# ECE421 - Winter 2022 Assignment 3: Unsupervised Learning and Probabilistic Models

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Code written in Google Colab: https://colab.research.google.com/drive/1TOGHI-snK5q5YR9Hac1PCcwV8NNDjeQ0

# 0. Helper Functions

# 0.1 Loading Data

```
from google.colab import drive
drive.mount('/content/gdrive', force_remount=True)
def load_2D(is_valid=True):
   data = np.load('/content/gdrive/My Drive/4-2/ECE421/data2D.npy')
   [num_pts, dim] = data.shape
   # getting validation set
   if is valid:
       valid_batch = int(num_pts / 3.0)
       np.random.seed(45689)
       rnd_idx = np.arange(num_pts)
       np.random.shuffle(rnd_idx)
       val_data = data[rnd_idx[:valid_batch]]
       train_data = data[rnd_idx[valid_batch:]]
       return train_data, val_data
   else:
        return data
def load_100D(is_valid=True):
   data = np.load('/content/gdrive/My Drive/4-2/ECE421/data100D.npy')
    [num_pts, dim] = data.shape
   # getting validation set
   if is_valid:
       valid_batch = int(num_pts / 3.0)
       np.random.seed(45689)
       rnd_idx = np.arange(num_pts)
        np.random.shuffle(rnd_idx)
        val_data = data[rnd_idx[:valid_batch]]
        train_data = data[rnd_idx[valid_batch:]]
        return train_data, val_data
        return data
```

# 0.2 K-means Helper Functions

```
def find_loss(X, MU):
    pair_dist = distance_func(X, MU)
    mins = tf.reduce_min(pair_dist, 1)
    loss = tf.reduce_sum(mins, 0)
    return loss

def get_cluster(K, MU, X):
    # getting square pairwise distances
    pair_dist = tf.Session().run(distance_func(X, MU))

    # getting most likely cluster by index
    index = np.argmin(pair_dist, axis=1)

    # getting list of actual data grouped by cluster
    cluster = K * [None]
    for i in range(K):
        cluster[i] = X[index == i]

    return cluster
```

# 0.3 GMM Helper Functions

```
def find_GMM_loss(pdf, prob):
   likelihood = reduce_logsumexp(pdf + tf.transpose(prob), 1)
   return - tf.reduce_sum(likelihood, axis=0)

def get_GMM_cluster(K, X, MU, log_pi, sigma):
    # getting posterior distribution
   pdf = tf.Session().run(log_gauss_pdf(X, MU, sigma))
    log_post = tf.Session().run(log_posterior(pdf, log_pi))

   # getting most likely cluster by index
   index = np.argmax(log_post, axis=1)

# getting list of actual data grouped by cluster
   cluster = K * [None]
   for i in range(K):
        cluster[i] = X[index == i]

   return cluster
```

# 0.4 Getting Percentages

```
def get_percentage(K, cluster):
   total = 0.0
   counts = np.zeros(K)
   for i in range(K):
      total += cluster[i].shape[0]
      counts[i] += cluster[i].shape[0]
   return counts / total
```

# 1. K-Means

# 1.1 Learning K-means

### 1.1.1 Model Implementation

Implemented function distance\_func()

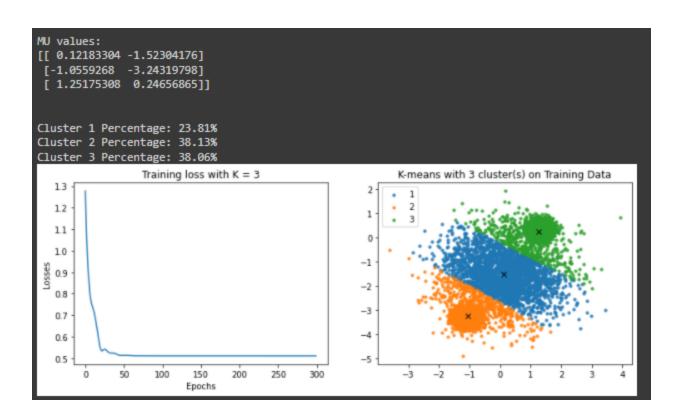
```
def distance_func(X, mu):
    """ Inputs:
        X: is an NxD matrix (N observations and D dimensions)
        mu: is an KxD matrix (K means and D dimensions)

Output:
        pair_dist: is the squared pairwise distance matrix (NxK)
    """

X = tf.expand_dims(X, 1)
    mu = tf.expand_dims(mu, 0)
    pair_dist = tf.reduce_sum(tf.square(tf.subtract(X, mu)), 2)
    return pair_dist
```

