Machine Learning Exercise Sheet 12

Clustering

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.

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

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

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

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

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*.

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Therefore, the optimal update is given as

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

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Gaussian Mixture Model

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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 $\mathcal{L} = \mathbb{E}_{\boldsymbol{Z}\sim\gamma_t(\boldsymbol{Z})}\left[\log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})\right]$ 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.

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

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

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

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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

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

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

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

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 $\boldsymbol{\theta} = \{\boldsymbol{\theta}_{kd} \mid k = 1, \dots, K, d = 1, \dots, D\}$ 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

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

which constitues the E-step.

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

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

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:

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

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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.

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

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

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

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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:

$$
\begin{aligned}
\mathrm{p}(\boldsymbol{z}_{ik} = 1 \mid \boldsymbol{x}_i, \boldsymbol{\theta}) &= \frac{\mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z}_{ik} = 1, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\, \mathrm{p}(\boldsymbol{z}_{ik} = 1 \mid \boldsymbol{\pi}_k)}{\int \mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z})\, \mathrm{p}(\boldsymbol{z})\, \mathrm{d}\boldsymbol{z}} && (1)\\
&= \frac{\boldsymbol{\pi}_k \mathcal{N}(\boldsymbol{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{l=1}^{K} \boldsymbol{\pi}_l \mathcal{N}(\boldsymbol{x}_i \mid \boldsymbol{\mu}_l, \boldsymbol{\Sigma}_l)} && (2)\\
&= \frac{\boldsymbol{\pi}_k \exp\left(\frac{-||\boldsymbol{x}_i - \boldsymbol{\mu}_k||^2}{2\sigma^2}\right)}{\sum_l \boldsymbol{\pi}_l \exp\left(\frac{-||\boldsymbol{x}_i - \boldsymbol{\mu}_l||^2}{2\sigma^2}\right)} && (3)\\
&= \frac{1}{\sum_l \frac{\boldsymbol{\pi}_l}{\boldsymbol{\pi}_k} \exp\left(\frac{-||\boldsymbol{x}_i - \boldsymbol{\mu}_l||^2 + ||\boldsymbol{x}_i - \boldsymbol{\mu}_k||^2}{2\sigma^2}\right)} && (4)
\end{aligned}
$$

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

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

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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.

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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

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

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Consequently, the denominator of Equation 4 diverges to ∞.

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 $\boldsymbol{z} = \boldsymbol{x} + \boldsymbol{y}$.

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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.

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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

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

Problem 8: Download the notebook `exercise_12_clustering.ipynb` from Moodle. Fill in the missing code and run the notebook. Convert the evaluated notebook to PDF and append it to your other solutions before uploading.