> Note: This report was made on `Hackmd.io` and restricted by the `.pdf` format, the `.gif` animation would not display. Please read it on Hackmd.io, 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`)

```python
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(u, v):
    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=0.0001):
    return np.exp(-1*g*euclidean(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_distance(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 naive_distance(u, v):
    return np.sum((u - v)**2)

def initial_clusters(size, data, method='default'):
    init_ck = np.zeros(size)
    n, k = size
    if method == 'kmeans++':
        centers = []
        centers.append(data[np.random.randint(n), :])

        for c_id in range(k - 1):
            dist = []
            for i in range(n):
                point = data[i, :]
                d = sys.maxsize
                for j in range(len(centers)):
                    temp_dist = naive_distance(point, centers[j])
                    d = min(d, temp_dist)
                dist.append(d)
            dist = np.array(dist)
            next_center = data[np.argmax(dist), :]
            centers.append(next_center)
            dist = []

        centers = np.array(centers)
        dist = euclidean(data, centers)
        init_ck[np.arange(dist.shape[0]), np.argmin(dist, axis=1)] = 1
    else:
        init_ck[np.arange(n), np.random.randint(k,size=n)] = 1
    return init_ck

def kernel_k_means(gram, k=2, method='default', max_iter=100):
    #initial clusters
    n = gram.shape[0]
    ck = initial_clusters((n, k), gram, method)

    record = []
    record.append(ck)
```

```
    iter_record = 0
    for r in range(max_iter):
        #E-step with kernel trick
        dis = get_distance(gram, ck)

        #M-step
        update_ck = np.zeros(dis.shape)
        update_ck[np.arange(dis.shape[0]),np.argmin(dis, axis=1)] = 1
        delta_ck = np.count_nonzero(np.abs(update_ck - ck))

        if delta_ck == 0 and iter_record == 0:
            iter_record = r+1
        record.append(update_ck)
        ck = update_ck
    return record, iter_record
```

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, k=2, 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, id):
    gif = []
    for i in range(len(gifs)):
        gif.append(imageio.get_reader(gifs[i]))

    new_gif = imageio.get_writer('image'+str(id)+'.gif')

    for frame_number in range(100):
        img = []
        for i in range(len(gif)):
            img.append(gif[i].get_next_data())
        new_image = np.hstack(img)
```

```python
            new_gif.append_data(new_image)
        for i in range(len(gif)):
            gif[i].close()
        new_gif.close()
```

Screen shot

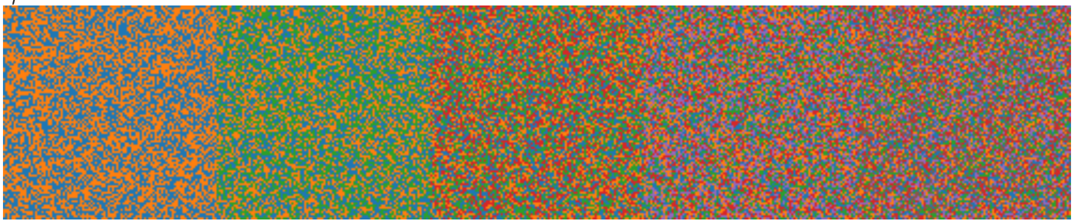
```
processing image1...
running kernel k-means (k = 2, default).........[complete at [12] iterations]
running kernel k-means (k = 2, kmeans++).........[complete at [8] iterations]
faster....................[kmeans++]
visualizing.........[complete]
running kernel k-means (k = 3, default).........[complete at [11] iterations]
running kernel k-means (k = 3, kmeans++).........[complete at [8] iterations]
faster....................[kmeans++]
visualizing.........[complete]
running kernel k-means (k = 4, default).........[complete at [23] iterations]
running kernel k-means (k = 4, kmeans++).........[complete at [28] iterations]
faster....................[tradition]
visualizing.........[complete]
running kernel k-means (k = 5, default).........[complete at [85] iterations]
running kernel k-means (k = 5, kmeans++).........[complete at [31] iterations]
faster....................[kmeans++]
visualizing.........[complete]
running kernel k-means (k = 6, default).........[complete at [64] iterations]
running kernel k-means (k = 6, kmeans++).........[complete at [29] iterations]
faster....................[kmeans++]
visualizing.........[complete]
processing image2...
