Mixture Models

- We will look at the mixture models, including Gaussian mixture models and mixture of Bernoulli.

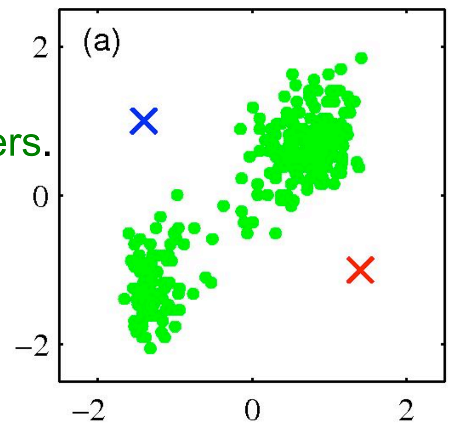
- The key idea is to introduce latent variables, which allows complicated distributions to be formed from simpler distributions.

- We will see that mixture models can be interpreted in terms of having discrete latent variables (in a directed graphical model).

- Later in class, we will also look at the continuous latent variables.

K-Means Clustering

- Let us first look at the following problem: Identify clusters, or groups, of data points in a multidimensional space.
- We observe the dataset $\{\mathbf{x_1}, ..., \mathbf{x}_N\}$ consisting of N D-dimensional observations
- We would like to partition the data into K clusters, where K is given.
- We next introduce D-dimensional vectors, prototypes, $\boldsymbol{\mu}_k, k = 1, ..., K.$
- We can think of μ_k as representing cluster centers.
- Our goal:
  - Find an assignment of data points to clusters.
  - Sum of squared distances of each data point to its closest prototype is at the minimum.



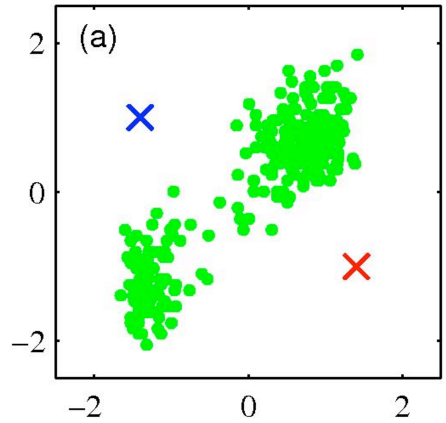
K-Means Clustering

- For each data point $\mathbf{x}_n$ we introduce a binary vector $\mathbf{r}_n$ of length K (1-of-K encoding), which indicates which of the K clusters the data point $\mathbf{x}_n$ is assigned to.
- Define objective (distortion measure):

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

- It represents the sum of squares of the distances of each data point to its assigned prototype μ_k.

- Our goal it find the values of r_{nk} and the cluster centers μ_k so as to minimize the objective J.



Iterative Algorithm

- Define iterative procedure to minimize:

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

- Given μ_k, minimize J with respect to r_{nk} (**E-step**):

Hard assignments of points to clusters.

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j ||\mathbf{x}_n - \boldsymbol{\mu}_j||^2 \\ 0 & \text{otherwise} \end{cases}$$

which simply says assign n^{th} data point $\mathbf{x}_n$ to its closest cluster center.

- Given r_{nk}, minimize J with respect to μ_k (**M-step**):

$$\boldsymbol{\mu}_k = \frac{\sum_n r_{nk} \mathbf{x}_n}{\sum_n r_{nk}}.$$

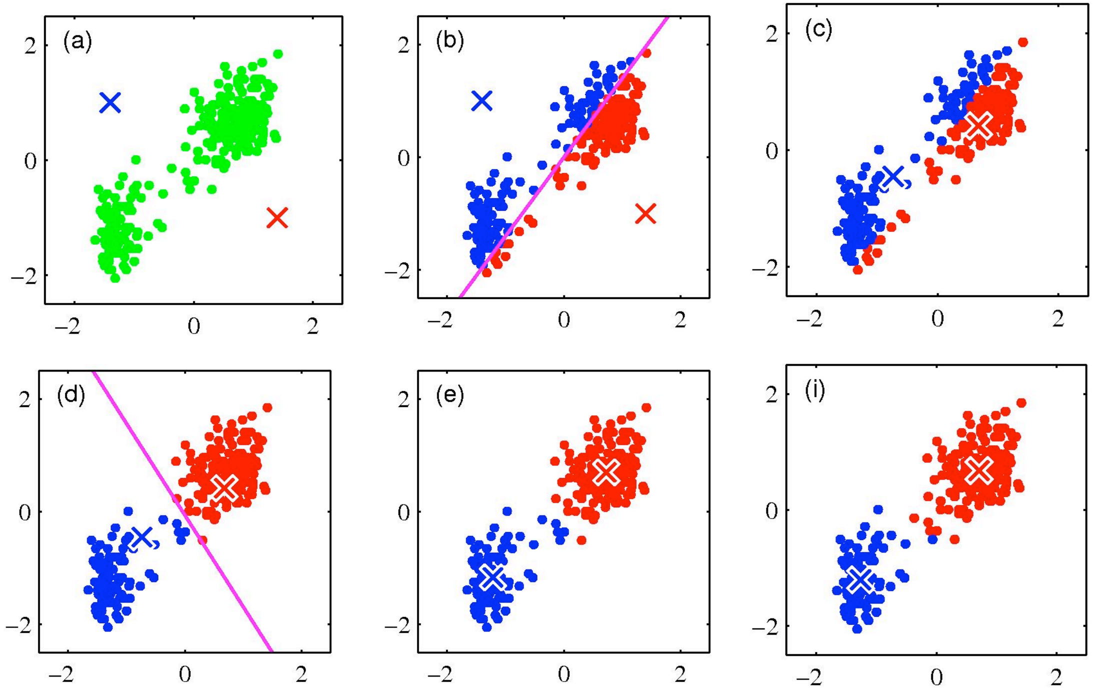
Number of points assigned to cluster k.

Set μ_k equal to the mean of all the data points assigned to cluster k.

- Guaranteed convergence to local minimum (not global minimum).

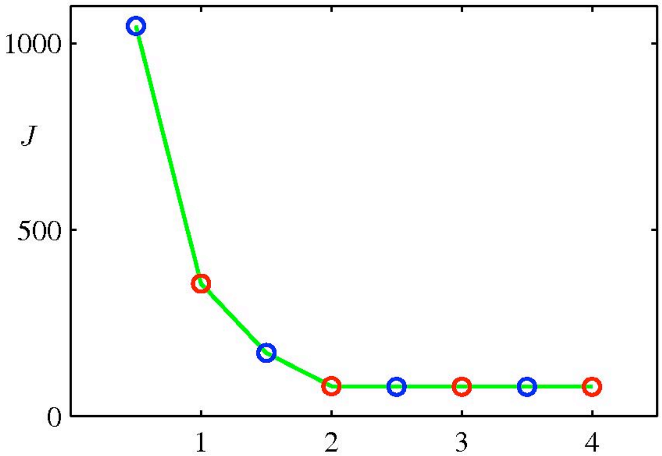
Example

- Example of using K-means (K=2) on Old Faithful dataset.



