PRML学习笔记——第九章

Mixture Models and EM

9.1 K-means Clustering

假设现在有一笔data set$\{\mathbf{x}_1,\ldots,\mathbf{x}_N\}$,我们的目标是将dataset划分成$K$(某个数)个clusters.直觉上,同一clusters内的data之间的距离应该比较小,属于不同clusters的data会有较大的距离.我们可以引入每个custer的中心$\boldsymbol{\mu}_k$,再引入一个符号r_{nk},如果第n个data point属于第k类,那么值就是1,其余为0.如此可以将我们的直觉用表达式写出:

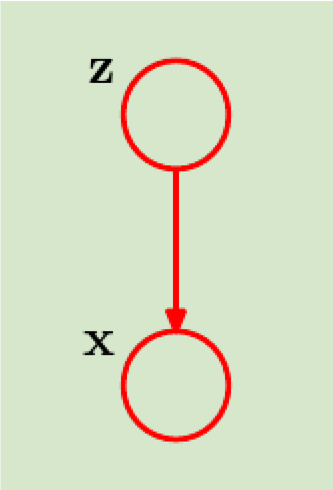
$$J=\sum_{n=1}^{N}\sum_{k=1}^{K}r_{nk}||\mathbf{x}_n-\boldsymbol{\mu}_k||^2$$

现在的目标就是minimize J.

对于这个优化问题可以采用交替优化.先固定$\boldsymbol{\mu}$,关于r_{nk}优化;再根据固定的r_{nk}优化$\boldsymbol{\mu}$.

然而Kmeans有个问题是硬聚类,无法体现某个data point属于某个类的概率,后面的GMM就能解决这个问题.

9.2. Mixtures of Gaussians



其中$\mathbf{z}$是一个1-of-K code:$z_k \in \{0,1\}$,并且$\sum_k z_k = 1$.,一个latent variable,$\mathbf{x}$是一个Gaussian.

设$p(z_k = 1) = \pi_k$,并且$\{\pi_k\}$满足:

$$\begin{array}{l} 0 \leqslant \pi_k \leqslant 1 \\ \sum_{k=1}^{K} \pi_k = 1 \end{array}$$

这样就能表示z的marginal distribution:

$$p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{zk}$$

$\mathbf{x}$的conditional distribution:

$$p(\mathbf{x} \mid \mathbf{z}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{zk}$$

有了这两个概率就能计算$\mathbf{x}$的marginal和$\mathbf{z}$的posterior(responsibility):

$$\begin{aligned} p(\mathbf{x}) &= \sum_{\mathbf{z}} p(\mathbf{z}) p(\mathbf{x} \mid \mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right) \\ \gamma\left(z_k\right) \equiv p\left(z_k = 1 \mid \mathbf{x}\right) &= \frac{p\left(z_k = 1\right) p\left(\mathbf{x} \mid z_k = 1\right)}{\sum_{j=1}^{K} p\left(z_j = 1\right) p\left(\mathbf{x} \mid z_j = 1\right)} \\ &= \frac{\pi_k \mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)}{\sum_{j=1}^{K} \pi_j \mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\right)} \end{aligned}$$

