Lecture 24. Expectation Maximization.

COMP90051 Statistical Machine Learning

Lecturer: Ben Rubinstein



This lecture

- EM intuition by GMM with recap
- Lower-bound $\log p(\pmb{X}|\pmb{\theta})$ by $\mathbb{E}_{\pmb{Z}}[\log p(\pmb{X},\pmb{Z}|\pmb{\theta})] \mathbb{E}_{\pmb{Z}}[\log p(\pmb{Z})]$
 - * Holds for any θ , $p(\mathbf{Z})$
 - Uses Jensen's inequality (concavity of log)
- Maximise not $\log p(X|\theta)$ but lower bound, alternating:
 - * E-Step: choose $p(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^*)$ raises lower bound up to log-likelihood, for any $\boldsymbol{\theta}^*$
 - * M-Step: θ^* by max'ing "completed" log-likelihood; ideally, easy MLE
- Proving the E-step
- Applying EM to GMM MLE-based training
 - Coming full circle back to comparison to k-means

Recap: EM for fitting the GMM

- Initialisation Step:
 - * Initialize K clusters: C_1 , ..., C_K (μ_i, Σ_i) and $P(C_i)$ for each cluster j.
- <u>Iteration Step</u>:
 - * Estimate the cluster of each datum $p(C_i | x_i)$



Re-estimate the cluster parameters



 $(\mu_j, \Sigma_j), p(C_j)$ for each cluster j

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

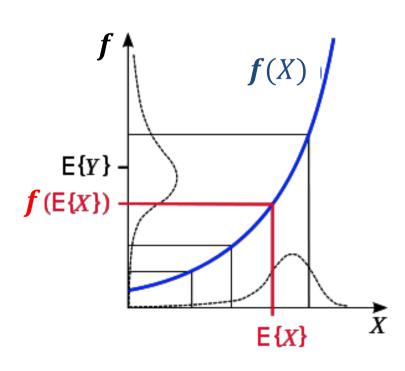
- EM is a general approach, goes beyond GMMs
 - Purpose: Implement MLE under latent variables Z
 ('latent' is fancy for 'missing')
- What are variables, parameters in GMMs?
 - Variables: Point locations X and cluster assignments Z
 - let z_i denote true cluster membership for each point x_i , computing the likelihood with known values 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: $f(Average(x)) \leq Average(f(x))$
- Example:
 - * Let f be some convex function, such as $f(x) = x^2$
 - * Consider x = [1,2,3,4,5]', then f(x) = [1,4,9,16,25]'
 - * Average of input Average(x) = 3
 - * f(Average(x)) = 9
 - * Average of output Average(f(x)) = 12.4
- Proof follows from the definition of convexity
 - Proof by induction

General statement:

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



Putting the latent variables to use

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

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

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

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

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

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

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

 \leftarrow Marginalisation (here \sum_{Z} ... iterates over all possible values of Z)

← Need **Z** to have non-zero marginal

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

Maximising the lower bound (1/2)

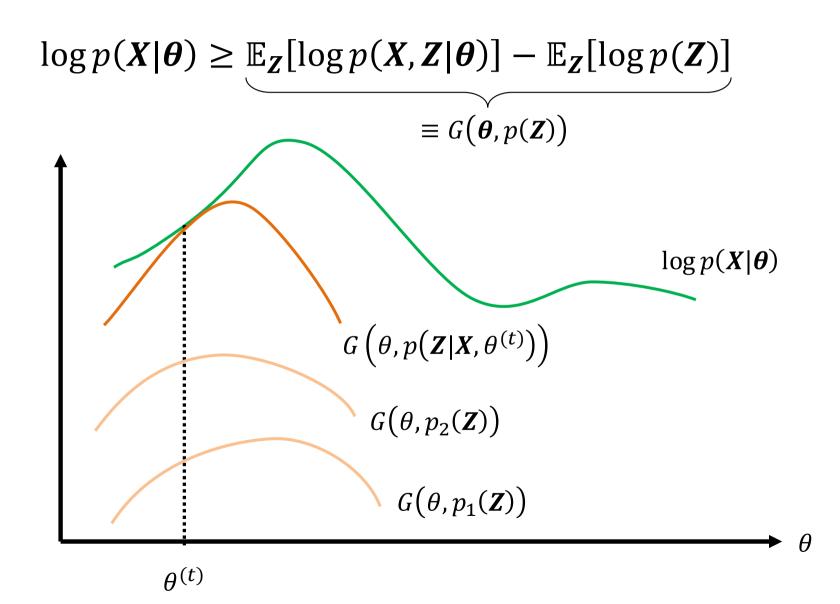
- $\log p(X|\theta) \ge \mathbb{E}_{Z}[\log p(X,Z|\theta)] \mathbb{E}_{Z}[\log p(Z)]$
- The right-hand side (RHS) is a lower bound on the original log likelihood
 - * This holds for any θ and any non-zero p(Z)
- Intuitively, we want to push the lower bound up
- This lower bound is a function of two "variables" θ and p(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)

