

Example solution

Minimize  $L(\sigma, \theta)$  by setting the gradient of  $L$  to  $\vec{0}$ .

$$\begin{aligned}
 \frac{\partial L}{\partial \theta_i} &= \frac{\partial}{\partial \theta_i} \left( \sum_{n=1}^N \sum_{k=1}^K r_{kn} \|x^{(n)} - \theta_k\|_2^2 \right) \\
 &= \frac{\partial}{\partial \theta_i} \left( \sum_{k=1}^K \sum_{n=1}^N r_{kn} (x^{(n)} - \theta_k)^T (x^{(n)} - \theta_k) \right) \\
 &= \frac{\partial}{\partial \theta_i} \left( \sum_{n=1}^N r_{in} (x^{(n)} - \theta_i)^T (x^{(n)} - \theta_i) \right) \\
 &= \sum_{n=1}^N r_{in} 2 (x^{(n)} - \theta_i) (-1) \\
 &= -2 \sum_{n=1}^N r_{in} x^{(n)} - 2 \sum_{n=1}^N r_{in} \theta_i \\
 &= -2 \sum_{n=1}^N r_{in} x^{(n)} - 2 \theta_i \sum_{n=1}^N r_{in} \stackrel{!}{=} 0 \\
 &\Rightarrow \hat{\theta}_i = \frac{\sum_{n=1}^N r_{in} x^{(n)}}{\sum_{n=1}^N r_{in}}
 \end{aligned}$$

- $\sum_{n=1}^N r_{in} x^{(n)}$  := the sum of the data point assigned to cluster  $i$
- $\sum_{n=1}^N r_{in}$  := the number //
- $\Rightarrow \hat{\theta}_i$  := the mean //

This is exactly the cluster update step in K-means.

Check if  $(\hat{\theta}_1, \dots, \hat{\theta}_K)$  is indeed a minimum. The Hessian of  $L$  is

$$\mathcal{H}(L) = \begin{bmatrix} \frac{\partial^2 L}{\partial \theta_1^2} & \dots & \frac{\partial^2 L}{\partial \theta_1 \partial \theta_K} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 L}{\partial \theta_K \partial \theta_1} & \dots & \frac{\partial^2 L}{\partial \theta_K^2} \end{bmatrix} = \begin{bmatrix} 2 \sum_{n=1}^N r_{1n} & & \\ & \ddots & \\ & & 2 \sum_{n=1}^N r_{Kn} \end{bmatrix}$$

$$\begin{aligned}
 \text{Since } \frac{\partial^2 L}{\partial \theta_i \partial \theta_j} &= \frac{\partial}{\partial \theta_j} \left( -2 \sum_{n=1}^N r_{in} x^{(n)} + 2 \theta_i \sum_{n=1}^N r_{in} \right) = 0 \\
 \frac{\partial^2 L}{\partial \theta_i^2} &= \frac{\partial}{\partial \theta_i} \left( \quad \quad \quad \right) = 2 \sum_{n=1}^N r_{in} .
 \end{aligned}$$

$$\sum_{n=1}^N r_{in} > 0 \text{ for all } i=1, \dots, K$$

- $\Rightarrow$  all the eigenvalues of  $\mathcal{H}(L) > 0$
- $\Rightarrow \mathcal{H}(L)$  is (symmetric) positive definite.
- $\Rightarrow (\hat{\theta}_1, \dots, \hat{\theta}_K)$  is a global minimum.