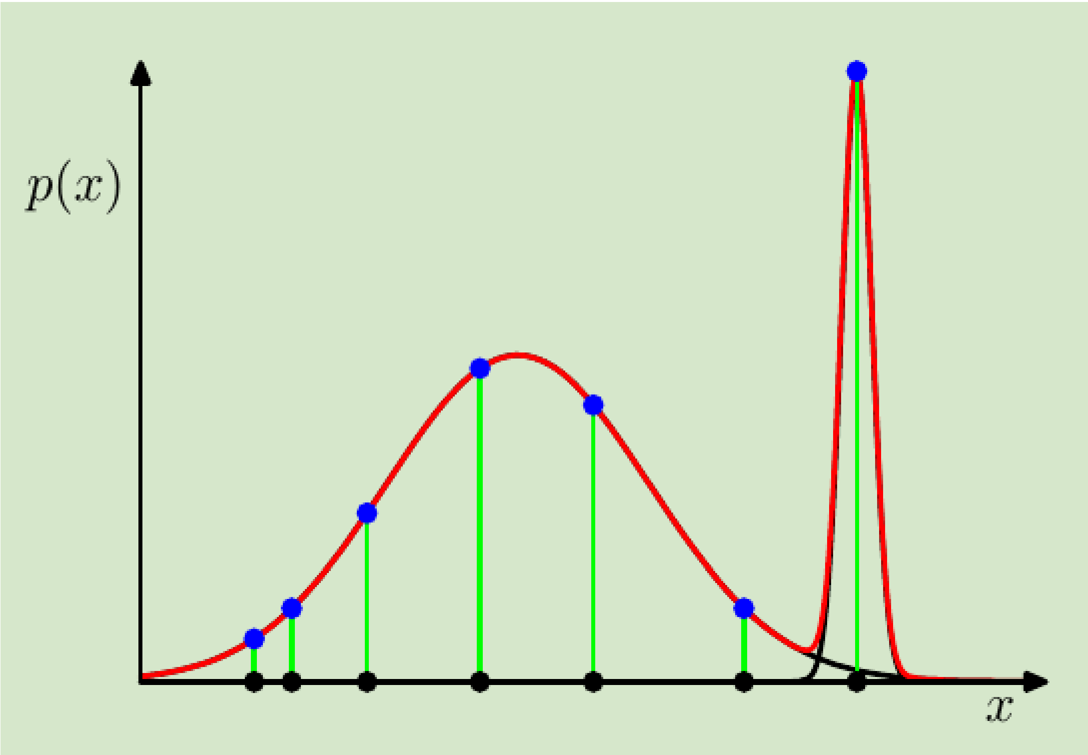
9.2.1 Maximum likelihood

简单的取logarithm会得到:

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

现在要考虑maximize这个式子的问题.

1. 当某一个子Gaussian的mean正好落在了某个data point上,只要将其$\sigma \to 0$就可以使likelihood无穷大,但这显然不是我们需要的solution(严重的over-fitting)
2. 有$K!$个对称solution
3. maximize这个likelihood无法得到closed form solution



严重over-fitting的一个demo

9.2.2 EM for Gaussian mixtures

前面已经给出了log of likelihood的表达式,如果我们直接对其关于参数($\boldsymbol{\mu}_k$)求导令为0:

$$0 = -\sum_{n=1}^{N} \underbrace{\frac{\pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}}_{\gamma(z_{nk})} \boldsymbol{\Sigma}_k (\mathbf{x}_n - \boldsymbol{\mu}_k)$$

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n$$

其中$N_k=\sum_{n=1}^{N} \gamma\left(z_{nk}\right)$.这里的$\gamma$其实就是上节中的posterior.尽管$\gamma$中也依赖于未知参数,我们可以把这个均值理解为对所有data point的weighted average,并且weight是这个data point属于这个类的posterior.这样一看其实就是kmeans的general情况!

类似地,对于其余参数($, \boldsymbol{\Sigma}_k, \pi_k$)求导,可以得到:

$$\boldsymbol{\Sigma}_k=\frac{1}{N_k} \sum_{n=1}^{N} \gamma\left(z_{nk}\right)\left(\mathbf{x}_n-\boldsymbol{\mu}_k\right)\left(\mathbf{x}_n-\boldsymbol{\mu}_k\right)^{\mathrm{T}}$$
$$\pi_k=\frac{N_k}{N}$$

虽然不能直接获得closed form solution,但用kmeans的求解过程,迭代可以解出local maximum solution.

9.3. An Alternative View of EM

再回顾含latent variable的MLE问题:

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

问题的关键就在于log内的sum导致表达式的特别复杂.所以现在的出发点就在于去掉这个log内的sum.

那么sum是怎么来的?是由于要marginal这个joint distribution得到$p(\mathbf{X})$,那么我们就先不考虑marginal这一步,直接让log计算这个joint distribution.那么就会有$\ln p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$.

但是不能直接求这个joint distribution最大,因为这里面的latent variable是unobversed.所以引入了一个期望函数:

$$\mathcal{Q}\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}\right)=\sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \boldsymbol{\theta}^{\text{old}}\right) \ln p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta}).$$

可以看到这里使用一个posterior(已知量)来求对$\ln p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$的期望.成功消去了$\mathbf{Z}$的影响,并且现在的表达式依然是trackable的.
最后再解出$\mathcal{Q}$的maximum.由于开始用的posterior是不准的,所以还得继续交替计算和更新.这就是EM算法.