Convergence

• Plot of the cost function after each E-step (blue points) and M-step (red points)



The algorithm has converged after 3 iterations.

• K-means can be generalized by introducing a more general dissimilarity measure:

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} K(\mathbf{x}_n, \boldsymbol{\mu}_k).$$

Image Segmentation

- Another application of K-means algorithm.
- Partition an image into regions corresponding, for example, to object parts.
- Each pixel in an image is a point in 3-D space, corresponding to R,G,B channels.

- For a given value of K, the algorithm represent an image using K colors.

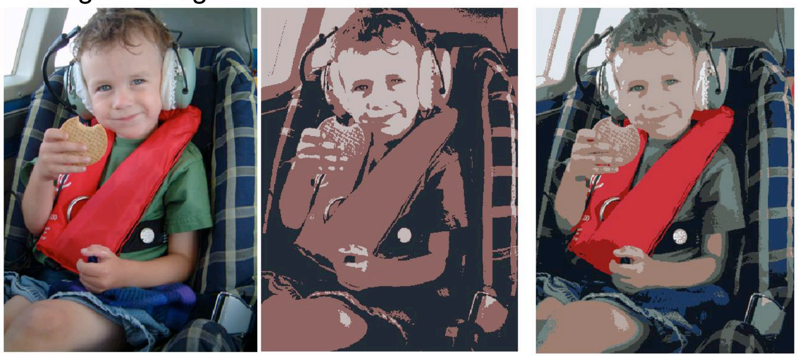
- Another application is image compression.

Image Compression

- For each data point, we store only the identity k of the assigned cluster.
- We also store the values of the cluster centers μ_k.
- Provided K $\ll$ N, we require significantly less data.

编码还能进一步压缩

Original image K=3 K=10



- The original image has 240 $\times$ 180 = 43,200 pixels.
- Each pixel contains {R,G,B} values, each of which requires 8 bits.

- Requires 43,200 $\times$ 24 = 1,036,800 bits to transmit directly.
- With K-means, we need to transmit K code-book vectors μ_k -- 24K bits.
- For each pixel we need to transmit $\log_2$K bits (as there are K vectors).
- Compressed image requires 43,248 (K=2), 86,472 (K=3), and 173,040 (K=10) bits, which amounts to compression rations of 4.2%, 8.3%, and 16.7%.

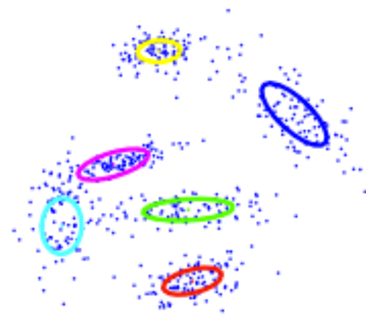
$$p(x) = \sum_{k=1}^{K} \pi_k N(x \mid \mu_k, \Sigma_k)$$

Mixture of Gaussians

- We will look at mixture of Gaussians in terms of discrete latent variables.

- The Gaussian mixture can be written as a linear superposition of Gaussians:

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_K).$$



- Introduce K-dimensional binary random variable **z** having a 1-of-K representation:

$$z_k \in \{0, 1\}, \quad \sum_k z_k = 1.$$ 表达属于哪个高斯

- We will specify the distribution over **z** in terms of mixing coefficients: 混合比

$$p(z_k = 1) = \pi_k, \quad 0 \le \pi_k \le 1, \quad \sum_k \pi_k = 1.$$

$$p(x, z) = p(z)\, p(x|z) = \pi_k N(\mu_k, \Sigma_k)$$

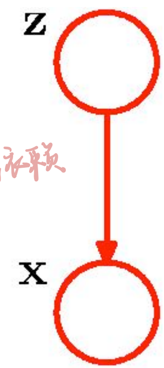
$$p(x|z) = N(\mu_k, \Sigma_k)$$

$$p(x) = \sum p(x, z) = \sum_k \pi_k N(\mu_k, \Sigma_k).$$

Mixture of Gaussians

- Because **z** uses 1-of-K encoding, we have:

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



互相依赖

- We can now specify the conditional distribution:

$$p(\mathbf{x}|z_k = 1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k), \text{ or } p(\mathbf{x}|\mathbf{z}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_k}.$$

- We have therefore specified the joint distribution: 联合

$$p(\mathbf{x}, \mathbf{z}) = p(\mathbf{x}|\mathbf{z})p(\mathbf{z}).$$

- The marginal distribution over **x** is given by: 边缘

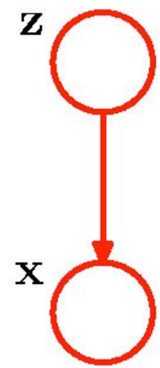
$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{z})p(\mathbf{x}|\mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).$$

- The marginal distribution over **x** is given by a Gaussian mixture.

Mixture of Gaussians

• The marginal distribution:

$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{z}) p(\mathbf{x}|\mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k).$$



• If we have several observations $\mathbf{x}_1,\ldots,\mathbf{x}_N$, it follows that for every observed data point $\mathbf{x}_n$, there is a corresponding latent variable $\mathbf{z}_n$.

• Let us look at the conditional p(**z**|**x**), responsibilities, which we will need for doing inference:

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

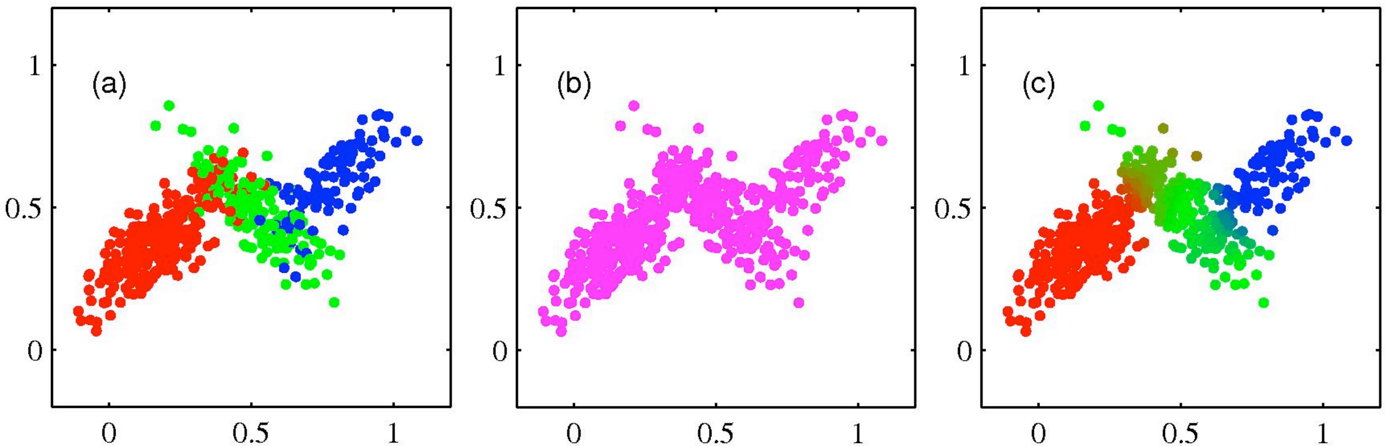
responsibility that component k takes for explaining the data x

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

• We will view π_k as prior probability that z_k=1, and $\gamma(z_k)$ is the corresponding posterior once we have observed the data.

