**Machine Learning Exercise Sheet 12**

# Clustering

Exercise sheets consist of two parts: In-class exercises and homework. The in-class exercises will be solved and discussed during the tutorial. The homework is for you to solve at home and further engage with the lecture content. There is no grade bonus and you do not have to upload any solutions. Note that the order of some exercises might have changed compared to last year's recordings.

## In-class Exercises

### K-Medians

**Problem 1:** Consider a modified version of the $K$-means objective, where we use $L_1$ distance instead.

$$\mathcal{J}(\boldsymbol{X}, \boldsymbol{Z}, \boldsymbol{\mu}) = \sum_{i=1}^{N} \sum_{k=1}^{K} \boldsymbol{z}_{ik} ||\boldsymbol{x}_i - \boldsymbol{\mu}_k||_1$$

This variation of the algorithm is called *$K$-medians*. Derive the Lloyd's algorithm for this model.

1. Updating the cluster assignments $\boldsymbol{z}_{ik}$ is the same as for the $K$-means algorithm:

$$\boldsymbol{z}_{ik}^{new} = \begin{cases} 1 & \text{if } \; k = \arg\min_j ||\boldsymbol{x}_i - \boldsymbol{\mu}_j||_1 \\ 0 & \text{else.} \end{cases}$$

2. The updates for $\boldsymbol{\mu}_k$'s should solve

$$\boldsymbol{\mu}_k^{new} = \arg\min_{\boldsymbol{\mu}_k} \sum_{i=1}^{N} \boldsymbol{z}_{ik} ||\boldsymbol{x}_i - \boldsymbol{\mu}_k||_1$$

   The objective for each single centroid $\boldsymbol{\mu}_k$ can be rewritten as

$$\begin{aligned} \mathcal{J}(\boldsymbol{X}, \boldsymbol{Z}, \boldsymbol{\mu}_k) &= \sum_{i=1}^{N} \boldsymbol{z}_{ik} ||\boldsymbol{x}_i - \boldsymbol{\mu}_k||_1 \\ &= \sum_{i=1}^{N} \boldsymbol{z}_{ik} \sum_{d=1}^{D} |\boldsymbol{x}_{id} - \boldsymbol{\mu}_{kd}| \end{aligned}$$

   Clearly, this is a convex function of $\boldsymbol{\mu}_k$, as it is a sum of piecewise linear functions. We can actually solve for each $\boldsymbol{\mu}_{kd}$ separately, as they do not interact in the objective, by finding the roots of the derivatives.

Observe, that

$$\frac{\partial}{\partial \boldsymbol{\mu}_{kd}} |\boldsymbol{x}_{id} - \boldsymbol{\mu}_{kd}| = \begin{cases} \frac{\partial}{\partial \boldsymbol{\mu}_{kd}} (\boldsymbol{\mu}_{kd} - \boldsymbol{x}_{id}) = 1 & \text{if } \boldsymbol{\mu}_{kd} > \boldsymbol{x}_{id} \\ \frac{\partial}{\partial \boldsymbol{\mu}_{kd}} (\boldsymbol{x}_{id} - \boldsymbol{\mu}_{kd}) = -1 & \text{if } \boldsymbol{\mu}_{kd} < \boldsymbol{x}_{id} \\ 0 & \text{if } \boldsymbol{\mu}_{kd} = \boldsymbol{x}_{id}. \end{cases}$$

(Note: actually the absolute value function is not differentiable at 0, so the derivative is undefined. A rigorous treatment of this problem would require us to use subgradients (see `https://web.stanford.edu/class/ee364b/lectures/subgradients_notes.pdf`), but just "pretending" that the gradient is 0 suffices for our purpose.)

Hence, the derivative of the entire objective is

$$\begin{aligned} \frac{\partial}{\partial \boldsymbol{\mu}_{kd}} \mathcal{J}(\boldsymbol{X}, \boldsymbol{Z}, \boldsymbol{\mu}) &= \sum_{i=1}^{N} \boldsymbol{z}_{ik} |\boldsymbol{x}_{id} - \boldsymbol{\mu}_{kd}| \\ &= \sum_{i=1}^{N} \boldsymbol{z}_{ik} \mathbb{I}[\boldsymbol{\mu}_{kd} > \boldsymbol{x}_{id}] - \sum_{i=1}^{N} \boldsymbol{z}_{ik} \mathbb{I}[\boldsymbol{\mu}_{kd} < \boldsymbol{x}_{id}] \stackrel{!}{=} 0 \end{aligned}$$

The first sum represents "number of points $\boldsymbol{x}_i$ assigned to class $k$, such that $\boldsymbol{x}_{id} < \boldsymbol{\mu}_{kd}$". Each of these sums represents the number of points in class $k$, that are located to the left (right) of the given value of $\boldsymbol{\mu}_{kd}$. Because we want to set the gradient to zero, we are looking for such a $\boldsymbol{\mu}_{kd}$, that along the axis $d$ exactly $N_k/2$ points are to left of it, and another $N_k/2$ points are to the right (where $N_k = \sum_{i=1}^{N} \boldsymbol{z}_{ik}$). This is exactly the definition of a *median*.