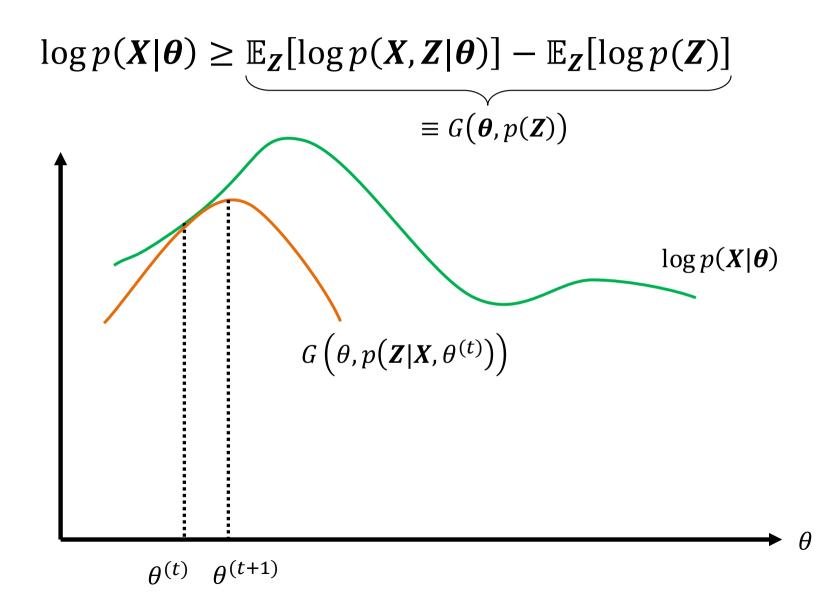
- $\log p(X|\theta) \ge \mathbb{E}_{Z}[\log p(X,Z|\theta)] \mathbb{E}_{Z}[\log p(Z)]$
- EM is essentially coordinate ascent:
 - * Fix θ and optimise the lower bound for $p(\mathbf{Z})$
 - * Fix $p(\mathbf{Z})$ and optimise for $\boldsymbol{\theta}$

- we will prove this shortly
- The convenience of EM comes from the following
- For any point θ^* , it can be shown that setting $p(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \theta^*)$ makes the lower bound tight
- For any $p(\mathbf{Z})$, the second term does not depend on $\boldsymbol{\theta}$
- When $p(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^*)$, 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

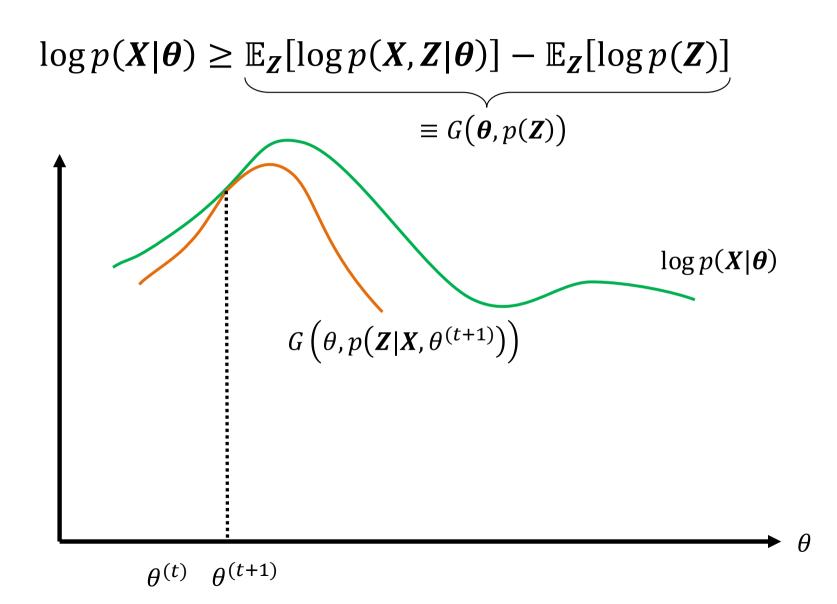
Example (1/3)



