Artificial Intelligence

Mixture Models and EM

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2015.4

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- K-means clustering
- Mixtures of Gaussians
- An alternative view of EM
- The EM algorithm in general

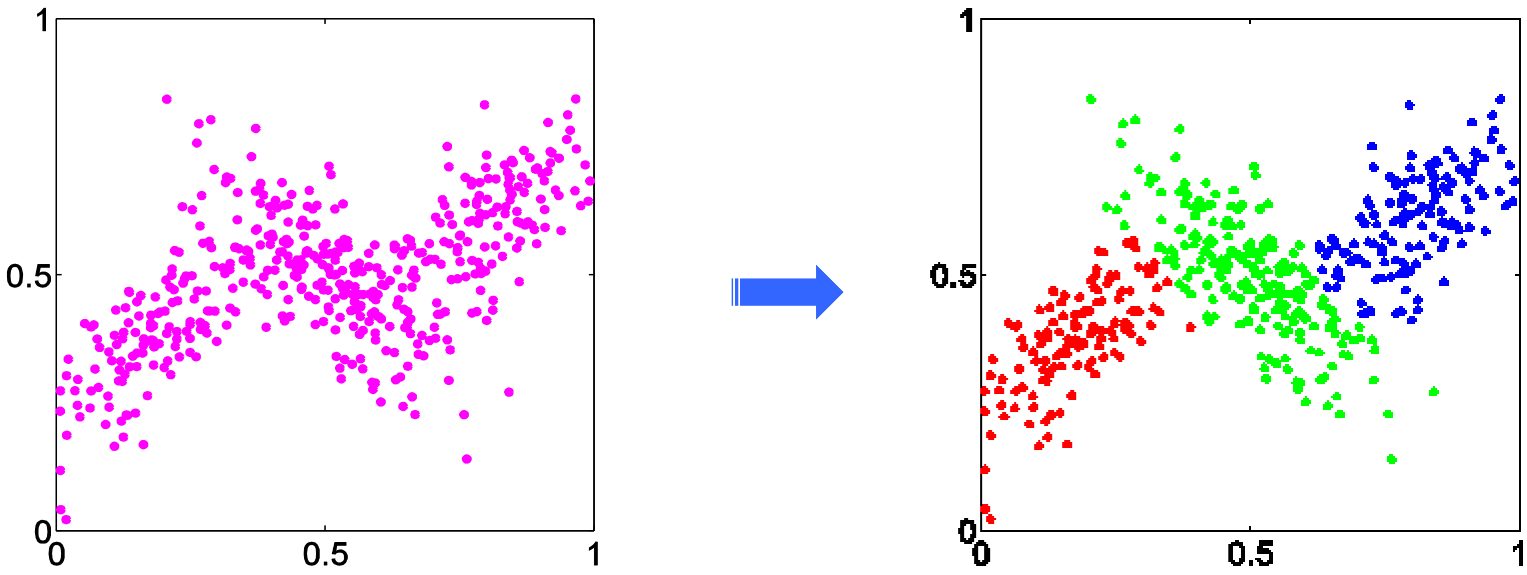
References:

1. *Bishop. “Pattern Recognition and Machine Learning”, Chapter 9. 2006.*

K-means clustering

K-means clustering

- Suppose we have a data set {$\mathbf{x}_1$, $\mathbf{x}_2$, …, $\mathbf{x}_N$} in D-dimensional space and these data points have an intrinsic structure of K clusters.
- We use $\boldsymbol{\mu}_k$ as a prototype associated with the k^{th} cluster.
- Goal: find an assignment of data points to clusters such that some objective function.