Therefore, the optimal update is given as

$$\boldsymbol{\mu}_{kd} = \text{median}\,\{\boldsymbol{x}_{id} \text{ such that } \boldsymbol{z}_{ik} = 1\}$$

## Gaussian Mixture Model

**Problem 2:** Derive the E-step update for the Gaussian mixture model.

In the E-step we have to evaluate the posterior distribution over the latent variables given the current parameters, i.e. $\gamma_t(\boldsymbol{Z})$. Because GMMs assume that the latent variables are independent, $\gamma_t(\boldsymbol{Z}) = \prod_{i=1}^{N} \gamma_t(\boldsymbol{z}_i)$ and it is enough to derive the E-step for a single data point. The update rule follows

directly from Bayes' theorem.

$$\begin{aligned}
\gamma_t(\boldsymbol{z}_i = k) &= \mathrm{p}(\boldsymbol{z}_i = k \mid \boldsymbol{x}_i, \boldsymbol{\pi}^{(t)}, \boldsymbol{\mu}^{(t)}, \boldsymbol{\Sigma}^{(t)}) \\
&= \frac{\mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z}_i = k, \boldsymbol{\mu}^{(t)}, \boldsymbol{\Sigma}^{(t)})\ \mathrm{p}(\boldsymbol{z}_i = k \mid \boldsymbol{\pi}^{(t)})}{\mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{\pi}^{(t)}, \boldsymbol{\mu}^{(t)}, \boldsymbol{\Sigma}^{(t)})} \\
&= \frac{\mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z}_i = k, \boldsymbol{\mu}^{(t)}, \boldsymbol{\Sigma}^{(t)})\ \mathrm{p}(\boldsymbol{z}_i = k \mid \boldsymbol{\pi}^{(t)})}{\sum_{j=1}^{K} \mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z}_i = j, \boldsymbol{\pi}^{(t)}, \boldsymbol{\mu}^{(t)}, \boldsymbol{\Sigma}^{(t)})\ \mathrm{p}(\boldsymbol{z}_i = j \mid \boldsymbol{\pi}^{(t)})} \\
&= \frac{\boldsymbol{\pi}_k^{(t)} \mathcal{N}\left(\boldsymbol{x}_i \mid \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)}\right)}{\sum_{j=1}^{K} \boldsymbol{\pi}_j^{(t)} \mathcal{N}\left(\boldsymbol{x}_i \mid \boldsymbol{\mu}_j^{(t)}, \boldsymbol{\Sigma}_j^{(t)}\right)}
\end{aligned}$$

**Problem 3:** Derive the M-step update for the Gaussian mixture model.

In the M-step we maximize $\mathcal{L} = \mathbb{E}_{\boldsymbol{Z} \sim \gamma_t(\boldsymbol{Z})} [\log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})]$ with respect to $\boldsymbol{\pi}$, $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$. When we plug in the definition of the expected value and expand, we get

$$\begin{aligned}
\mathcal{L} &= \sum_{i=1}^{N} \sum_{k=1}^{K} \gamma_t(\boldsymbol{z}_i = k)\ \log \mathrm{p}(\boldsymbol{x}_i, \boldsymbol{z}_i = k \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) \\
&= \sum_{i=1}^{N} \sum_{k=1}^{K} \gamma_t(\boldsymbol{z}_i = k)\ \log \mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z}_i = k, \boldsymbol{\mu}, \boldsymbol{\Sigma})\ \mathrm{p}(\boldsymbol{z}_i = k \mid \boldsymbol{\pi}) \\
&= \underbrace{\sum_{i=1}^{N} \sum_{k=1}^{K} \gamma_t(\boldsymbol{z}_i = k)\ \log \mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z}_i = k, \boldsymbol{\mu}, \boldsymbol{\Sigma})}_{\mathcal{L}_{\boldsymbol{x}}} + \underbrace{\sum_{i=1}^{N} \sum_{k=1}^{K} \gamma_t(\boldsymbol{z}_i = k)\ \log \mathrm{p}(\boldsymbol{z}_i = k \mid \boldsymbol{\pi})}_{\mathcal{L}_{\boldsymbol{z}}}
\end{aligned}$$

where $\mathcal{L}_{\boldsymbol{z}}$ only depends on $\boldsymbol{\pi}$ and $\mathcal{L}_{\boldsymbol{x}}$ only depends on $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$. To find the optimal $\boldsymbol{\pi}$, we need to maximize $\mathcal{L}_{\boldsymbol{z}}$ with respect to $\boldsymbol{\pi}$. Since $\boldsymbol{\pi}$ has several constraints placed on it, we will have to solve the following convex optimization problem.

