COMS30035, Machine learning: The EM algorithm

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MLE for a Gaussian mixture

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

- No closed form for the MLE
- (At least $K!$ solutions)
- So have to resort to an iterative algorithm where we are only guaranteed a local maximum.
- The algorithm is called the *Expectation-Maximization (EM) algorithm*.

Settings derivatives to zero

$$
\begin{aligned}
\boldsymbol{\mu}_k &= \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\mathbf{x}_n \\
\boldsymbol{\Sigma}_k &= \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})(\mathbf{x}_n-\boldsymbol{\mu}_k)(\mathbf{x}_n-\boldsymbol{\mu}_k)^T \\
\pi_k &= \frac{N_k}{N}
\end{aligned}
$$

where $\gamma(z_{nk}) = p(z_k = 1|\mathbf{x}_n)$ and $N_k = \sum_{n=1}^{N}\gamma(z_{nk})$.

- See [Bis06, §9.22] for the derivation.

EM for Gaussian mixtures

- To initialise the EM algorithm we choose starting values for $\boldsymbol{\mu}$, $\boldsymbol{\Sigma}$ and π.

E step Compute the values for the responsibilities $\gamma(z_{nk})$ given the current parameter values:

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

M step Re-estimate the parameters using the current responsibilities:

$$\begin{aligned}
\boldsymbol{\mu}_k^{\text{new}} &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n \\
\boldsymbol{\Sigma}_k^{\text{new}} &= \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}})^T \\
\pi_k^{\text{new}} &= \frac{N_k}{N}
\end{aligned}$$

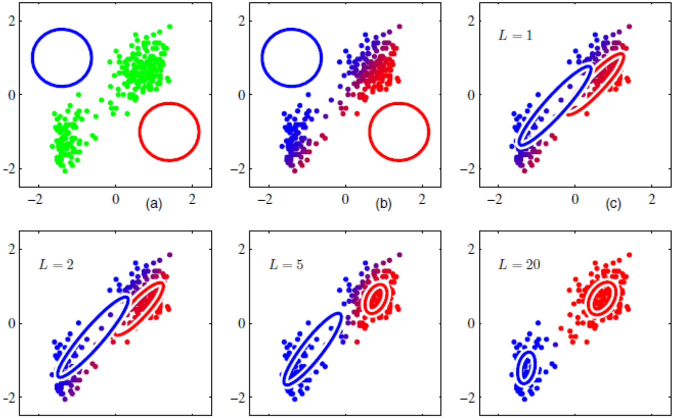
This E-step is just Bayes theorem

$$p(z_k = 1|\mathbf{x}_n) = \frac{p(z_k = 1)p(\mathbf{x}_n|z_k = 1)}{p(\mathbf{x}_n)} = \frac{p(z_k = 1)p(\mathbf{x}_n|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(\mathbf{x}_n|z_j = 1)}$$

The same equation in different notation is:

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

EM in pictures



Why does EM work?

- We have yet to show that each iteration of the EM algorithm increases the log-likelihood $\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$.
- We will do this for the general case:

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

- Z are hidden variables (i.e. not observed) also called *latent variables*.
- $\{X, Z\}$ is the *complete data*. Assume that if we had the complete data then MLE would be easy.
- $\{X\}$ is the *incomplete data*.

Decomposing the log-likelihood

- Let $q(\mathbf{Z})$ be any distribution over the hidden variables.
- We have the following key decomposition of the log-likelihood:

$$\ln p(\mathbf{X}|\boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + \mathrm{KL}(q||p)$$

where

$$\begin{aligned}
\mathcal{L}(q, \boldsymbol{\theta}) &= \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})}{q(\mathbf{Z})} \right\} \\
\mathrm{KL}(q||p) &= -\sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta})}{q(\mathbf{Z})} \right\}
\end{aligned}$$

- An exercise for you: prove that this decomposition is correct (Exercise 9.24 in Bishop). Use the tip Bishop gives on p.451.