K-means clustering

- Distortion measure (responsibilities):

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

$$\frac{\partial J}{\partial \boldsymbol{\mu}_k} = 2\sum_{n=1}^{N} r_{nk}(\mathbf{x}_n - \boldsymbol{\mu}_k) = 0$$

Responsibilities

Data

Prototypes (expected value)

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

$$r_{n,k} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

Example: 5 data points and 3 clusters

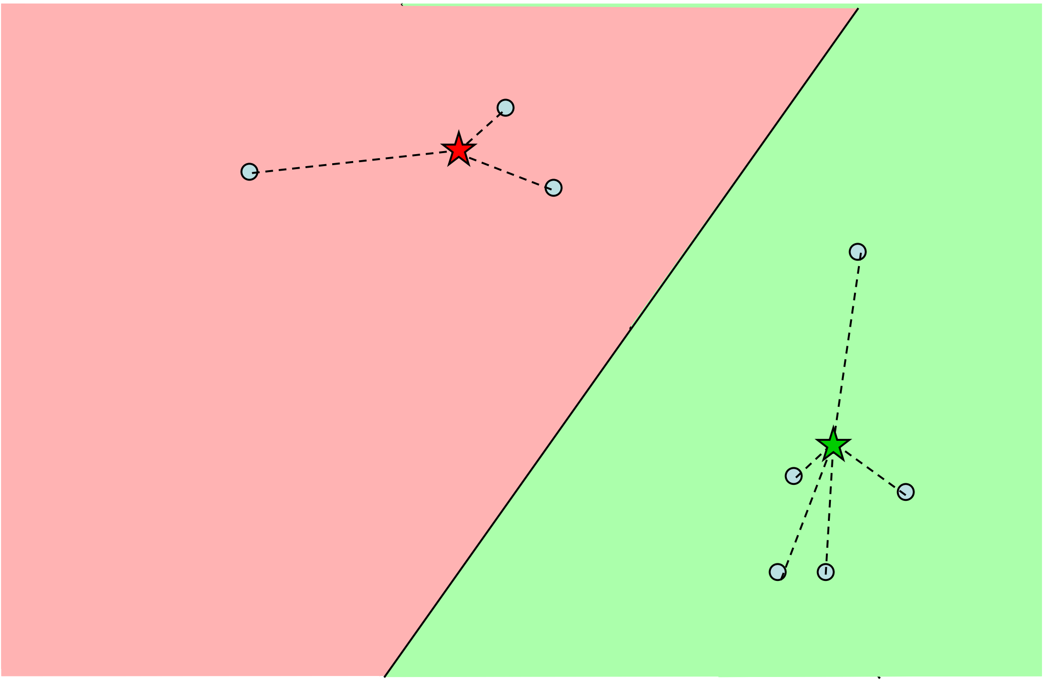
K-means algorithm (batch version):

1. Pick number of clusters *k*
2. Randomly scatter *k* “cluster centers” in data space
3. Repeat:
   a. Assign each data point to its closest cluster center
   b. Move each cluster center to the mean of the points assigned to it

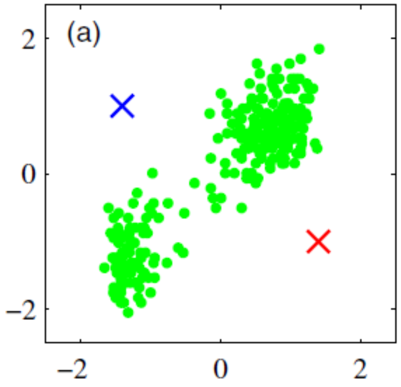
K-means clustering

- The procedure of k-means algorithm:

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

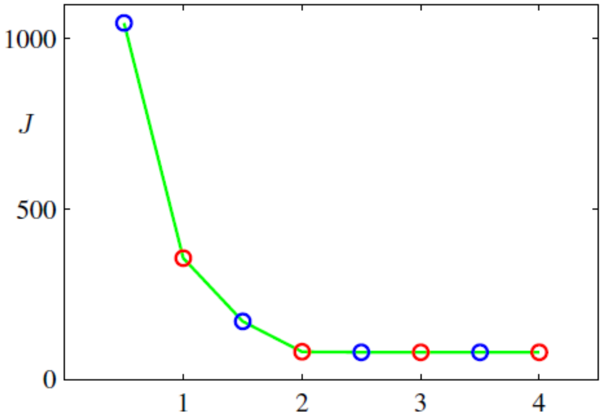


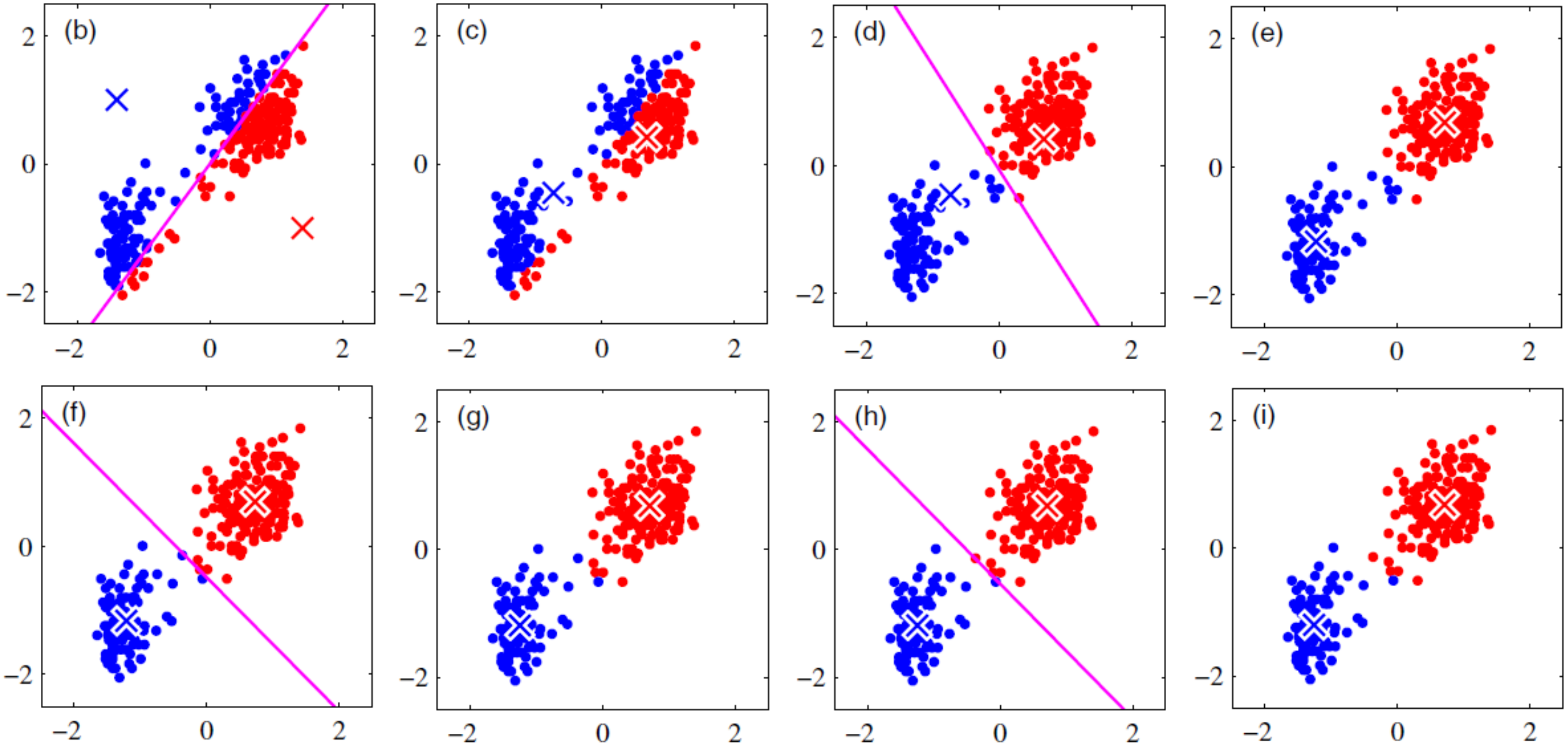
K-means clustering



- The convergence of J:

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





K-means clustering

- Online k-means algorithm (sequential k-means):

