Lecture 24. Expectation Maximization.

COMP90051 Statistical Machine Learning

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MLE vs EM

- MLE is a frequentist *principle* that suggests that given a dataset, the "best" parameters to use are the ones that maximise the probability of the data
  - MLE is a way *to formally pose* the problem
- EM is an *algorithm*
  - EM is a way *to solve* the problem posed by MLE
  - Especially convenient under unobserved latent variables
- MLE can be found by other methods such as gradient descent (but gradient descent is not always the most convenient method)

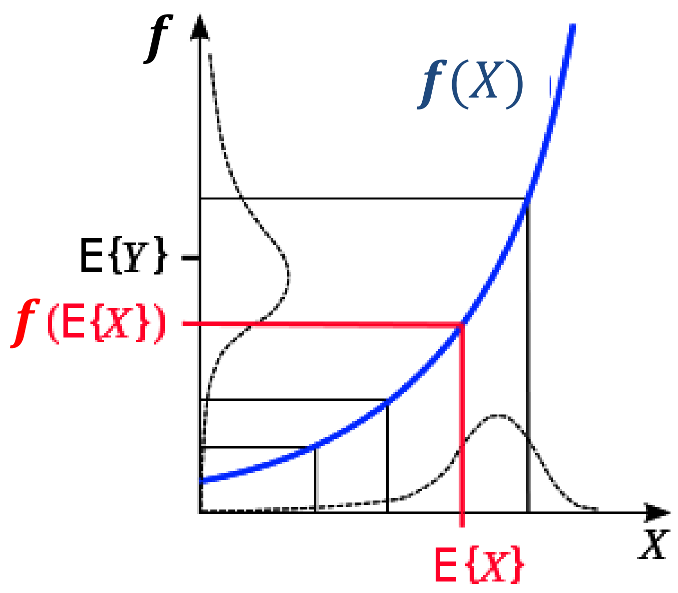
EM for GMM and generally

- EM is a general approach, goes beyond GMMs
  - Purpose: Implement MLE under latent variables **Z** ('latent' is fancy for 'missing')
- What are variables, parameters in GMMs?
  - Variables: Point locations **X** and cluster assignments **Z**
    - let z_i denote true cluster membership for each point $\boldsymbol{x}_i$, computing the likelihood with known values $\boldsymbol{z}$ is simplified (see next section)
  - Parameters: **θ** are cluster locations and scales
- What is EM really doing?
  - Coordinate ascent on a lower bound on the log-likelihood
    - M-step: ascent in modeled parameters **θ**
    - E-step: ascent in the marginal likelihood P(**Z**)
  - Each step moves towards a ***local*** optimum
  - Can get stuck, can need random restarts

Using convexity: Jensen's inequality

- Compares effect of averaging before and after applying a convex function: $f\left(Average(\boldsymbol{x})\right) \leq Average\left(f(\boldsymbol{x})\right)$
- Example:
  - Let f be some convex function, such as $f(x) = x^2$
  - Consider $\boldsymbol{x} = [1,2,3,4,5]'$, then $f(\boldsymbol{x}) = [1,4,9,16,25]'$
  - Average of input $Average(\boldsymbol{x}) = 3$
  - $f\left(Average(\boldsymbol{x})\right) = 9$
  - Average of output $Average\left(f(\boldsymbol{x})\right) = 12.4$
- Proof follows from the definition of convexity
  - Proof by induction

General statement:
- If $\boldsymbol{X}$ random variable, f is a convex function
- $f(\mathbb{E}[\boldsymbol{X}]) \leq \mathbb{E}[f(\boldsymbol{X})]$



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Putting the latent variables to use

We want to maximise $\log p(\boldsymbol{X}|\boldsymbol{\theta})$. We don't observe $\boldsymbol{Z}$ (here discrete), but can (re)introduce it nonetheless.

$$\boxed{\log p(\boldsymbol{X}|\boldsymbol{\theta})} = \log \sum_{\boldsymbol{Z}} p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})$$

← Marginalisation (here $\sum_{\boldsymbol{Z}} \dots$ iterates over all possible values of $\boldsymbol{Z}$)

$$= \log \sum_{\boldsymbol{Z}} \left(p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta}) \frac{p(\boldsymbol{Z})}{p(\boldsymbol{Z})} \right)$$

