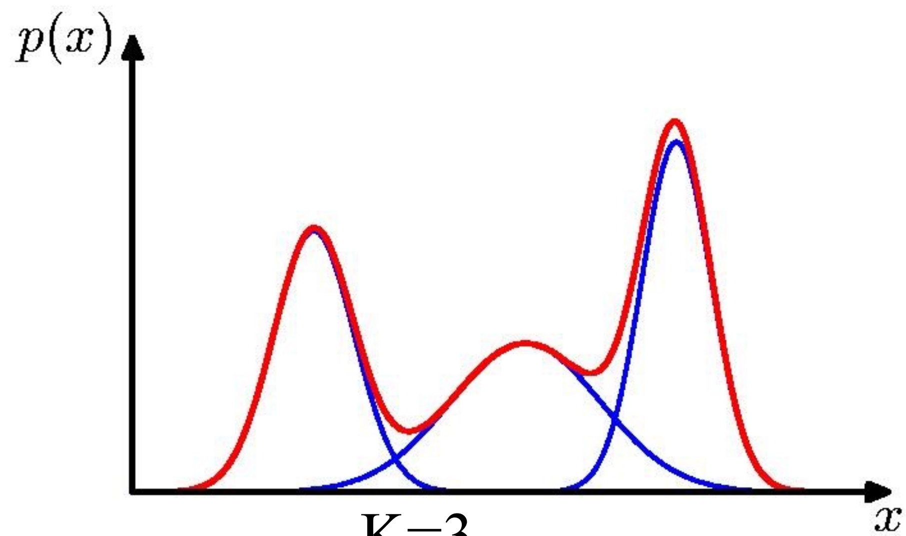
Mixture of Gaussians

• We combine simple models into a complex model by defining a superposition of K Gaussian densities of the form:

$$p(\mathbf{x}) = \sum_{k=1}^{K} \underbrace{\pi_k}_{\text{Mixing coefficient}} \underbrace{\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}_{\text{Component}}$$

$$\forall k : \pi_k \geqslant 0 \qquad \sum_{k=1}^{K} \pi_k = 1$$



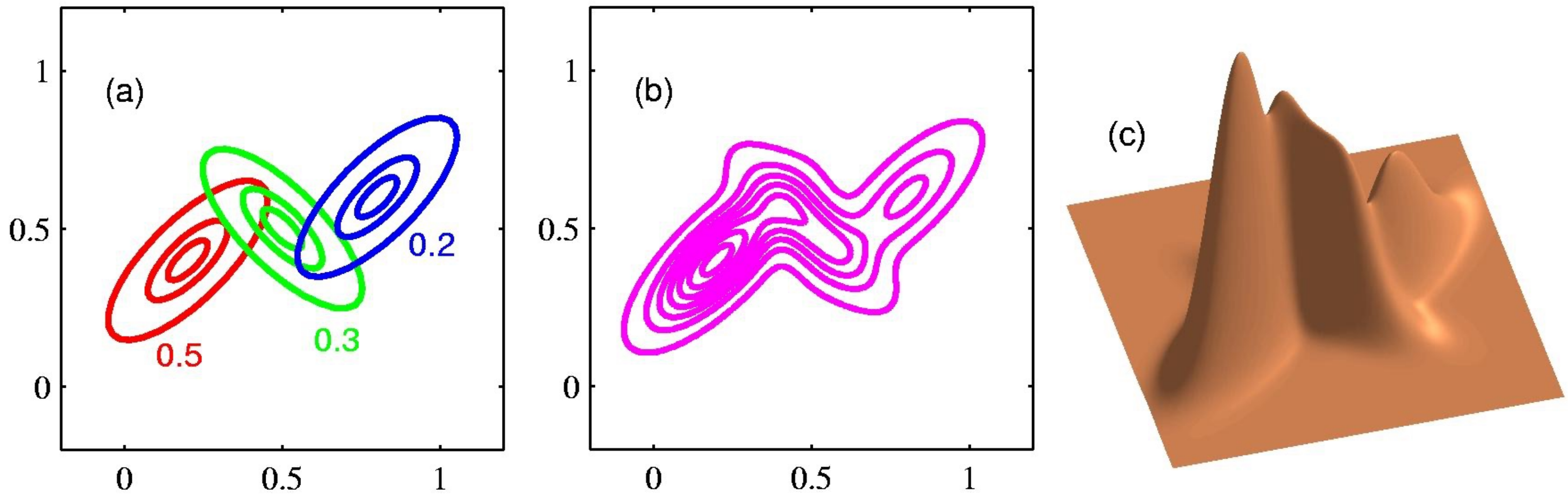
K=3

• Note that each Gaussian component has its own mean and covariance. The parameters π_k are called mixing coefficients.