### 1.1.2 K-means Clusters when K = 3

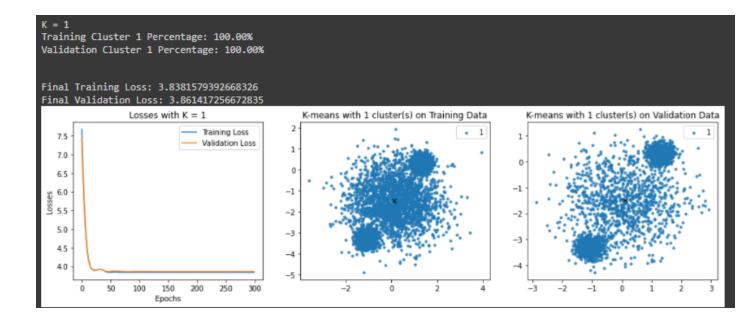
```
K = 3
# load training data
train_data = load_2D(is_valid=False)
[num_pts, dim] = train_data.shape
# get kmeans loss
train_loss, valid_loss, MU = kMeans(K, train_data)
print("MU values: ")
print(MU)
print("\n")
# get clusters
cluster = get_cluster(K, MU, train_data)
# get percentage of each cluster
percentages = get_percentage(K, cluster)
# plotting
plt.figure(figsize=(12,4))
# plotting loss
plt.subplot(121)
plt.xlabel('Epochs')
plt.ylabel('Losses')
plt.plot(train_loss)
plt.title('Training loss with K = {}'.format(K))
# plotting scatters
plt.subplot(122)
for i in range(K):
  x ,y = cluster[i][:, 0], cluster[i][:, 1]
 # print percentage of each cluster
  print("Cluster {} Percentage: {:.2%}".format(i + 1,percentages[i]))
  plt.scatter(x, y, s=10, alpha=0.8, label=str(i+1) )
plt.plot(MU[:, 0], MU[:, 1], 'x', color='black')
plt.title('K-means with {} cluster(s) on Training Data'.format(K))
plt.legend()
plt.show()
```

