ECE421 – Introduction to Machine Learning

Assignment 3

Unsupervised Learning and Probabilistic Models

Hard Copy Due: Friday, March 27 @ 3:00 PM, at BA3128 Code Submission Due: Friday, March 27 @ 5:00 PM, on Quercus

General Notes:

- Attach this cover page to your hard copy submission
- Please post assignment related questions on Piazza.

Please check section to which you would like the assignment returned.

Tutorial Sections:

☐ Tutorial 1: Thursdays 3-5pm (SF2202)				
☐ Tutorial 2: Thursdays 3-5pm (GB304)				
☐ Tutorial 3: Tuesdays 10-12 (SF2202)				
☐ Tutorial 4: Fridays 9-11 (BA1230)				
Group Members				
Name	Student ID			

0 Setup

```
[1]: # ignore all future warnings
from warnings import simplefilter
simplefilter(action='ignore', category=FutureWarning)

[2]: # imports
import numpy as np
import matplotlib.pyplot as plt
import tensorflow as tf
assert tf.__version__ == "1.13.1"

# ignore tensorflow depreciation warnings
import tensorflow.python.util.deprecation as deprecation
deprecation._PRINT_DEPRECATION_WARNINGS = False
```

0.1 Plotting Functions

```
[3]: def plot_loss(train_loss, valid_loss=None, title=None, ax=None):
         ax = plt.gca() if ax == None else ax
         x = np.arange(0, len(train_loss), 1)
         ax.plot(x, train_loss, label="Training Loss")
         if not valid_loss is None:
             ax.plot(x, valid_loss, label="Valdation Loss")
         ax.set title("Loss" if title == None else title)
         ax.set_xlabel("Updates")
         ax.set xlim(left=0)
         ax.set_ylabel("Loss")
         ax.set ylim(bottom=0)
         ax.legend(loc="upper right")
     def plot_cluster(K, MU, S, colors=None, title=None, ax=None):
         ax = plt.gca() if ax == None else ax
         colors = [None]*K if colors is None else colors
         for i in range(K):
             x, y = S[i][:,0], S[i][:,1]
             ax.scatter(x, y, c=colors[i], alpha=0.5, label=str(i+1), zorder=0)
             ax.scatter(MU[i][0], MU[i][1], c='black', marker='x', s=50, zorder=100)
         ax.set_title(title)
         ax.legend(fontsize="small")
```

0.2 Helper Functions

```
[4]: def reduce_logsumexp(input_tensor, reduction_indices=1, keep_dims=False):
         """Computes the sum of elements across dimensions of a tensor in log domain.
          It uses a similar API to tf.reduce_sum.
         Arqs:
             input_tensor: The tensor to reduce. Should have numeric type.
             reduction_indices: The dimensions to reduce.
             keep_dims: If true, retains reduced dimensions with length 1.
         Returns:
             The reduced tensor.
         max_input_tensor1 = tf.reduce_max(input_tensor, reduction_indices,_
      →keep_dims=keep_dims)
         max_input_tensor2 = max_input_tensor1
         if not keep_dims:
             max_input_tensor2 = tf.expand_dims(max_input_tensor2, reduction_indices)
         return tf.log(
                 tf.reduce_sum(
                   tf.exp(input_tensor - max_input_tensor2),
                   reduction indices,
                   keep_dims=keep_dims)) + max_input_tensor1
     def logsoftmax(input_tensor):
         """Computes normal softmax nonlinearity in log domain.
          It can be used to normalize log probability.
          The softmax is always computed along the second dimension of the input_\sqcup
      \hookrightarrow Tensor.
         Args:
             input_tensor: Unnormalized log probability.
         Returns:
             normalized log probability.
         return input_tensor - reduce_logsumexp(input_tensor, reduction_indices=0,_
      →keep_dims=True)
```

```
[5]: def get_clusters_Kmeans(K, MU, X):
         """ Given a set of MUs, computes optimal clusters of X
         # getting square pairwise distances
         pair_dist = tf.Session().run(distanceFunc_Kmeans(X, MU))
         # getting most likely cluster by index
         S_indices = np.argmin(pair_dist, axis=1)
         # getting list of actual data grouped by cluster
         S = [None] *K
         for i in range(K):
             S[i] = X[S_indices == i]
         return S
[6]: def get_clusters_GMM(K, MU, sigma, log_pi, X):
         """ Given a set of MUs, computes most likely clusters of X
         nnn
         # getting posterior distribution
         log_PDF = tf.Session().run(log_GaussPDF(X, MU, sigma))
         log_post = tf.Session().run(log_posterior(log_PDF, log_pi))
         # getting most likely cluster by index
         S_indices = np.argmax(log_post, axis=1)
         # getting list of actual data grouped by cluster
         S = [None] *K
         for i in range(K):
             S[i] = X[S_indices == i]
         return S
[7]: def cluster_percentages(K, S):
         """ Computes percentage of data in each cluster S[i]
         n n n
         total = 0.0
         percentages = np.zeros(K)
         for i in range(K):
             total += S[i].shape[0]
             percentages[i] += S[i].shape[0]
         return percentages / total
```