← Need $\boldsymbol{Z}$ to have non-zero marginal

$$= \log \sum_{\boldsymbol{Z}} \left(p(\boldsymbol{Z}) \frac{p(\boldsymbol{X},\boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})} \right)$$

$$= \log \mathbb{E}_{\boldsymbol{Z}} \left[\frac{p(\boldsymbol{X},\boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})} \right]$$

$$\geq \mathbb{E}_{\boldsymbol{Z}} \left[\log \frac{p(\boldsymbol{X},\boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})} \right]$$

← Jensen's inequality holds in this direction since $\log(\dots)$ is a concave function

$$= \boxed{\mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]}$$

Maximising the lower bound (1/2)

- $\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]$
- The right-hand side (RHS) is a lower bound on the original log likelihood
  - This holds for any $\boldsymbol{\theta}$ and any non-zero $p(\boldsymbol{Z})$
- Intuitively, we want to push the lower bound up
- This lower bound is a function of two "variables" $\boldsymbol{\theta}$ and $p(\boldsymbol{Z})$. We want to maximise the RHS as a function of these two "variables"
- It is hard to optimise with respect to both at the same time, so EM resorts to an iterative procedure

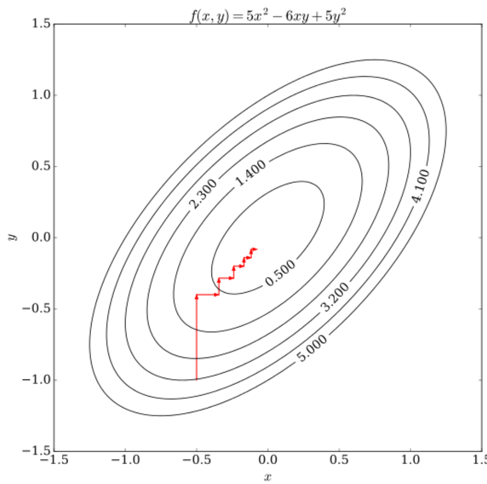
Maximising the lower bound (2/2)

- $\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X},\boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]$
- EM is essentially coordinate ascent:
  - Fix $\boldsymbol{\theta}$ and optimise the lower bound for $p(\boldsymbol{Z})$
  - Fix $p(\boldsymbol{Z})$ and optimise for $\boldsymbol{\theta}$
- The convenience of EM comes from the following

we will prove this shortly

- For any point $\boldsymbol{\theta}^*$, it can be shown that setting $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta}^*)$ makes the lower bound tight
- For any $p(\boldsymbol{Z})$, the second term does not depend on $\boldsymbol{\theta}$
- When $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta}^*)$, the first term can usually be maximised as a function of $\boldsymbol{\theta}$ in a closed-form
  - If not, then probably don't use EM

Mini Summary



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- EM intuition by GMM with recap
- Lower-bound $\log p(\boldsymbol{X}|\boldsymbol{\theta})$ by $\mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X},\boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]$
  - Holds for any $\boldsymbol{\theta}, p(\boldsymbol{Z})$
  - Uses Jensen's inequality (concavity of $\log$)
- Maximise not $\log p(\boldsymbol{X}|\boldsymbol{\theta})$ but lower bound, alternating:
  - E-Step: choose $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta}^*)$ raises lower bound up to log-likelihood, for any $\boldsymbol{\theta}^*$
  - M-Step: $\boldsymbol{\theta}^*$ by max'ing "completed" log-likelihood; ideally, easy MLE
- The E- and M-steps implement coordinate ascent

Next: Proving the E-step

EM as iterative (coordinate) ascent

1. Initialisation: choose (random) initial values of $\boldsymbol{\theta}^{(1)}$

2. Update:
   * E-step: compute $Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}\right) \equiv \mathbb{E}_{\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta}^{(t)}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})]$
   * M-step: $\boldsymbol{\theta}^{(t+1)} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}\right)$

3. Termination: if no change then stop

4. Go to Step 2

This algorithm will eventually stop (converge), but the resulting estimate can be only a local maximum

Maximising the lower bound (2/2)

- $\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]$
- EM is essentially coordinate descent:
  * Fix $\boldsymbol{\theta}$ and optimise the lower bound for $p(\boldsymbol{Z})$
  * Fix $p(\boldsymbol{Z})$ and optimise for $\boldsymbol{\theta}$
- The convenience of EM follows from the following
- For any point $\boldsymbol{\theta}^*$, it can be shown that setting $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X}, \boldsymbol{\theta}^*)$ makes the lower bound tight
- For any $p(\boldsymbol{Z})$, the second term does not depend on $\boldsymbol{\theta}$
- When $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X}, \boldsymbol{\theta}^*)$, the first term can usually be maximised as a function of $\boldsymbol{\theta}$ in a closed-form
  * If not, then probably don't use EM

we will prove this now

Putting the latent variables in use

We want to maximise $\log p(\boldsymbol{X}|\boldsymbol{\theta})$. We don't know $\boldsymbol{Z}$, but consider an arbitrary non-zero distribution $p(\boldsymbol{Z})$

$$\boxed{\log p(\boldsymbol{X}|\boldsymbol{\theta})} = \log \textstyle\sum_{\boldsymbol{Z}} p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})$$