• More generally, mixture models can comprise linear combinations of other distributions.

Mixture of Gaussians

- Illustration of a mixture of 3 Gaussians in a 2-dimensional space:



(a) Contours of constant density of each of the mixture components, along with the mixing coefficients

(b) Contours of marginal probability density $p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$

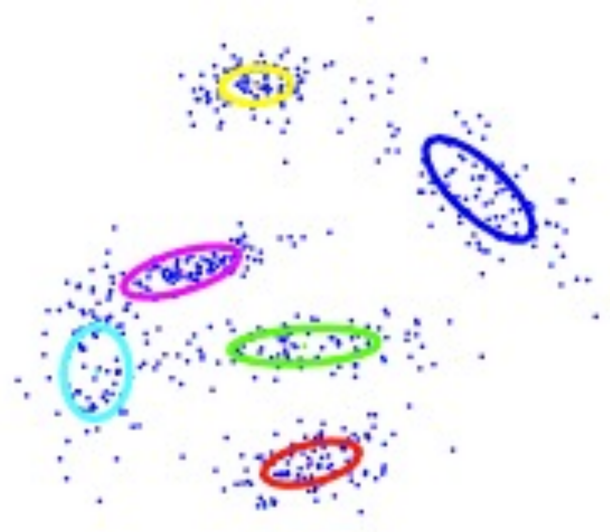
(c) A surface plot of the distribution p(x).

Mixture of Gaussians

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

• The Gaussian mixture:

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



•K-dimensional binary random variable **z** having a 1-of-K representation is the latent variable:

$$\mathbf{z} = [0, 0, .., 1, 0]^T \qquad z_k \in \{0, 1\}, \quad \sum_k z_k = 1.$$

• We will specify the distribution over **z** in terms of mixing coefficients:

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

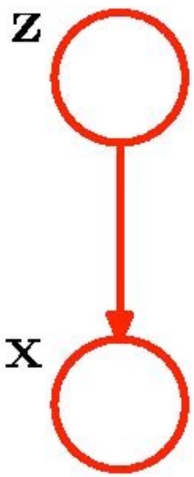
Mixture of Gaussians

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

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

- We can now specify the conditional distribution:

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



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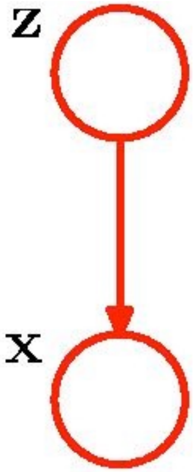

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- We have therefore specified the joint distribution:

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

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

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

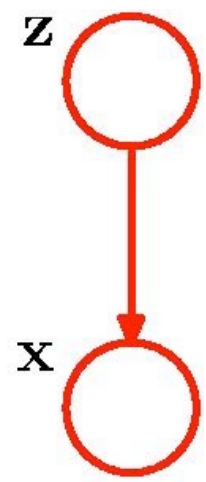
- The marginal distribution over **x** is given by a Gaussian mixture.

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 $\mathbf{x_1,\ldots,x_N}$, it follows that for every observed data point $\mathbf{x_n}$, there is a corresponding latent variable $\mathbf{z_n}$.



Mixture of Gaussians

- The marginal distribution:

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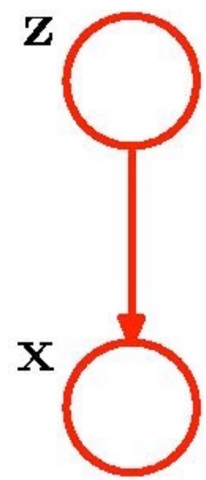


- If we have several observations $\mathbf{x_1,\ldots,x_N}$, it follows that for every observed data point $\mathbf{x_n}$, there is a corresponding latent variable $\mathbf{z_n}$.