0.3 Data Loaders

```
[8]: def load 2D(valid=True):
         data = np.load('data2D.npy')
         [num_pts, dim] = data.shape
         # getting validation set
         if valid:
             valid_batch = int(num_pts / 3.0)
             np.random.seed(69)
             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(valid=True):
         data = np.load('data100D.npy')
         [num_pts, dim] = data.shape
         # getting validation set
         if valid:
             valid_batch = int(num_pts / 3.0)
             np.random.seed(69)
             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
```

1 K-means

1.1 Learning K-means

1.1.1 Creating Model

```
[9]: # Distance function
def distanceFunc_Kmeans(X, MU):
    # Inputs
    # X: is an NxD matrix (N observations and D dimensions)
    # MU: is an KxD matrix (K means and D dimensions)

# Outputs
    # pair_dist: is the squared pairwise distance matrix (NxK)

# expand dimensions to properly subract the two
    X_expanded = tf.expand_dims(X, 1)
    MU_expanded = tf.expand_dims(MU, 0)

# uses broadcasting to do the subtraction
    pair_dist = tf.reduce_sum(tf.square(tf.subtract(X_expanded, MU_expanded)),u
    axis=2)

return pair_dist
```

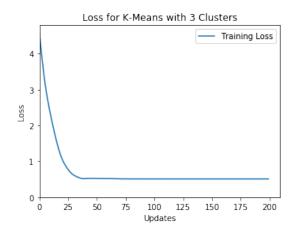
```
[10]: # loss function
      def L_Kmeans(X, MU):
          # calculate pairwise distances
          pair_dist = distanceFunc_Kmeans(X, MU)
          # assign clusters to min val and sum
          return tf.reduce_sum(tf.reduce_min(pair_dist, axis=1))
      # tensorflow training loop
      def load Kmeans(K, dims):
          N, D = dims
          X = tf.placeholder(tf.float64, shape=(None,D))
          with tf.variable_scope("Part1", reuse=tf.AUTO_REUSE):
              # init with random MU
              MU = tf.Variable(tf.truncated normal((K, D), mean=0, stddev=1, dtype=tf.
      →float64), trainable=True)
             loss = L_Kmeans(X, MU) # loss function
              # set up Adam optimizer
```

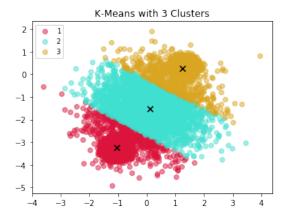
```
optimizer = tf.train.AdamOptimizer(learning_rate=0.1, beta1=0.9, __
 →beta2=0.99, epsilon=1e-5).minimize(loss)
   return optimizer, loss, X, MU
# Kmean solver
def Kmeans(K, train_data, valid_data=None, epochs=10):
   train_loss = []
   valid_loss = []
    # load model
   optimizer, loss, X, MU = load_Kmeans(K, train_data.shape)
   # train
   with tf.Session() as sess:
        # init all variables (needed for Adam)
       sess.run(tf.global_variables_initializer())
       for epoch in range(epochs):
            # print("Epoch {}".format(epoch+1))
            # run through optimizer and update loss values
            sess.run(optimizer, feed_dict={X: train_data})
            train_loss.append(sess.run(loss, feed_dict={X: train_data}))
            if not valid_data is None:
                valid_loss.append(sess.run(loss, feed_dict={X: valid_data}))
        # get final MUs
       MU_optim = sess.run(MU, feed_dict={X: train_data})
   statistics = (np.array(train_loss) / train_data.shape[0], )
   if not valid data is None:
        statistics += (np.array(valid_loss) / valid_data.shape[0], )
    # returning optimal values of parameters and loss statistics
   out = (MU_optim, *statistics)
   return out
```