$$\begin{aligned}
&\text{maximize} && \mathcal{L}_{\boldsymbol{z}} \\
&\text{subject to} && \sum_{k=1}^{K} \boldsymbol{\pi}_k - 1 = 0
\end{aligned}$$

Before we formulate the Lagrangian, we simplify $\mathcal{L}_{\boldsymbol{z}}$ as

$$\mathcal{L}_{\boldsymbol{z}} = \sum_{i=1}^{N} \sum_{k=1}^{K} \gamma_t(\boldsymbol{z}_i = k)\ \log \mathrm{p}(\boldsymbol{z}_i = k \mid \boldsymbol{\pi}) = \sum_{k=1}^{K} N_k \log \boldsymbol{\pi}_k$$

where $N_k = \sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_i = k)$ is the size of the $k$-th cluster. The Lagrangian is given by

$$f(\boldsymbol{\pi}, \lambda) = \sum_{k=1}^{K} N_k \log \boldsymbol{\pi}_k + \lambda \left(1 - \sum_{k=1}^{K} \boldsymbol{\pi}_k\right)$$

and it has its maximum in $\boldsymbol{\pi}$ at

$$\frac{\partial f}{\partial \boldsymbol{\pi}_k} = \frac{N_k}{\boldsymbol{\pi}_k} - \lambda \stackrel{!}{=} 0 \Leftrightarrow \boldsymbol{\pi}_k = \frac{N_k}{\lambda}$$

because $f$ is concave as a function of $\boldsymbol{\pi}$. This gives us the dual function as

$$g(\lambda) = \max_{\boldsymbol{\pi}} f(\boldsymbol{\pi}, \lambda) = f\left(\left(\frac{N_1}{\lambda}, \ldots, \frac{N_K}{\lambda}\right), \lambda\right) = \sum_{k=1}^{K} N_k \log \frac{N_k}{\lambda} + \lambda - N.$$

When $f$ is concave, the dual is convex and we find the minimum of $g$ at

$$\frac{\partial g}{\partial \lambda} = \sum_{k=1}^{K} N_k \frac{\lambda}{N_k}\left(-\frac{N_k}{\lambda^2}\right) + 1 = 1 - \frac{N}{\lambda} \stackrel{!}{=} 0 \Leftrightarrow \lambda = N.$$

This means that the M-step for $\boldsymbol{\pi}$ is $\boldsymbol{\pi}_k^{(t+1)} = \frac{N_k}{N}$.

To find the M-step rules for $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$, we need to examine $\mathcal{L}_{\boldsymbol{x}}$.

$$\begin{aligned}
\mathcal{L}_{\boldsymbol{x}} &= \sum_{i=1}^{N}\sum_{k=1}^{K} \gamma_t(\boldsymbol{z}_i = k)\, \log\left(\mathcal{N}\left(\boldsymbol{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)\right) \\
&= -\frac{1}{2}\sum_{i=1}^{N}\sum_{k=1}^{K} \gamma_t(\boldsymbol{z}_i = k)\left((\boldsymbol{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x}_i - \boldsymbol{\mu}_k) + D\log(2\pi) + \log\det\boldsymbol{\Sigma}_k\right).
\end{aligned}$$

where $D$ is the feature dimension. We can take the derivative with respect to $\boldsymbol{\mu}_k$

$$\frac{\partial \mathcal{L}_{\boldsymbol{x}}}{\partial \boldsymbol{\mu}_k} = -\frac{1}{2}\sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_i = k)\left((-1)\cdot\left(\boldsymbol{\Sigma}_k^{-1} + \boldsymbol{\Sigma}_k^{-T}\right)(\boldsymbol{x}_i - \boldsymbol{\mu}_k)\right) = \sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_i = k)\left(\boldsymbol{\Sigma}_k^{-1}(\boldsymbol{x}_i - \boldsymbol{\mu}_k)\right)$$

and then find its root

$$\frac{\partial \mathcal{L}_{\boldsymbol{x}}}{\partial \boldsymbol{\mu}_k} = 0 \Leftrightarrow \sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_i = k)\boldsymbol{\Sigma}_k^{-1}\boldsymbol{x}_i = N_k\boldsymbol{\Sigma}_k^{-1}\boldsymbol{\mu}_k \Leftrightarrow \boldsymbol{\mu}_k = \frac{1}{N_k}\sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_i = k)\boldsymbol{x}_i$$

which gives us the update rule

$$\boldsymbol{\mu}_k^{(t+1)} = \frac{1}{N_k}\sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_i = k)\boldsymbol{x}_i.$$