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

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

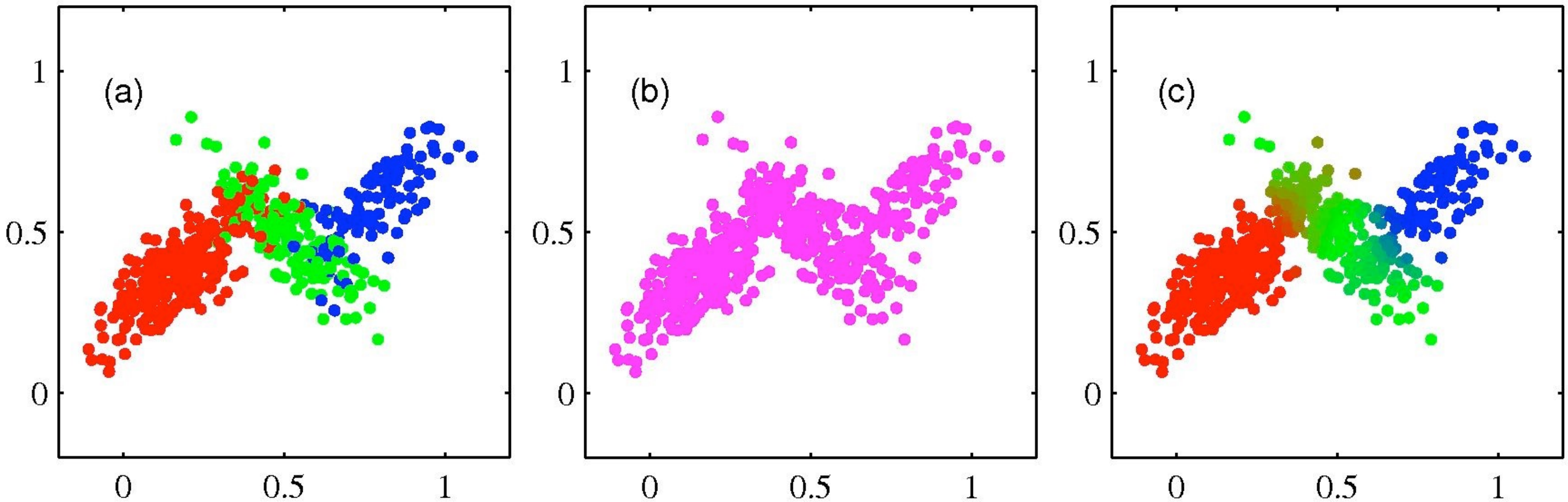
responsibility that component k takes for explaining the data x

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

- 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.

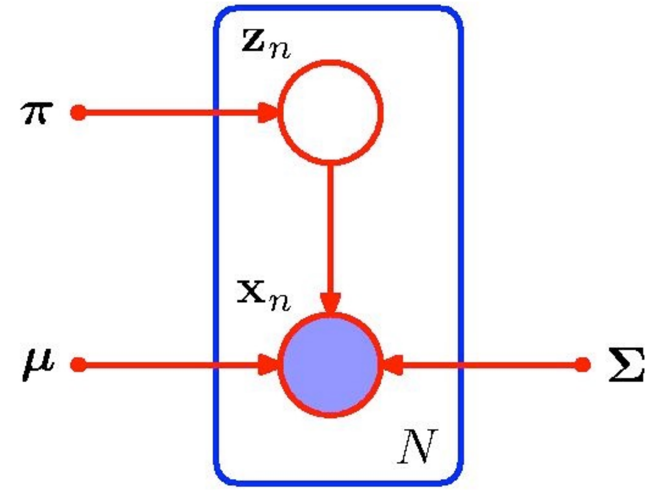
Maximum Likelihood

- Suppose we observe a dataset $\{x_1,\ldots,x_N\}$, 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 as an N by K matrix **Z**.