Training

```
[11]: K = 3
      # getting data
      train_data = load_2D(valid=False)
      # compute optimal model parameters
      MU, train_loss = Kmeans(K, train_data, epochs=200)
      # getting clusters
      S = get_clusters_Kmeans(K, MU, train_data)
      # displaying model parameters
      print("MU:")
      print(MU)
      print("\n")
      # plotting
      fig, ax = plt.subplots(1, 2, figsize=(12, 4))
      colors = ['crimson', 'turquoise', 'goldenrod', 'lightcoral', 'yellowgreen']
      plot_loss(train_loss, title=f"Loss for K-Means with {K} Clusters", ax=ax[0])
      plot_cluster(K, MU, S, title=f"K-Means with {K} Clusters", colors=colors, u
       \rightarrowax=ax[1])
```

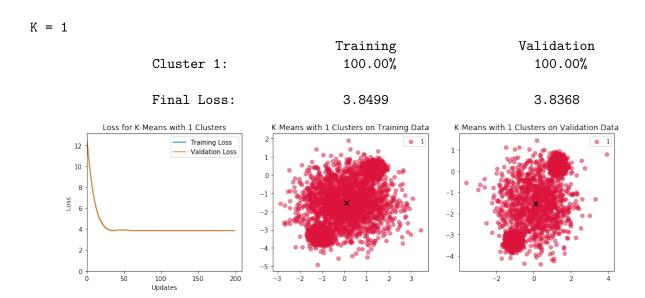
MU:





1.1.2 Varying K and 1.1.3 Validation

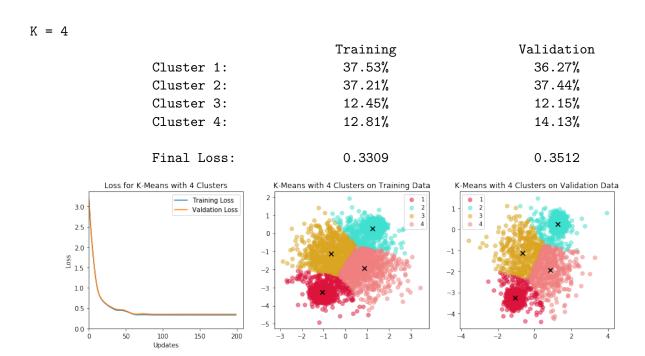
```
[12]: # getting data
      train_data, valid_data = load_2D()
      print("\n\n\n\n\n\n") # this just makes things look better in the pdf
      # Iterate through values of K
      for K in [1, 2, 3, 4, 5]:
          print("K =", K)
          # compute optimal model parameters
          MU, train_loss, valid_loss = Kmeans(K, train_data, valid_data, epochs=200)
          # getting clusters
          S_train = get_clusters_Kmeans(K, MU, train_data)
          S_valid = get_clusters_Kmeans(K, MU, valid_data)
          # computer percentages
          train_percentages = cluster_percentages(K, S_train)
          valid percentages = cluster percentages(K, S valid)
          print("\t\t\t\t\tTraining\t\tValidation")
          for i in range(K):
             print(f"\t\tCluster {i+1}:\t\t {train_percentages[i]:.2%} \t\t \_
      →{valid_percentages[i]:.2%}")
          print()
          print(f"\t\tFinal Loss:\t\t {train_loss[-1]:.4f} \t\t {valid_loss[-1]:.
      \hookrightarrow4f}")
          # plot
          fig, ax = plt.subplots(1, 3, figsize=(15, 4))
          colors = ['crimson', 'turquoise', 'goldenrod', 'lightcoral', 'yellowgreen']
          plot_loss(train_loss, valid_loss, title=f"Loss for K-Means with {K}_{LI}
      plot_cluster(K, MU, S_train, title=f"K-Means with {K} Clusters on Training_
       →Data", colors=colors, ax=ax[1])
          plot_cluster(K, MU, S_valid, title=f"K-Means with {K} Clusters on_
      →Validation Data", colors=colors, ax=ax[2])
          plt.show()
          plt.close()
```