Example

- 500 points drawn from a mixture of 3 Gaussians.



Samples from the joint distribution p(**x**,**z**).

Samples from the marginal distribution p(**x**).

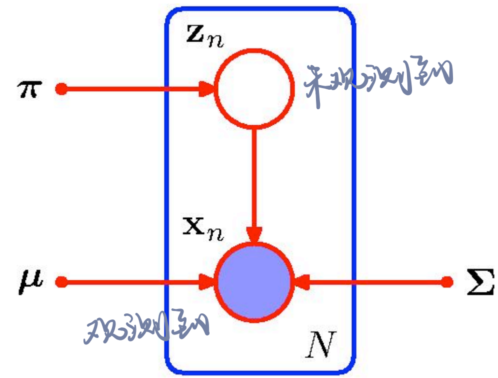
Same samples where colors represent the value of responsibilities.

Maximum Likelihood

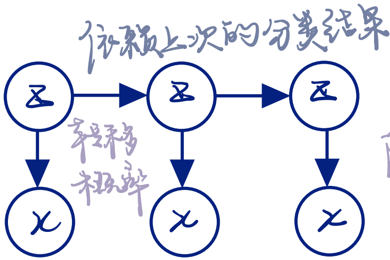
- Suppose we observe a dataset $\{\mathbf{x}_1,\ldots,\mathbf{x}_N\}$, and we model the data using mixture of Gaussians.
- We represent the dataset as an N by D matrix **X**.
- The corresponding latent variables will be represented and an N by K matrix **Z**.
- The log-likelihood takes form:

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

Model parameters



Graphical model for a Gaussian mixture model for a set of i.i.d. data point $\{\mathbf{x}_n\}$, and corresponding latent variables $\{\mathbf{z}_n\}$.



隐马尔可夫

n x x_dim

n x x_dim

Maximum Likelihood

- The log-likelihood:

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

- Differentiating with respect to μ_k and setting to zero:

无约束,较好优化

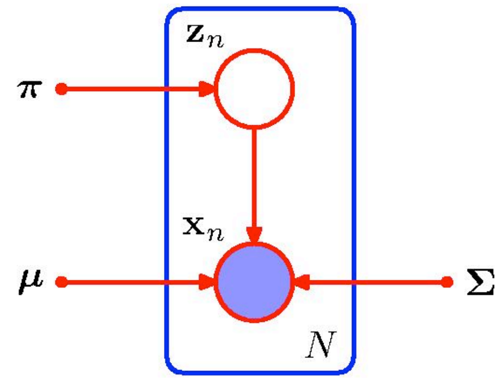
$$0 = \sum_{n} \underbrace{\frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}}_{\gamma(z_{nk})} \boldsymbol{\Sigma}_K^{-1}(\mathbf{x}_n - \boldsymbol{\mu}_k).$$

自己算一下

Soft assignment

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

γ和μ
互相依赖
⇒ 迭代



- We can interpret N_k as effective number of points assigned to cluster k.

- The mean μ_k is given by the mean of all the data points weighted by the posterior $\gamma(z_{nk})$ that component k was responsible for generating $\mathbf{x}_n$.

kMeans实际上是特殊的GMM

高斯混合模型

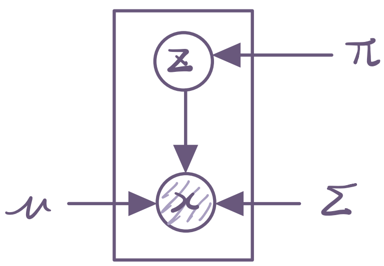
1、定义

几何角度 $p(x) = \sum_k \pi_k N(x \mid \mu_k, \Sigma_k)$

$$\begin{cases} 0 \le \pi_k \le 1 \\ \sum_k \pi_k = 1 \end{cases}$$

生成角度

概率图 z：隐变量



x：观测变量

$$p(z_k=1) = \pi_k$$

$$p(x \mid z_k=1) = N(x \mid \mu_k, \Sigma_k)$$

$$p(x) = \sum_k p(x, z) = \sum_k p(z_k=1)\, p(x \mid z_k=1)$$

$$= \sum_k \pi_k N(x \mid \mu_k, \Sigma_k)$$

2、极大似然

$$\theta = \{\mu_1, \mu_2, \dots, \mu_k; \Sigma_1, \Sigma_2, \dots, \Sigma_k; \pi_1, \pi_2, \dots, \pi_k\}$$

$$\hat{\theta}_{MLE} = \arg\max_\theta \ln p(x)$$

$$= \arg\max_\theta \sum_{n=1}^{N} \ln p(x_n)$$

$$= \arg\max_\theta \sum_{n=1}^{N} \ln \sum_k \pi_k N(x_n \mid \mu_k, \Sigma_k)$$

注：单一高斯分布可以用MLE求出解析解

$$\hat{\theta}_{MLE} = \arg\max_\theta \sum_{n=1}^{N} \ln N(x_n \mid \mu, \Sigma)$$

$$= \arg\max_\theta \sum_{n=1}^{N} \ln (2\pi)^{-\frac{D}{2}} |\Sigma|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(x_n-\mu)^T \Sigma^{-1} (x_n-\mu)\right)$$

$$= \arg\max_\theta \sum_{n=1}^{N} -\frac{D}{2}\ln(2\pi) - \frac{1}{2}\ln|\Sigma| - \frac{1}{2}(x_n-\mu)^T \Sigma^{-1} (x_n-\mu)$$

分别关于 μ, Σ 偏导为0，可以求得解析解

但高斯混合模型无法用MLE求解析解

$$\sum_{i=1}^{N} \ln \sum_{k} \pi_k N(x_n \mid \mu_k, \Sigma_k)$$

对数内是求和形式，形式复杂，求偏导后无法求解方程组

(算不出来！)

GMM不能用MLE求解析解，但可以用EM算法迭代求解

- 为什么单一高斯没有奇异性问题？混合高斯就有？

我应该是懂了！

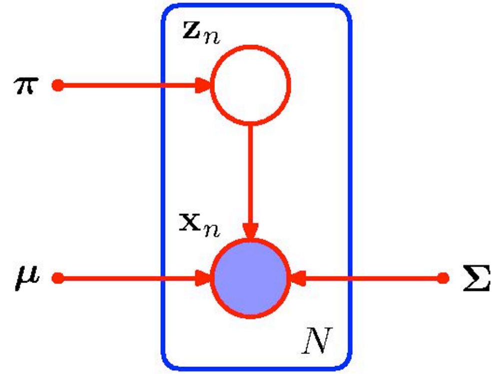
Maximum Likelihood

- The log-likelihood:

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

- Differentiating with respect to Σ_k and setting to zero:

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



- Note that the data points are weighted by the posterior probabilities.
- Maximizing log-likelihood with respect to mixing proportions:

$$\pi_k = \frac{N_k}{N}.$$

- Mixing proportion for the kth component is given by the average responsibility which that component takes for explaining the data.