- The log-likelihood takes form:

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

Model parameters



Graphical model for a Gaussian mixture model for a set of i.i.d. data point $\{x_n\}$, and corresponding latent variables $\{z_n\}$.

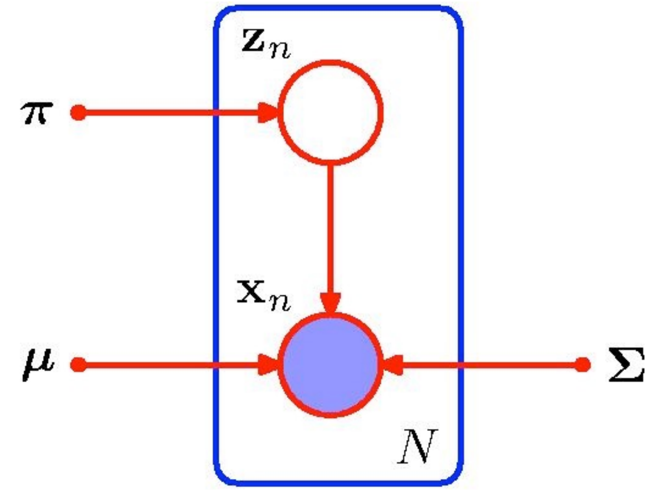
Maximum Likelihood

- The log-likelihood takes form:

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

- Differentiating with respect to $\boldsymbol{\mu}_k$ and setting to zero:

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



Maximum Likelihood

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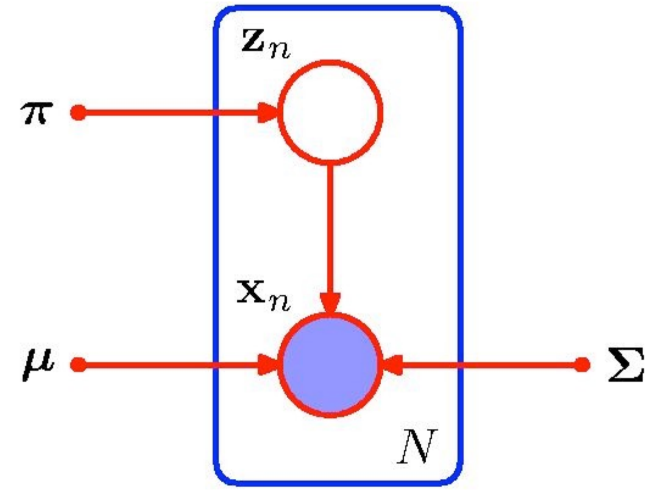


Soft assignment

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

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

- The mean $\boldsymbol{\mu}_k$ is given by the mean of all the data points weighted by the posterior $\gamma(z_{nk})$ that component k was responsible for generating x_n.

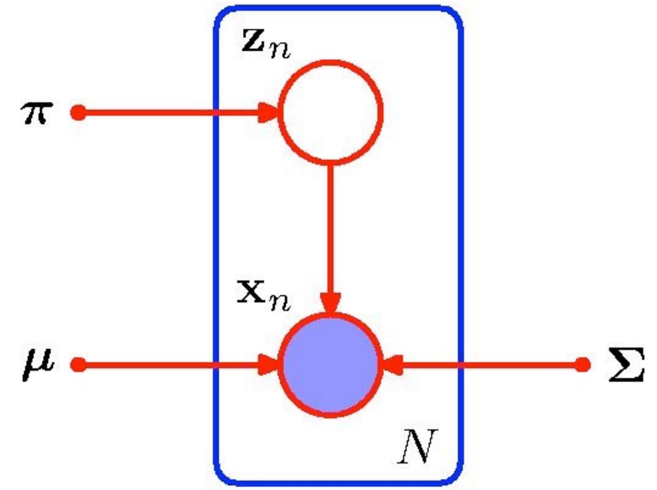
Maximum Likelihood

- The log-likelihood takes form:

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

- Differentiating with respect to Σ_k and setting to zero:

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



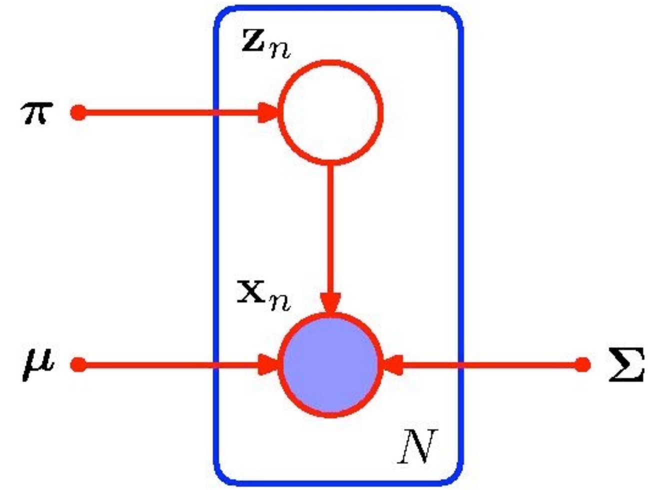
Maximum Likelihood

- The log-likelihood takes form:

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

- 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

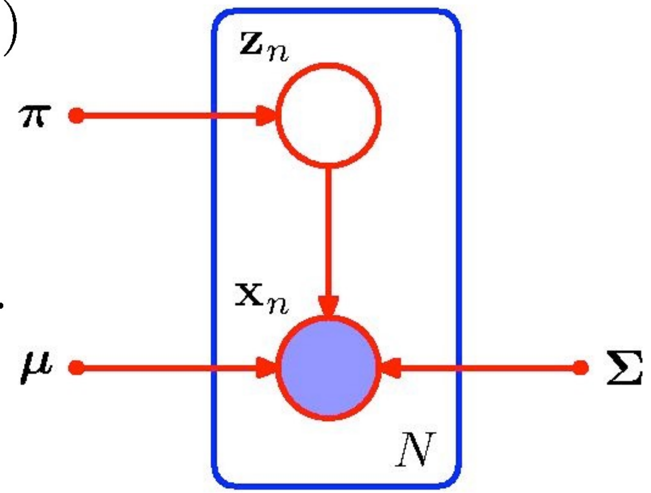
- The log-likelihood takes form:

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

- 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:

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



Maximum Likelihood

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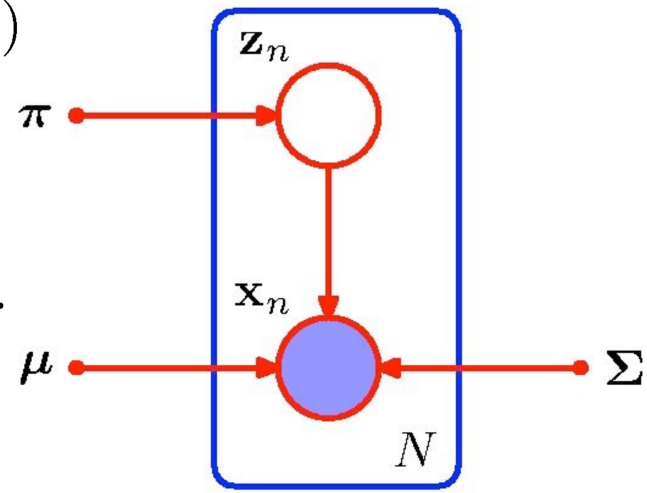

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- Iterative Solution:

  E-step: Update responsibilities $\gamma(z_{nk})$
  M-step: Update model parameters: μ_k Σ_k π_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:

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

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

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

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

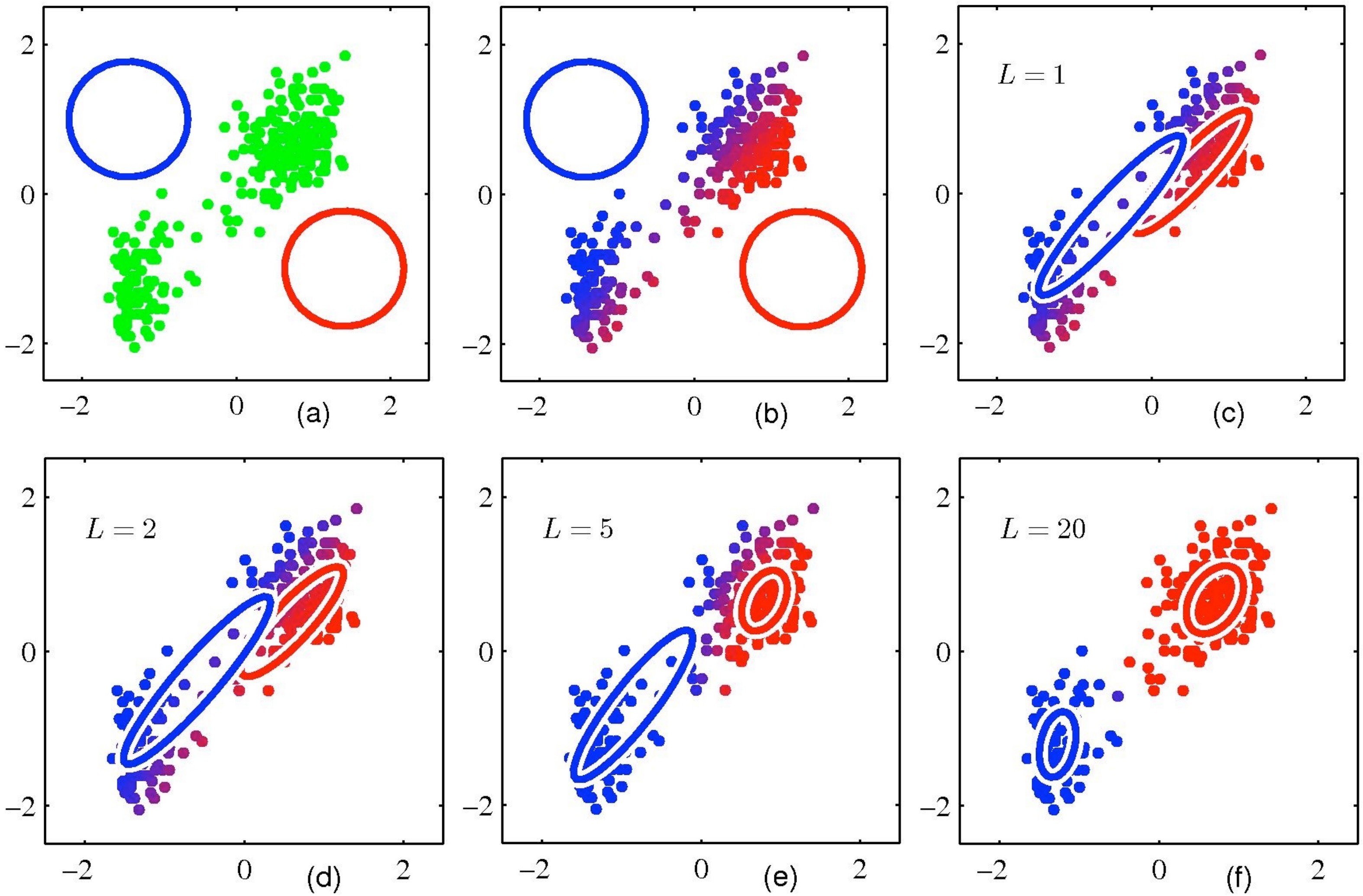
$$\pi_k^{new} = \frac{N_k}{N}.$$

$\boldsymbol{\mu}_k^{new}$

- Evaluate the log-likelihood and check for convergence.

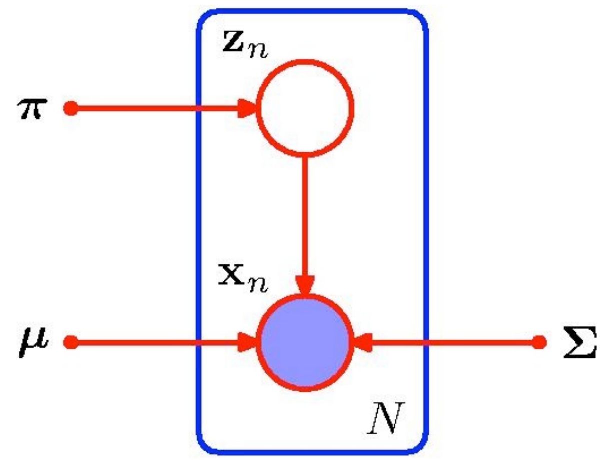
Mixture of Gaussians: Example

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



General EM formulation

- 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.