Example (2/3)

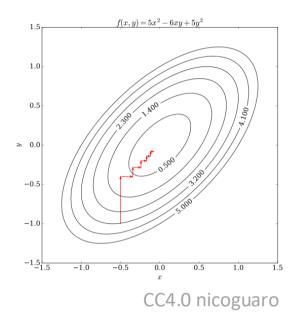


Example (3/3)



Mini Summary

- EM intuition by GMM with recap
- Lower-bound $\log p(\pmb{X}|\pmb{\theta})$ by $\mathbb{E}_{\pmb{Z}}[\log p(\pmb{X},\pmb{Z}|\pmb{\theta})] \mathbb{E}_{\pmb{Z}}[\log p(\pmb{Z})]$
 - * Holds for any θ , p(Z)
 - Uses Jensen's inequality (concavity of log)



- Maximise not $\log p(X|\boldsymbol{\theta})$ but lower bound, alternating:
 - * E-Step: choose $p(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^*)$ raises lower bound up to log-likelihood, for any $\boldsymbol{\theta}^*$
 - * M-Step: θ^* 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. <u>Update</u>:
 - * E-step: compute $Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)}) \equiv \mathbb{E}_{\boldsymbol{Z}|\boldsymbol{X},\boldsymbol{\theta}^{(t)}}[\log p(\boldsymbol{X}, \boldsymbol{Z}|\boldsymbol{\theta})]$
 - * M-step: $\boldsymbol{\theta}^{(t+1)} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{(t)})$
- 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)

- $\log p(X|\theta) \ge \mathbb{E}_{Z}[\log p(X,Z|\theta)] \mathbb{E}_{Z}[\log p(Z)]$
- EM is essentially coordinate descent:
 - * Fix θ and optimise the lower bound for $p(\mathbf{Z})$
 - * Fix $p(\mathbf{Z})$ and optimise for $\boldsymbol{\theta}$

- we will prove this now
- The convenience of EM follows from the following
- For any point θ^* , it can be shown that setting $p(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \theta^*)$ makes the lower bound tight
- For any $p(\mathbf{Z})$, the second term does not depend on $\boldsymbol{\theta}$
- When $p(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^*)$, 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

Putting the latent variables in use

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

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

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

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

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

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

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

 \leftarrow Rule of marginal distribution (here \sum_{Z} ... iterates over all possible values of Z)

← Jensen's inequality holds since log(...) is a concave function

Setting a tight lower bound (1/2)

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

$$= \mathbb{E}_{Z} \left[\log \frac{p(Z|X,\theta)p(X|\theta)}{p(Z)}\right] \qquad \leftarrow \text{Chain rule of probability}$$

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

$$= \mathbb{E}_{Z} \left[\log \frac{p(Z|X,\theta)}{p(Z)}\right] + \mathbb{E}_{Z} [\log p(X|\theta)] \qquad \leftarrow \text{Linearity of } \mathbb{E}[.]$$

$$= \mathbb{E}_{Z} \left[\log \frac{p(Z|X,\theta)}{p(Z)}\right] + \log p(X|\theta) \qquad \leftarrow \mathbb{E}[.] \text{ of a constant}$$
• $\log p(X|\theta) \ge \mathbb{E}_{Z} \left[\log \frac{p(Z|X,\theta)}{p(Z)}\right] + \log p(X|\theta)$

Setting a tight lower bound (2/2)

Ultimate aim: Lower bound of what maximise this we want to maximise

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

First, note that this term* ≤ 0

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

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

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

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 $\mathbb{E}_{\pmb{Z}} \left[\log \frac{p(\pmb{Z}|\pmb{X},\pmb{\theta})}{p(\pmb{Z})} \right] + \log p(\pmb{X}|\pmb{\theta})$
- And that setting $p(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta})$
 - * Makes this RHS as big as possible
 - * Makes this RHS equal to $\log p(X|\theta)$
 - * \rightarrow 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 $z_1, ..., z_n$ denote true origins of the corresponding points $x_1, ..., x_n$. Each z_i is a discrete variable that takes values in 1, ..., k, where k is a number of clusters
- Now compare the original log likelihood

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

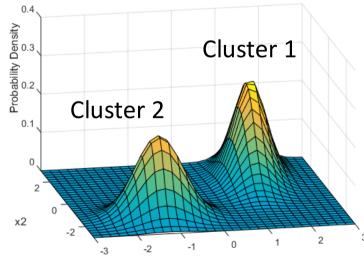
With complete log likelihood (if we knew z)