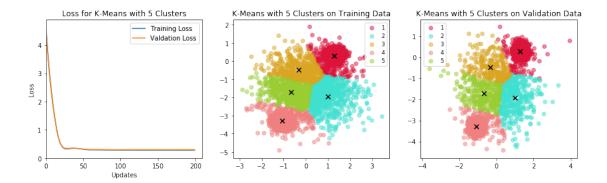


	opatics		
K = 3			
		Training	Validation
	Cluster 1:	23.77%	24.00%
	Cluster 2:	38.40%	37.53%
	Cluster 3:	37.83%	38.46%
	Final Loss:	0.5032	0.5271





K = 5			
		Training	Validation
	Cluster 1:	35.98%	36.18%
	Cluster 2:	11.11%	11.76%
	Cluster 3:	6.94%	7.59%
	Cluster 4:	36.76%	35.34%
	Cluster 5:	9.19%	9.12%
	Final Loss:	0.2818	0.2994



Discussion The "best" number of clusters seems to be 3. Looking at the data, we see two highly dense clusters: one on the top right and one in the bottom left. Aside from these two distinct clusters, the rest of the data seems to be a noisy cluster centered around (0, -1). For all the plots where we choose $K \geq 3$, the two dense clusters always seem to appear. Increasing K beyond 3 only partitions the big middle cluster. For plots with K > 3, however, the cluster centers don't appear to be near any centered bunch of data. Instead, they seem to only split up a larger cluster.

Considering K < 3, K = 1 misses distinguish between the two highly dense clusters. Also, K = 2 appears to include points beyond the highly dense cluster (i.e. around half of the points which appear to be outside of the main two clusters are accidentally included).

2 Mixtures of Gaussians

2.1 The Guassian Cluster Model

```
[13]: def distanceFunc_GMM(X, MU):
          # Inputs
          \# X: is an NxD matrix (N observations and D dimensions)
          # MU: is an KxD matrix (K means and D dimensions)
          # Outputs
          # pair_dist: is the pairwise distance matrix (NxK)
          # expand dimensions to properly subract the two
          X_expanded = tf.expand_dims(X, 1)
          MU_expanded = tf.expand_dims(MU, 0)
          # uses broadcasting to do the subtraction
          pair_dist = tf.reduce_sum(tf.square(tf.subtract(X_expanded, MU_expanded)),__
       \rightarrowaxis=2)
          return tf.sqrt(pair_dist)
      def log_GaussPDF(X, MU, sigma):
          # Inputs
          # X: N X D
          # mu: K X D
          # sigma: K X 1
          # Outputs:
          # log Gaussian PDF N X K
          _{\text{,}} D = X.shape
              D = D.value # D is a tensorflow variable
          except:
              pass
          constants = -(D/2) * tf.log(2 * np.pi * tf.transpose(sigma)**2)
          pair_dist = distanceFunc_GMM(X, MU)
          return constants - tf.square(pair_dist) / (2 * tf.transpose(sigma)**2)
      def log_posterior(log_PDF, log_pi):
          # Input
          # log PDF: log Gaussian PDF N X K
          # log_pi: K X 1
          # Outputs
```

```
# log_post: N X K

log_post = tf.add(log_PDF, tf.transpose(log_pi))
correction = reduce_logsumexp(log_post, keep_dims=True)
return tf.subtract(log_post, correction)
```

Importance of logsumexp: For numerical stability computational efficiency, we deal with the log of the probabilities instead of the actual probabilities themselves (i.e. we deal with the probabilities in log-domain). In order to computer the posterior, we must take a sum of the actual probabilities. In general, we are looking for some operation \odot which we can do in log-domain which will be able to give us the result $(P_1 + P_2)$ in log-domain. Specifically, we want an operation \odot such that $\log(P_1) \odot \log(P_2) = \log(P_1 + P_2)$. Unfortunately, we don't know of a simple \odot that meets this condition. So, we will perform this summation outside of log-domain. The function logsumexp will first perform e^x for each term x to get out of log-domain. Then, it will perform the desired sum. Finally, it will perform $\log(x)$ for each term x to get back into log-domain.