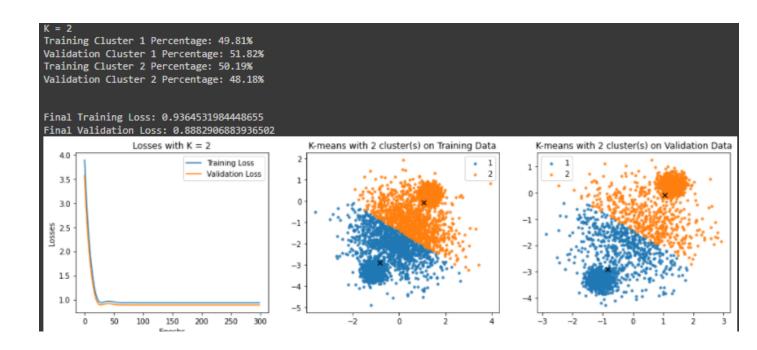


### 1.1.3 Varying K with Validation

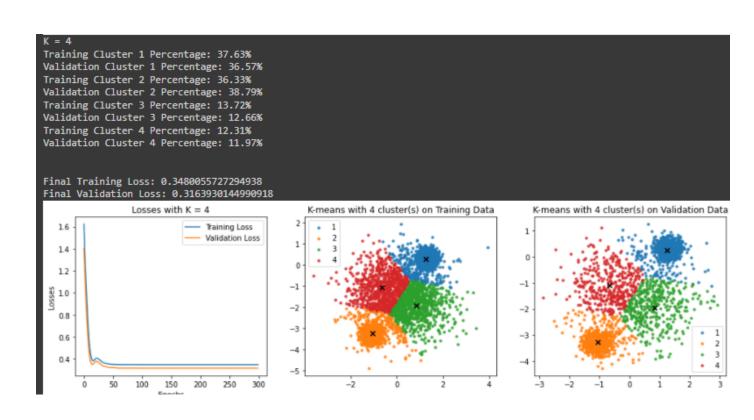
Trained the K-means model for K = 1,2,3,4,5.

```
# train K-means model for 1,2,3,4,5
for K in range(1,6):
  print("K = {}".format(K))
  train_loss, valid_loss, MU = kMeans(K, train_data, valid_data, is_valid=True)
  # get clusters
 train_cluster = get_cluster(K, MU, train_data)
  valid_cluster = get_cluster(K, MU, valid_data)
  # get percentage of each cluster
  train_percentages = get_percentage(K, train_cluster)
  valid_percentages = get_percentage(K, valid_cluster)
  # plotting
  fig, ax = plt.subplots(1, 3, figsize=(16,4))
  # plotting loss
  ax[0].set_xlabel('Epochs')
  ax[0].set_ylabel('Losses')
  ax[0].plot(train_loss, label = "Training Loss")
  ax[0].plot(valid_loss, label = "Validation Loss")
  ax[0].set_title('Losses with K = {}'.format(K))
  ax[0].legend()
  # plotting scatters
  for i in range(K):
    train_x, train_y = train_cluster[i][:, 0], train_cluster[i][:, 1]
    valid_x, valid_y = valid_cluster[i][:, 0], valid_cluster[i][:, 1]
    # print percentage of each cluster
    print("Training Cluster {} Percentage: {:.2%}".format(i + 1,train_percentages[i]))
    print("Validation Cluster {} Percentage: {:.2%}".format(i + 1,valid_percentages[i]))
    # plot training scatter
    ax[1].scatter(train_x, train_y, s=10, alpha=0.8, label=str(i+1) )
    ax[1].plot(MU[:, 0], MU[:, 1], 'x', color='black')
    ax[1].set_title('K-means with {} cluster(s) on Training Data'.format(K))
    ax[1].legend()
    # plot validation scatter
    ax[2].scatter(valid_x, valid_y, s=10, alpha=0.8, label=str(i+1) )
    ax[2].plot(MU[:, 0], MU[:, 1], 'x', color='black')
    ax[2].set_title('K-means with {} cluster(s) on Validation Data'.format(K))
    ax[2].legend()
  print("\n")
  print("Final Training Loss: {}".format(train_loss[-1]))
  print("Final Validation Loss: {}".format(valid_loss[-1]))
 plt.show()
```



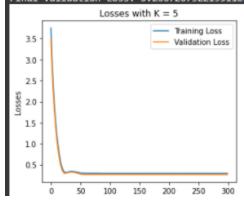


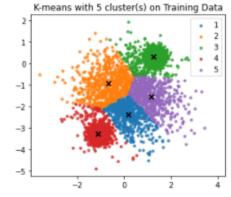
Training Cluster 1 Percentage: 37.51% Validation Cluster 1 Percentage: 39.78% Training Cluster 2 Percentage: 38.41% Validation Cluster 2 Percentage: 37.35% Training Cluster 3 Percentage: 24.07% Validation Cluster 3 Percentage: 22.86% Final Training Loss: 0.5233501591809401 Final Validation Loss: 0.488841713259277 Losses with K = 3 K-means with 3 cluster(s) on Training Data K-means with 3 cluster(s) on Validation Data Training Loss 2.5 Validation Loss 0 2.0 -1 25 15 -2-3 1.0 100 150 200 250 300

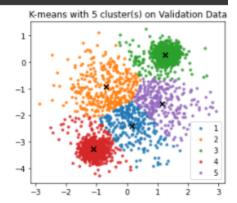


# Training Cluster 1 Percentage: 8.83% Validation Cluster 1 Percentage: 8.31% Training Cluster 2 Percentage: 10.68% Validation Cluster 2 Percentage: 10.68% Training Cluster 3 Percentage: 36.70% Validation Cluster 3 Percentage: 35.76% Training Cluster 4 Percentage: 34.89% Validation Cluster 4 Percentage: 37.38% Training Cluster 5 Percentage: 8.89% Validation Cluster 5 Percentage: 7.86%