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

The nearest prototype to $\mathbf{x}_n$

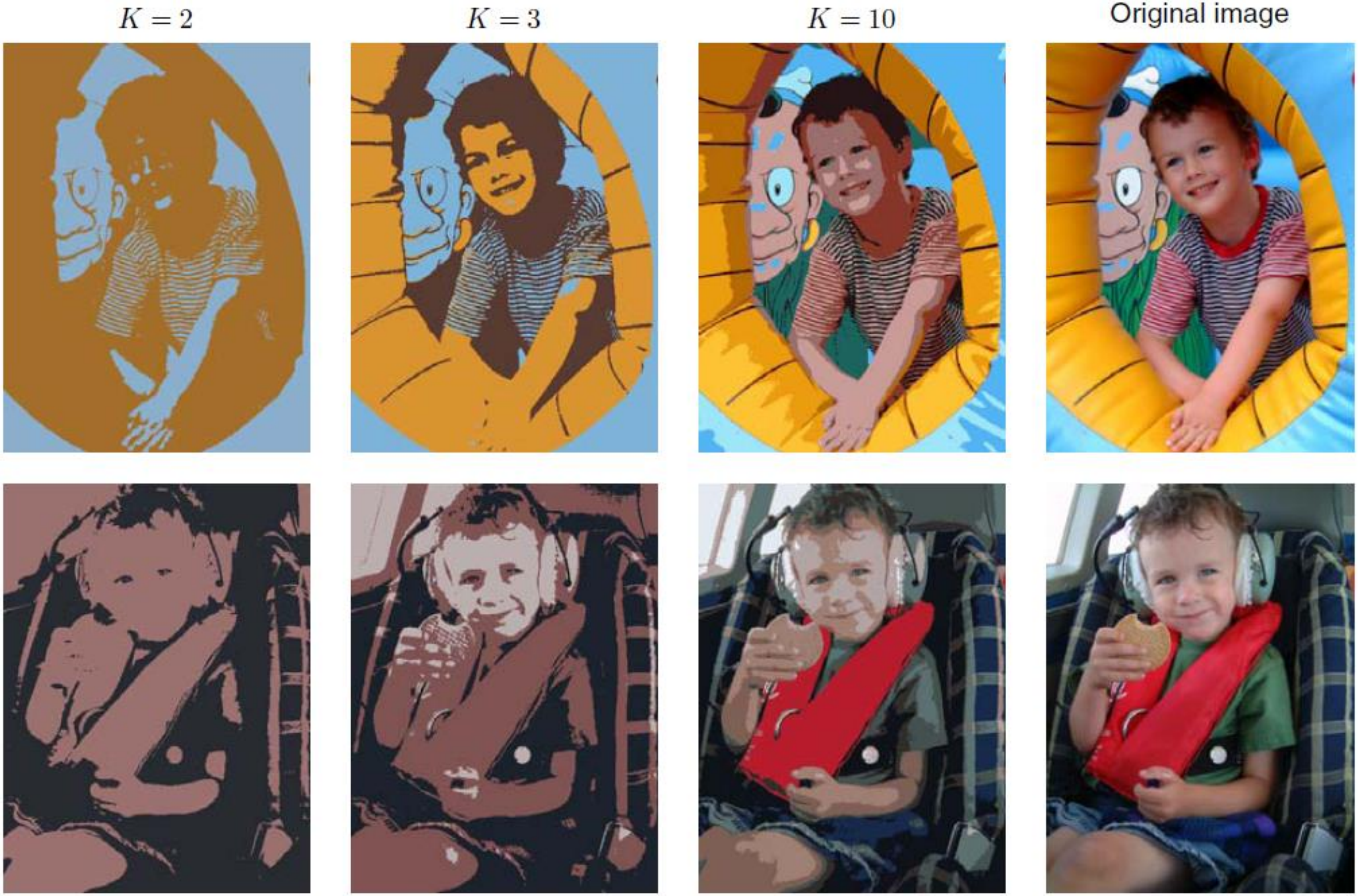
$$\boldsymbol{\mu}_k = \frac{\sum_n r_{nk} \mathbf{x}_n}{\sum_n r_{nk}} \Rightarrow \boldsymbol{\mu}_k^{\text{new}} = \boldsymbol{\mu}_k^{\text{old}} + \eta_n (\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{old}})$$

