1. Consider the following unlabeled training data:

| | $y_1$ | $y_2$ |
|---|---|---|
| $x_1$ | 0 | 0 |
| $x_2$ | 1 | 0 |
| $x_3$ | 0 | 2 |
| $x_4$ | 2 | 2 |

Consider also the following initialization centroids:

$$\mu_1 = \begin{bmatrix} 2 \\ 0 \end{bmatrix}, \quad \mu_2 = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

(a) Apply $k$-means until convergence. What are the final centroids?

(b) Plot the data points and draw the clusters (with their respective centroids).

(c) Compute the silhouette score for sample $x_1$, cluster $c_1$ and for the overall solution.

(d) As the ground truth, take $x_3$ as a "negative" sample and the rest as "positive". Compute the error classification rate (ECR) of $k$-means here against the ground truth.

For starters, it's probably worth it to write a general explanation of how $k$-means works. Basically, $k$-means is a clustering algorithm which, given a set of $n$ data points $\{x_1, \ldots, x_n\}$, tries to assign each data point to one of $k$ clusters. Each cluster is centered around a centroid $\mu_i$; while other clustering algorithms may create clusters of different shapes, $k$-means clusters are always circular/spherical. The algorithm works as follows:

(a) Initialize the centroids $\mu_1, \ldots, \mu_n$.

(b) Assign each data point to the closest centroid.

(c) Recompute the centroids based on the assigned data points.

(d) Repeat steps b) and c) until convergence - that is, until the centroids don't change anymore (or until the change is below a certain threshold).

In $k$-means solution implementations, we usually perform a series of runs with different centroid initializations and pick the best one (where the *best* here is defined by a combination of metrics, which we'll discuss later). In the following exercises, though, we'll just use a single run. We'll also be using the Euclidean distance here, the most common distance metric used in this algorithm.

For starters, let's assign each sample to the closest centroid. We can do this by computing the distance (squared or not is irrelevant) between each sample and each centroid, and then picking the centroid with the smallest distance:

$$\|x_1 - \mu_1\| = \left\| \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 2 \\ 0 \end{bmatrix} \right\|^2 = 4, \quad \|x_1 - \mu_2\| = \left\| \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 2 \\ 1 \end{bmatrix} \right\|^2 = 5$$

$c = \text{argmin}_{k \in \{1,2\}} \|x_1 - \mu_n\|$ is, therefore, $k = 1$, and $x_1$ is assigned to cluster $c_1$.

Performing similar computations for the other samples, we get the following:

$$\begin{aligned}
\text{argmin}_{k\in\{1,2\}} \|x_2 - \mu_n\|^2 &= \text{argmin}_{k\in\{1,2\}}\{1, 2\} = c_1 \\
\text{argmin}_{k\in\{1,2\}} \|x_3 - \mu_n\|^2 &= \text{argmin}_{k\in\{1,2\}}\{8, 5\} = c_2 \\
\text{argmin}_{k\in\{1,2\}} \|x_4 - \mu_n\|^2 &= \text{argmin}_{k\in\{1,2\}}\{4, 1\} = c_2
\end{aligned}$$

Now, we'll want to adjust our centroids: for each cluster, we'll compute the mean of all the samples assigned to it, and use that as the new centroid. $k$-means differs from other clustering algorithms here: EM, for example, utilizes every single sample in the dataset to compute the new centroids' parameters. $k$-means, on the other hand, by nature of working with hard assignments ends up using only a subset of the samples in the dataset to compute the new centroids.

$$\mu_1 = \frac{1}{2}(x_1 + x_2) = \frac{1}{2}\left(\begin{bmatrix}0\\0\end{bmatrix} + \begin{bmatrix}1\\0\end{bmatrix}\right) = \begin{bmatrix}0.5\\0\end{bmatrix}, \quad \mu_2 = \frac{1}{2}(x_3 + x_4) = \frac{1}{2}\left(\begin{bmatrix}0\\2\end{bmatrix} + \begin{bmatrix}2\\2\end{bmatrix}\right) = \begin{bmatrix}1\\2\end{bmatrix}$$

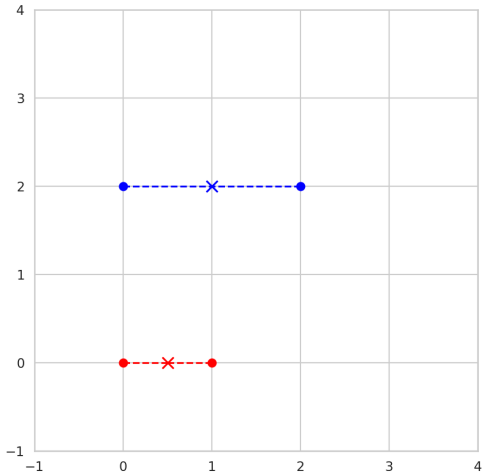
The centroids have moved, so we'll have to repeat steps b) and c).