Maximum Likelihood

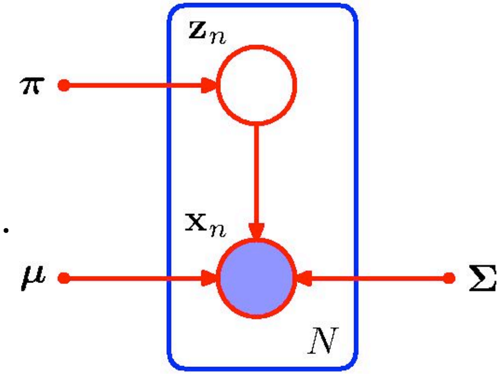
- The log-likelihood:

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

- Note that the maximum likelihood does not have a closed form solution.

- Parameter updates depend on responsibilities $\gamma(z_{nk})$, which themselves depend on those parameters:

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



- Iterative Solution:

  E-step: Update responsibilities $\gamma(z_{nk})$.
  M-step: Update model parameters π_k, μ_k, Σ_k, for k=1,…,K.

EM algorithm

- Initialize the means μ_k, covariances Σ_k, and mixing proportions π_k.
- E-step: Evaluate responsibilities using current parameter values:

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

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

$$\boldsymbol{\mu}_k^{new} = \frac{1}{N_k} \sum_n \gamma(z_{nk}) \mathbf{x}_n, \quad N_k = \sum_n \gamma(z_{nk}),$$

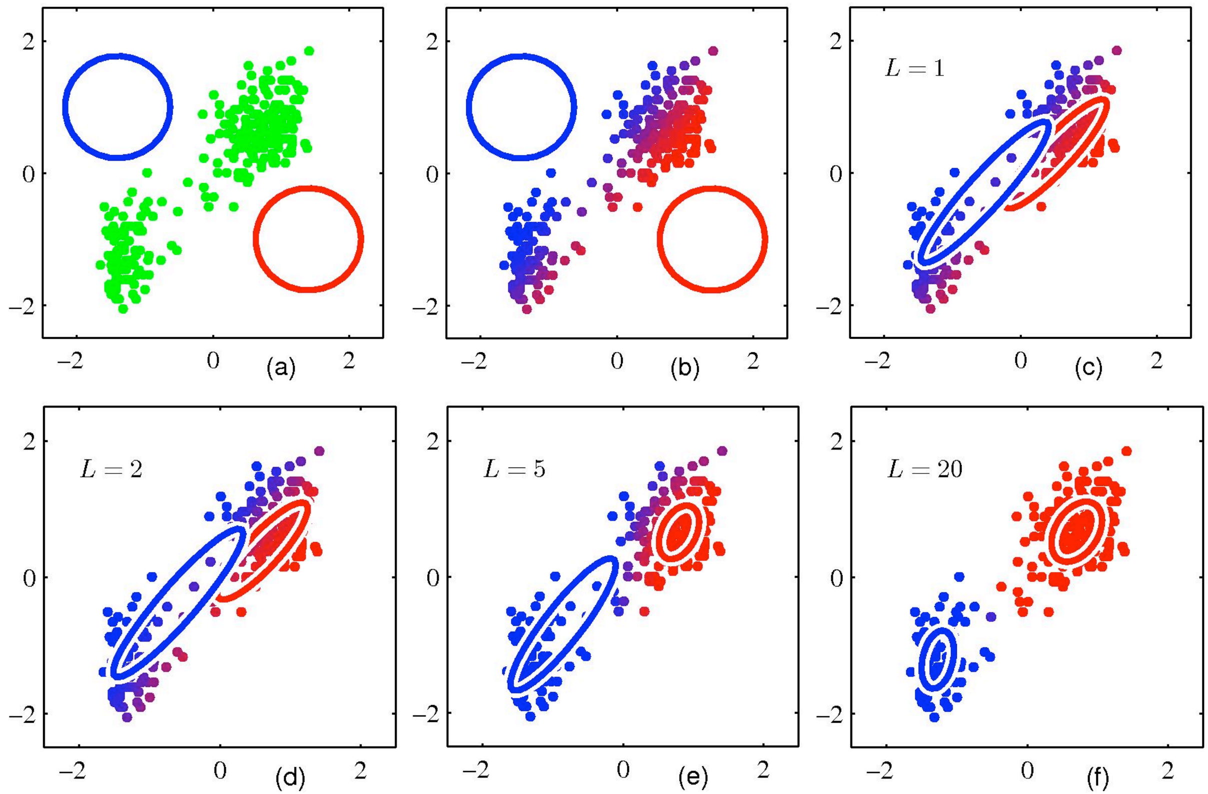
$$\boldsymbol{\Sigma}_k^{new} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(y_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T,$$

$$\pi_k^{new} = \frac{N_k}{N}.$$

- Evaluate the log-likelihood and check for convergence.

Mixture of Gaussians: Example

- Illustration of the EM algorithm (much slower convergence compared to K-means)

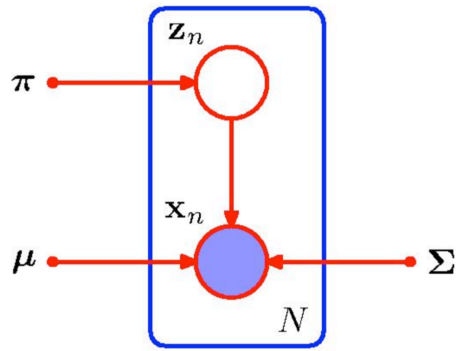


一个高斯只解释了一个样本：崩塌

An Alternative View of EM

- The goal of EM is to find maximum likelihood solutions for models with latent variables.
- We represent the observed dataset as an N by D matrix **X**.
- Latent variables will be represented and an N by K matrix **Z**.
- The set of all model parameters is denoted by θ.
- The log-likelihood takes form:

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



- Note: even if the joint distribution belongs to exponential family, the marginal typically does not!
- We will call:

$\{\mathbf{X}, \mathbf{Z}\}$ as complete dataset.

$\{\mathbf{X}\}$ as incomplete dataset.

An Alternative View of EM

• In practice, we are not given a complete dataset {**X**,**Z**}, but only incomplete dataset {**X**}.

• Our knowledge about the latent variables is given only by the posterior distribution p(**Z**|**X**,θ).