← Rule of marginal distribution (here $\sum_{\boldsymbol{Z}} \dots$ iterates over all possible values of $\boldsymbol{Z}$)

$$= \log \textstyle\sum_{\boldsymbol{Z}} \left(p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta}) \frac{p(\boldsymbol{Z})}{p(\boldsymbol{Z})} \right)$$

$$= \log \textstyle\sum_{\boldsymbol{Z}} \left(p(\boldsymbol{Z}) \frac{p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})} \right)$$

$$= \log \mathbb{E}_{\boldsymbol{Z}} \left[\frac{p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})} \right]$$

← Jensen's inequality holds since $\log(\dots)$ is a concave function

$$\boxed{\geq \mathbb{E}_{\boldsymbol{Z}} \left[\log \frac{p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})} \right]}$$

$$= \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})] - \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{Z})]$$

Setting a tight lower bound (1/2)

- $\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \mathbb{E}_{\boldsymbol{Z}}\left[\log\frac{p(\boldsymbol{X},\boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right]$

$$= \mathbb{E}_{\boldsymbol{Z}}\left[\log\frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})p(\boldsymbol{X}|\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right]$$

← Chain rule of probability

$$= \mathbb{E}_{\boldsymbol{Z}}\left[\log\frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z})} + \log p(\boldsymbol{X}|\boldsymbol{\theta})\right]$$

$$= \mathbb{E}_{\boldsymbol{Z}}\left[\log\frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right] + \mathbb{E}_{\boldsymbol{Z}}[\log p(\boldsymbol{X}|\boldsymbol{\theta})]$$

← Linearity of $\mathbb{E}[.]$

$$= \mathbb{E}_{\boldsymbol{Z}}\left[\log\frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right] + \log p(\boldsymbol{X}|\boldsymbol{\theta})$$

← $\mathbb{E}[.]$ of a constant

- $\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \mathbb{E}_{\boldsymbol{Z}}\left[\log\frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right] + \log p(\boldsymbol{X}|\boldsymbol{\theta})$

Setting a tight lower bound (2/2)

$$\overbrace{\log p(\boldsymbol{X}|\boldsymbol{\theta})}^{\text{Ultimate aim: maximise this}} \geq \overbrace{\underbrace{\mathbb{E}_{\boldsymbol{Z}}\left[\log\frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right]}_{\text{First, note that this term* } \leq 0} + \log p(\boldsymbol{X}|\boldsymbol{\theta})}^{\text{Lower bound of what we want to maximise}}$$

Second, note that if $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})$, then

$$\mathbb{E}_{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}\left[\log\frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}\right] = \mathbb{E}_{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}[\log 1] = 0$$

For any $\boldsymbol{\theta}^*$, setting $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta}^*)$ maximises the lower bound on $\log p(\boldsymbol{X}|\boldsymbol{\theta}^*)$ and makes it tight

*Negative Kullback-Leibler divergence between $p(\boldsymbol{Z})$ and $p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})$

Mini Summary

- We're wanting to maximise the lower bound
$$\log p(\boldsymbol{X}|\boldsymbol{\theta}) \geq \mathbb{E}_{\boldsymbol{Z}}\left[\log \frac{p(\boldsymbol{X},\boldsymbol{Z}|\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right]$$
- We've shown RHS is $\mathbb{E}_{\boldsymbol{Z}}\left[\log \frac{p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})}{p(\boldsymbol{Z})}\right] + \log p(\boldsymbol{X}|\boldsymbol{\theta})$
- And that setting $p(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta})$
  * Makes this RHS as big as possible
  * Makes this RHS equal to $\log p(\boldsymbol{X}|\boldsymbol{\theta})$
  * → maximises the lower bound as desired!

Next: Application of EM to GMM learning

Estimating Parameters of Gaussian Mixture Model

Classical application of the Expectation-Maximisation algorithm. Completes previous lecture.