It remains to find the M-step for $\boldsymbol{\Sigma}$. Again we proceed by taking the derivative with respect to $\boldsymbol{\Sigma}_k$

$$\begin{aligned}
\frac{\partial \mathcal{L}_{\boldsymbol{x}}}{\partial \boldsymbol{\Sigma}_k} &= -\frac{1}{2}\sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_i = k)\left[-\boldsymbol{\Sigma}_k^{-T}(\boldsymbol{x}_i - \boldsymbol{\mu}_k)(\boldsymbol{x}_i - \boldsymbol{\mu}_k)^T\boldsymbol{\Sigma}_k^{-T} + \boldsymbol{\Sigma}_k^{-T}\right] \\
&= -\frac{1}{2}\left(N_k I_D - \sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_i = k)\left[\boldsymbol{\Sigma}_k^{-T}(\boldsymbol{x}_i - \boldsymbol{\mu}_k)(\boldsymbol{x}_i - \boldsymbol{\mu}_k)^T\right]\right)\boldsymbol{\Sigma}_k^{-T}
\end{aligned}$$

where $I_D$ is the $D$-dimensional identity matrix. We finish by finding its root

$$\frac{\partial \mathcal{L}_{\boldsymbol{x}}}{\partial \boldsymbol{\Sigma}_k} = 0 \Leftrightarrow N_k I_D = \boldsymbol{\Sigma}_k^{-T} \sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_i = k)(\boldsymbol{x}_i - \boldsymbol{\mu}_k)(\boldsymbol{x}_i - \boldsymbol{\mu}_k)^T$$

which produces the final update rule

$$\boldsymbol{\Sigma}_k^{(t+1)} = \frac{1}{N_k} \sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_i = k)(\boldsymbol{x}_i - \boldsymbol{\mu}_k)(\boldsymbol{x}_i - \boldsymbol{\mu}_k)^T.$$

In this exercise we have used the following matrix calculus rules which you can look up in the matrix cookbook.

$$\frac{\partial \boldsymbol{a}^T \boldsymbol{X} \boldsymbol{a}}{\partial \boldsymbol{a}} = \left(\boldsymbol{X} + \boldsymbol{X}^T\right) \boldsymbol{a}^T \qquad \frac{\partial \boldsymbol{a}^T \boldsymbol{X}^{-1} \boldsymbol{b}}{\partial \boldsymbol{X}} = -\boldsymbol{X}^{-T} \boldsymbol{b} \boldsymbol{a}^T \boldsymbol{X}^{-T} \qquad \frac{\partial \log |\det \boldsymbol{X}|}{\partial \boldsymbol{X}} = \boldsymbol{X}^{-T}$$

## Expectation Maximization Algorithm

**Problem 4:** Consider a mixture model where the components are given by independent Bernoulli variables. This is useful when modelling, e.g., binary images, where each of the $D$ dimensions of the image $\boldsymbol{x}$ corresponds to a different pixel that is either black or white. More formally, we have

$$\mathrm{p}(\boldsymbol{x} \mid \boldsymbol{z} = k) = \prod_{d=1}^{D} \boldsymbol{\theta}_{kd}^{x_d} (1 - \boldsymbol{\theta}_{kd})^{1 - x_d}.$$

That is, for a given mixture index $\boldsymbol{z} = k$, we have a product of independent Bernoullis, where $\boldsymbol{\theta}_{kd}$ denotes the Bernoulli parameter for component $k$ at pixel $d$.

Derive the EM algorithm for the parameters $\boldsymbol{\theta} = \{\boldsymbol{\theta}_{kd} \mid k = 1, \ldots, K, d = 1, \ldots, D\}$ of a mixture of Bernoullis.

Assume here for simplicity, that the distribution of components $\mathrm{p}(\boldsymbol{z})$ is uniform: $\mathrm{p}(\boldsymbol{z}) = \prod_{k=1}^{K} \boldsymbol{\pi}_k^{z_k} = \prod_{k=1}^{K} \left(\frac{1}{K}\right)^{z_k}$.