• Because we cannot use the complete data log-likelihood, we can consider expected complete-data log-likelihood:

May seem ad-hoc.

$$\mathcal{Q}(\theta, \theta^{old}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{old}) \ln p(\mathbf{X}, \mathbf{Z}|\theta).$$

联合似然

$p(x,z|\theta)=p(z|x,\theta)p(x|\theta)$

• In the E-step, we use the current parameters θ^{old} to compute the posterior over the latent variables p(**Z**|**X**,θ^{old}).

• We use this posterior to compute expected complete log-likelihood.

• In the M-step, we find the revised parameter estimate θ^{new} by maximizing the expected complete log-likelihood:

$$\theta^{new} = \arg\max_{\theta} \mathcal{Q}(\theta, \theta^{old}).$$

Tractable

The General EM algorithm

- Given a joint distribution p(**Z**,**X**|θ) over observed and latent variables governed by parameters θ, the goal is to maximize the likelihood function p(**X**|θ) with respect to θ.
- Initialize parameters θ^{old}.
- E-step: Compute posterior over latent variables: p(**Z**|**X**,θ^{old}).
- M-step: Find the new estimate of parameters θ^{new}:

$$\theta^{new} = \arg\max_{\theta} \mathcal{Q}(\theta, \theta^{old}).$$

where

$$\mathcal{Q}(\theta, \theta^{old}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{old}) \ln p(\mathbf{X}, \mathbf{Z}|\theta).$$

- Check for convergence of either log-likelihood or the parameter values. Otherwise:

$$\theta^{new} \leftarrow \theta^{old}, \qquad \text{and iterate.}$$

- We will next show that each step of EM algorithm maximizes the log-likelihood function.

Variational Bound 变分界

- Given a joint distribution p(**Z**,**X**|θ) over observed and latent variables governed by parameters θ, the goal is to maximize the likelihood function p(**X**|θ) with respect to θ:

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

目标

- We will assume that **Z** is discrete, although derivations are identical if **Z** contains continuous, or a combination of discrete and continuous variables.
- For any distribution q(**Z**) over latent variables we can derive the following variational lower bound:

$$\ln p(\mathbf{X}|\theta) = \ln \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta) = \ln \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})}$$

Jensen's inequality

$$\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \frac{p(\mathbf{X}, \mathbf{Z}|\theta)}{q(\mathbf{Z})} = \mathcal{L}(q, \theta).$$

找下界

Variational Bound

- Variational lower-bound:

$$
\begin{aligned}
\ln p(\mathbf{X}|\theta) &= \ln \sum_{\mathbf{Z}} p(\mathbf{X},\mathbf{Z}|\theta) = \ln \sum_{\mathbf{Z}} q(\mathbf{Z}) \frac{p(\mathbf{X},\mathbf{Z}|\theta)}{q(\mathbf{Z})} \\
&\geq \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \frac{p(\mathbf{X},\mathbf{Z}|\theta)}{q(\mathbf{Z})} \\
&= \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln p(\mathbf{X},\mathbf{Z}|\theta) + \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \frac{1}{q(\mathbf{Z})} \\
&= \mathbb{E}_{q(\mathbf{Z})}\big[\ln p(\mathbf{X},\mathbf{Z}|\theta)\big] + \mathcal{H}(q(\mathbf{Z})) = \mathcal{L}(q,\theta).
\end{aligned}
$$

$E_{q(z)} f(z) = \sum q(z) f(z)$

Expected complete log-likelihood

Entropy functional.

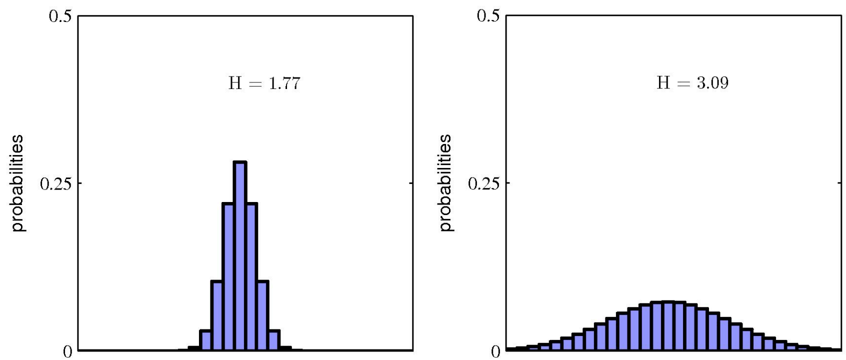
Variational lower-bound

Entropy

- For a discrete random variable X, where $P(X=x_i) = p(x_i)$, the entropy of a random variable is:

$$\mathcal{H}(p) = -\sum_i p(x_i) \log p(x_i).$$

- Distributions that are sharply picked around a few values will have a relatively low entropy, whereas those that are spread more evenly across many values will have higher entropy



- Histograms of two probability distributions over 30 bins.

- The largest entropy will arise from a uniform distribution $H = -\ln(1/30) = 3.40$.

- For a density defined over continuous random variable, the differential entropy is given by:

$$\mathcal{H}(p) = -\int p(x) \log p(x) \mathrm{d}x.$$

Variational Bound

- We saw:

$$\ln p(\mathbf{X}|\theta) \geq \mathbb{E}_{q(\mathbf{Z})}\big[\ln p(\mathbf{X}, \mathbf{Z}|\theta)\big] + \mathcal{H}(q(\mathbf{Z})) = \mathcal{L}(q, \theta).$$

- We also note that the following decomposition also holds:

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

where

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

Variational lower-bound

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

Kullback-Leibler (KL) divergence.

Also known as Relative Entropy.

- KL divergence is not symmetric.
- KL(q||p) $\geq$ 0 with equality iff p(x) = q(x).
- Intuitively, it measures the “distance” between the two distributions.

Variational Bound

- Let us derive that:

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

- We can write:

$$\ln p(\mathbf{X},\mathbf{Z}|\theta) = \ln p(\mathbf{Z}|\mathbf{X},\theta) + \ln p(\mathbf{X}|\theta),$$

and plugging into the definition of $\mathcal{L}(q,\theta),$ gives the desired result.

- Note that variational bound becomes tight iff q(**Z**) = p(**Z** | **X**,θ).
- In other words the distribution q(**Z**) is equal to the true posterior distribution over the latent variables, so that KL(q||p) = 0.
- As KL(q||p) $\geq$ 0, it immediately follows that:

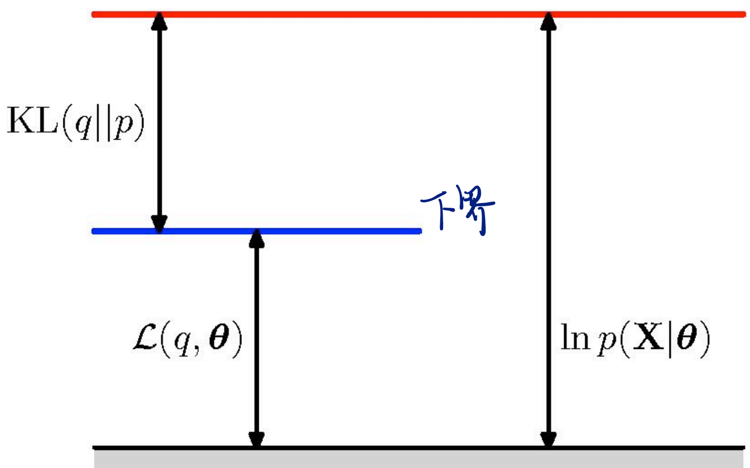
$$\ln p(\mathbf{X}|\theta) \geq \mathcal{L}(q,\theta),$$

which also showed using Jensen's inequality.