### Final Training Loss: 0.2940552930347517 Final Validation Loss: 0.26672073221951187







The resulting percentages and final losses for each K is demonstrated here:

K	1	2	3	4	5
Final Training Loss	3.8381579 392668326	0.9364531 984448655	0.5233501 591809401	0.3480055 727294938	0.2940552 930347517
Final Validation Loss	3.8614172 56672835	0.8882906 883936502	0.4888417 13259277	0.3163930 144990918	0.2667207 322195118 7
Training Cluster Percentage	Cluster 1: 100 %	Cluster 1: 49.81%	Cluster 1: 37.51%	Cluster 1: 37.63%	Cluster 1: 8.83%
		Cluster 2: 50.19%	Cluster 2: 38.41%	Cluster 2: 36.33%	Cluster 2: 10.68%
			Cluster 3: 24.07%	Cluster 3: 13.72%	Cluster 3: 36.70%
				Cluster 4: 12.31%	Cluster 4: 34.89%
					Cluster 5: 8.89%
Validation Cluster Percentage	Cluster 1: 100%	Cluster 1: 51.82%	Cluster 1: 39.78%	Cluster 1: 36.57%	Cluster 1: 8.31%
1 ordentage		Cluster 2: 48.18%	Cluster 2: 37.35%	Cluster 2: 38.79%	Cluster 2: 10.68%
			Cluster 3: 22.86%	Cluster 3: 12.66%	Cluster 3: 35.76%
				Cluster 4: 11.97%	Cluster 4: 37.38%
					Cluster 5: 7.86%

# **Discussion**

The best number of clusters to use is 3. There are two highly populated areas on the top right and left bottom corners of the scatter plots. Other than these two areas, data scatters across the board. When K > 3, the 2 areas on the corners stay, and only the middle part splits into smaller parts. This is not too accurate as the scattered area in the middle should not have multiple centers. In addition, when K < 3, the scatter plot fails to capture the significant difference between the 3 parts. Therefore, 3 is the best number of clusters to use.

# 2. Mixtures of Gaussians

### 2.1 The Gaussian Cluster Mode

```
import math
def log_gauss_pdf(X, mu, sigma):
   """ Inputs:
           X: N X D
           mu: K X D
           sigma: K X 1
       Outputs:
           log Gaussian PDF (N X K)
   num_pts, dim = X.shape
   try:
     dim = dim.value
   except:
   const = - (dim / 2) * tf.log(2 * math.pi * tf.transpose(sigma) ** 2)
   pair_dist = distance_func(X, mu)
   exp = - tf.divide(pair_dist, 2 * tf.transpose(sigma) ** 2)
   return tf.add(const, exp)
def log_posterior(log_PDF, log_pi):
   """ Inputs:
           log_PDF: log Gaussian PDF N X K
           log pi: K X 1
       Outputs
           log_post: N X K
   numerator_log = tf.add(log_PDF, tf.transpose(log_pi))
   denominator_log = - reduce_logsumexp(numerator_log, 1, keep_dims=True)
   return tf.add(numerator_log, denominator_log)
```