$$\begin{aligned}
\text{argmin}_{k\in\{1,2\}} \|x_1 - \mu_n\|^2 &= \text{argmin}_{k\in\{1,2\}}\{0.25, 5\} = c_1 \\
\text{argmin}_{k\in\{1,2\}} \|x_2 - \mu_n\|^2 &= \text{argmin}_{k\in\{1,2\}}\{0.25, 4\} = c_1 \\
\text{argmin}_{k\in\{1,2\}} \|x_3 - \mu_n\|^2 &= \text{argmin}_{k\in\{1,2\}}\{4.25, 1\} = c_2 \\
\text{argmin}_{k\in\{1,2\}} \|x_4 - \mu_n\|^2 &= \text{argmin}_{k\in\{1,2\}}\{6.25, 1\} = c_2
\end{aligned}$$

$$\mu_1 = \frac{1}{2}(x_1 + x_2) = \frac{1}{2}\left(\begin{bmatrix}0\\0\end{bmatrix} + \begin{bmatrix}1\\0\end{bmatrix}\right) = \begin{bmatrix}0.5\\0\end{bmatrix}, \quad \mu_2 = \frac{1}{2}(x_3 + x_4) = \frac{1}{2}\left(\begin{bmatrix}0\\2\end{bmatrix} + \begin{bmatrix}2\\2\end{bmatrix}\right) = \begin{bmatrix}1\\2\end{bmatrix}$$

The centroids haven't moved, so we're done. At the end of the algorithm's run, the cluster assignments are as follows: $c_1 = \{x_1, x_2\}$, $c_2 = \{x_3, x_4\}$.

Afterward, we can plot the clusters and the centroids (we can pretend that the cluster's circle is actually drawn and such), with $c_1$ in red and $c_2$ in blue:



Finally, regarding the **silhouette scores** of observations, we can compute them as follows (considering $s_n$ to be the silhouette of sample $x_n$ and $c_N$ to be its assigned cluster):

$$
\begin{aligned}
s_n &= \frac{b_n - a_n}{\max\{a_n, b_n\}} \\
a_n &= \frac{1}{|c_N| - 1} \sum_{x_i \in c_n, x_i \neq x_n} \|x_i - x_n\| \\
b_n &= \min_{n' \in \{1, \cdots, k\}, n' \neq N} \frac{1}{|c_{n'}|} \sum_{x_i \in c_{k'}} \|x_i - x_n\|
\end{aligned}
$$

Essentially, the silhouette score of a sample will take into account how close it is to the other samples in its cluster (in average), and how far it is from the samples in its most neighboring cluster (in average).

$$
\begin{aligned}
a_1 &= \frac{1}{1}\left(\|x_2 - x_1\|\right) = 1, \quad a_2 &&= \frac{1}{1}\left(\|x_1 - x_2\|\right) = 1 \\
a_3 &= \frac{1}{1}\left(\|x_4 - x_3\|\right) = 2, \quad a_4 &&= \frac{1}{1}\left(\|x_3 - x_4\|\right) = 2
\end{aligned}
$$

$$
\begin{aligned}
b_1 &= \min_{n' \in \{1,2\}, n' \neq 1} \frac{1}{2}\left(\|x_3 - x_1\| + \|x_4 - x_1\|\right) = 2.414, \quad b_2 &&= \min_{n' \in \{1,2\}, n' \neq 1} \frac{1}{2}\left(\|x_3 - x_2\| + \|x_4 - x_2\|\right) = 2.236 \\
b_3 &= \min_{n' \in \{1,2\}, n' \neq 2} \frac{1}{2}\left(\|x_1 - x_3\| + \|x_2 - x_3\|\right) = 2.118, \quad b_4 &&= \min_{n' \in \{1,2\}, n' \neq 2} \frac{1}{2}\left(\|x_1 - x_4\| + \|x_2 - x_4\|\right) = 2.532
\end{aligned}
$$

$$
\begin{aligned}
s_1 &= \frac{2.414 - 1}{\max\{1, 2.414\}} = 0.5858, \quad s_2 &&= \frac{2.236 - 1}{\max\{1, 2.236\}} = 0.5528 \\
s_3 &= \frac{2.118 - 2}{\max\{2, 2.118\}} = 0.0557, \quad s_4 &&= \frac{2.532 - 2}{\max\{2, 2.532\}} = 0.2102
\end{aligned}
$$