Due to the uniform prior on $\boldsymbol{z}_i$, the $\mathrm{p}(\boldsymbol{z}_i)$ cancel and the responsibilities compute as

$$\gamma_t(\boldsymbol{z}_i = k) = \frac{\mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z}_i = k, \boldsymbol{\theta}) \cdot \mathrm{p}(\boldsymbol{z}_i = k)}{\sum_{l=1}^{K} \mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z}_i = l, \boldsymbol{\theta}) \cdot \mathrm{p}(\boldsymbol{z}_i = l)} = \frac{\mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z}_i = k, \boldsymbol{\theta})}{\sum_{l=1}^{K} \mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z}_i = l, \boldsymbol{\theta})}$$

which constitues the E-step.

It remains to derive the M-step. Similiar to mixture of Gaussians:

$$\begin{aligned}\mathop{\mathbb{E}}_{\boldsymbol{z}\sim\gamma_t(\boldsymbol{z})}[\log \mathrm{p}(\boldsymbol{X},\boldsymbol{z}\mid\boldsymbol{\theta}^{(t)})] &= \sum_{i=1}^{N}\sum_{k=1}^{K}\gamma_t(\boldsymbol{z}_i=k)\log\left(\frac{1}{K}\prod_{d=1}^{D}\boldsymbol{\theta}_{kd}^{\boldsymbol{x}_{id}}(1-\boldsymbol{\theta}_{kd})^{1-\boldsymbol{x}_{id}}\right)\\ &= C+\sum_{i=1}^{N}\underbrace{\sum_{k=1}^{K}\gamma_t(\boldsymbol{z}_i=k)\sum_{d=1}^{D}\left(\boldsymbol{x}_{id}\log\boldsymbol{\theta}_{kd}+(1-\boldsymbol{x}_{id})\log(1-\boldsymbol{\theta}_{kd})\right)}_{=:\mathcal{L}_i}\end{aligned}$$

The constant $C$ collects all terms independent of $\boldsymbol{\theta}$ and hence irrelevant for further optimization.

We now need to take derivatives with respect to $\boldsymbol{\theta}$.

$$\begin{aligned}\frac{\partial\mathcal{L}_i}{\partial\boldsymbol{\theta}_{k',d'}} &= \sum_{k=1}^{K}\gamma_t(\boldsymbol{z}_i=k)\sum_{d=1}^{D}\left(\boldsymbol{x}_{id}\frac{\partial\log\boldsymbol{\theta}_{kd}}{\partial\boldsymbol{\theta}_{k',d'}}+(1-\boldsymbol{x}_{id})\frac{\partial\log(1-\boldsymbol{\theta}_{kd})}{\partial\boldsymbol{\theta}_{k',d'}}\right)\\ &= \gamma_t(\boldsymbol{z}_i=k)\left(\frac{\boldsymbol{x}_{id}}{\boldsymbol{\theta}_{k',d'}}-\frac{1-\boldsymbol{x}_{id}}{1-\boldsymbol{\theta}_{k',d'}}\right)\end{aligned}$$

We observe that the $\boldsymbol{\theta}_{kd}$ do not interact, so their optimal values are independent from each other and we can handle them individually.

$$\frac{\partial\ \mathbb{E}_{\boldsymbol{z}\sim\gamma_t(\boldsymbol{z})}[\log \mathrm{p}(\boldsymbol{X},\boldsymbol{z}\mid\boldsymbol{\theta})]}{\partial\boldsymbol{\theta}_{kd}} = \sum_{i=1}^{N}\frac{\partial\mathcal{L}_i}{\partial\boldsymbol{\theta}_{kd}} = \sum_{i=1}^{N}\gamma_t(\boldsymbol{z}_i=k)\left(\frac{\boldsymbol{x}_{id}}{\boldsymbol{\theta}_{kd}}-\frac{1-\boldsymbol{x}_{id}}{1-\boldsymbol{\theta}_{kd}}\right)$$

By finding the roots $\frac{\partial\ \mathbb{E}_{\boldsymbol{z}\sim\gamma_t(\boldsymbol{z})}[\log \mathrm{p}(\boldsymbol{X},\boldsymbol{z}|\boldsymbol{\theta})]}{\partial\boldsymbol{\theta}_{kd}}=0$, we obtain the optimal update in a similar fashion as in the standard Bernoulli MLE:

$$\boldsymbol{\theta}_{kd} = \frac{\sum_{i=1}^{N}\gamma_t(\boldsymbol{z}_i=k)\,\boldsymbol{x}_{id}}{\sum_{i=1}^{N}\gamma_t(\boldsymbol{z}_i=k)}$$

# Homework

## Gaussian Mixture Model

**Problem 5:** Consider a mixture of $K$ Gaussians

$$\mathrm{p}(\boldsymbol{x}) = \sum_k \boldsymbol{\pi}_k \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).$$

Derive the expected value $\mathbb{E}[\boldsymbol{x}]$ and the covariance $\mathrm{Cov}[\boldsymbol{x}]$.