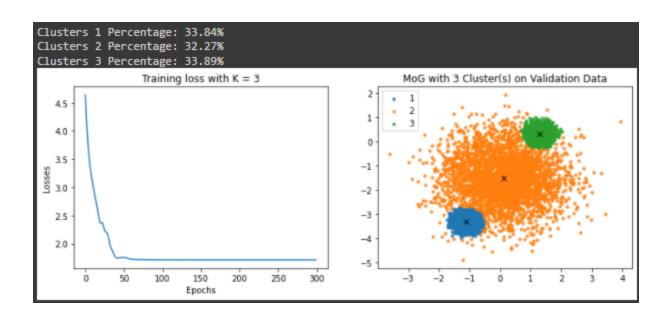
# 2.2 Learning the MoG

### 2.2.1 Model Implementation

```
def GMM(K, train_data, valid_data=None, is_valid=False):
 [num_pts, dim] = train_data.shape
 X = tf.placeholder(tf.float64, [None, dim])
 MU = tf.Variable(tf.truncated_normal([K, dim], dtype=tf.float64))
 phi = tf.Variable(tf.truncated_normal([K, 1], dtype=tf.float64))
 psi = tf.Variable(tf.truncated_normal([K, 1], dtype=tf.float64))
 sigma = tf.exp(phi)
 log_pi = logsoftmax(psi)
 logGaussPdf = log_gauss_pdf(X, MU, sigma)
 loss = find_GMM_loss(logGaussPdf, log_pi)
 adam_op = tf.train.AdamOptimizer(learning_rate=0.1, beta1=0.9, beta2=0.99, epsilon=1e-5).minimize(loss)
 train_loss = []
 valid_loss = []
 with tf.Session() as sess:
   sess.run(tf.global_variables_initializer())
   for i in range(300):
     sess.run(adam_op, feed_dict={X: train_data})
     train_loss.append(sess.run(loss, feed_dict={X: train_data}))
     if is_valid:
       valid_loss.append(sess.run(loss, feed_dict={X: valid_data}))
   MUs, sigmas, log_pis = sess.run([MU, sigma, log_pi], feed_dict={X: train_data})
   train_loss = np.array(train_loss)/ train_data.shape[0]
   if is_valid:
       valid_loss = np.array(valid_loss)/valid_data.shape[0]
  return train_loss, valid_loss, MUs, sigmas, log_pis
```

### 2.2.2 MoG Clusters with K = 3

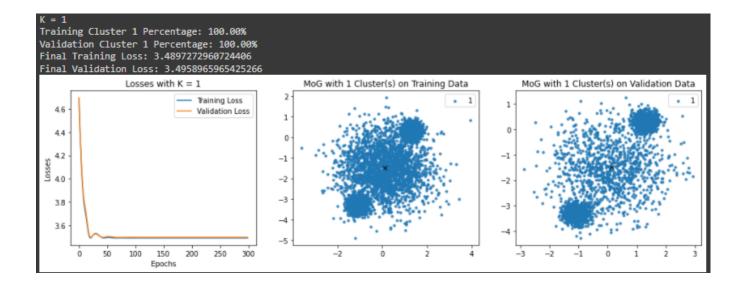
```
K = 3
# load training data
train_data = load_2D(is_valid=False)
[num_pts, dim] = train_data.shape
# get GMM loss
train_loss, valid_loss, MU, sigma, log_pi = GMM(K, train_data)
# get clusters
clusters = get_GMM_cluster(K, train_data, MU, log_pi, sigma)
# get percentage of each cluster
percentages = get_percentage(K, clusters)
# plotting
plt.figure(figsize=(12,4))
# plotting loss
plt.subplot(121)
plt.xlabel('Epochs')
plt.ylabel('Losses')
plt.plot(train_loss)
plt.title('Training loss with K = {}'.format(K))
# plotting scatters
plt.subplot(122)
for i in range(K):
  x , y = clusters[i][:, 0], clusters[i][:, 1]
  # print percentage of each clusters
  print("Clusters {} Percentage: {:.2%}".format(i + 1,percentages[i]))
  plt.scatter(x, y, s=10, alpha=0.8, label=str(i+1) )
plt.plot(MU[:, 0], MU[:, 1], 'x', color='black')
plt.title('MoG with {} Cluster(s) on Validation Data'.format(K))
plt.legend()
plt.show()
```