The silhouette scores for each cluster are given by the average of the silhouette scores of its samples:

$$
s_1 = \frac{1}{2}\left(0.5858 + 0.5528\right) = 0.5693, \quad s_2 = \frac{1}{2}\left(0.0557 + 0.2102\right) = 0.1329
$$

The overall silhouette score is given by the average of the silhouette scores of each cluster:

$$
s = \frac{1}{2}\left(0.5693 + 0.1329\right) = 0.3511
$$

Finally, the **error classification rate** measures the proportion of misclassified samples in the dataset. If we think about the confusion matrix of the problem, we can write down the expression as:

$$
ECR = \frac{FP + FN}{FP + FN + TP + TN} = \frac{(2-2) + (2-1)}{2 + 2} = 0.25
$$

2. Consider the following unlabeled training data:

| | $y_1$ | $y_2$ | $y_3$ |
|---|---|---|---|
| $x_1$ | 1 | 0 | 0 |
| $x_2$ | 8 | 8 | 4 |
| $x_3$ | 3 | 3 | 0 |
| $x_4$ | 0 | 0 | 1 |
| $x_5$ | 0 | 1 | 0 |
| $x_6$ | 3 | 2 | 1 |

and let the initial $k$ centroids be the first $k$ samples.

(a) Apply $k$-means until convergence, for $k \in \{2, 3\}$. What are the final centroids?

(b) Which $k$ provides a better clustering regarding **cohesion** (i.e the intra-cluster distance - the sum of the distances from every point to their centroid)?

(c) Which $k$ provides a better clustering regarding **separation** (i.e the inter-cluster distance - the average distance of every centroid to every other centroid)?

Won't be doing the first question since it's basically repeating the last question's exercise (twice), and it's also in the teacher's solutions. We'll need the **post-convergence** centroids, though, so I'll write them down here (plus each cluster's assigned samples):

$k = 2$:

$$\mu_1 = \begin{bmatrix} 1.4 \\ 1.2 \\ 0.4 \end{bmatrix}, \quad \mu_2 = \begin{bmatrix} 8 \\ 8 \\ 4 \end{bmatrix}$$

$$k_1 = \{x_1, x_3, x_4, x_5, x_6\}, \quad k_2 = \{x_2\}$$

$k = 3$:

$$\mu_1 = \begin{bmatrix} 0.333333 \\ 0.333333 \\ 0.333333 \end{bmatrix}, \quad \mu_2 = \begin{bmatrix} 8 \\ 8 \\ 4 \end{bmatrix}, \quad \mu_3 = \begin{bmatrix} 3 \\ 2.5 \\ 0.5 \end{bmatrix}$$

$$k_1 = \{x_1, x_4, x_5\}, \quad k_2 = \{x_2\}, \quad k_3 = \{x_3, x_6\}$$

Regarding **cohesion**, we measure it as the sum of the distances from every point to their centroid. We can write down the expression as:

$$\text{Cohesion}(k) = \sum_{i=1}^{k} \sum_{x \in k_i} \|x - \mu_i\|^2$$

$$\text{Cohesion}(2) = \|x_1 - \mu_1\|^2 + \|x_2 - \mu_2\|^2 + \|x_3 - \mu_1\|^2 + \|x_4 - \mu_1\|^2 + \|x_5 - \mu_1\|^2 + \|x_6 - \mu_1\|^2 \approx 17.2$$

$$\text{Cohesion}(3) = \|x_1 - \mu_1\|^2 + \|x_2 - \mu_2\|^2 + \|x_3 - \mu_3\|^2 + \|x_4 - \mu_1\|^2 + \|x_5 - \mu_1\|^2 + \|x_6 - \mu_3\|^2 \approx 3.0$$

Our goal is, ideally, to minimize this cohesion value: the closer the points are to their centroids, the better the clustering. We can see that $k = 3$ provides a better clustering in this regard, as expected: if there are more clusters, the points (generally speaking) should be able to better fit into them.