*Hint: it is helpful to remember the identity* $\mathrm{Cov}[\boldsymbol{x}] = \mathbb{E}[\boldsymbol{x}\boldsymbol{x}^T] - \mathbb{E}[\boldsymbol{x}]\,\mathbb{E}[\boldsymbol{x}]^T$.

For $\mathbb{E}[\boldsymbol{x}]$ we use the law of iterated expectations.

$$\mathbb{E}[\boldsymbol{x}] = \mathop{\mathbb{E}}_{\boldsymbol{z}}\Big[\mathop{\mathbb{E}}_{\boldsymbol{x}}[\boldsymbol{x} \mid \boldsymbol{z}]\Big] = \sum_{k=1}^{K} \boldsymbol{\pi}_k\, \mathbb{E}[\boldsymbol{x} \mid \boldsymbol{z} = k] = \sum_{k=1}^{K} \boldsymbol{\pi}_k \boldsymbol{\mu}_k$$

For covariance, we first compute $\mathbb{E}[\boldsymbol{x}\boldsymbol{x}^T]$ again using the law of iterated expectations

$$\begin{aligned}
\mathbb{E}[\boldsymbol{x}\boldsymbol{x}^T] &= \mathop{\mathbb{E}}_{\boldsymbol{z}}\Big[\mathop{\mathbb{E}}_{\boldsymbol{x}}[\boldsymbol{x}\boldsymbol{x}^T \mid \boldsymbol{z}]\Big] \\
&= \sum_{k=1}^{K} \boldsymbol{\pi}_k\, \mathbb{E}[\boldsymbol{x}\boldsymbol{x}^T \mid \boldsymbol{z} = k] \\
&= \sum_{k=1}^{K} \boldsymbol{\pi}_k \left(\mathrm{Cov}[\boldsymbol{x} \mid \boldsymbol{z} = k] + \mathbb{E}[\boldsymbol{x} \mid \boldsymbol{z} = k]\,\mathbb{E}[\boldsymbol{x} \mid \boldsymbol{z} = k]^T\right) \\
&= \sum_{k=1}^{K} \boldsymbol{\pi}_k \left(\boldsymbol{\Sigma}_k + \boldsymbol{\mu}_k \boldsymbol{\mu}_k^T\right)
\end{aligned}$$

and thus

$$\mathrm{Cov}[\boldsymbol{x}] = \mathbb{E}[\boldsymbol{x}\boldsymbol{x}^T] - \mathbb{E}[\boldsymbol{x}]\,\mathbb{E}[\boldsymbol{x}]^T = \sum_{k=1}^{K} \boldsymbol{\pi}_k(\boldsymbol{\Sigma}_k + \boldsymbol{\mu}_k\boldsymbol{\mu}_k^T) - \sum_{k=1}^{K}\sum_{j=1}^{K} \boldsymbol{\pi}_k\boldsymbol{\pi}_j\boldsymbol{\mu}_k\boldsymbol{\mu}_j^T$$

**Problem 6:** Consider a mixture of $K$ isotropic Gaussians, all with the same *known* covariances $\boldsymbol{\Sigma}_k = \sigma^2\boldsymbol{I}$.

Derive the EM algorithm for the case when $\sigma^2 \to 0$, and show that it's equivalent to Lloyd's algorithm for $K$-means.

We consider a GMM with identical, isotropic covariances. In that case, the responsibilities take the following form:

$$\mathrm{p}(\boldsymbol{z}_{ik} = 1 \mid \boldsymbol{x}_i, \boldsymbol{\theta}) = \frac{\mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z}_{ik} = 1, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\,\mathrm{p}(\boldsymbol{z}_{ik} = 1 \mid \boldsymbol{\pi}_k)}{\int \mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z})\,\mathrm{p}(\boldsymbol{z})\,\mathrm{d}\boldsymbol{z}} \tag{1}$$

$$= \frac{\boldsymbol{\pi}_k \mathcal{N}(\boldsymbol{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{l=1}^{K} \boldsymbol{\pi}_l \mathcal{N}(\boldsymbol{x}_i \mid \boldsymbol{\mu}_l, \boldsymbol{\Sigma}_l)} \tag{2}$$

$$= \frac{\boldsymbol{\pi}_k \exp\left(\frac{-||\boldsymbol{x}_i - \boldsymbol{\mu}_k||^2}{2\sigma^2}\right)}{\sum_l \boldsymbol{\pi}_l \exp\left(\frac{-||\boldsymbol{x}_i - \boldsymbol{\mu}_l||^2}{2\sigma^2}\right)} \tag{3}$$

$$= \frac{1}{\sum_l \frac{\boldsymbol{\pi}_l}{\boldsymbol{\pi}_k} \exp\left(\frac{-||\boldsymbol{x}_i - \boldsymbol{\mu}_l||^2 + ||\boldsymbol{x}_i - \boldsymbol{\mu}_k||^2}{2\sigma^2}\right)} \tag{4}$$