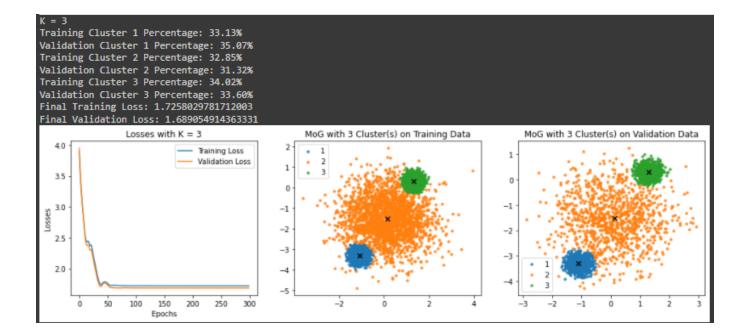
### 2.2.3 Varying K with Validation

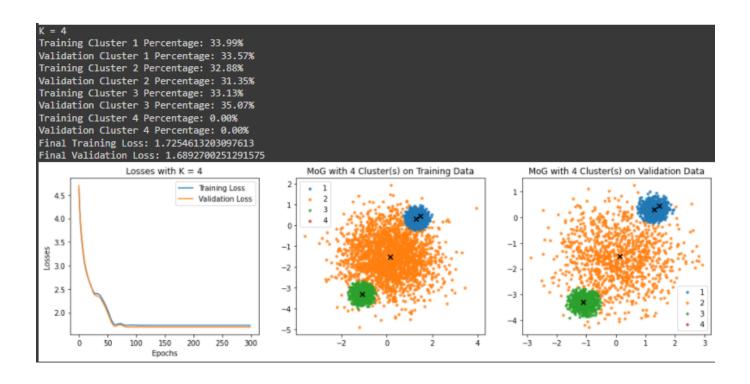
Trained the MoG model for K = 1,2,3,4,5.

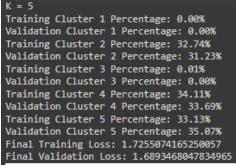
```
train_data, valid_data = load_2D(is_valid=True)
# train MoG model for 1,2,3,4,5
for K in range(1,6):
 print("K = {}".format(K))
  # compute losses
 train_loss, valid_loss, MU, sigma, log_pi= GMM(K, train_data, valid_data, is_valid=True
  # get clusters
 train_cluster = get_GMM_cluster(K, train_data, MU, log_pi, sigma)
 valid_cluster = get_GMM_cluster(K, valid_data, MU, log_pi, sigma)
 # get percentage of each cluster
 train_percentages = get_percentage(K, train_cluster)
 valid_percentages = get_percentage(K, valid_cluster)
  # plotting
 fig, ax = plt.subplots(1, 3, figsize=(16,4))
  # plotting loss
 ax[0].set_xlabel('Epochs')
  ax[0].set_ylabel('Losses')
  ax[0].plot(train_loss, label = "Training Loss")
  ax[0].plot(valid_loss, label = "Validation Loss")
  ax[0].set_title('Losses with K = {}'.format(K))
  ax[0].legend()
  # plotting scatters
  for i in range(K):
    train_x, train_y = train_cluster[i][:, 0], train_cluster[i][:, 1]
   valid_x, valid_y = valid_cluster[i][:, 0], valid_cluster[i][:, 1]
    # print percentage of each cluster
    print("Training Cluster {} Percentage: {:.2%}".format(i + 1,train_percentages[i]))
    print("Validation Cluster {} Percentage: {:.2%}".format(i + 1,valid_percentages[i]))
    # plot training scatter
    ax[1].scatter(train_x, train_y, s=10, alpha=0.8, label=str(i+1) )
    ax[1].plot(MU[:, 0], MU[:, 1], 'x', color='black')
    ax[1].set_title('MoG with {} Cluster(s) on Training Data'.format(K))
    ax[1].legend()
    # plot validation scatter
    ax[2].scatter(valid_x, valid_y, s=10, alpha=0.8, label=str(i+1) )
    ax[2].plot(MU[:, 0], MU[:, 1], 'x', color='black')
    ax[2].set_title('MoG with {} Cluster(s) on Validation Data'.format(K))
    ax[2].legend()
  print("Final Training Loss: {}".format(train_loss[-1]))
  print("Final Validation Loss: {}".format(valid_loss[-1]))
  plt.show()
```

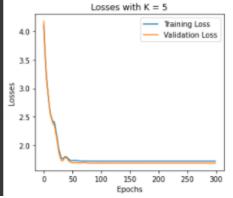




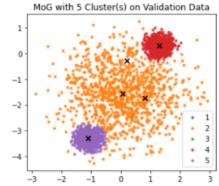












The resulting percentages and final losses for each K is demonstrated here:

K	1	2	3	4	5
Final Training Loss	3.4897272 960724406	2.4387798 408841848	1.7258029 781712003	1.7254613 203097613	1.7255074 165250057
Final Validation Loss	3.4958965 965425266	2.4043988 79191213	1.6890549 14363331	1.6892700 251291575	1.6893468 047834965
Training Cluster Percentage	Cluster 1: 100 %	Cluster 1: 66.40% Cluster 2:	Cluster 1: 33.13%	Cluster 1: 33.99%	Cluster 1: 0.00%
		33.60%	32.85%	32.88%	32.74%
			Cluster 3: 34.02%	Cluster 3: 33.13%	Cluster 3: 0.01%
				Cluster 4: 0.00%	Cluster 4: 34.11%
					Cluster 5: 33.13%
Validation Cluster Percentage	Cluster 1: 100%	Cluster 1: 64.30%	Cluster 1: 35.07%	Cluster 1: 33.57%	Cluster 1: 0.00%
		Cluster 2: 35.70%	Cluster 2: 31.32%	Cluster 2: 32.88%	Cluster 2: 31.23%
			Cluster 3: 33.60%	Cluster 3: 33.13%	Cluster 3: 0.00%
				Cluster 4: 0%	Cluster 4: 33.69%
					Cluster 5: 35.07%

### **Discussion**

The best number of clusters to use is 3.

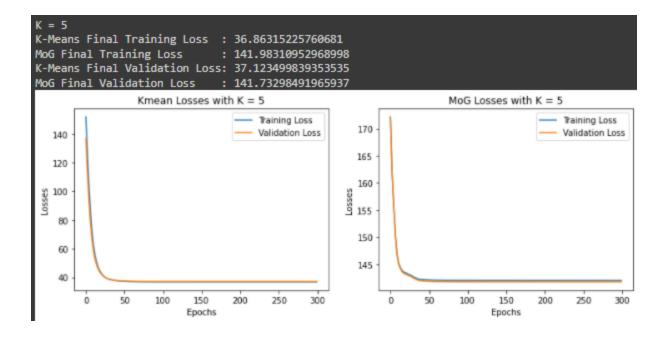
When K =2, MoG model accurately determines one of the dense areas of the dataset. Despite the location of the dense cluster center, some data closer to this center actually belongs to the other cluster. This is how MoG is different from K-means.

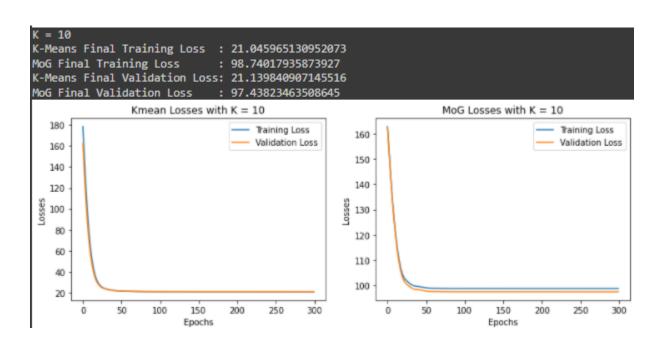
When K = 3, MoG model has 3 easily identifiable clusters with 2 on the corners and 1 scattered in the middle. However, for K > 3, the new clusters (specifically #4 and #5) are just added to the same location. The clusters beyond K = 3 would be redundant clusters