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

 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 $oldsymbol{Z}$
- EM algorithm handles this uncertainty replacing $\log p(\pmb{X}, \pmb{z}|\pmb{\theta})$ with expectation $\mathbb{E}_{\pmb{Z}|\pmb{X},\pmb{\theta}^{(t)}}[\log p(\pmb{X},\pmb{Z}|\pmb{\theta})]$
- This in turn requires the distribution of $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{(t)})$ given current parameter estimates
- Assuming that Z_i are pairwise independent, we need $P(Z_i = c | \mathbf{x}_i, \boldsymbol{\theta}^{(t)})$
- E.g., suppose $x_i = (-2, -2)$. What is the probability that this point originated from Cluster 1



х1

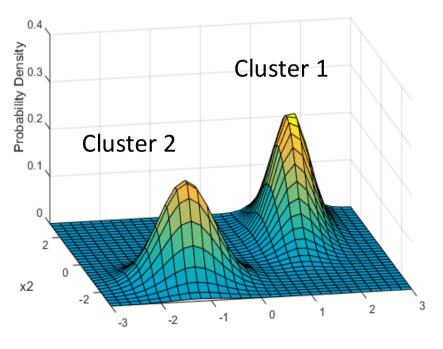
E-step: Cluster responsibilities

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

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

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

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



Expectation step for GMM

To simplify notation, we denote $x_1, ..., x_n$ as X

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

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

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

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

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

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

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

Maximisation step for GMM

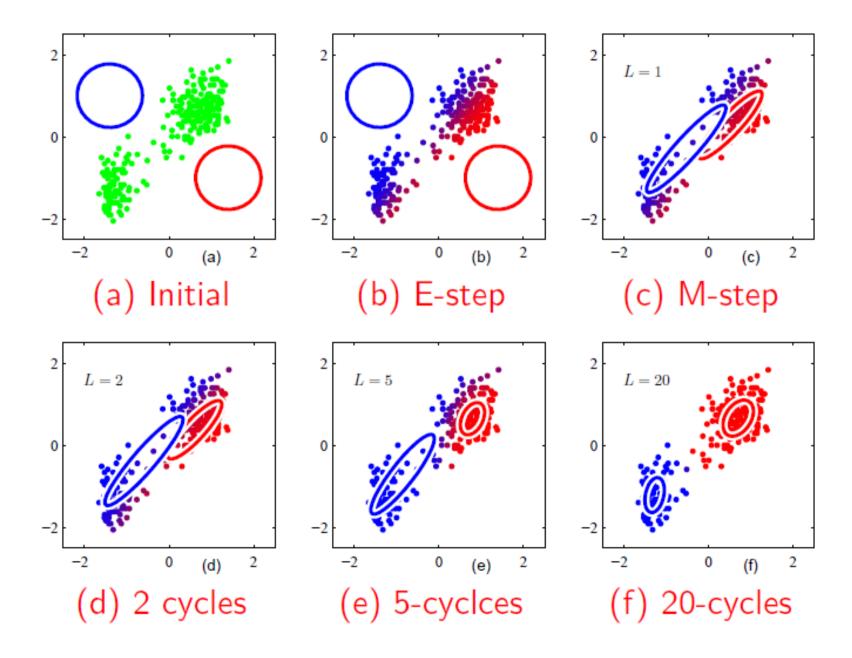
• In the maximisation step, take partial derivatives of $Q(\theta, \theta^{(t)})$ with respect to each of the parameters and set the derivatives to zero to obtain new parameter estimates

•
$$w_c^{(t+1)} = \frac{1}{n} \sum_{i=1}^n r_{ic}$$

•
$$\mu_c^{(t+1)} = \frac{\sum_{i=1}^n r_{ic} x_i}{r_c}$$
* Here $r_c \equiv \sum_{i=1}^n r_{ic}$

• Note that these are the estimates for step (t+1)

Example of fitting Gaussian Mixture model



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 $\Sigma_c = \sigma^2 I$, where I is the identity matrix
- In such a model, only component centroids $oldsymbol{\mu}_c$ 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 μ_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!!!

Summary

- EM as MLE algorithm under latent variables
- Maximise not $\log p(X|\theta)$ but lower bound, alternating:
 - * E-Step: choose $p(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^*)$ raises lower bound up to log-likelihood, for any $\boldsymbol{\theta}^*$
 - * M-Step: θ^* by max'ing "completed" log-likelihood; ideally, easy MLE
- Applying EM to GMM MLE-based training
 - * "New" interpretation of k-means as MLE with constraints