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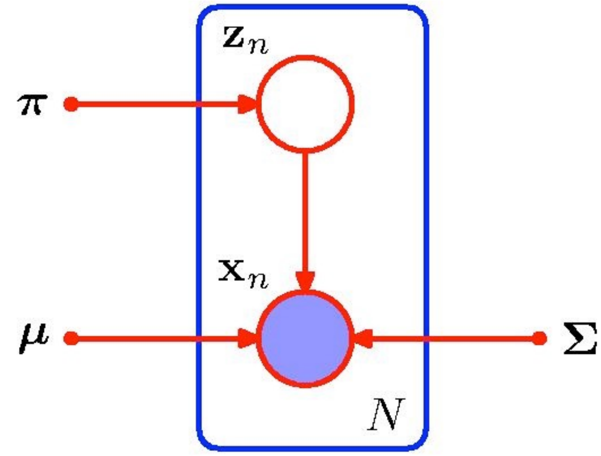
- The log-likelihood takes form:

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



- We will call:

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

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

General EM formulation

- In practice, we are not given a complete dataset $\{\mathbf{X}, \mathbf{Z}\}$, but only incomplete dataset $\{\mathbf{X}\}$.
- 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:

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

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- 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, 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}) and $\mathcal{Q}(\theta, \theta^{old})$.
- M-step: Find the new estimate of parameters θ^{new}:

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

where

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

The General EM algorithm

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

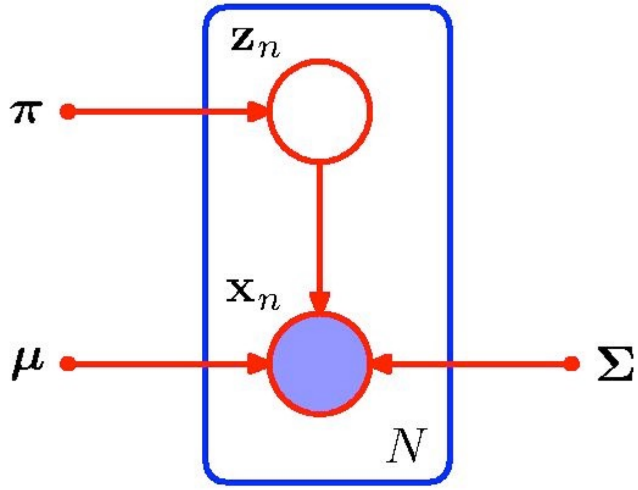
Otherwise:

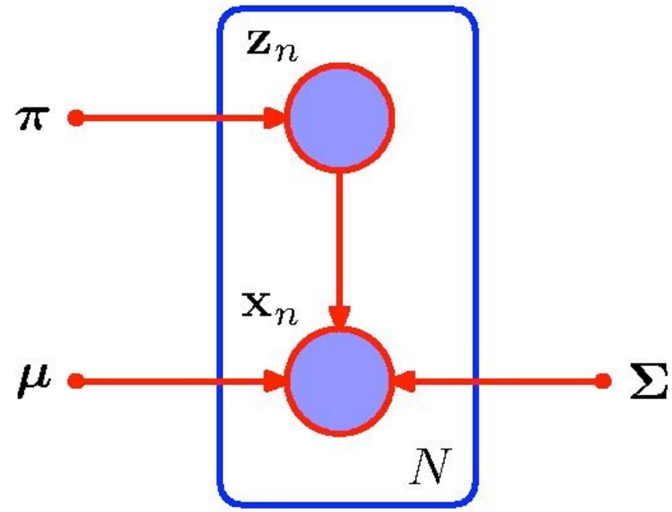
$$\theta^{new} \leftarrow \theta^{old}, \qquad \text{and iterate.}$$

Gaussian Mixtures Revisited

- We now consider the application of the latent variable view of EM to 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.