If $\boldsymbol{\mu}_k$ denotes the center that is closest to $\boldsymbol{x}_i$, then

$$\frac{-||\boldsymbol{x}_i - \boldsymbol{\mu}_l||^2 + ||\boldsymbol{x}_i - \boldsymbol{\mu}_k||^2}{2\sigma^2} \leq 0$$

for all $l$, with equality if and only if $k = l$. For $\sigma \to 0$, the denominator of Equation 4 converges to 1: If $k = l$, the argument of $\exp(\cdot)$ is exactly zero, while for $k \neq l$ we are exponentiating increasingly negative arguments.

If $\boldsymbol{\mu}_k$ denotes a center that is *not* closest to $\boldsymbol{x}_i$, there is at least one $l \neq k$ for which

$$0 < \frac{-||\boldsymbol{x}_i - \boldsymbol{\mu}_l||^2 + ||\boldsymbol{x}_i - \boldsymbol{\mu}_k||^2}{2\sigma^2} \longrightarrow \infty \qquad \text{as } \sigma \to 0.$$

Consequently, the denominator of Equation 4 diverges to $\infty$.

This means that the responsibilities degenerate to a hard one-hot assignment of the data point $\boldsymbol{x}_i$ to the component closest to $\boldsymbol{x}_i$. This coincides with step 1 of Lloyd's algorithm.

Inserting one-hot responsibilities into the general GMM M-step immediately yields step 2 in Lloyd's algorithm. Notice that we do not learn covariances, they are assumed fixed. Moreover, we don't have to worry about $\boldsymbol{\pi}_k$s, because they are irrelevant as the term $\boldsymbol{\pi}_l / \boldsymbol{\pi}_k$ always gets overshadowed by the $\exp(\cdot)$ next to it.

We can conclude that Lloyd's algorithm for $K$-Means is a special case of the more general EM algorithm for GMM.

**Problem 7:** Consider two random variables $\boldsymbol{x} \in \mathbb{R}^D$ and $\boldsymbol{y} \in \mathbb{R}^D$ distributed according to two different Gaussian mixture models with $\boldsymbol{\theta}^x = \{\boldsymbol{\pi}^x, \boldsymbol{\mu}^x, \boldsymbol{\Sigma}^x\}$ and $\boldsymbol{\theta}^y = \{\boldsymbol{\pi}^y, \boldsymbol{\mu}^y, \boldsymbol{\Sigma}^y\}$, i.e.

$$\mathrm{p}(\boldsymbol{x} \mid \boldsymbol{\theta}^x) = \sum_{k=1}^{K_x} \boldsymbol{\pi}_k^x \, \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_k^x, \boldsymbol{\Sigma}_k^x),$$
$$\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{\theta}^y) = \sum_{l=1}^{K_y} \boldsymbol{\pi}_l^y \, \mathcal{N}(\boldsymbol{y} \mid \boldsymbol{\mu}_l^y, \boldsymbol{\Sigma}_l^y),$$

and the random variable $\boldsymbol{z} = \boldsymbol{x} + \boldsymbol{y}$.

a) Describe a generative process (process of drawing samples) for $\boldsymbol{z}$.

b) Explain in a few sentences why $\mathrm{p}(\boldsymbol{z} \mid \boldsymbol{\theta}^x, \boldsymbol{\theta}^y)$ is again a mixture of Gaussians.

c) State the probability density function $\mathrm{p}(\boldsymbol{z} \mid \boldsymbol{\theta}^x, \boldsymbol{\theta}^y)$ of $\boldsymbol{z}$.

a) Draw a sample $\boldsymbol{x}$ from $\mathrm{p}(\boldsymbol{x} \mid \boldsymbol{\theta}^x)$ with the usual GMM sampling method and the same for $\boldsymbol{y}$ from $\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{\theta}^y)$. Now add them together to get $\boldsymbol{z} = \boldsymbol{x} + \boldsymbol{y}$.