Essentially, logsumexp is a way of adding two numbers in log-domain while ensuring the result is also in log-domain.

2.2 Learning the MoG

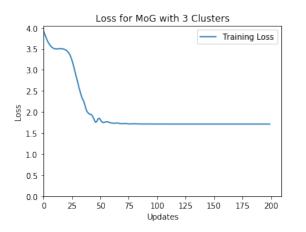
2.2.1 Creating Model

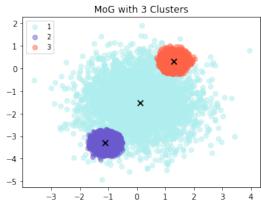
```
[14]: # loss function
      def L_GMM(log_PDF, log_pi):
          likelihood = reduce_logsumexp(tf.add(log_PDF, tf.transpose(log_pi)))
          return -tf.reduce_sum(likelihood)
      def load_GMM(K, dims):
          N, D = dims
          X = tf.placeholder(tf.float64, shape=(None,D))
          with tf.variable_scope("Part2", reuse=tf.AUTO_REUSE):
              # init with random MU
              MU = tf.Variable(tf.truncated_normal((K, D), mean=0, stddev=1, dtype=tf.
       →float64), trainable=True)
              phi = tf.Variable(tf.truncated_normal((K,), mean=0, stddev=1, dtype=tf.
       →float64), trainable=True)
              psi = tf.Variable(tf.truncated_normal((K,), mean=0, stddev=1, dtype=tf.
       →float64), trainable=True)
              # turing the unconstrained parameters into the constrained ones
              sigma = tf.exp(phi)
              log_pi = logsoftmax(psi)
              # computing log probability distributions
              log_PDF = log_GaussPDF(X, MU, sigma)
              loss = L_GMM(log_PDF, log_pi) # loss function
              # set up Adam optimizer
              optimizer = tf.train.AdamOptimizer(learning_rate=0.1, beta1=0.9,__
       →beta2=0.99, epsilon=1e-5).minimize(loss)
          return optimizer, loss, X, MU, sigma, log_pi
      def GMM(K, train_data, valid_data=None, epochs=10):
          train loss = []
          valid_loss = []
          # load model
          optimizer, loss, X, MU, sigma, log_pi = load_GMM(K, train_data.shape)
          # train
          with tf.Session() as sess:
              # init all variables (needed for Adam)
```

```
sess.run(tf.global_variables_initializer())
      for epoch in range(epochs):
           # print("Epoch {}".format(epoch+1))
           # run through optimizer and update loss values
           sess.run(optimizer, feed_dict={X: train_data})
           train_loss.append(sess.run(loss, feed_dict={X: train_data}))
           if not valid data is None:
               valid_loss.append(sess.run(loss, feed_dict={X: valid_data}))
       # get final MUs
      MU_optim, sigma_optim, log_pi_optim = sess.run([MU, sigma, log_pi],_
→feed_dict={X: train_data})
   train_loss = np.array(train_loss) / train_data.shape[0] # normalizing_
→ loss
   statistics = (train_loss, )
   if not valid_data is None:
      valid_loss = np.array(valid_loss) / valid_data.shape[0] # normalizing_
→ loss
      statistics += (valid_loss, )
   # returning optimal values of parameters and loss statistics
   out = (MU_optim, sigma_optim, log_pi_optim, *statistics)
   return out
```