Kullback-Leibler divergence

$$\mathrm{KL}(q||p) = -\sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta})}{q(\mathbf{Z})} \right\}$$

- $\mathrm{KL}(p_1||p_2)$ denotes the *Kullback-Leibler divergence* between probability distributions p_1 and p_2.
- KL-divergence is important in, e.g., information theory.
- It's a bit like a 'distance' between two distributions.
- But it is not a true distance since, for example, it is not symmetric.
- $\mathrm{KL}(p_1||p_2) \geq 0$ and $\mathrm{KL}(p_1||p_2) = 0$ if and only if $p_1 = p_2$.

EM: key ideas

$$\ln p(\mathbf{X}|\boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + \mathrm{KL}(q||p)$$

- $\mathrm{KL}(q||p) \geq 0$ for any choice of q, so $\mathcal{L}(q, \boldsymbol{\theta}) \leq \ln p(\mathbf{X}|\boldsymbol{\theta})$.
- In the E-step we increase $\mathcal{L}(q, \boldsymbol{\theta})$ by updating q (and leaving $\boldsymbol{\theta}$ fixed).
- In the M-step we increase $\mathcal{L}(q, \boldsymbol{\theta})$ by updating $\boldsymbol{\theta}$ (and leaving q fixed).
- After the E-step we have $\mathcal{L}(q, \boldsymbol{\theta}) = \ln p(\mathbf{X}|\boldsymbol{\theta})$, so that in the following M-step increasing $\mathcal{L}(q, \boldsymbol{\theta})$ will also increase $\ln p(\mathbf{X}|\boldsymbol{\theta})$.

The E-step

$$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\text{old}}) = \mathcal{L}(q, \boldsymbol{\theta}^{\text{old}}) + \mathrm{KL}(q||p)$$

- In the E-step we update q but leave $\boldsymbol{\theta}^{\text{old}}$ fixed.
- $\mathrm{KL}(q||p) = 0$ when $q = p$, so to maximise $\mathcal{L}(q, \boldsymbol{\theta}^{\text{old}})$ we set $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})$.
- This increases $\mathcal{L}(q, \boldsymbol{\theta}^{\text{old}})$ but not $\ln p(\mathbf{X}|\boldsymbol{\theta}^{\text{old}})$.
- [Bis06, Fig 9.12] illustrates the E-step.

The M-step

$$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\text{new}}) = \mathcal{L}(q, \boldsymbol{\theta}^{\text{new}}) + \mathrm{KL}(q||p)$$

$$\mathcal{L}(q, \boldsymbol{\theta}) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})}{q(\mathbf{Z})} \right\} = \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \; p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}) - \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln q(\mathbf{Z})$$

- In the M-step we find parameters $\boldsymbol{\theta}^{\text{new}}$ which maximise $\mathcal{L}(q, \boldsymbol{\theta})$, while leaving q fixed.
- This will necessarily increase $\ln p(\mathbf{X}|\boldsymbol{\theta})$ since $\mathrm{KL}(q||p) \geq 0$.
- In fact we get a 'bonus' since changing p from $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})$ to $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{new}})$ will (typically) lead $\mathrm{KL}(q||p)$ to increase from 0 to some positive value.
- [Bis06, Fig 9.13] illustrates the M-step.

Visualising EM

- David Barber (from UCL) provides a nice visualisation for EM (where the latent variable is binary).
- It's Fig 11.2 on p.259 of his book [Bar12].

Back to Gaussian mixtures

- In the standard case of independent and identically distributed (i.i.d.) dataset $\mathbf{X}$, we get:

$$p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}) = \prod_{n=1}^{N} p(\mathbf{z}_n|\mathbf{x}_n, \boldsymbol{\theta})$$

- In the case of Gaussian mixtures the responsibilities $\gamma(z_{nk})$ define the $p(\mathbf{z}_n|\mathbf{x}_n, \boldsymbol{\theta})$.
- So computing the responsibilities is the E-step.
- And the M-step we saw on slide 4 does indeed maximise $\mathcal{L}(q, \boldsymbol{\theta})$ given the current responsibilities.
- Proving this is Exercises 9.8 and 9.9 in Bishop.

David Barber.
Bayesian Reasoning and Machine Learning.
Cambridge University Press, 2012.

Christopher M. Bishop.
Pattern Recognition and Machine Learning.
Springer, 2006.