b) Let $\boldsymbol{x}$ be drawn from the component $k$ of $\mathrm{p}(\boldsymbol{x} \mid \boldsymbol{\theta}^x)$ and $\boldsymbol{y}$ be drawn from the component $l$ of $\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{\theta}^y)$. Then $\boldsymbol{z}$ is the sum of two normally distributed random variables $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}_k^x, \boldsymbol{\Sigma}_k^x)$ and $\boldsymbol{y} \sim \mathcal{N}(\boldsymbol{\mu}_l^y, \boldsymbol{\Sigma}_l^y)$. Therefore, it also follows a normal distribution $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{\mu}_k^x + \boldsymbol{\mu}_l^y, \boldsymbol{\Sigma}_k^x + \boldsymbol{\Sigma}_l^y)$. There are $K_x \cdot K_y$ such possible $(k, l)$ combinations, each having probability $\boldsymbol{\pi}_k^x \boldsymbol{\pi}_l^y$ respectively.

That is, $\mathrm{p}(\boldsymbol{z} \mid \boldsymbol{\theta}^x, \boldsymbol{\theta}^y)$ is a mixture of $K_x K_y$ Gaussians.

c) It follows from the argument in b) that the probability density function of $\boldsymbol{z}$ is

$$\mathrm{p}(\boldsymbol{z} \mid \boldsymbol{\theta}^x, \boldsymbol{\theta}^y) = \sum_{k=1}^{K_x} \sum_{l=1}^{K_y} \boldsymbol{\pi}_k^x \boldsymbol{\pi}_l^y \, \mathcal{N}(\boldsymbol{z} \mid \boldsymbol{\mu}_k^x + \boldsymbol{\mu}_l^y, \boldsymbol{\Sigma}_k^x + \boldsymbol{\Sigma}_l^y).$$

**Problem 8:**

a) Given is the dataset displayed in the figure below. Apply the K-means algorithm to this data using $K = 2$ and using the circled points as initial centroids.

What are the clusters after K-Means converges? Draw your solution in the figure above, i.e. mark the location of the centroids with $\times$'s and show the clusters by drawing two bounding boxes around the points assigned to each cluster.

How many iterations did it take for K-Means to converge in the above problem?

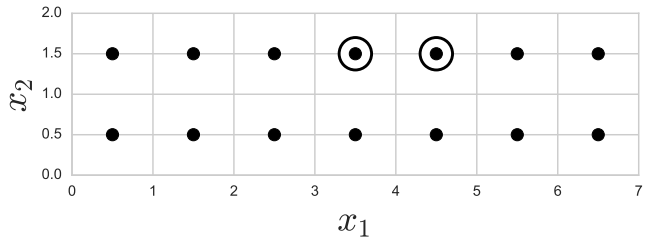
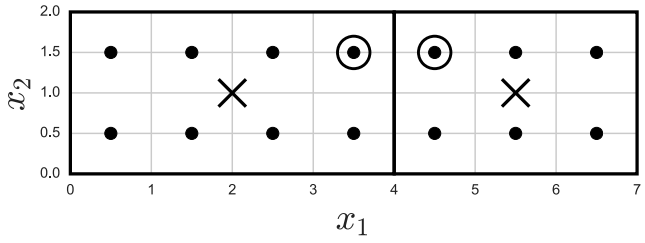



Figure 1: K-Means Dataset




K-means takes one iteration to converge.

b) Provide a different initialization, for which the algorithm will take **more** iterations to converge to the **same** solution. Make sure that your initialization does not lead to ties. Circle the initial centroids in the figure below.

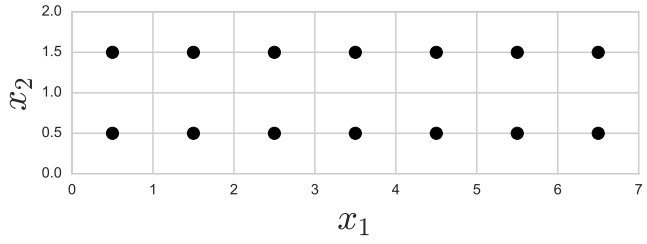
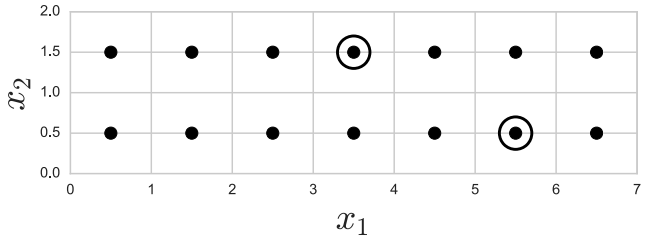



Figure 2: Provide your initialization




**Problem 9:** Download the notebook `exercise_12_clustering.ipynb` from Moodle. Fill in the missing code and run the notebook.