Decomposition

- Illustration of the decomposition which holds for any distribution q(**Z**).

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



Alternative View of EM

- We can use our decomposition to define the EM algorithm and show that it maximizes the log-likelihood function.

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

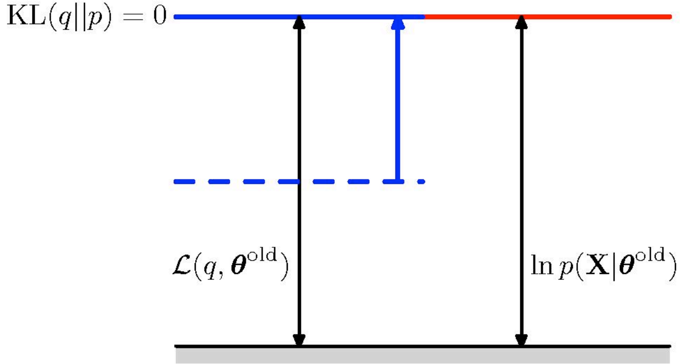
- Summary:
  - In the E-step, the lower bound $\mathcal{L}(q,\theta)$ is maximized with respect to distribution q while holding parameters θ fixed.
  - In the M-step, the lower bound $\mathcal{L}(q,\theta)$ is maximized with respect to parameters θ while holding the distribution q fixed.
- These steps will increase the corresponding log-likelihood.

E-step

- Suppose that the current value of the parameter vector is θ^{old}.
- In the E-step, we maximize the lower with respect to q while holding parameters θ^{old} fixed.

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

does not depend on q



- The lower-bound is maximized when KL term turns to zero.
- In other words, when q(**Z**) is equal to the true posterior:

$$q(\mathbf{Z}) = \mathbf{p}(\mathbf{Z}|\mathbf{X}, \theta^{\mathbf{old}}).$$

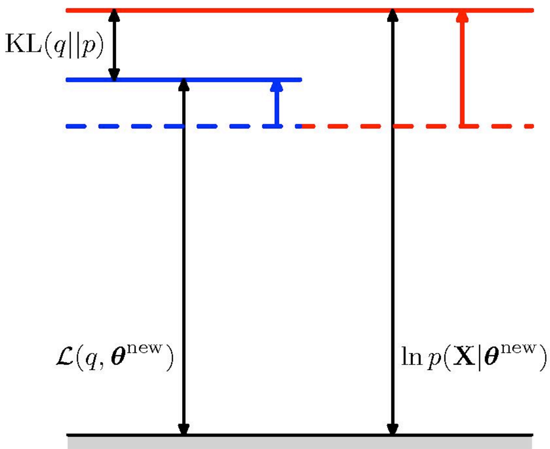
- The lower bound will become equal to the log-likelihood.

M-step

• In the M-step, the lower bound is maximized with respect to parameters θ while holding the distribution q fixed.

does not depend on θ.

$$\mathcal{L}(q,\theta) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\theta^{old}) \ln p(\mathbf{X},\mathbf{Z}|\theta) + \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\theta^{old}) \ln \frac{1}{p(\mathbf{Z}|\mathbf{X},\theta^{old})}.$$



$$\mathcal{L}(q,\theta) = Q(\theta,\theta^{old}) + \text{const.}$$

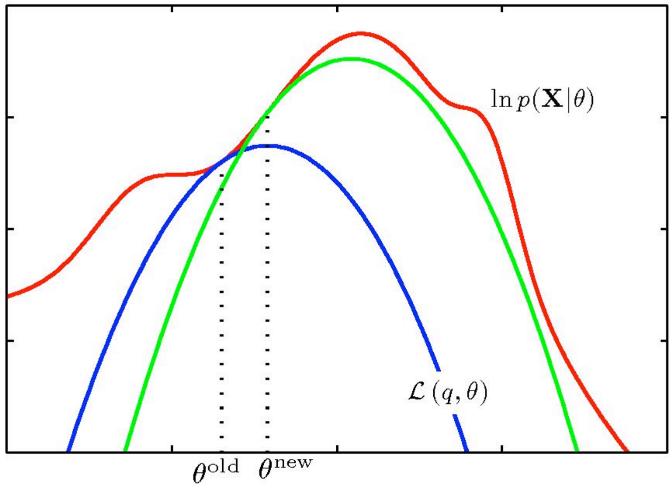
• Hence the M-step amounts to maximizing the expected complete log-likelihood.

$$\theta^{new} = \arg\max_{\theta} Q(\theta,\theta^{old}).$$

• Because KL divergence is non-negative, this causes the log-likelihood log p($\mathbf{X}$ | θ) to increase by at least as much as the lower bound does.

Bound Optimization

• The EM algorithm belongs to the general class of bound optimization methods:



• At each step, we compute:

- E-step: a lower bound on the log-likelihood function for the current parameter values. The bound is concave with unique global optimum.
- M-step: maximize the lower-bound to obtain the new parameter values.

tractable $\rightarrow$ intractable

$q(z)$ $\quad$ $q_\beta(z)$ $\quad$ VAE

$p(z|x,q)$ $\quad$ $p(z|x,\theta_\beta)$

Extensions

- For some complex problems, it maybe the case that either E-step or M-step, or both remain intractable.
- This leads to two possible extensions.
- The Generalized EM deals with intractability of the M-step.
- Instead of maximizing the lower-bound in the M-step, we instead seek to change parameters so as to increase its value (e.g. using nonlinear optimization, conjugate gradient, etc.).
- We can also generalize the E-step by performing a partial, rather than complete, optimization of the lower-bound with respect to q.
- For example, we can use an incremental form of EM, in which at each EM step only one data point is processed at a time.
- In the E-step, instead of recomputing the responsibilities for all the data points, we just re-evaluate the responsibilities for one data point, and proceed with the M-step.

Maximizing the Posterior

- We can also use EM to maximize the posterior p(θ | **X**) for models ih which we have introduced the prior p(θ).

- To see this, note that:

$$\ln p(\theta|\mathbf{X}) = \ln p(\mathbf{X}|\theta) + \ln p(\theta) - \ln p(\mathbf{X}).$$

- Decomposing the log-likelihood into lower-bound and KL terms, we have:

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

- Hence

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

where lnp(**X**) is a constant.