**Separation**, on the other hand, is the average distance of every centroid to every other centroid. We can write down the expression as:

$$\text{Separation}(k) = \frac{1}{k^2} \sum_{i=1}^{k} \sum_{j=1}^{k} \left\| \mu_i - \mu_j \right\|^2$$

$$\text{Separation}(2) = \frac{1}{4}(\|\mu_1 - \mu_1\|^2 + \|\mu_1 - \mu_2\|^2 + \|\mu_2 - \mu_1\|^2 + \|\mu_2 - \mu_2\|^2) = \frac{1}{2}\|\mu_1 - \mu_2\|^2 \approx 51.38$$

$$\text{Separation}(3) = \frac{1}{9}(\|\mu_1 - \mu_1\|^2 + \|\mu_1 - \mu_2\|^2 + \cdots \|\mu_3 - \mu_2\|^2 + \|\mu_3 - \mu_3\|^2) \approx 46.74$$

As we've seen above, our previous goal was to minimize the cohesion value (for a better clustering solution); intuitively, we can say that growing separation values should lead to a better clustering solution, as well: the more separated the centroids are, (ideally) the better the clustering. We can see that $k = 3$ provides a worse clustering solution in this regard: the centroids are closer to each other, which means that the points could be more likely to be assigned to the wrong cluster.

In the end, choosing the best $k$ value is a matter of balancing these (and other) metrics.

3. Consider the following data points:

$$x_1 = (4), \quad x_2 = (0), \quad x_3 = (1)$$

Moreover, consider a mixture of two normal distributions with the following initialization of likelihoods and priors:

$$\pi_1 = P(c = k_1) = 0.5, \qquad P(x|c = k_1) = \mathcal{N}(x; \mu_1, \sigma_1^2) = \mathcal{N}(x; 1, 1)$$
$$\pi_2 = P(c = k_2) = 0.5, \qquad P(x|c = k_2) = \mathcal{N}(x; \mu_2, \sigma_2^2) = \mathcal{N}(x; 0, 1)$$

Plot the clusters after a single iteration of the EM algorithm.

The Expectation-Maximization (EM) algorithm is a powerful tool for cluster creation, learning the parameters of a distribution/mixture of distributions. It is a two-step iterative algorithm that alternates between two steps: the **Expectation** step and the **Maximization** step.

Here, our centroids are precisely the means of each distribution; if in $k$-means we directly assigned the points to a cluster (and centroid updates would only take into account the samples assigned to them), in EM points aren't "assigned" to a given cluster, having rather a probability of belonging to each one of them. This way, parameter updates will always take into account **all** the points in the dataset (which should, ideally, lead us to a better clustering solution). This way, with each centroid being associated with a given distribution, we're not only able to know where the cluster's centroid is, but also its shape.

In the **E-step**, we calculate the **posteriors** (i.e the probability/*expectation* of a point belonging to each cluster), given the current parameters of the distributions. As we know, these probabilities can be written in function of the likelihoods and priors:

$$\gamma_{ni} = P(c = k_i|x_n) = \frac{P(x_n|c = k_i)\pi_i}{\sum_{j=1}^{k} P(x|c = k_j)\pi_j}$$

Since we know the priors in advance, we'll only need to calculate the likelihoods here. From the question's statement, we know that we can write down the likelihoods as:

$$P(x|c = k_i) = \mathcal{N}(x; \mu_i, \sigma_i^2)$$

Computing this for each sample (and, for each one of them, for each cluster), we'll be able to gather the following (calculations will be shown in their entirety for the first sample, only final results for the remaining ones):

$$\begin{aligned}
\mathcal{N}(x_1; \mu_1, \sigma_1^2) &= \frac{1}{\sqrt{2\pi\sigma_1^2}} \exp\left(-\frac{(x_1 - \mu_1)^2}{2\sigma_1^2}\right) \\
&= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x_1 - 1)^2}{2}\right) = 0.004432 \\
\mathcal{N}(x_1; \mu_2, \sigma_2^2) &= \frac{1}{\sqrt{2\pi\sigma_2^2}} \exp\left(-\frac{(x_1 - \mu_2)^2}{2\sigma_2^2}\right) \\
&= \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x_1 - 0)^2}{2}\right) = 0.0001338
\end{aligned}$$

$$\gamma_{11} = \frac{0.004432 \cdot 0.5}{0.004432 \cdot 0.5 + 0.0001338 \cdot 0.5} = 0.9707, \quad \gamma_{12} = \frac{0.0001338 \cdot 0.5}{0.004432 \cdot 0.5 + 0.0001338 \cdot 0.5} = 0.02931$$

Performing similar computations for the following samples, we're able to gather the following results:

$$\mathcal{N}(x_2; \mu_1, \sigma_1^2) = 0.242, \quad \mathcal{N}(x_2; \mu_2, \sigma_2^2) = 0.3989, \quad \mathcal{N}(x_3; \mu_1, \sigma_1^2) = 0.3989, \quad \mathcal{N}(x_3; \mu_2, \sigma_2^2) = 0.242$$