running kernel k-means (k = 2, default).........[complete at [17] iterations]
running kernel k-means (k = 2, kmeans++).........[complete at [15] iterations]
faster....................[kmeans++]
visualizing.........[complete]
running kernel k-means (k = 3, default).........[complete at [19] iterations]
running kernel k-means (k = 3, kmeans++).........[complete at [22] iterations]
faster....................[tradition]
visualizing.........[complete]
running kernel k-means (k = 4, default).........[complete at [53] iterations]
running kernel k-means (k = 4, kmeans++).........[complete at [23] iterations]
faster....................[kmeans++]
visualizing.........[complete]
running kernel k-means (k = 5, default).........[complete at [35] iterations]
running kernel k-means (k = 5, kmeans++).........[complete at [40] iterations]
faster....................[tradition]
visualizing.........[complete]
running kernel k-means (k = 6, default).........[complete at [34] iterations]
running kernel k-means (k = 6, kmeans++).........[complete at [27] iterations]
faster....................[kmeans++]
visualizing.........[complete]
```

Result

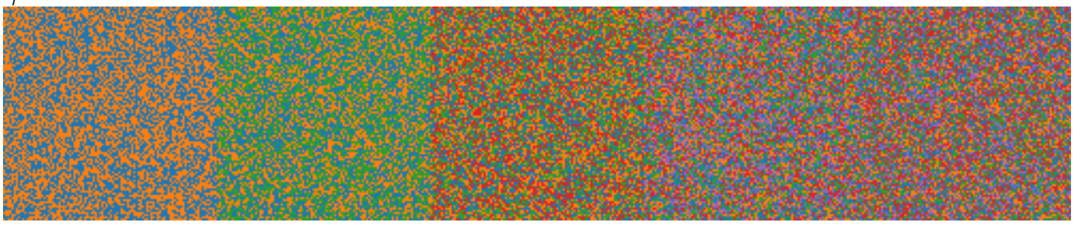
- image1 (k=2, 3, 4, 5, 6)

Original image:

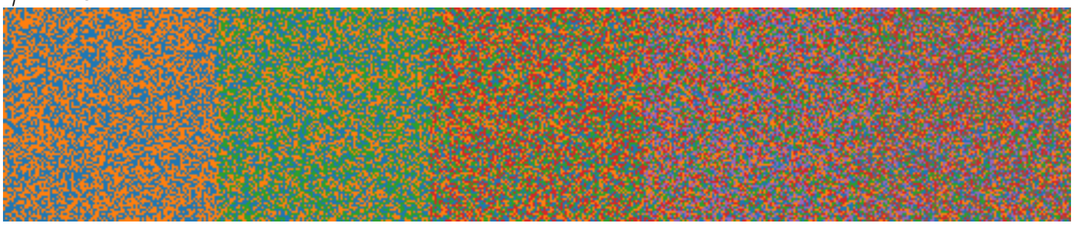
$\gamma = 10^{-6}$:



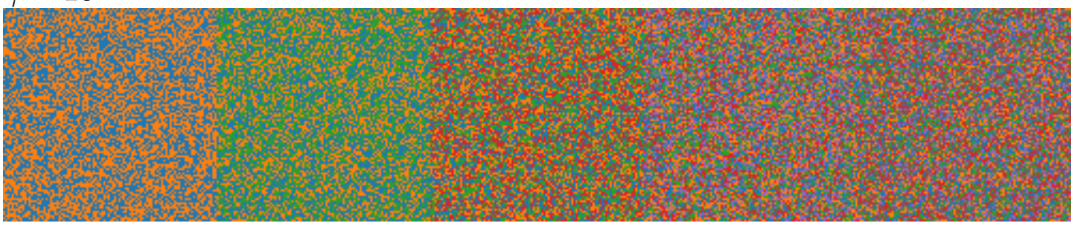
$\gamma = 10^{-5}$:



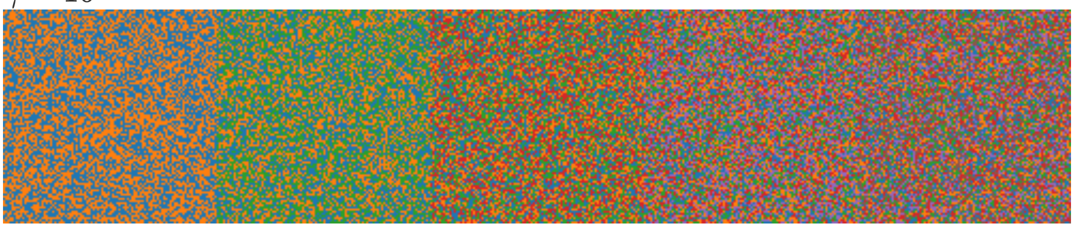
$\gamma = 10^{-4}$:



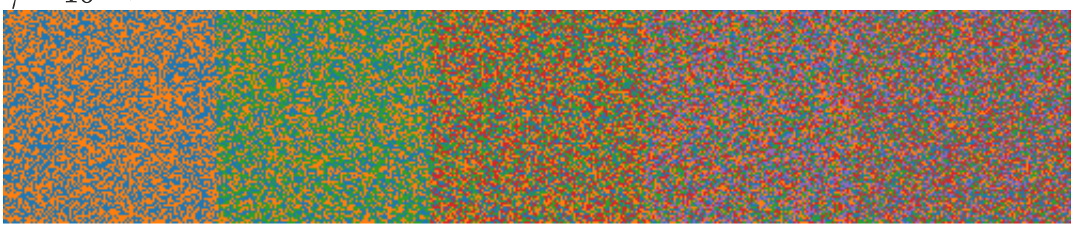
$\gamma = 10^{-3}$:



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

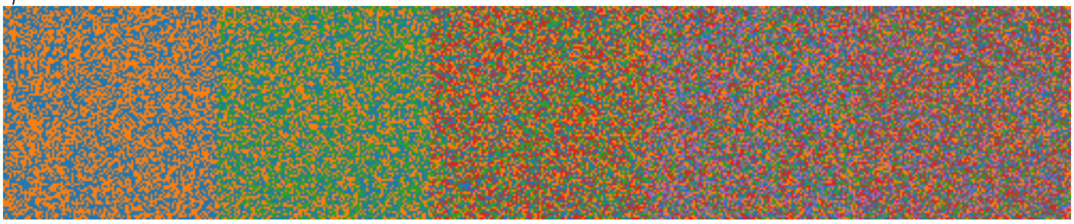


$\gamma = 10^{-1}$:

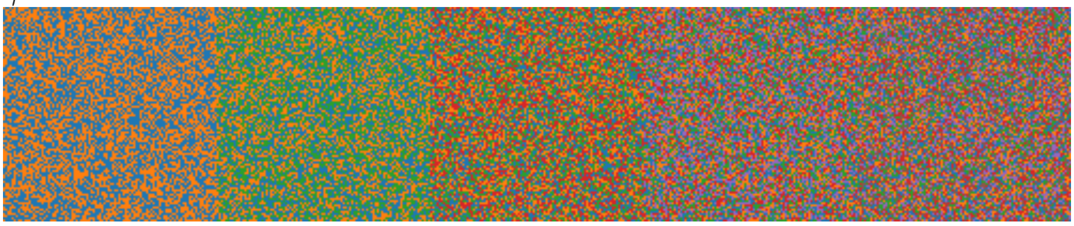


- image2 (k=2, 3, 4, 5, 6)

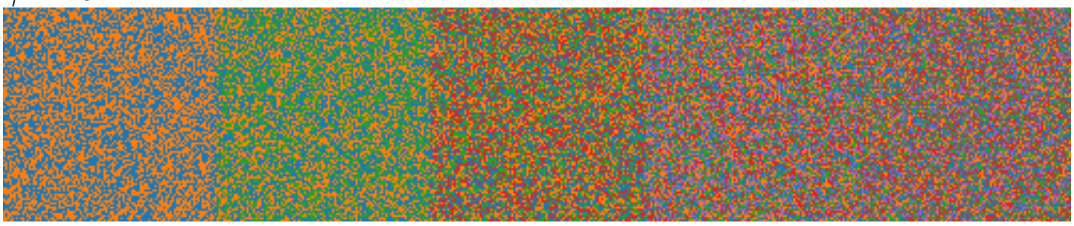
$\gamma = 10^{-6}$:



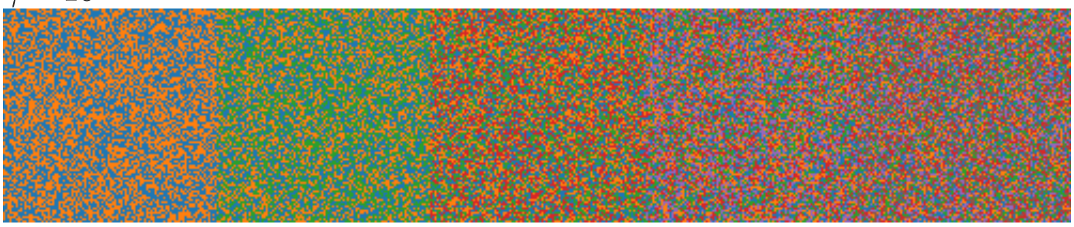
$\gamma = 10^{-5}$:



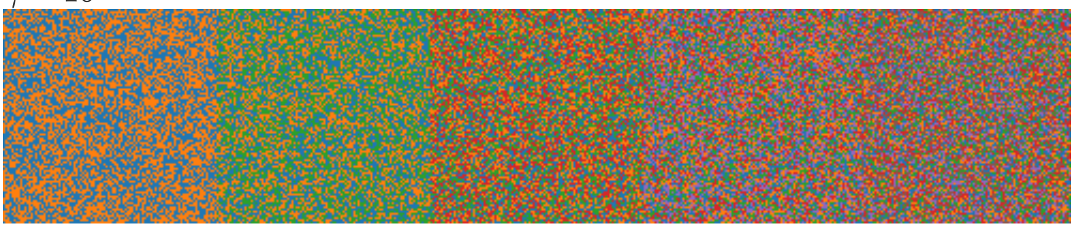
$\gamma = 10^{-4}$:



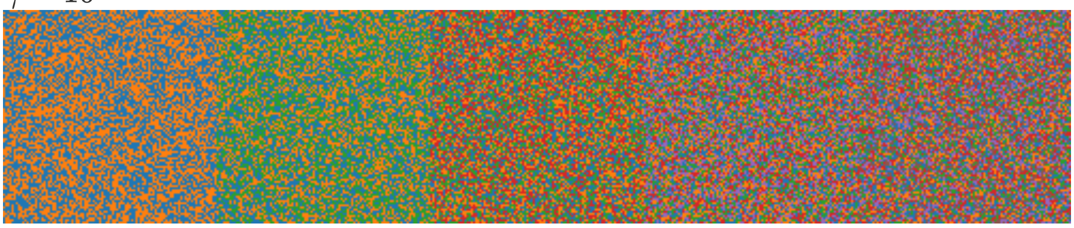
$\gamma = 10^{-3}$:



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



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

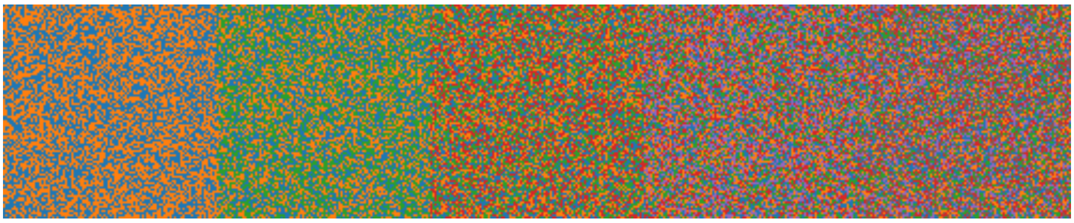


For the value of γ parameter in the RBF kernel, I found that when γ is lower, the effect of clustering is larger.

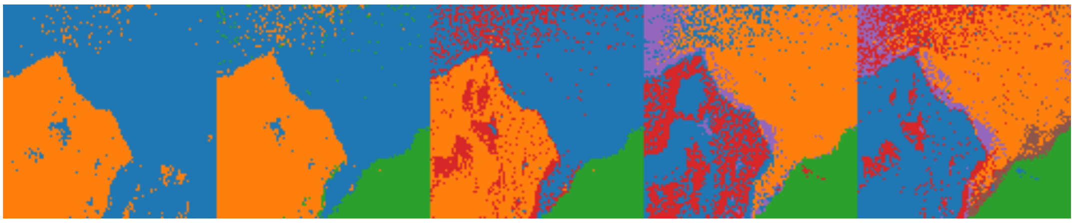
The reason I thought is that the lower γ hints that the higer σ of the Gaussion distribution (i.e., In this work, this distribution is the distance between the point and the center of the cluster.), but too lower γ (i.e., higher σ) may cause underfitting.

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

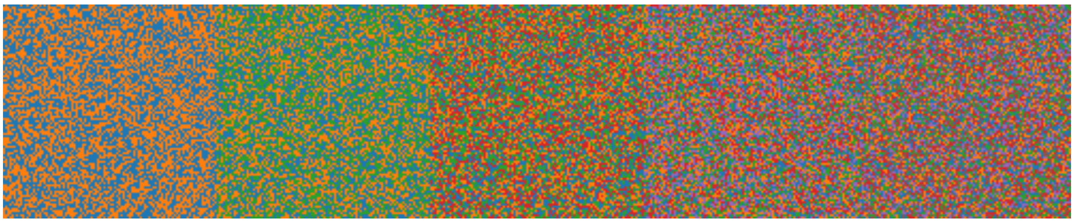
Traditional:



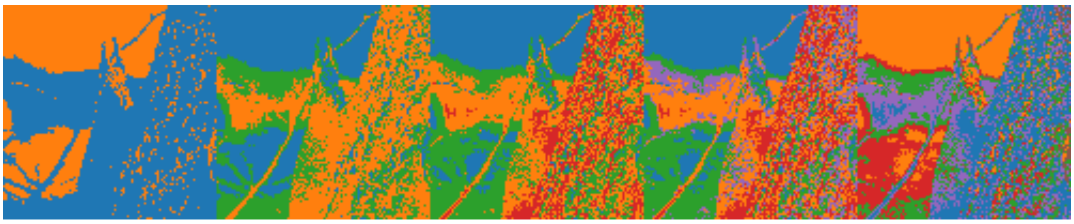
K-means++:



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.