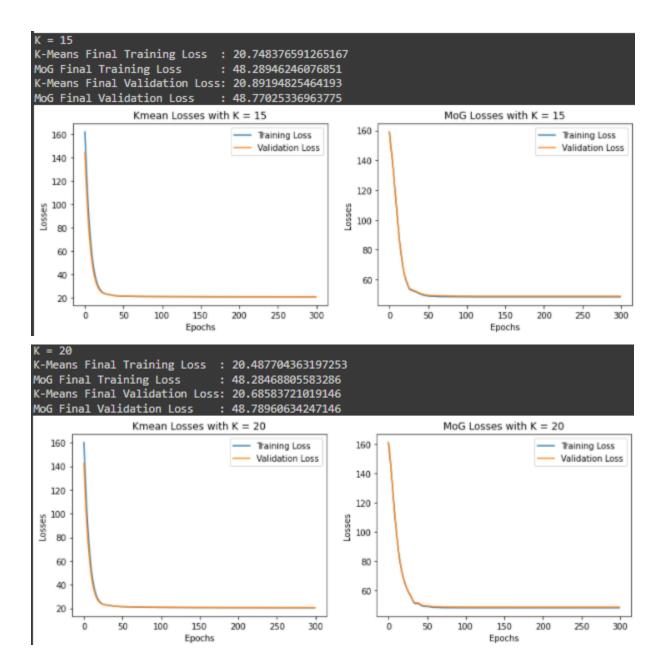
### 2.2.3 K-means vs. MoG

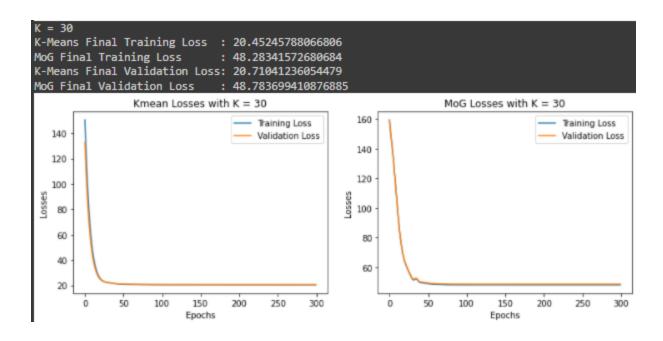
Run both the K-means and the MoG learning algorithms on data100D.npy for K = 5, 10, 15, 20, 30 while holding out  $\frac{1}{3}$  of the data for validation. Find the losses for both models.

```
# getting data
train_data, valid_data = load_100D(is_valid=True)
for K in [5, 10, 15, 20, 30]:
    print("K = {}".format(K))
    # compute models
    Kmeans_train_loss, Kmeans_valid_loss, MU = kMeans(K, train_data, valid_data, is_valid=True)
    MoG_train_loss, MoG_valid_loss, MU , sigma, log_pi= GMM(K, train_data, valid_data, is_valid=True)
    print("K-Means Final Training Loss : {}".format(Kmeans_train_loss[-1]))
    print("MoG Final Training Loss : {}".format(MoG_train_loss[-1]))
    print("K-Means Final Validation Loss: {}".format(Kmeans_valid_loss[-1]))
    print("MoG Final Validation Loss : {}".format(MoG_valid_loss[-1]))
    # plotting
    fig, ax = plt.subplots(1, 2, figsize=(12, 4))
    # plotting losses
    ax[0].set_xlabel('Epochs')
    ax[0].set_ylabel('Losses')
    ax[0].plot(Kmeans_train_loss, label = "Training Loss")
    ax[0].plot(Kmeans_valid_loss, label = "Validation Loss")
    ax[0].set_title('Kmean Losses with K = {}'.format(K))
    ax[0].legend()
    ax[1].set_xlabel('Epochs')
    ax[1].set_ylabel('Losses')
    ax[1].plot(MoG_train_loss, label = "Training Loss")
    ax[1].plot(MoG_valid_loss, label = "Validation Loss")
    ax[1].set_title('MoG Losses with K = {}'.format(K))
    ax[1].legend()
    plt.show()
```









### **Discussion**

I think there are **15** clusters within the 100D dataset.

For the K-means models, a larger K would allow better partition of the input data. The average distance from each data point to its cluster center is decreased since there are more clusters.

The MoG models can be more helpful in determining the number of clusters. Unlike the K-means models in which data are split evenly by a hyperplane bisecting the 2 nearest clusters, MoG models assign data to the cluster with the higher probability. From the 2D dataset, we observed that K increases beyond the desired number of clusters. Extra clusters are just added to the same location repeatedly after the desired number is reached. Thus, increasing K beyond optimal cluster number would not result in better loss values for MoG models. As we can see in the output plots, when K=5 or 10, we do not have enough clusters. For K= 15, 20, or 30, the losses all converge around 48. This means increasing K beyond 15 does not have a significant decrease in loss which infers the extra clusters are all redundant.

MoG models appear to have worse losses for smaller K since K-means can partition unidentifiable clusters better. However, even though K-means models have lower loss values from MoG models, K-Means can have its drawbacks. For

example, if K = # of data points in the dataset, K-means would achieve a loss = 0 which means it assigns each data point to its own cluster. This is overfitting and should be prevented. On the other hand, MoG models would give similar results for K > 15 and beyond. In conclusion, K-Means models are better for smaller K and MoG models are better for larger K.