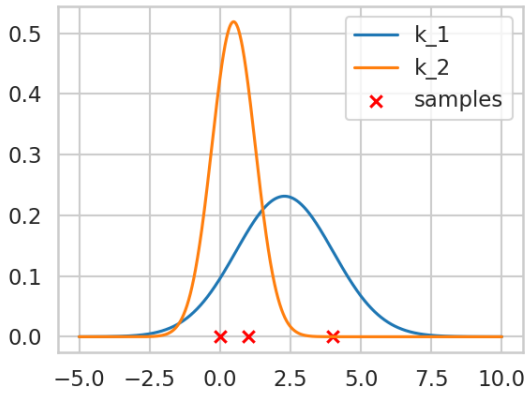
$$\gamma_{21} = 0.3775, \quad \gamma_{22} = 0.6225, \quad \gamma_{31} = 0.6225, \quad \gamma_{32} = 0.3775$$

Having calculated the posteriors (and, subsequently, being able to perform an *estimate of the probabilities of a sample belonging to each cluster*), we can move on to the **M-step**, where we'll update the parameters of the distributions, utilizing these new estimations. In this case, we'll be updating the means and std. deviations of each distribution, plus updating the priors afterward (note that when updating $\sigma$, we use the newly updated means).

$$\mu_k = \frac{\sum_{n=1}^{N} \gamma_{nk} x_n}{\sum_{n=1}^{N} \gamma_{nk}}, \quad \sigma_k = \sqrt{\frac{\sum_{n=1}^{N} \gamma_{nk}(x_n - \mu_k)^2}{\sum_{n=1}^{N} \gamma_{nk}}}, \quad \pi_k = \frac{1}{N} \sum_{n=1}^{N} \gamma_{nk}$$

| $k_1$: | $k_2$: |
|---|---|
| $\mu_1 = \frac{0.9707 \cdot 4 + 0 + 0.6225 \cdot 1}{0.9707 + 0.3775 + 0.6225} = 2.286$ | $\mu_2 = \frac{0.02931 \cdot 4 + 0 + 0.3775 \cdot 1}{0.02931 + 0.6225 + 0.3775} = 0.4807$ |
| $\sigma_1 = 1.724,$ | $\sigma_2 = 0.769,$ |
| $\pi_1 = 0.6569$ | $\pi_2 = 0.3431$ |

After one EM epoch, we'll have the following:




*Note: even though the original question's statement doesn't mention the fact that the distributions are uniformly initialized, it's needed to solve this exercise.*

4. Consider the following boolean data:

| | $y_1$ | $y_2$ | $y_3$ | $y_4$ |
|---|---|---|---|---|
| $x_1$ | 1 | 0 | 0 | 0 |
| $x_2$ | 0 | 1 | 1 | 1 |
| $x_3$ | 0 | 1 | 0 | 1 |
| $x_4$ | 0 | 0 | 1 | 1 |
| $x_5$ | 1 | 1 | 0 | 0 |

Assuming the presence of 3 clusters, variables to be conditionally independent, and the following priors:

| | $P(y_1 = 1 \mid k = c)$ | $P(y_2 = 1 \mid k = c)$ | $P(y_3 = 1 \mid k = c)$ | $P(y_4 = 1 \mid k = c)$ |
|---|---|---|---|---|
| $c = 1$ | 0.8 | 0.5 | 0.1 | 0.1 |
| $c = 2$ | 0.1 | 0.5 | 0.4 | 0.8 |
| $c = 3$ | 0.1 | 0.1 | 0.9 | 0.2 |

(a) Perform one EM iteration

(b) Verify that, after one iteration, the probability of the data increased

Given that the distributions are uniformly initialized, we can assume that the priors are equal to $\frac{1}{K} = \frac{1}{3}$, with $K$ being the number of clusters of course.

Moreover, given that all features all conditionally independent, all likelihoods can be computed as the product of the individual likelihoods:

$$P(x_n \mid k = c) = \prod_{i=1}^{4} P(x_{ni} \mid k = c), \quad x_{ni} = x_n\text{'s } y_i$$

Let's perform the **E-step**. As usual, all steps are performed for the first sample (for both clusters), while for the remaining samples only the intermediate steps' results are shown.