Training

```
[20]: K = 3
      # getting data
      train_data = load_2D(valid=False)
      # compute optimal model parameters
      MU, sigma, log_pi, train_loss = GMM(K, train_data, epochs=200)
      # getting clusters
      #S = get_clusters_Kmeans(K, MU, train_data)
      S = get_clusters_GMM(K, MU, sigma, log_pi, train_data)
      # displaying model parameters
      print("MU:")
      print(MU)
      print("\n")
      print("sigma:", sigma)
      print("\n")
      print("pi:", np.exp(log_pi))
      print("\n")
      # plotting
      fig, ax = plt.subplots(1, 2, figsize=(12, 4))
      colors = ['paleturquoise', 'slateblue', 'tomato', 'orange', 'darkcyan']
      plot_loss(train_loss, title=f"Loss for MoG with {K} Clusters", ax=ax[0])
     plot_cluster(K, MU, S, title=f"MoG with {K} Clusters", colors=colors, ax=ax[1])
     MU:
     [[ 0.10584793 -1.52744683]
      [-1.10171464 -3.30615532]
      [ 1.29863453  0.30921863]]
     sigma: [0.99358419 0.1976946 0.19712042]
     pi: [0.33463062 0.33190656 0.33346282]
```



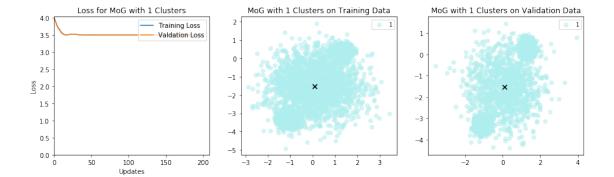


2.2.2 Varying K

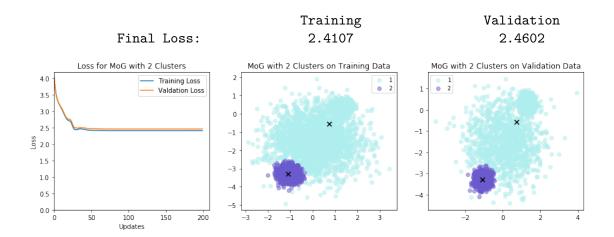
```
[30]: # getting data
      train_data, valid_data = load_2D()
      # Iterate through values of K
      for K in [1, 2, 3, 4, 5]:
          print("K =", K)
          # compute optimal model parameters
          MU, sigma, log_pi, train_loss, valid_loss = GMM(K, train_data, valid_data, u
       ⇒epochs=200)
          # getting clusters
          S_train = get_clusters_GMM(K, MU, sigma, log_pi, train_data)
          S_valid = get_clusters_GMM(K, MU, sigma, log_pi, valid_data)
          print("\n")
          print("\t\t\t\t\tTraining\t\tValidation")
          print(f"\t\tFinal Loss:\t\t {train_loss[-1]:.4f} \t\t {valid_loss[-1]:.
       \hookrightarrow4f}")
          # plot
          fig, ax = plt.subplots(1, 3, figsize=(15, 4))
          colors = ['paleturquoise', 'slateblue', 'tomato', 'orange', 'darkcyan']
          plot_loss(train_loss, valid_loss, title=f"Loss for MoG with {K} Clusters", u
       \rightarrowax=ax[0])
          plot_cluster(K, MU, S_train, title=f"MoG with {K} Clusters on Training⊔
       →Data", colors=colors, ax=ax[1])
          plot_cluster(K, MU, S_valid, title=f"MoG with {K} Clusters on Validation⊔
       →Data", colors=colors, ax=ax[2])
          plt.show()
          plt.close()
```

K = 1

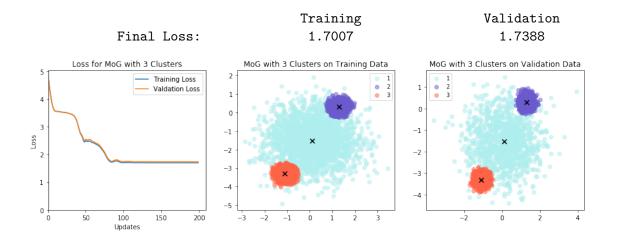
Training Validation Final Loss: 3.4928 3.4894



K = 2



K = 3





K = 5



Discussion In the plots with the GMM (Gaussian Mixture Model), we see a similar result as compared to the K-means result but considerably more pronounced since the GMM clusters take in the adjustable prior and are probabilistic instead of forcing each data point to be assigned to the closest cluster. This allows for a more well defined clusters than when compared with the K-means case.