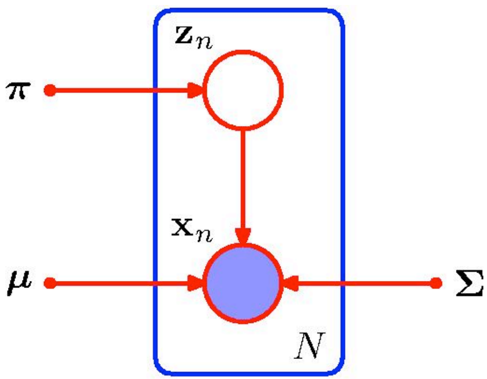
- Optimizing with respect to q gives rise to the same E-step as for the standard EM algorithm.

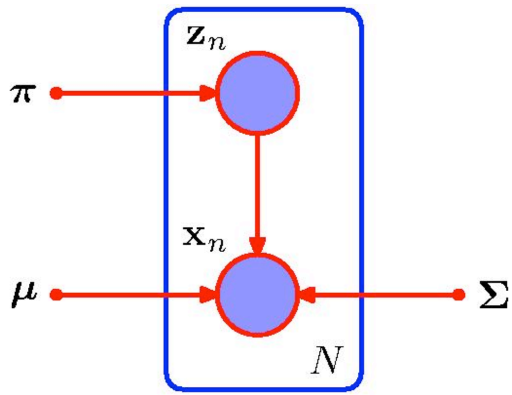
- The M-step equations are modified through introduction of the prior term, which typically amounts to only a small modification to the standard ML M-step equations.

Gaussian Mixtures Revisited

- We now consider the application of the latent variable view of EM the case of Gaussian mixture model.
- Recall:

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





$\{\mathbf{X}\}$ -- incomplete dataset. $\{\mathbf{X}, \mathbf{Z}\}$ -- complete dataset.

Maximizing Complete Data

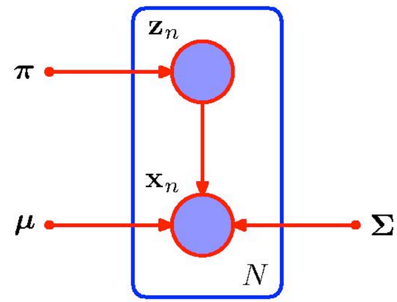
- Consider the problem of maximizing the likelihood for the complete data:

联合分布是与z有关的，z别忘了次数！

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

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

Sum of K independent contributions, one for each mixture component.



$\{\mathbf{X}, \mathbf{Z}\}$

-- complete dataset.

- Maximizing with respect to mixing proportions yields:

$$\pi_k = \frac{1}{N} \sum_{n=1}^{N} z_{nk}.$$

- And similarly for the means and covariances.

Posterior Over Latent Variables

- Remember:

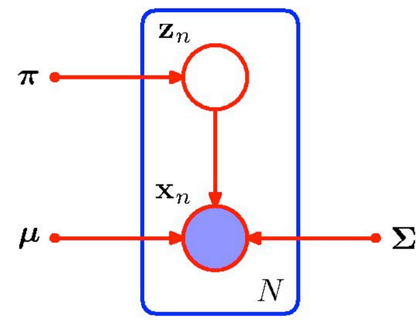
$$p(\mathbf{x}|\mathbf{z}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_k}, \quad p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k}.$$

- The posterior over latent variables takes form:

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

- Note that the posterior factorizes over n points, so that under the posterior distribution $\{\mathbf{z}_n\}$ are independent.

- This can be verified by inspection of directed graph and making use of the d-separation property.



Expected Complete Log-Likelihood

- The expected value of indicator variable z_{nk} under the posterior distribution is:

$$\mathbb{E}[z_{nk}] = \frac{\sum_{\mathbf{z}_n} z_{nk} \prod_j \left[\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)\right]^{z_{nj}}}{\sum_{\mathbf{z}_n} \prod_j \left[\pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)\right]^{z_{nj}}}$$

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

- This represent the responsibility of component k for data point x_n.
- The complete-data log-likelihood:

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

- The expected complete data log-likelihood is:

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

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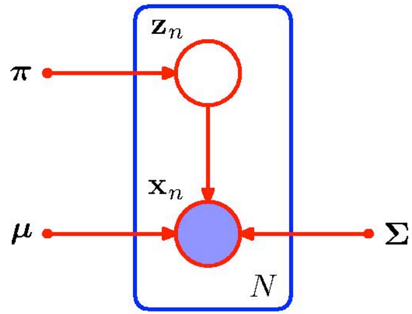
- Maximizing the respect to model parameters we obtain:

$$\boldsymbol{\mu}_k^{new} = \frac{1}{N_k} \sum_n \gamma(z_{nk}) \mathbf{x}_n, \quad N_k = \sum_n \gamma(z_{nk}),$$

$$\boldsymbol{\Sigma}_k^{new} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(y_{nk}) (\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T,$$

$$\pi_k^{new} = \frac{N_k}{N}.$$



Relationship to K-Means

- Consider a Gaussian mixture model in which covariances are shared and are given by $\epsilon \boldsymbol{I}$.

$$p(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) = \frac{1}{(2\pi\epsilon)^{D/2}} \exp\left[-\frac{1}{2\epsilon}||\mathbf{x} - \boldsymbol{\mu}_k||^2 \right].$$

- Consider EM algorithm for a mixture of K Gaussians, in which we treat ϵ as a fixed constant. The posterior responsibilities take form:

$$\gamma(z_{nk}) = \frac{\pi_k \exp(-||\mathbf{x}_n - \boldsymbol{\mu}_k||^2/2\epsilon)}{\sum_{j=1}^{K} \pi_j \exp(-||\mathbf{x}_n - \boldsymbol{\mu}_j||^2/2\epsilon)}.$$

- Consider the limit $\epsilon \to 0$.
- In the denominator, the term for which $||\mathbf{x}_n - \boldsymbol{\mu}_j||^2$ is smallest will go to zero most slowly. Hence $\gamma(z_{nk}) \to r_{nk}$, where

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j ||\mathbf{x}_n - \boldsymbol{\mu}_j||^2 \\ 0 & \text{otherwise} \end{cases}$$

Relationship to K-Means

- Consider EM algorithm for a mixture of K Gaussians, in which we treat ϵ as a fixed constant. The posterior responsibilities take form:

$$\gamma(z_{nk}) = \frac{\pi_k \exp(-||\mathbf{x}_n - \boldsymbol{\mu}_k||^2/2\epsilon)}{\sum_{j=1}^{K} \pi_j \exp(-||\mathbf{x}_n - \boldsymbol{\mu}_j||^2/2\epsilon)}.$$

- Finally, in the limit $\epsilon \to 0$, the expected complete log-likelihood becomes:

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

- Hence in the limit, maximizing the expected complete log-likelihood is equivalent to minimizing the distortion measure J for the K-means algorithm.

