

Suppose we have a dataset with  $n$  observations  $\mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$  and a (log) likelihood function:

$$\ln p(\mathbf{X}|\boldsymbol{\theta}) \quad (1)$$

I can get the Maximum Likelihood Estimators of the parameter, which I call  $\hat{\boldsymbol{\theta}}_0$ . I denote the achieved likelihood  $\mathcal{L}_0$ .

Now I want to fit the same model using mixtures, assuming that there are  $K$  groups of points with parameters  $\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_K$ . For that, we introduce the a matrix  $\mathbf{Z}$  of latent variables where  $z_{nk} = 1$  if point  $n$  belongs to cluster  $k$ .

The likelihood can be re-expressed as:

$$\ln p(\mathbf{X}|\boldsymbol{\theta}) = \ln \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})$$

Because optimizing with that sum is usually hard, we do a couple of tricks:

$$\ln p(\mathbf{X}|\boldsymbol{\theta}) = \ln \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})}{q(\mathbf{Z})} = \ln \mathbb{E}_q \left( \frac{p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})}{q(\mathbf{Z})} \right)$$

which is the logarithm of a expected value. By Jennsenn inequality, we know that:

$$\ln \mathbb{E}[x] \geq \mathbb{E}[\ln(x)]$$

and then:

$$\ln p(\mathbf{X}|\boldsymbol{\theta}) = \ln \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})}{q(\mathbf{Z})} \geq \overbrace{\sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \frac{p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})}{q(\mathbf{Z})}}^{\mathcal{L}}$$

The equality holds if the function inside the logarithm is constant. And this happens when  $q(\mathbf{Z})$  is the posterior of  $\mathbf{Z}$ . Therefore we have the general EM expression of the lower bound:

$$\mathcal{L} = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}) \ln \overbrace{\frac{p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})}{p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta})}}^{p(\mathbf{X}|\boldsymbol{\theta})} = \overbrace{\sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}) \ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})}^Q - \overbrace{\sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}) \ln p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta})}^{H(\mathbf{Z}) \text{ (entropy)}}$$

**k=1**

If there is only one cluster,  $p(\mathbf{Z}|\cdot)$  can be thought of as a constant, and

$$\mathcal{L} = \ln p(\mathbf{X}|\boldsymbol{\theta}) = \mathcal{L}_0$$

and if the plug the estimators  $\hat{\boldsymbol{\theta}}_0$  we obtain:

$$\ln p(\mathbf{X}|\hat{\boldsymbol{\theta}}_0) = \mathcal{L}_0$$

**K overlapped clusters**

The likelihood of  $K$  clusters completely overlapped, all sharing the same parameters  $\hat{\theta}_0$  we have that  $p(\mathbf{X}|\theta)$  does not depend on  $\mathbf{Z}$ , therefore

$$\mathcal{L} = \ln p(\mathbf{X}|\theta) \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta) = \ln p(\mathbf{X}|\theta)$$

Let us demonstrate it again using  $Q$  and  $H(\mathbf{Z})$ .

$$\mathcal{L} = \overbrace{\sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta) \ln p(\mathbf{X}, \mathbf{Z}|\theta)}^Q - \overbrace{\sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta) \ln p(\mathbf{Z}|\mathbf{X}, \theta)}^{H(\mathbf{Z}) \text{ (entropy)}}$$

Since the  $\theta$  are equal for every cluster, then:

$$\begin{aligned} \mathcal{L} &= \overbrace{\ln p(\mathbf{X}, \mathbf{Z}|\theta) \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta)}^Q - \overbrace{\ln p(\mathbf{Z}|\mathbf{X}, \theta) \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta)}^{H(\mathbf{Z}) \text{ (entropy)}} \\ &\quad \underbrace{\hspace{1.5cm}}_1 \quad \underbrace{\hspace{1.5cm}}_1 \\ &= \overbrace{\ln p(\mathbf{X}, \mathbf{Z}|\theta)}^Q - \overbrace{\ln p(\mathbf{Z}|\mathbf{X}, \theta)}^{H(\mathbf{Z}) \text{ (entropy)}} = \ln p(\mathbf{X}|\theta) \end{aligned}$$