Regarding the first sample, we have the following likelihoods:

$$\begin{aligned} P(x_1 \mid c = k_1) &= P(y_1 = 1 \mid c = k_1) \cdot P(y_2 = 0 \mid c = k_1) \cdot P(y_3 = 0 \mid c = k_1) \cdot P(y_4 = 0 \mid c = k_1) \\ &= 0.8 \cdot (1 - 0.5) \cdot (1 - 0.1) \cdot (1 - 0.1) = 0.324 \end{aligned}$$

$$\begin{aligned} P(x_1 \mid c = k_2) &= P(y_1 = 1 \mid c = k_2) \cdot P(y_2 = 0 \mid c = k_2) \cdot P(y_3 = 0 \mid c = k_2) \cdot P(y_4 = 0 \mid c = k_2) \\ &= 0.1 \cdot (1 - 0.5) \cdot (1 - 0.4) \cdot (1 - 0.8) = 0.006 \end{aligned}$$

$$\begin{aligned} P(x_1 \mid c = k_3) &= P(y_1 = 1 \mid c = k_3) \cdot P(y_2 = 0 \mid c = k_3) \cdot P(y_3 = 0 \mid c = k_3) \cdot P(y_4 = 0 \mid c = k_3) \\ &= 0.1 \cdot (1 - 0.1) \cdot (1 - 0.9) \cdot (1 - 0.2) = 0.0072 \end{aligned}$$

Having gathered previously that all priors are equal to $\frac{1}{3}$, we can compute the (normalized) posterior probabilities as follows:

$$\begin{aligned} \gamma_{11} &= \frac{P(x_1 \mid c = k_1) \cdot P(c = k_1)}{P(x_1)} = \frac{0.324 \cdot 1/3}{0.324 \cdot 1/3 + 0.006 \cdot 1/3 + 0.0072 \cdot 1/3} = 0.9609 \\ \gamma_{12} &= \frac{P(x_1 \mid c = k_2) \cdot P(c = k_2)}{P(x_1)} = \frac{0.006 \cdot 1/3}{0.324 \cdot 1/3 + 0.006 \cdot 1/3 + 0.0072 \cdot 1/3} = 0.01779 \\ \gamma_{13} &= \frac{P(x_1 \mid c = k_3) \cdot P(c = k_3)}{P(x_1)} = \frac{0.0072 \cdot 1/3}{0.324 \cdot 1/3 + 0.006 \cdot 1/3 + 0.0072 \cdot 1/3} = 0.02135 \end{aligned}$$

Performing similar computations for the remaining samples, we obtain the following results:

$$P(x_2 \mid c = k_1) = 0.001, \quad P(x_2 \mid c = k_2) = 0.144, \quad P(x_2 \mid c = k_3) = 0.0162$$

$$P(x_3 \mid c = k_1) = 0.009, \quad P(x_3 \mid c = k_2) = 0.216, \quad P(x_3 \mid c = k_3) = 0.0018$$

$$P(x_4 \mid c = k_1) = 0.001, \quad P(x_4 \mid c = k_2) = 0.144, \quad P(x_4 \mid c = k_3) = 0.1458$$

$$P(x_5 \mid c = k_1) = 0.324, \quad P(x_5 \mid c = k_2) = 0.006, \quad P(x_5 \mid c = k_3) = 0.0008$$

$$\gamma_{21} = 0.006203, \quad \gamma_{22} = 0.8933, \quad \gamma_{23} = 0.1005$$
$$\gamma_{31} = 0.03968, \quad \gamma_{32} = 0.9524, \quad \gamma_{33} = 0.007937$$
$$\gamma_{41} = 0.003439, \quad \gamma_{42} = 0.4952, \quad \gamma_{43} = 0.5014$$
$$\gamma_{51} = 0.9794, \quad \gamma_{52} = 0.01814, \quad \gamma_{53} = 0.002418$$

Regarding the **M-step**, we'll of course want to re-estimate the parameters according to the newly found posterior probabilities. In this case, however, we're no longer working with a Gaussian distribution representing the data; our parameters here will be the likelihoods and priors. The likelihoods, in particular, will be estimated using the following formula (considering that they're all conditionally independent):

$$P(y_n \mid c = k_i) = \frac{\sum_{j=1}^{N} \gamma_{ji} x_{jn}}{\sum_{i=1}^{N} \gamma_{ji}}$$

The priors will be updated the same way as in the previous exercise.

Regarding the first cluster, let's first compute each feature's prior likelihood:

$$P(y_1 \mid c = k_1) = \frac{\sum_{j=1}^{N} \gamma_{j1} x_{j1}}{\sum_{j=1}^{N} \gamma_{j1}}$$
$$= \frac{0.9609 \cdot 1 + 0.006203 \cdot 0 + 0.03968 \cdot 0 + 0.003439 \cdot 0 + 0.9794 \cdot 1}{0.9609 + 0.006203 + 0.03968 + 0.003439 + 0.9794} = 0.9752$$

$$P(y_2 \mid c = k_1) = 0.5153, \quad P(y_3 \mid c = k_1) = 0.0048, \quad P(y_4 \mid c = k_1) = 0.02479$$

