Expectation Maximization and Gaussian Mixture Models

To be completed individually or in groups of two people. **Please be sure that matriculation numbers are clearly included at the top of your submission.** Submissions can be handwritten or in LaTeX formatting, but hard-to-read handwritten submissions will not be graded. Please submit via Ilias. Submissions should be a single PDF document (note that Jupyter notebooks can and should also be downloaded as PDFs, and not submitted as .ipynb files). Each question will be graded "pass" (full points) or "fail" (no points). We award 0.5 bonus points for the exam for each theory and practical question solved. You must complete 50% of all exercises to enter the final exam.

1. **EXAMple Question — Expectation Maximization (EM)**

   Let's say we want to find the maximum likelihood estimate for a model: $\arg\max_\theta \log p(x|\theta)$.

   We can use EM, if introducing a latent variable z, makes maximizing the complete-data log-likelihood $\log p(x, z|\theta)$ possible. EM allows us to maximize the marginal log-likelihood $\log p(x|\theta)$ by iteratively computing:

   1. E-step: $p(z|x, \theta_{old})$ to derive $\mathbb{E}_{p(z|x,\theta_{old})} \log p(x, z|\theta)$
   2. M-step: $\arg\max_\theta \mathbb{E}_{p(z|x,\theta_{old})} \log p(x, z|\theta)$.

   It is however, non-obvious how this scheme maximizes the marginal log-likelihood. Here, you will show that repeatedly running these two steps guarantees that one monotonically increases $\log p(x|\theta)$. To make the argument in part (c), you will derive the required tools in parts (a) and (b).

   (a) Show that for any distribution $q(z)$ over latent variables, $\mathcal{L}(q) = \mathbb{E}_q \left[\log \frac{p(x,z|\theta)}{q(z)}\right]$ lower bounds the marginal log-likelihood.
   Hint: You can use Jensen's inequality for that.
   ***Jensen's inequality**: Let ϕ be a convex function and X a random variable, then:*

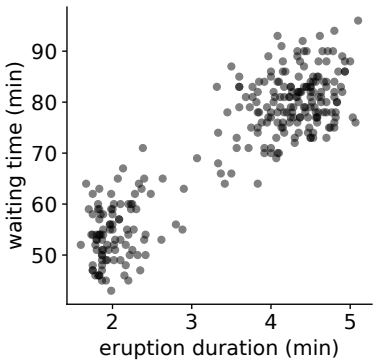
   $$\phi(\mathbb{E}[X]) \leq \mathbb{E}[\phi(X)]$$

   (b) We can write the marginal log-likelihood as the sum of the previously derived lower bound and an additional term : $\log p(x|\theta) = \mathcal{L}(q) + ...$. Derive the additional term.
   Hint: Start by splitting $\mathcal{L}(q)$ into the terms depending on z and the terms not depending on z. Note that the answer will take the form of the KL-divergence D_{KL}.

   (c) Now argue that EM monotonically increases the marginal log-likelihood. Think about what happens to $\mathcal{L}$, as well as to the D_{KL}, during the E and M steps. Your answer should only require a few sentences.
   Hint: The KL divergence satisfies $D_{KL}(q(z)||p(z)) = 0 \iff q = p$.

2. **Theory Question — EM for Gaussian Mixtures**

   The plot below shows a classic dataset that you already saw in lecture 15: the interval between eruptions of the *Old Faithful* geyser in Yellowstone National Park in the US, plotted against the duration of the eruption following the waiting time. Datasets like this, which show a "cluster" structure, are often modelled with *Gaussian mixture models* (GMMs): each datum $\boldsymbol{x}_i \in \mathbb{R}^d$ for $i = 1, \ldots, n$ is a real vector. The data are assumed to come from k separate Gaussian distributions (in this concrete case, $n = 272, d = 2, k = 2$), according to the following generative process:



For each datum $i \in [1, \ldots, n]$:

- draw a discrete cluster identity $\boldsymbol{z}_i \in \{0,1\}^k, \sum_j z_{ij} = 1$ ("one-hot") with

$$p(\boldsymbol{z}_i \mid \pi) = \prod_{j=1}^{k} \pi_j^{z_{ij}}$$

- draw the datum $x_i \in \mathbb{R}^d$ from one of k Gaussian distributions, selected by $\boldsymbol{z}_i$ with probability

$$p(\boldsymbol{x}_i \mid \boldsymbol{z}_i, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \prod_{j=1}^{k} \mathcal{N}(\boldsymbol{x}_i; \mu_j, \Sigma_j)^{z_{ij}}$$

This process involves the following parameters: a probability $\pi \in \mathbb{R}^k_{+,0}, \sum_j^k \pi_j = 1$, and cluster parameters $\mu_j \in \mathbb{R}^d, \Sigma_j \in \mathbb{R}^{d \times d}$.

Write down an EM algorithm for the GMM above that finds a maximum likelihood assignment for the parameters π_j, μ_j, Σ_j defined above. To do so, proceed according to the example in lecture 15, including all derivations, and not just the final result. Write down each step incl. the assumptions, rules etc. that you make/apply:

1. For the E-step, compute the expectation of the complete-data likelihood $p(\boldsymbol{z}, \boldsymbol{x} \mid \mu, \Sigma, \pi)$ under the posterior $p(\boldsymbol{z} \mid \mu, \Sigma, \boldsymbol{x})$.
2. For the M-step, analytically maximize this expression in π, μ, Σ.

Hints:
***Constrained optimization**: You may need to enforce constraints within the M-step of π, an easy technique to do so is to use Lagrange multipliers.*

***Matrix calculus**: These identities may be helpful:*

- *Let $f : \mathbb{R}^{n \times n} \to \mathbb{R},\ f(A) = x^T A^{-1} x$, then $\nabla_A f(A) = -A^{-T} x x^T A^{-T}$.*
- *Let $f : \mathbb{R}^{n \times n} \to \mathbb{R},\ f(A) = det(A)$, then $\nabla_A f(A) = det(A)(A^{-1})^T$.*

3. **Practical Question** In this week's practical question, we will implement such an EM algorithm for a very common dataset that also shows a "cluster" structure, namely the iris dataset. You will find the required information in notebook `Exercise_09.ipynb`, which can be solved without solving the questions above.