CS280 Fall 2022 Assignment 1
Part A

Basics & MLP

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1. *Gradient descent for fitting GMM* (10 points).

Consider the Gaussian mixture model

$$p(\mathbf{x}|\theta) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

where $\pi_j \geq 0, \sum_{j=1}^{K} \pi_j = 1$. (Assume $\mathbf{x}, \boldsymbol{\mu}_k \in \mathbb{R}^d, \boldsymbol{\Sigma}_k \in \mathbb{R}^{d\times d}$)

Define the log likelihood as

$$l(\theta) = \sum_{n=1}^{N} \log p(\mathbf{x}_n|\theta)$$

Denote the posterior responsibility that cluster k has for datapoint n as follows:

$$r_{nk} := p(z_n = k|\mathbf{x}_n, \theta) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{k'} \pi_{k'} \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_{k'}, \boldsymbol{\Sigma}_{k'})}$$

(a) Show that the gradient of the log-likelihood wrt $\boldsymbol{\mu}_k$ is

$$\frac{d}{d\boldsymbol{\mu}_k} l(\theta) = \sum_n r_{nk} \boldsymbol{\Sigma}_k^{-1}(\mathbf{x}_n - \boldsymbol{\mu}_k)$$

Proof. By the *chain rule*, we have

$$\begin{aligned}
\frac{\partial l(\theta)}{\partial \boldsymbol{\mu}_k} &= \sum_{n=1}^{N} \frac{1}{p(\boldsymbol{x}_n|\theta)} \frac{\partial p(\boldsymbol{x}_n|\theta)}{\partial \boldsymbol{\mu}_k} \\
&= \sum_{n=1}^{N} \frac{1}{p(\boldsymbol{x}_n|\theta)} \frac{\partial \pi_k \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\partial \boldsymbol{\mu}_k} \\
&= \sum_{n=1}^{N} \frac{\pi_k \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{p(\boldsymbol{x}_n|\theta)} \frac{\partial(-\frac{1}{2}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}_n - \boldsymbol{\mu}_k))}{\partial \boldsymbol{\mu}_k} \\
&= \sum_{n=1}^{N} r_{nk} \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}_n - \boldsymbol{\mu}_k)
\end{aligned}$$

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(b) Derive the gradient of the log-likelihood wrt π_k without considering any constraint on π_k. (bonus 2 points: with constraint $\sum_k \pi_k = 1$.)

Proof. For the case without any constriant on π_k, by the *chain rule*, we have:

$$\begin{aligned}
\frac{\partial l(\theta)}{\partial \pi_k} &= \sum_{n=1}^{N} \frac{1}{p(\boldsymbol{x}_n|\theta)} \frac{\partial p(\boldsymbol{x}_n|\theta)}{\partial \pi_k} \\
&= \sum_{n=1}^{N} \frac{1}{p(\boldsymbol{x}_n|\theta)} \mathcal{N}(\boldsymbol{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \\
&= \sum_{n=1}^{n} \frac{r_{nk}}{\pi_k}
\end{aligned}$$

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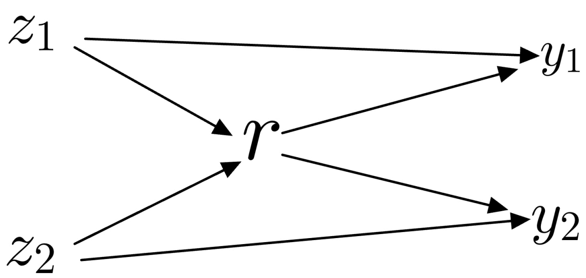
2. ***Sotfmax & Computation Graph*** **(10 points).**

Recall that the softmax function takes in a vector $(z_1, \ldots, z_D)$ and returns a vector $(y_1, \ldots, y_D)$. We can express it in the following form:

$$r = \sum_j e^{z_j} \qquad y = \frac{e^{z_j}}{r}$$

(a) Consider $D = 2$, i.e. just two inputs and outputs to the softmax. Draw the computation graph relating z_1, z_2, r, y_1, and y_2.

Solution:



(b) Determine the backprop updates for computing the $\bar{z}_j$ when given the $\bar{y}_i$. You need to justify your answer. (You may give your answer either for $D = 2$ or for the more general case.)

Solution:

By the *chain rule* and the forward precess, we have the backprop updates as follows:

$$\bar{r} = \sum_{i=1}^{D} \bar{y}_i \frac{\partial y_i}{\partial r} = -\sum_{i=1}^{D} \bar{y}_i \frac{e^{z_i}}{r^2}$$
$$\bar{z}_i = \bar{y}_i \frac{\partial y_i}{\partial z_i} + \bar{r} \frac{\partial r}{\partial z_i} = \bar{y}_i \frac{e^{z_i}}{r} + \bar{r} e^{z_i}$$

(c) Write a function to implement the vector-Jacobian product (VJP) for the softmax function based on your answer from part (b). For efficiency, it should operate on a mini-batch. The inputs are:

- a matrix $\boldsymbol{Z}$ of size $N \times D$ giving a batch of input vectors. N is the batch size and D is the number of dimensions. Each row gives one input vector $z = (z_1, \ldots, z_D)$.
- A matrix $\mathbf{Y_{bar}}$ giving the output error signals. It is also $N \times D$

The output should be the error signal $\mathbf{Z_{bar}}$. Do not use a for loop.