The prior probability for this cluster will be computed as follows:

$$P(c = k_1) = \frac{\sum_{j=1}^{N} \gamma_{j1}}{N} = \frac{0.9609 + 0.006203 + 0.03968 + 0.003439 + 0.9794}{5} = 0.3979$$

We're able to perform similar computations for the remaining clusters, gathering the following results:

$$P(y_1 \mid c = k_2) = 0.0151, \quad P(y_2 \mid c = k_2) = 0.784, \quad P(y_3 \mid c = k_2) = 0.5842, \quad P(y_4 \mid c = k_2) = 0.9849$$
$$P(y_1 \mid c = k_3) = 0.0375, \quad P(y_2 \mid c = k_3) = 0.175, \quad P(y_3 \mid c = k_3) = 0.9500, \quad P(y_4 \mid c = k_3) = 0.9625$$

$$P(c = k_2) = 0.4754, \quad P(c = k_3) = 0.1267$$

Regarding the second section of the exercise, we'll want to check whether, after an EM epoch, the **probability of the data increased** - that is, whether or not our distribution mixture is more likely to generate the data we're working with. Note that this is also a synonym of checking whether the **fitting probability** increasing. Considering conditionally independent variables, we're able to write this probability as the product of the probabilities of each sample:

$$P(\mathbf{X}) = \prod_{n=1}^{N} P(\mathbf{x_n})$$

Moreover, we can also write the following:

$$P(\mathbf{x_n}) = \sum_{i=1}^{K} \prod_{j=1}^{M} P(c = k_i) P(x_{nj} \mid c = k_i)$$

We have already calculated the likelihoods for each sample in the previous section; having done so, and since we also know the priors, we're able to easily compute $P(\mathbf{X})$ for before the EM epoch:

$$P(\mathbf{X}) = \left(\frac{1}{3}\right)^5 (0.324 + 0.006 + 0.0072) \times \cdots \times (0.324 + 0.006 + 0.0008) = 4.88 \cdot 10^{-6}$$

Regarding the probability after the EM epoch, we'll need the feature-wise likelihood priors (which we have already calculated):

$$\begin{aligned} P(\mathbf{X}) &= (0.3979 \cdot 0.9752 + 0.4754 \cdot 0.0151 + 0.1267 \cdot 0.0375) \times \cdots \times (\cdots + 0.1267 \cdot 0.9625) \\ &= 0.000186 \end{aligned}$$

We can see that the probability of the data increased after the EM epoch: the mixture model has, then, become better at describing the data we're working with.

*Won't be doing the fifth question here since it's basically a copy of the third but with multivariate Gaussians, which are also covered in the fourth homework.*

5. Consider the following dataset (and an Euclidean distance space):

| | $y_1$ | $y_2$ |
|---|---|---|
| $x_1$ | 2 | 10 |
| $x_2$ | 2 | 5 |
| $x_3$ | 8 | 4 |
| $x_4$ | 5 | 8 |
| $x_5$ | 7 | 5 |
| $x_6$ | 6 | 4 |
| $x_7$ | 1 | 2 |
| $x_8$ | 4 | 9 |

(a) Assuming observations $x_1$, $x_4$ and $x_7$ to be the initial seeds, identify the centroids after the first epoch using both $k$-means and $k$-medians.

(b) When is the median preferred over the mean?

For starters, it's worth noting that, as expected, the variation between $k$-means and $k$-medians is exclusively related to the way the centroids are updated: instead of updating them utilizing the mean distance between each centroid and its assigned observations, $k$-medians will update them by taking the median distance between each centroid and its assigned observations - this way, the centroids shouldn't be affected by outliers as much as if they were updated using a mean.

Let's start by assigning the samples to each cluster in the usual manner (note that, just as referenced in the question's statement, $k_1 = x_1$, $k_2 = x_4$ and $k_3 = x_7$, and that we're using the Euclidean distance):

$$k_1 = \{x_1\}, \quad k_2 = \{x_3, x_4, x_5, x_6, x_8\}, \quad k_3 = \{x_2, x_7\}$$

We can now calculate the centroids for each cluster, using both $k$-means and $k$-medians. Regarding the former:

$$\begin{aligned} \bar{x}_1 &= \frac{2}{1} = 2, & \bar{y}_1 &= \frac{10}{1} = 10 \\ \bar{x}_2 &= \frac{8+5+7+6+4}{5} = 6, & \bar{y}_2 &= \frac{4+8+5+4+9}{5} = 6 \\ \bar{x}_3 &= \frac{2+1}{2} = 1.5, & \bar{y}_3 &= \frac{5+2}{2} = 3.5 \end{aligned}$$

$$k_1' = \begin{pmatrix} 2 \\ 10 \end{pmatrix}, \quad k_2' = \begin{pmatrix} 6 \\ 6 \end{pmatrix}, \quad k_3' = \begin{pmatrix} 1.5 \\ 3.5 \end{pmatrix}$$

