

Machine Learning Worksheet 11

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Problem 1

Consider a Gaussian Mixture Model that describes the data points \mathbf{x}

$$p(x|\theta) = \sum_{k=0}^K \pi_k \mathcal{N}(x|\mu_k, \sigma^2 \mathbf{I})$$

with some $\sigma \in \mathbb{R}$. Let us define $\pi_k = \frac{|C_k|}{N}$ with $|C_k|$ being the number of data point belonging to a cluster k and N the total number of data points.

Since we cannot easily optimize

$$\arg \max_{\theta} \ln p(\mathcal{D}|\theta) = \sum_{n=1}^N \ln \sum_{k=0}^K \frac{|C_k|}{N} \mathcal{N}(x_n|\mu_k, \sigma^2 \mathbf{I})$$

we use the EM algorithm. In EM, we are doing alternate coordinate ascent on $\mathcal{L}_{ELBO}(q, \theta)$ for some posterior distribution $q(z)$, i.e. two steps:

1. Optimization w.r.t. q :

$$\arg \max_q \mathcal{L}_{ELBO}(q, \theta) = \arg \max_q \mathbb{E}_{q(z)}[\ln p(x, z|\theta)] + H(q)$$

With

$$\mathbb{E}_{q(z)}[\ln p(x, z|\theta)] = \mathbb{E}_{q(z)}[\ln p(z|x, \theta)] + \mathbb{E}_{q(z)}[\ln p(x|\theta)]$$

one arrives at

$$\arg \max_q \mathcal{L}_{ELBO}(q, \theta) = \arg \max_q (\mathbb{E}_{q(z)}[\ln p(z|x, \theta)] + \mathbb{E}_{q(z)}[\ln p(x|\theta)] + H(q))$$

2. Optimization w.r.t. parameters θ :

$$\begin{aligned} \arg \max_{\theta} \mathcal{L}_{ELBO}(q, \theta) &= \arg \max_{\theta} (\mathbb{E}_{q(z)}[\ln p(x, z|\theta)] + H(q)) \\ &= \arg \max_{\theta} (\mathbb{E}_{q(z)}[\ln p(x, z|\theta)]) \\ &= \arg \max_{\theta} (\mathbb{E}_{q(z)}[\ln p(z|x, \theta)] + \mathbb{E}_{q(z)}[\ln p(x|\theta)]) \end{aligned}$$

The *K-Means algorithm* is an instance of the EM-algorithm. In the first step (E-Step), using

$$p(z|x, \theta) = r_{nk}(\theta) \sim \mathcal{N}(d(x_n, \mu_k) | \mu_k, \sigma^2 \mathbf{I}) \quad \text{with} \quad d(x_n, \mu_k) = \|x_n - \mu_k\|_2$$

and taking σ towards 0, one can see that $\mathcal{L}_{ELBO}(q, \theta)$ is maximized by picking a j for every x_n such that $d(x_n, \mu_j)$ is minimized, which corresponds to the step of "calculating clusters" in *K-Means*. [Euclidean distance puts equidistant points on a circle (2D) resp. sphere (3D), so does a Gaussian with $\Sigma = \sigma^2 \mathbf{I}$]

In the second step (M-step) the optimization of the arguments θ is done, namely the μ_k are updated as follows:

$$\mu_k \leftarrow \frac{1}{|C_k|} \sum_{x \in C_k} x$$

and thus maximizing $\mathcal{L}_{ELBO}(q, \theta)$, which corresponds to the step "recalibrating the cluster mean".