Latent variables of GMM

- Let $z_1, \dots, z_n$ denote true origins of the corresponding points $\boldsymbol{x}_1, \dots, \boldsymbol{x}_n$. Each z_i is a discrete variable that takes values in $1, \dots, k$, where k is a number of clusters

- Now compare the original log likelihood

$$\log p(\boldsymbol{x}_1, \dots, \boldsymbol{x}_n) = \sum_{i=1}^{n} \log\left(\sum_{c=1}^{k} w_c \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)\right)$$

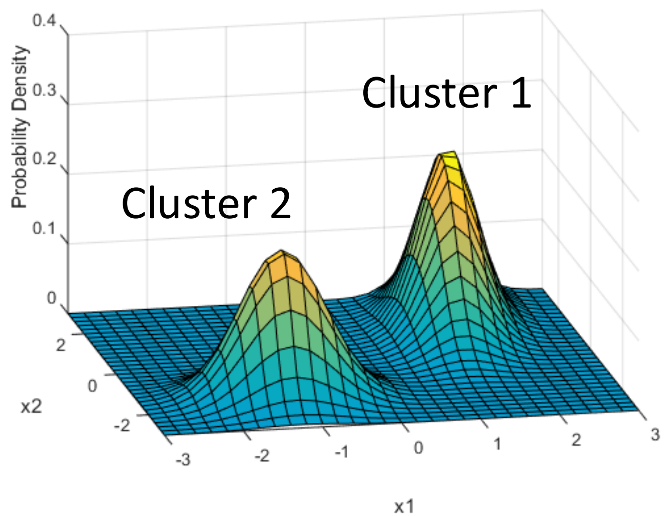
- With *complete log likelihood* (if we knew $\boldsymbol{z}$)

$$\log p(\boldsymbol{x}_1, \dots, \boldsymbol{x}_n, \boldsymbol{z}) = \sum_{i=1}^{n} \log\left(w_{z_i} \mathcal{N}\left(\boldsymbol{x}_i | \boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i}\right)\right)$$

- Recall that taking a log of a normal density function results in a tractable expression

Handling uncertainty about Z

- We cannot compute complete log likelihood because we don't know $\boldsymbol{Z}$
- EM algorithm handles this uncertainty replacing $\log p(\boldsymbol{X}, \boldsymbol{z}|\boldsymbol{\theta})$ with expectation $\mathbb{E}_{\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta}^{(t)}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})]$
- This in turn requires the distribution of $p\left(\boldsymbol{Z}|\boldsymbol{X}, \boldsymbol{\theta}^{(t)}\right)$ given current parameter estimates
- Assuming that Z_i are pairwise independent, we need $P\left(Z_i = c|\boldsymbol{x}_i, \boldsymbol{\theta}^{(t)}\right)$
- E.g., suppose $\boldsymbol{x}_i = (-2, -2)$. What is the probability that this point originated from Cluster 1



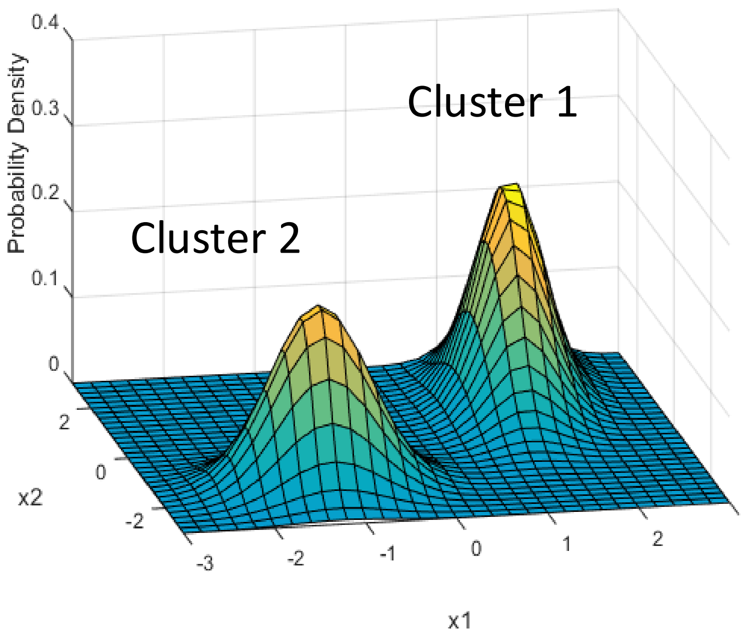
E-step: Cluster responsibilities

- Setting latent Z as originating cluster, yields (via Bayes rule)

$$P\left(z_i = c|\boldsymbol{x}_i, \boldsymbol{\theta}^{(t)}\right) = \frac{w_c \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_c, \boldsymbol{\Sigma}_c)}{\sum_{l=1}^{k} w_l \mathcal{N}(\boldsymbol{x}_i|\boldsymbol{\mu}_l, \boldsymbol{\Sigma}_l)}$$