Bernoulli Distribution

- So far we focused on distributions over continuous variables.
- We will now look at mixture of discrete binary variables described by Bernoulli distributions.
- Consider a set of binary random variables x_i, i=1,…,D, each of which is governed by a Bernoulli distribution with μ_i.

$$p(\mathbf{x}|\boldsymbol{\mu}) = \prod_{i=1}^{D} \mu_i^{x_i}(1-\mu_i)^{1-x_i}.$$

- The mean and covariance of this distribution are:

$$\mathbb{E}[\mathbf{x}] = \boldsymbol{\mu}, \qquad \mathrm{cov}[\mathbf{x}] = \mathrm{diag}(\mu_i(1-\mu_i)).$$

Mixture of Bernoulli Distributions

- Consider a finite mixture of Bernoulli distributions:

$$p(\mathbf{x}|\boldsymbol{\pi}, \boldsymbol{\mu}) = \sum_{k=1}^{K} \pi_k p(\mathbf{x}|\boldsymbol{\mu}_k),$$

$$p(\mathbf{x}|\boldsymbol{\mu}_k) = \prod_{i=1}^{D} \mu_{ki}^{x_i}(1-\mu_{ki})^{1-x_i}.$$

- The mean and covariance of this mixture distribution are:

$$\mathbb{E}[\mathbf{x}] = \sum_{k=1}^{K} \pi_k \boldsymbol{\mu}_k, \quad \mathrm{cov}[\mathbf{x}] = \sum_{k=1}^{K} \pi_k \left(\boldsymbol{\Sigma}_k + \boldsymbol{\mu}_k \boldsymbol{\mu}_k^T\right) - \mathbb{E}[\mathbf{x}]\mathbb{E}[\mathbf{x}]^T,$$

where $\boldsymbol{\Sigma}_k = \mathrm{diag}(\mu_{ki}(1-\mu_{ki}))$.

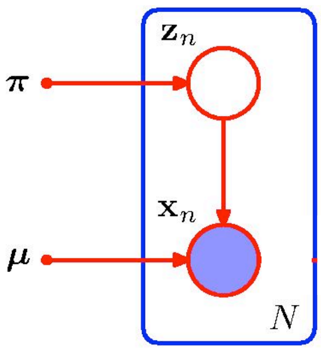
- The covariance matrix is no longer diagonal, so the mixture distribution can capture correlations between the variables, unlike a single Bernoulli distribution.

Maximum Likelihood

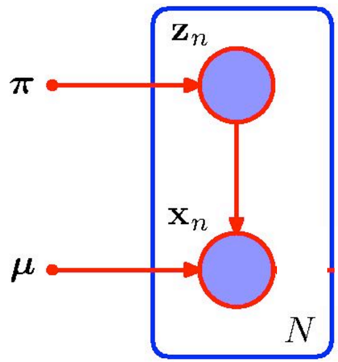
- Given a dataset **X** = {$\mathbf{x}_1,\ldots,\mathbf{x}_N$}, the log-likelihood takes form:

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

- Again, we see the sum inside the log, so the maximum likelihood solution no longer has a closed form solution.
- We will now derive EM for maximizing this likelihood function.



$\{\mathbf{X}\}$ -- incomplete dataset.



$\{\mathbf{X}, \mathbf{Z}\}$ -- complete dataset.

Complete Log-Likelihood

- By introducing latent discrete random variables, we have:

$$p(\mathbf{z}|\boldsymbol{\pi}) = \prod_{k=1}^{K} \pi_k^{z_k}, \qquad p(\mathbf{x}|\mathbf{z}, \boldsymbol{\mu}) = \prod_{k=1}^{K} p(\mathbf{x}|\boldsymbol{\mu}_k)^{z_k}.$$

- We can write down the complete log-likelihood

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

- The expected complete-data log-likelihood:

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

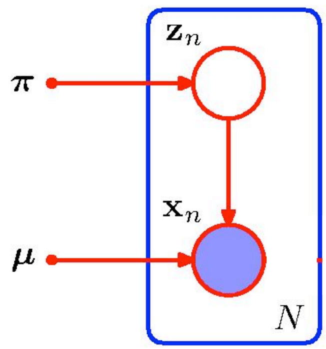
where $\mathbb{E}[z_{nk}] = \gamma(z_{nk})$.

E-step

• Similar to the mixture of Gaussians, in the E-step, we evaluate responsibilities using Bayes' rule:

$$\mathbb{E}[z_{nk}] = \frac{\sum_{\mathbf{z}_n} z_{nk} \prod_{k} \left[\pi_{k'} p(\mathbf{x}_n | \boldsymbol{\mu}_{k'})\right]^{z_{nk'}}}{\sum_{\mathbf{z}_n} \prod_{j} \left[\pi_j p(\mathbf{x}_n | \boldsymbol{\mu}_j)\right]^{z_{nj}}}$$

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



M-step

- The expected complete-data log-likelihood:

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

- Maximizing the expected complete-data log-likelihood:

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

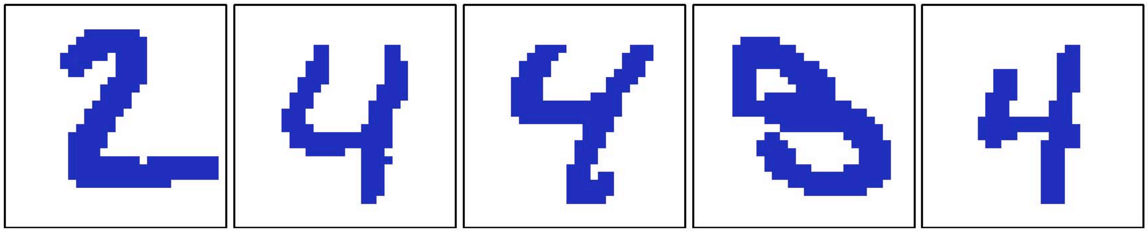
where N_k is the effective number of data points associated with component k.

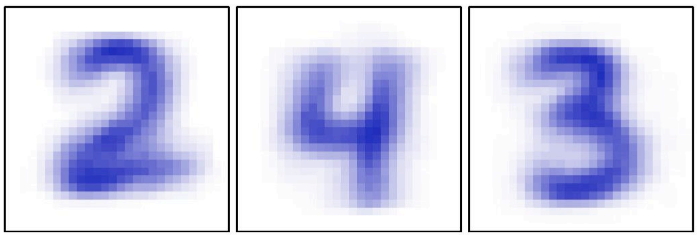
- Note that the mean of component k is equal to the weighted mean of the data, with weights given by the responsibilities that component k takes for explaining the data points.

Example

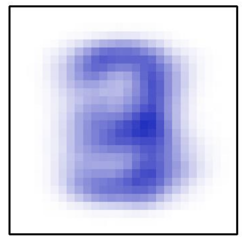
- Illustration of the Bernoulli mixture model

Training data





Learned μ_k for the first three components.



A single multinomial Bernoulli distribution fit to the full data.