9.3.1 Gaussian mixtures revisited

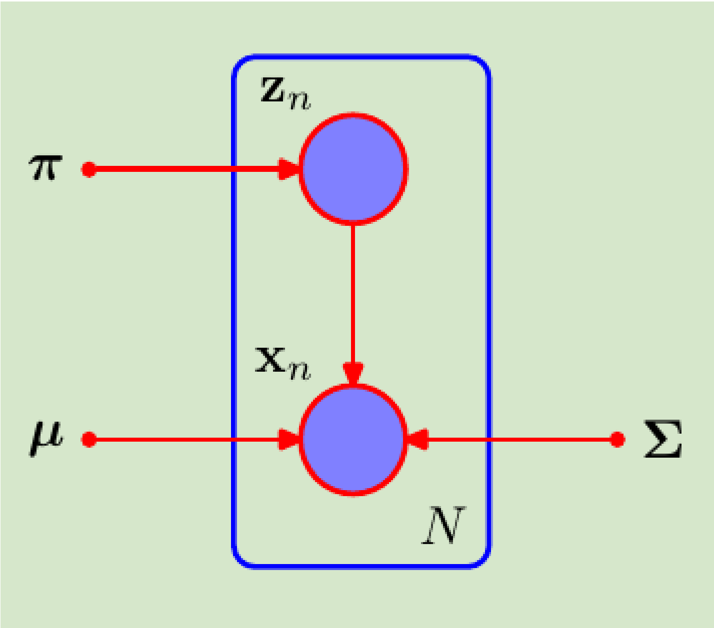
我们如果假设latent variable z也被观测,那么likelihood就变为:

$$p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi})=\prod_{n=1}^{N} \prod_{k=1}^{K} \pi_k^{z_{nk}} \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)^{z_{nk}}$$

如果我们对现在这个likelihood做logarithm:

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

容易知道现在这个maximum问题是可以获得closed form的,其中z_{nk}是binary variable.



当latent variable也被观测时对应的PG

我们假设了z已被观测,但实际上z取值是没有被观测的,但我们可以表示z的posterior:

$$p(\mathbf{Z} \mid \mathbf{X}, \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) \propto \prod_{n=1}^{N} \prod_{k=1}^{K} \left[\pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)\right]^{z_{nk}}$$

利用这个posterior可以对log likelihood取期望.利用$\{\mathbf{z}_n\}$之间是independent可以将求和的期望交换到最内层就是对z_{nk}求期望:

$$\begin{aligned}
\mathbb{E}\left[z_{nk}\right] &= \frac{\sum_{z_{nk}} z_{nk}\left[\pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)\right]^{z_{nk}}}{\sum_{z_{nj}}\left[\pi_j \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\right)\right]^{z_{nj}}} \\
&= \frac{\pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)}{\sum_{j=1}^{K} \pi_j \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\right)} = \gamma\left(z_{nk}\right)
\end{aligned}$$

完整的maximum式子为:

$$\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi})] = \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma\left(z_{nk}\right)\left\{\ln \pi_k + \ln \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)\right\}$$

可以看到这和之前求解GMM的式子是一样的.

9.3.2 Relation to K-means

假设GMM中的每一个Gaussian component的covariance都是同样一个数量矩阵$\epsilon\mathbf{I}$,那么当这个$\epsilon \rightarrow 0$时,
γ的分母中除了$||\mathbf{x}_n-\boldsymbol{\mu}_j||$最小的项趋于0最慢,其余项都是0,所以最后$\gamma$就变成了kmeans中的$r_{nk}$.同样地,complete-data的期望也会和kmenas的目标函数等价:

$$\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi})] \rightarrow -\frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk}\left\|\mathbf{x}_{n}-\boldsymbol{\mu}_{k}\right\|^{2}+\text{ const. }$$

9.3.3 Mixtures of Bernoulli distributions

这节将GMM的Gaussian变为discrete的bernoulli distribution:

$$p(\mathbf{x} \mid \boldsymbol{\mu})=\prod_{i=1}^{D} \mu_{i}^{x_{i}}\left(1-\mu_{i}\right)^{\left(1-x_{i}\right)}$$

引入和GMM一样的latent variable:

$$p(\mathbf{z} \mid \boldsymbol{\pi})=\prod_{k=1}^{K} \pi_{k}^{z_{k}}$$

conditional distribution为:

$$p(\mathbf{x} \mid \mathbf{z}, \boldsymbol{\mu})=\prod_{k=1}^{K} p\left(\mathbf{x} \mid \boldsymbol{\mu}_{k}\right)^{z_{k}}$$