Clearly, with only one cluster, everything is assigned to the same cluster. With K = 2, we see

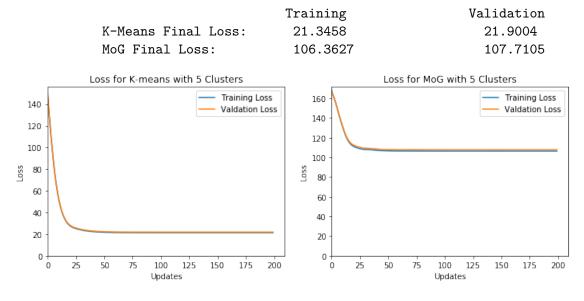
something more interesting. The GMM is able to very accurately find one of the two highly dense clusters (in our example, it found the bottom left one). Despite the location of the dense cluster center, we observe that some points which are closer to the dense cluster center are actually assigned to the other cluster! This is very different from the K-means case. The GMM model here seems to represent the situation much better as these far points are more likely just outliers of the center cluster than points belonging to the dense cluster.

With K=3, we see the GMM clearly find the two highly dense clusters and also identify the other points to the central cluster, as we expected the data to be labelled. Increasing beyond K=3, we only see that new cluster centers are being assigned to the central cluster. This seems redundant as the two centers appear to refer to the same central cluster (the one identified by K=3. This problem only gets worse with increasing K. As such, K=3 appears to be the best choice for this data.

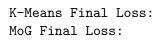
2.2.3 Big Dataset

```
[27]: # getting data
      train_data, valid_data = load_100D()
      # Iterate through values of K
      for K in [5, 10, 15, 20, 30]:
          print("K =", K)
          # compute optimal model parameters
          MU, Kmeans_train_loss, Kmeans_valid_loss = Kmeans(K, train_data,__
       →valid_data, epochs=200)
          MU, sigma, log_pi, MoG_train_loss, MoG_valid_loss = GMM(K, train_data,_
       →valid_data, epochs=200)
          print("\t\t\t\t\tTraining\t\tValidation")
          print(f"\t\tK-Means Final Loss:\t {Kmeans_train_loss[-1]:.4f} \t\t __
       \hookrightarrow {Kmeans_valid_loss[-1]:.4f}")
          print(f"\t\tMoG Final Loss:\t\t {MoG_train_loss[-1]:.4f} \t\t __
       \hookrightarrow{MoG valid loss[-1]:.4f}")
          # plot
          fig, ax = plt.subplots(1, 2, figsize=(12, 4))
          plot_loss(Kmeans_train_loss, Kmeans_valid_loss, title=f"Loss for K-means_u
       →with {K} Clusters", ax=ax[0])
          plot_loss(MoG_train_loss, MoG_valid_loss, title=f"Loss for MoG with {K}_u
       plt.show()
          plt.close()
```