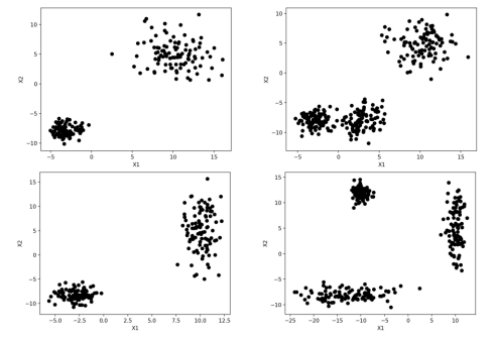
Regarding the latter:

$$\begin{aligned} m_x(1) &= 2, & m_y(1) &= 10 \\ m_x(2) &= \text{median}(8,5,7,6,4) = 6, & m_y(2) &= \text{median}(4,8,5,4,9) = 5 \\ m_x(3) &= \text{median}(2,1) = 1.5, & m_y(3) &= \text{median}(5,2) = 3.5 \end{aligned}$$

$$k_1'' = \begin{pmatrix} 2 \\ 10 \end{pmatrix}, \quad k_2'' = \begin{pmatrix} 6 \\ 5 \end{pmatrix}, \quad k_3'' = \begin{pmatrix} 1.5 \\ 3.5 \end{pmatrix}$$

(Note how the centroid remained the same, bar the $y$-coordinate of $k_2$'s centroid, which was updated from 6 to 5.)

Consider the following four scenarios of plotted data sets:



(a) For each scenario, justify whether $k$-means is suitable.

(b) Assuming EM clustering is applied to model all scenarios, what would the means and variances look like? For simplicity, assume that the covariance matrix is diagonal.

(c) When moving from numeric to ordinal data spaces, is the Hamming distance proper to handle ordinal data with high cardinality?

As mentioned in this sheet's introduction, $k$-means is a clustering algorithm that creates circle/spherical-like clusters (while EM tends creates clusters shaped like its data's distributions). This way, if we have data where the clusters are not circular/spherical, $k$-means probably won't be the most suitable algorithm to use.

(a) **Top-left**: we can clearly create a circle-like cluster for the bottom-left data points, while for the top-right ones, although not as clear, it does look like it's also possible to create a circle-like cluster for them; this way, we can say that $k$-means is suitable for this scenario (with $k = 2$).

(b) **Top-right**: in the same manner as the previous scenario, we can create a circle-like cluster for the top-right data points; however, regarding the bottom-left data points, $k$-means will only be suitable if we're willing to split the points into left and right sections (otherwise we get an ellipse-like cluster). This way, $k$-means is only suitable here if we're working with $k = 3$.

(c) **Bottom-left**: we can clearly create a circle-like cluster for the bottom-left data points, once again. However, there does not seem to be a way to avoid having an ellipse-like cluster for the right-most data points, hence $k$-means is not suitable for this scenario.

(d) **Bottom-right**: both the right-most and bottom-most data point clusters are clearly not circular/-spherical, hence $k$-means is not suitable for this scenario.

Regarding the second part of the question, the means will generally be wherever the data's distributions are centered, while the covariance matrices will be diagonal, with the diagonal values being the variances of each dimension - considering ellipse-like clusters, for example, the variance will be obviously higher in the "horizontal" (i.e the "first" in $\Sigma$) dimension, while it will be lower in the "vertical" (i.e the "second" in $\Sigma$) dimension (vice-versa for vertically elongated ellipses). Considering circle-like clusters, the variances will generally be the same in both dimensions, with more spread out data points having higher associated variances.

Finally, regarding whether the Hamming distance is suitable for ordinal data with high cardinality, the answer is no. The Hamming distance is the most suitable distance metric for data where there's no sense of "distance" between the values of each dimension (e.g. the values of each dimension are just labels, like blood types). Once we enter any type of data space where there's an intrinsic sense of "distance" between the values of a given dimension, Hamming distance ends up being less and less suitable for data with higher cardinality. Considering an example of ordinal data with low cardinality, like "High", "Medium" and "Low", the Hamming distance between "High" and "Medium" is 1, just like between "High" and "Low": while there should clearly be a bigger difference between them (which would only be accentuated with higher and higher cardinality).