根据EM算法的思想,首先是求complete-data的log likelihood:

$$\begin{array}{l}\ln p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\mu}, \boldsymbol{\pi})=\sum_{n=1}^{N} \sum_{k=1}^{K} z_{n k}\left\{\ln \pi_{k}\right. \\ \left.+\sum_{i=1}^{D}\left[x_{n i} \ln \mu_{k i}+\left(1-x_{n i}\right) \ln \left(1-\mu_{k i}\right)\right]\right\}\end{array}$$

$\mathbf{E}$-Step:

$$\gamma\left(z_{nk}\right)=\mathbb{E}\left[z_{nk}\right]=\frac{\sum_{z_{nk}} z_{nk}\left[\pi_k p\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k\right)\right]^{z_{nk}}}{\sum_{z_{nj}}\left[\pi_j p\left(\mathbf{x}_n \mid \boldsymbol{\mu}_j\right)\right]^{z_{nj}}}$$
$$=\frac{\pi_k p\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k\right)}{\sum_{j=1}^K \pi_j p\left(\mathbf{x}_n \mid \boldsymbol{\mu}_j\right)}$$

$\mathbf{M}$-Step:
求maximum:

$$\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\mu}, \boldsymbol{\pi})]=\sum_{n=1}^N \sum_{k=1}^K \gamma\left(z_{nk}\right)\left\{\ln \pi_k\right.$$
$$\left.+\sum_{i=1}^D\left[x_{ni} \ln \mu_{ki}+\left(1-x_{ni}\right) \ln \left(1-\mu_{ki}\right)\right]\right\}$$

9.4. The EM Algorithm in General

我们要优化的目标是这样一个likelihood:

$$p(\mathbf{X} \mid \boldsymbol{\theta})=\sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta})$$

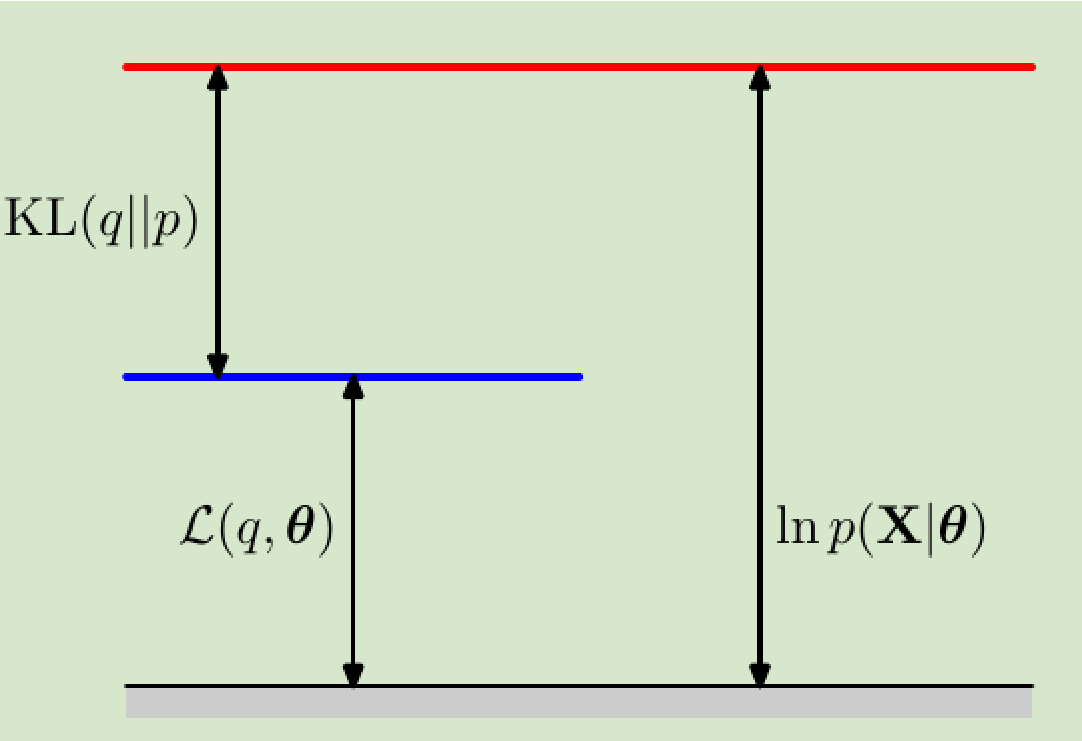
直接优化是困难的,但通过分解:

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

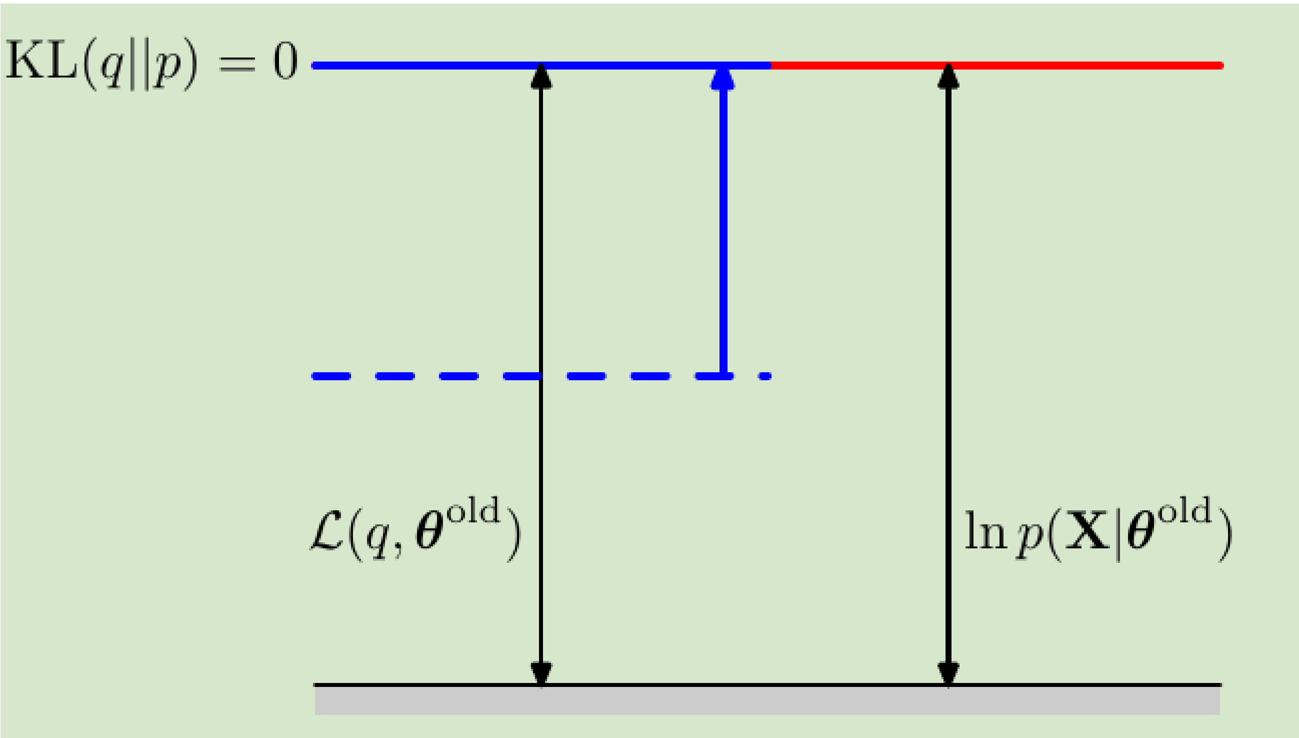
其中

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

其中KL的性质是大于等于0,当且仅当$q(\mathbf{Z})=p(\mathbf{Z} \mid \mathbf{X}, \boldsymbol{\theta})$时为0.



分解图示,$\mathcal{L}$是优化目标的一个lower bound,E-step得到的posterior就是q,使得lower bound等于优化目标.