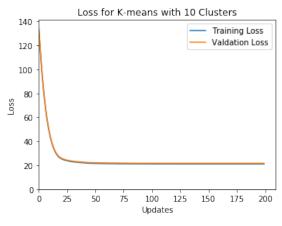


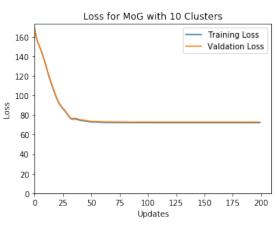




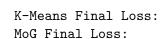


Training 21.0835 72.1040 Validation 21.6736 72.7620

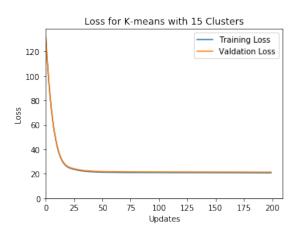


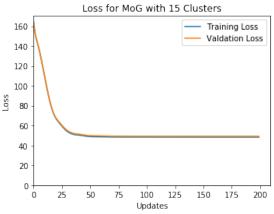


K = 15



Training 20.7694 48.3243 Validation 21.3852 49.3481

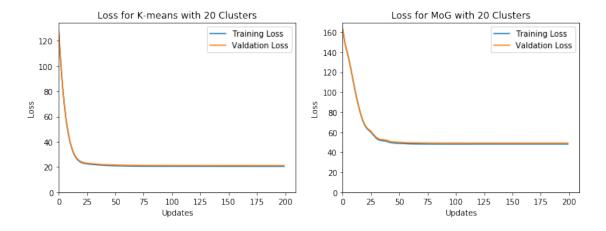


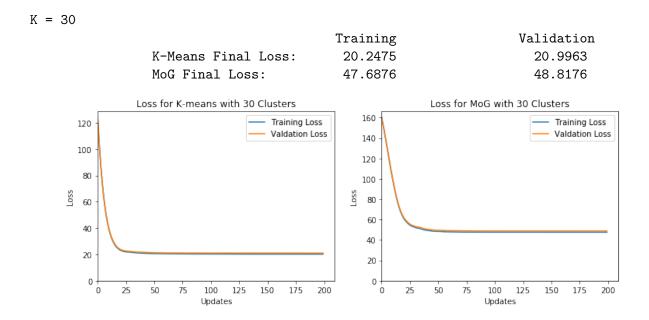


K = 20

K-Means Final Loss:
MoG Final Loss:

Training 20.5086 48.1003 Validation 21.1730 49.1542





Discussion - K Means From the plots above, we notice that the results for K-means shows a similar pattern regardless of the number of clusters. As the number of clusters increases, however, we see the final loss values to continue decreasing (or staying approximately the same). This makes sense for the K-means algorithm. Allowing the algorithm to find more clusters would allow finer partition of the input space. We expect this to decrease the average distance from each data point to its respective cluster center since there are more cluster centers and the data points are simply assigned to the cluster whose center is closest to them. Indeed, this is exactly what we see with the K-means graphs

Discussion - Mixture of Gaussians For the MoG (Mixture of Gaussian) models, we expect the different results as we increase K. From the 2D data set, we noticed that as K increased greatly

beyond the desired number of clusters, the MoG model starts adding the extra cluster centers to be approximately in the same location as one of the other cluster centers. The redundant clusters seem to follow a similar location and distribution as the cluster which they mirror but are assigned significantly lower π_k (prior probability). As such, increasing K shouldn't see much better loss values since the redundant extra clusters should be assigned very few points and have low overall probability.

In the case that K is too low, we expect the loss to be significantly higher than optimal. Extrapolating from the 2D case when we set K=2, we noticed that the MoG model identified and converged on one dense cluster, but was unable to converge on the second dense cluster since there were not enough clusters. Consequently, all points outside of the identified cluster were labelled to the remaining cluster. Unlike the K-means case where the "unidentifiable" (we use unidentifiable to mean points which should have been assigned to their own cluster but could not be due to K being set too low) points are split evenly by a hyperplane bisecting the two nearest clusters, the MoG will assign (almost) all of these unidentifiable points to the cluster which gives them higher probability. This incurrs a high loss.

These expectations align with what we see in the MoG plots. With K=5, we see the loss values converging at just over 100 (significantly higher than some higher K where convergence happened around 50). This aligns with the K=5 case not having enough clusters for the dataset. A similar thing happens for K=10. However, the plots for K=15, K=20, and K=30 all converge with loss values around 49. We notice that increasing K beyond 15 did not cause a significant decrease in loss. This aligns with the cases where K is set too high, and we can infer that K beyond 15 has some redundant clusters. From this, we conclude that the 100D dataset likely has around 15 clusters.

Discussion - Comparison Aside from the specific results mentioned above, it appears that the MoG model appears to have worse performance (in terms of loss) for lower values of K since K-means clustering is able to partition unidentifiable clusters better. However, despite that K-means sees lower loss values for higher K, we must be cautious when interpreting this result as more successful. In the extreme case, K=N (N being the number of data points), K-means would achieve a perfect loss at zero by overfitting and assign each data point to its own cluster. But, this does not mean it did better! By contrast, the MoG model should give similar results to the cases K>15 above.

In conclusion, we see that K-means seems to perform better for small K since it's not restricted to gaussian probabilities for splitting data into clusters. However, we also observe that the MoG model performs better for large K.