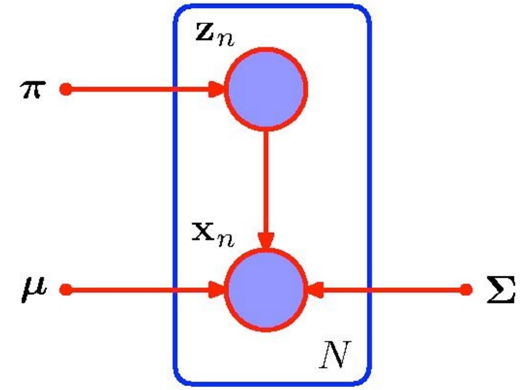
Maximizing Complete Data

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

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

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

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



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

-- complete dataset.

- Maximizing with respect to mixing proportions yields:

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

Posterior Over Latent Variables

- Remember:

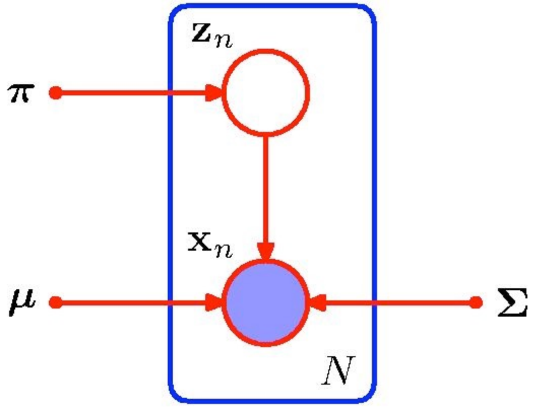
$$p(\mathbf{x}|\mathbf{z}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_k}, \quad p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k}.$$

- The posterior over latent variables takes form:

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

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

$$p(z_{nk} = 1|\mathbf{X}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{\pi_k \mathcal{N}(x_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(x_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$



Expected Complete Log-Likelihood

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

$$\mathbb{E}[z_{nk}] = \frac{\sum_{z_{nk}} z_{nk}[\pi_k \mathcal{N}(\mathbf{x}_n|\mu_k, \mathbf{\Sigma}_k)]^{z_{nk}}}{\sum_{z_{nj}} [\pi_j \mathcal{N}(\mathbf{x}_n|\mu_j, \mathbf{\Sigma}_j)]^{z_{nj}}}$$

Under posterior

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

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Under posterior

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

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

- The expected complete data log-likelihood is:

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

Expected Complete Log-Likelihood

- The expected complete data log-likelihood is:

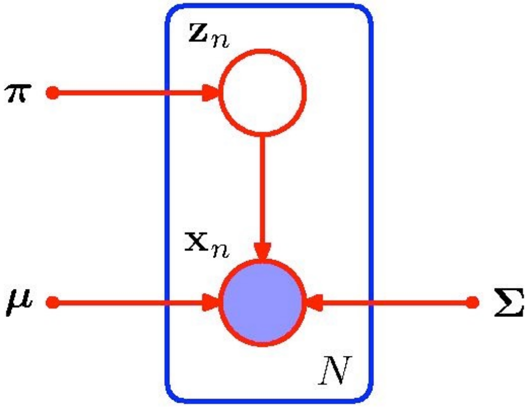
$$\mathbb{E}_{\mathbf{Z}}\left[\ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})\right] = \sum_{n=1}^{N}\sum_{k=1}^{K}\gamma(z_{nk})\Big[\ln \pi_k + \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\Big].$$

- Maximizing with 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 ϵI

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

- Consider EM algorithm for a mixture of K Gaussians, in which we treat $\boldsymbol{\Sigma}_k$ as a fixed constant. The posterior responsibilities take form:

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

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• Consider the limit ϵ goes 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 $\gamma(z_{nk})$ goes to r_{nk} where

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

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- Finally, in the limit ϵ goes to 0, the expected complete log-likelihood becomes:

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

- Hence in the limit, maximizing the expected complete log-likelihood is equivalent to minimizing the distortion measure in the K-means algorithm.
- This is why assignment step in k-Means is called E-step, and finding the cluster centers is called the M-step.