Define the complete data for this problem to be $D = \{(\mathbf{x}_i, \mathbf{z}_i)\}_{i=1}^n$. Write out the complete-data (negative) log likelihood.

$$\mathcal{L}(\boldsymbol{\theta}, \{\mu_k, \Sigma_k\}_{k=1}^c) = -\ln p(D \mid \boldsymbol{\theta}, \{\mu_k, \Sigma_k\}_{k=1}^c).$$

- **Expectation Step** Our next step is to introduce a mathematical expression for \mathbf{q}_i , the posterior over the hidden topic variables \mathbf{z}_i conditioned on the observed data \mathbf{x}_i with fixed parameters, i.e $p(\mathbf{z}_i|\mathbf{x}_i;\boldsymbol{\theta},\{\mu_k,\Sigma_k\}_{k=1}^c)$.
 - Write down and simplify the expression for \mathbf{q}_i .
 - Find an expression for θ that maximizes this expected complete-data log likelihood. You may find it helpful to use Lagrange multipliers in order to force the constraint $\sum \theta_k = 1$. Why does this optimized θ make intuitive sense?

To maximize given a constraint, we will use the method of Lagrangian multipliers. As we are maximizing with respect to θ_k , we may also drop the terms (on the right) not including θ . Previously, in homework 2, we had z_{ik} as our indicator variable. However, we now treat z as a latent variable, and instead we have a "soft estimate" q variable.

$$\mathcal{L}(\theta_{\mathbf{k}}, \lambda) = \sum_{i=1}^{n} \sum_{k=1}^{c} q_{ik} \ln \theta_k + \lambda (\sum_{k=1}^{c} \theta_k - 1)$$
(1)

Take the partial derivative of $\mathcal L$ with respect to θ_k and set it equal to zero, and noting that

$$\sum_{i} q_{ik} = n_k \tag{2}$$

(see homework 2 problem 2.2 for more details)

$$0 = \sum_{i=1}^{n} \frac{q_{ik}}{\theta_k} - \lambda \tag{3}$$

$$\theta_k = \frac{n_k}{\lambda} \tag{4}$$

Take the partial derivative with respect to λ and set it equal to zero to get

$$0 = \sum_{k=1}^{c} \theta_k - 1 \tag{5}$$

(6)

Now let's solve from lambda by combining ?? and ??

$$0 = \sum_{k=1}^{c} \frac{n_k}{\lambda} - 1 \tag{7}$$

$$\lambda = n_k \tag{8}$$

Returning to ?? we now see that

$$\theta_k = \frac{n_k}{n} \tag{9}$$

(Note that since we are actually estimating θ_k , it would be clearer to write $\hat{\theta_k}$)

This solution for $\hat{\theta}_k$ makes sense: the optimal (prior) probability of a given x_i belong to a class k is equal to the proportion of observations (we've estimated in this iteration) that come from class k.

– Apply a similar argument to find the value of the (μ_k, Σ_k) 's that maximizes the expected complete-data log likelihood. For μ_k case.

$$= \sum_{i=1}^{n} \sum_{k=1}^{c} q_{ik} \left(\ln \theta_k + \ln \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right)$$
 (10)

To solve for optimal μ_k , taking the derivative of $\ref{eq:main_k}$ with respect to μ_k and set to zero. Note that the left hand terms drop out. Furthermore, we remove terms in the log gaussian without μ_k

$$\begin{split} &= \sum_{i=1}^{n} \sum_{k=1}^{c} q_{ik} \left(\ln \theta_k + \ln \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right) \\ &= \sum_{i=1}^{n} \sum_{k=1}^{c} q_{ik} \ln \mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \end{split} \tag{\ref{eq:posterior}}$$

The natural log of the Gaussian is equal to

$$= -\frac{1}{2} \left(D \ln 2\pi + \ln |\mathbf{\Sigma}| + (\mathbf{x}_i - \boldsymbol{\mu}_k)^T \mathbf{\Sigma}^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) \right)$$
(11)

$$= -\frac{1}{2}(\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k)$$
(12)

Thus we get that we are solving for μ_k s.t.

$$\frac{\partial L}{\partial \boldsymbol{\mu}_k} = -\frac{1}{2} \sum_{i=1}^n \sum_{k=1}^c q_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k) + const$$
 (13)

$$=0 (14)$$

Carrying the derivative out:

$$0 = -\frac{1}{2} (\mathbf{\Sigma}^{-1} + \mathbf{\Sigma}^{-T}) \sum_{i=1}^{n} \sum_{k=1}^{c} q_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)$$
 (15)

$$0 = \sum_{i=1}^{n} \sum_{k=1}^{c} q_{ik} (\mathbf{x}_i - \boldsymbol{\mu}_k)$$
 (16)

$$0 = \sum_{i=1}^{n} \sum_{k=1}^{c} q_{ik} \mathbf{x}_i - q_{ik} \boldsymbol{\mu}_k$$

$$\tag{17}$$

$$\sum_{i=1}^{n} \sum_{k=1}^{c} q_{ik} \boldsymbol{\mu}_{k} = \sum_{i=1}^{n} \sum_{k=1}^{c} q_{ik} \mathbf{x}_{i}$$
(18)

(19)

As the μ_k is the same for all points in the class, $\sum_{k=1}^c q_{ik} \mu_k$ is simply $n_k \mu_k$. Thus we get that

$$\boldsymbol{\mu}_k = \frac{1}{n_k} \sum_{i=1}^n q_{ik} \mathbf{x}_i \tag{20}$$

– Apply a similar argument to find the value of the (μ_k, Σ_k) 's that maximizes the expected complete-data log likelihood. Σ_k case.

$$\hat{\boldsymbol{\Sigma}_k} = \frac{1}{n_k} \sum_{i=1}^n q_{ik} (x_i - \hat{\boldsymbol{\mu}_k}) (x_i - \hat{\boldsymbol{\mu}_k})^T$$
(21)

Dropping terms without Σ

$$\mathcal{L} = \sum_{i=1}^{n} \sum_{k=1}^{c} \left[-\frac{1}{2} (\ln |\mathbf{\Sigma}| + (\mathbf{x}_i - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k)) \right]$$
(22)

Taking the partial derivative and collapsing sums, we get

$$\frac{\partial \mathcal{L}}{\partial \mathbf{\Sigma}_k} = \frac{n_k}{\mathbf{\Sigma}^2} - \frac{1}{2} \sum_{i=1}^n q_{ik} (x_i - \hat{\boldsymbol{\mu}}_k) (x_i - \hat{\boldsymbol{\mu}}_k)^T$$
(23)

$$\Sigma_k = \frac{1}{n_k} \sum_{i=1}^n q_{ik} (x_i - \boldsymbol{\mu}_k) (x_i - \boldsymbol{\mu}_k)^T$$
(24)