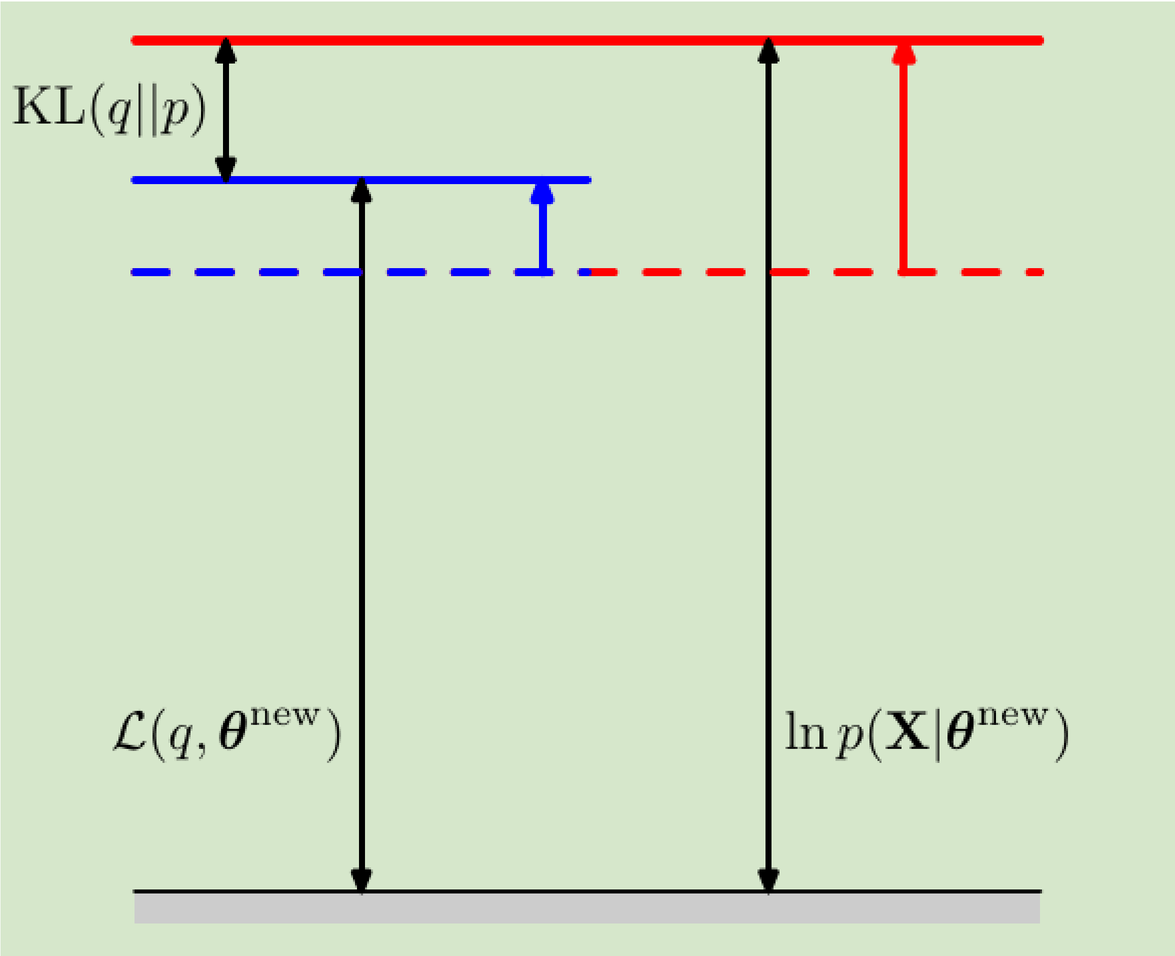


E-step结束后,KL=0了

对于lower bound,如果将E-step得到的posterior带入q:

$$\begin{aligned}\mathcal{L}(q, \boldsymbol{\theta}) &= \sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \boldsymbol{\theta}^{\mathrm{old}}\right) \ln p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta}) - \sum_{\mathbf{Z}} p\left(\mathbf{Z} \mid \mathbf{X}, \boldsymbol{\theta}^{\mathrm{old}}\right) \ln p\left(\mathbf{Z} \mid \mathbf{X}, \boldsymbol{\theta}^{\mathrm{old}}\right) \\ &= \mathcal{Q}\left(\boldsymbol{\theta}, \boldsymbol{\theta}^{\mathrm{old}}\right) + \text{const}\end{aligned}$$

那么在M-step优化Q实际就是在优化lower bound.



M-step优化lower bound,使得$\mathcal{L}$达到最大,值得注意的是,KL项用的还是旧的θ此时KL>0

这样交替更新,确保了最终优化目标始终increase(除非达到local maximum).

EM算法还能被用于maximize posterior:

$$\ln p(\boldsymbol{\theta} \mid \mathbf{X}) = \ln p(\boldsymbol{\theta}, \mathbf{X}) - \ln p(\mathbf{X})$$

套用前面的分解结果:

$$\begin{aligned}\ln p(\boldsymbol{\theta} \mid \mathbf{X}) &= \mathcal{L}(q, \boldsymbol{\theta}) + \mathrm{KL}(q\|p) + \ln p(\boldsymbol{\theta}) - \ln p(\mathbf{X}) \\ &\geqslant \mathcal{L}(q, \boldsymbol{\theta}) + \ln p(\boldsymbol{\theta}) - \ln p(\mathbf{X}).\end{aligned}$$

这里优化的parameter是θ,$\ln p(\mathbf{x})$就可以看作constant,那么相比于之前的EM算法,这里更新的时候只会在M-step增加一项prior $p(\theta)$.