- This probability is called *responsibility* that cluster c takes for data point i

$$r_{ic} \equiv P\left(z_i = c|\boldsymbol{x}_i, \boldsymbol{\theta}^{(t)}\right)$$



Expectation step for GMM

To simplify notation, we denote $\boldsymbol{x}_1, \dots, \boldsymbol{x}_n$ as $\boldsymbol{X}$

$$Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}\right) \equiv \mathbb{E}_{\boldsymbol{z}|\boldsymbol{X},\boldsymbol{\theta}^{(t)}}[\log p(\boldsymbol{X}, \boldsymbol{z}|\boldsymbol{\theta})]$$

$$= \sum_{\boldsymbol{z}} p\left(\boldsymbol{z}|\boldsymbol{X}, \boldsymbol{\theta}^{(t)}\right) \log p(\boldsymbol{X}, \boldsymbol{z}|\boldsymbol{\theta})$$

$$= \sum_{\boldsymbol{z}} p\left(\boldsymbol{z}|\boldsymbol{X}, \boldsymbol{\theta}^{(t)}\right) \sum_{i=1}^{n} \log w_{z_i} \mathcal{N}\left(\boldsymbol{x}_i|\boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i}\right)$$

$$= \sum_{i=1}^{n} \sum_{\boldsymbol{z}} p\left(\boldsymbol{z}|\boldsymbol{X}, \boldsymbol{\theta}^{(t)}\right) \log w_{z_i} \mathcal{N}\left(\boldsymbol{x}_i|\boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i}\right)$$

$$= \sum_{i=1}^{n} \sum_{c=1}^{k} r_{ic} \log w_{z_i} \mathcal{N}\left(\boldsymbol{x}_i|\boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i}\right)$$

$$= \sum_{i=1}^{n} \sum_{c=1}^{k} r_{ic} \log w_{z_i}$$

$$+ \sum_{i=1}^{n} \sum_{c=1}^{k} r_{ic} \log \mathcal{N}\left(\boldsymbol{x}_i|\boldsymbol{\mu}_{z_i}, \boldsymbol{\Sigma}_{z_i}\right)$$

Maximisation step for GMM

- In the maximisation step, take partial derivatives of $Q\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}\right)$ with respect to each of the parameters and set the derivatives to zero to obtain new parameter estimates
- $w_c^{(t+1)} = \frac{1}{n}\sum_{i=1}^{n} r_{ic}$
- $\boldsymbol{\mu}_c^{(t+1)} = \frac{\sum_{i=1}^{n} r_{ic}\boldsymbol{x}_i}{r_c}$
  * Here $r_c \equiv \sum_{i=1}^{n} r_{ic}$
- $\boldsymbol{\Sigma}_c^{(t+1)} = \frac{\sum_{i=1}^{n} r_{ic}\boldsymbol{x}_i\boldsymbol{x}_i'}{r_c} - \boldsymbol{\mu}_c^{(t)}\left(\boldsymbol{\mu}_c^{(t)}\right)'$
- Note that these are the estimates for step $(t+1)$

k-means as EM for a restricted GMM

- Consider a GMM model in which all components have the same fixed probability $w_c = 1/k$, and each Gaussian has the same fixed covariance matrix $\boldsymbol{\Sigma}_c = \sigma^2 \boldsymbol{I}$, where $\boldsymbol{I}$ is the identity matrix
- In such a model, only component centroids $\boldsymbol{\mu}_c$ need to be estimated
- Next approximate a probabilistic cluster responsibility $r_{ic} = P\left(z_i = c | \boldsymbol{x}_i, \boldsymbol{\mu}_c^{(t)}\right)$ with a deterministic assignment $r_{ic} = 1$ if centroid $\boldsymbol{\mu}_c^{(t)}$ is closest to point $\boldsymbol{x}_i$, and $r_{ic} = 0$ otherwise (E-step)
- Such a formulation results in a M-step where $\boldsymbol{\mu}_c$ should be set as a centroid of points assigned to cluster c
- In other words, k-means algorithm is an EM algorithm for the restricted GMM model described above*!!!*