:



$\gamma = 10^{-2}$:



$\gamma = 10^{-1}$:

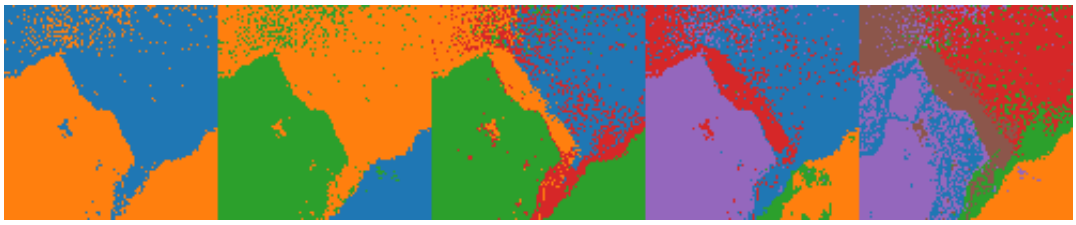


For the value of γ parameter in the RBF kernel, I found that when γ is lower, the effect of clustering is larger.

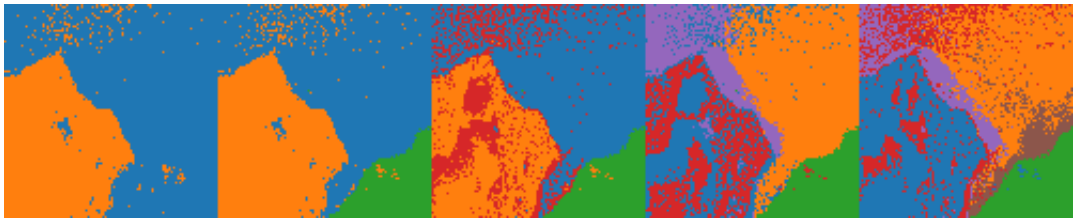
The reason I thought is that the lower γ hints that the higer σ of the Gaussion distribution (i.e., In this work, this distribution is the distance between the point and the center of the cluster.), but too lower γ (i.e., higher σ) may cause underfitting.

- Traditional v.s. K-means++
  - Both two image are $\gamma = 10^{-4}$:

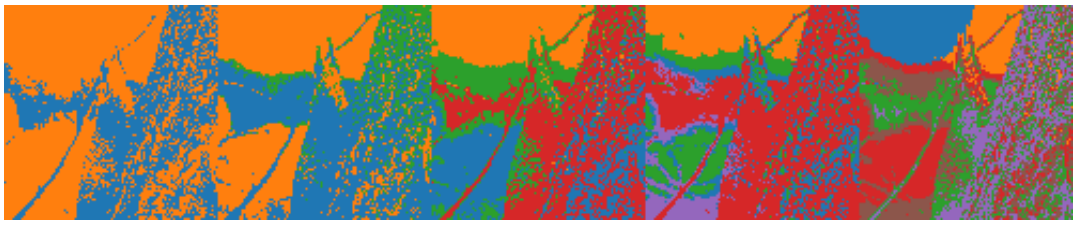
Traditional:



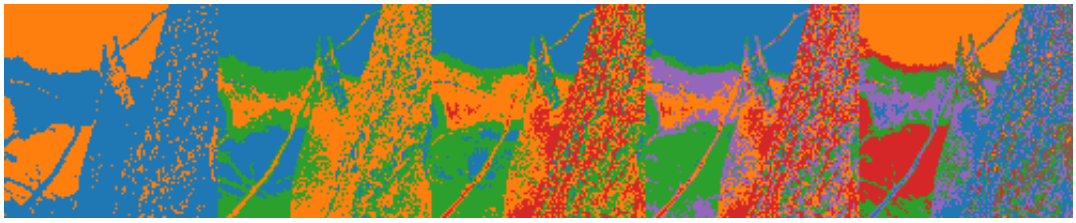
K-means++:



Traditional:



K-means++:



At first, I thought that the K-mean++ just more faster than the tradition according the number of iteration (shown at Screen shot part). But when the result of image2 produced, we could see that the sky area and the rabbit could be clustered in the different when `k=6`! So I believe that Kmeans++ is more powerful in this work.