- K-medoids algorithm:
  - Chooses input data points as centers;
  - Works with an arbitrary matrix of distances between data points instead of Euclidean distance.
    - E.g. Manhattan distance or Minkowski distance

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \| \mathbf{x}_n - \boldsymbol{\mu}_k \|^2 \Rightarrow \widetilde{J} = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \mathcal{V}(\mathbf{x}_n, \boldsymbol{\mu}_k)$$

The applications of K-means algorithm

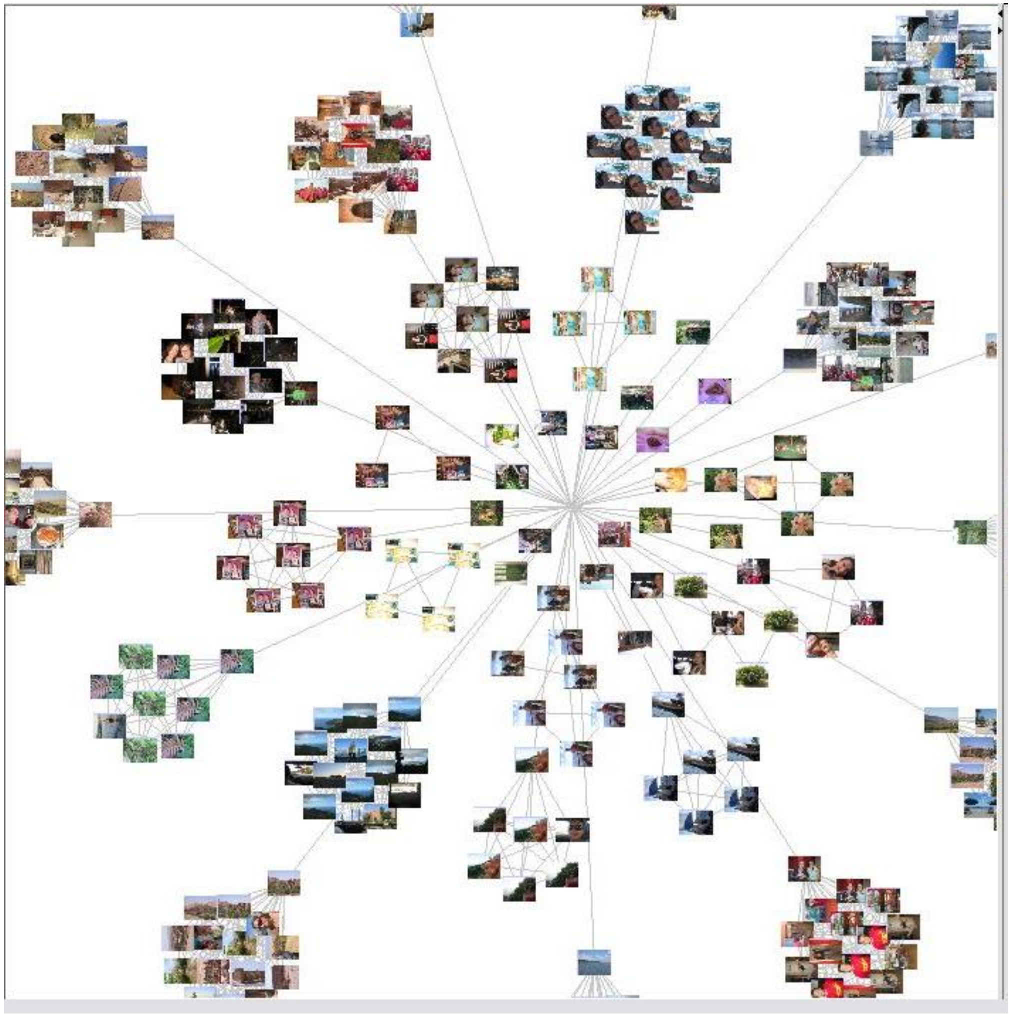
- Image segmentation:

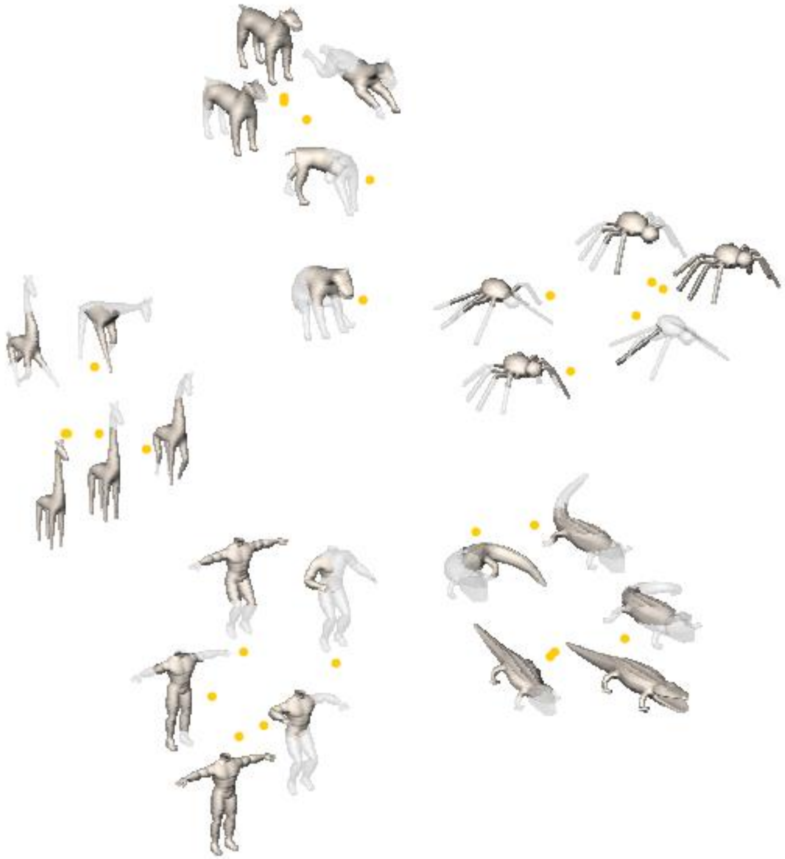


$K = 2$ $K = 3$ $K = 10$ Original image

The applications of K-means algorithm

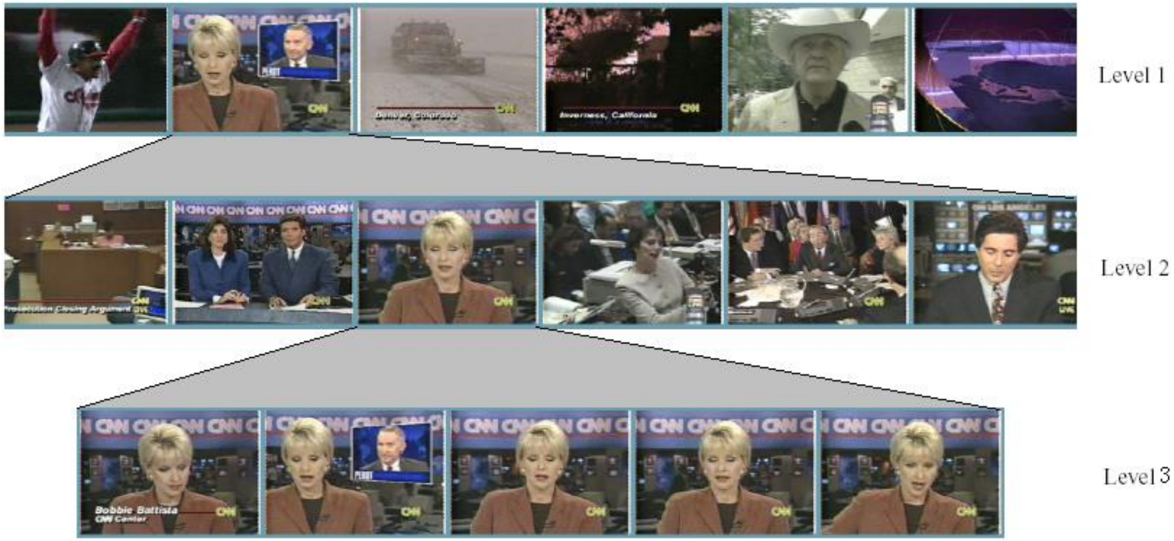
- Image clustering and 3D objects clustering:





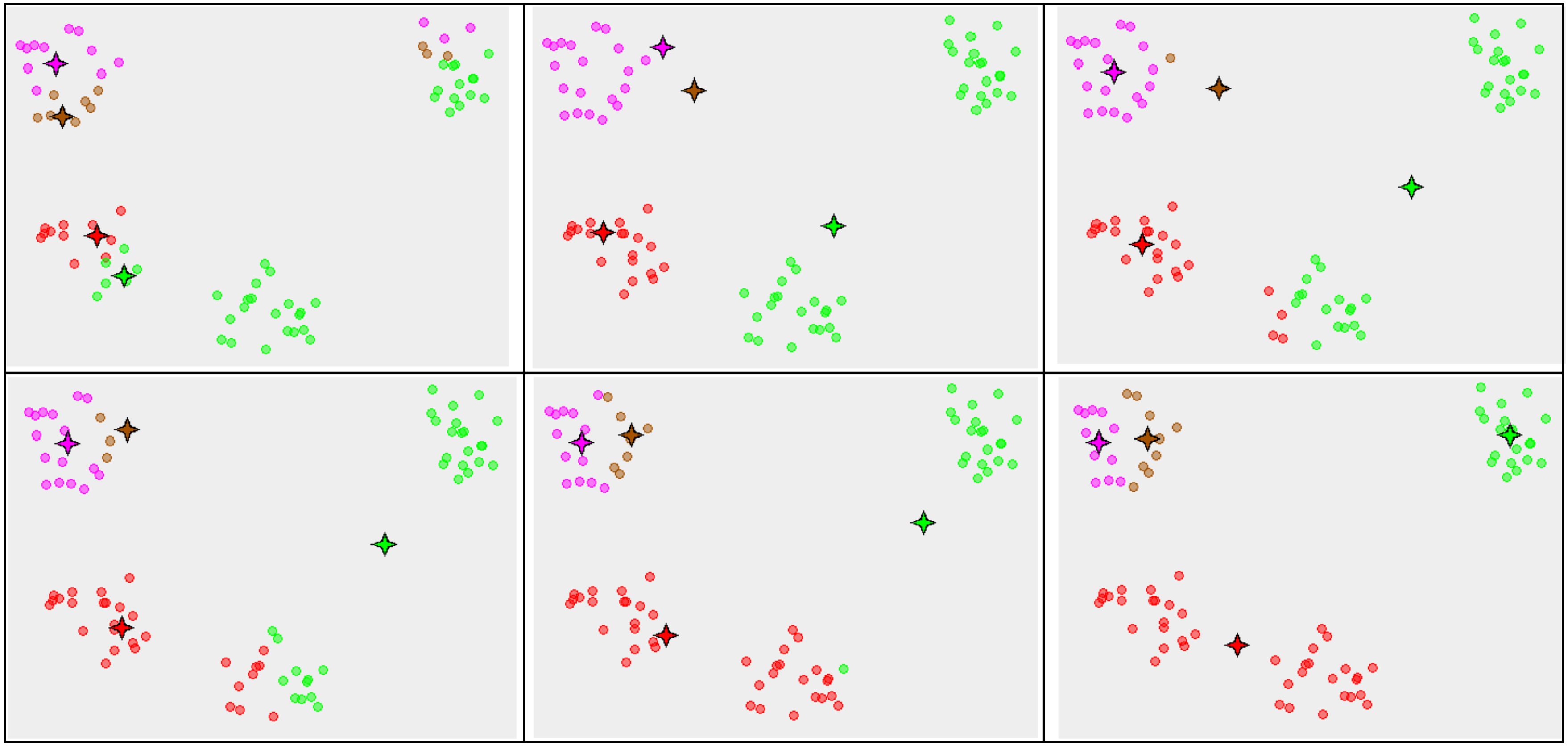
The applications of K-means algorithm

- News video clustering and video key frame extraction:



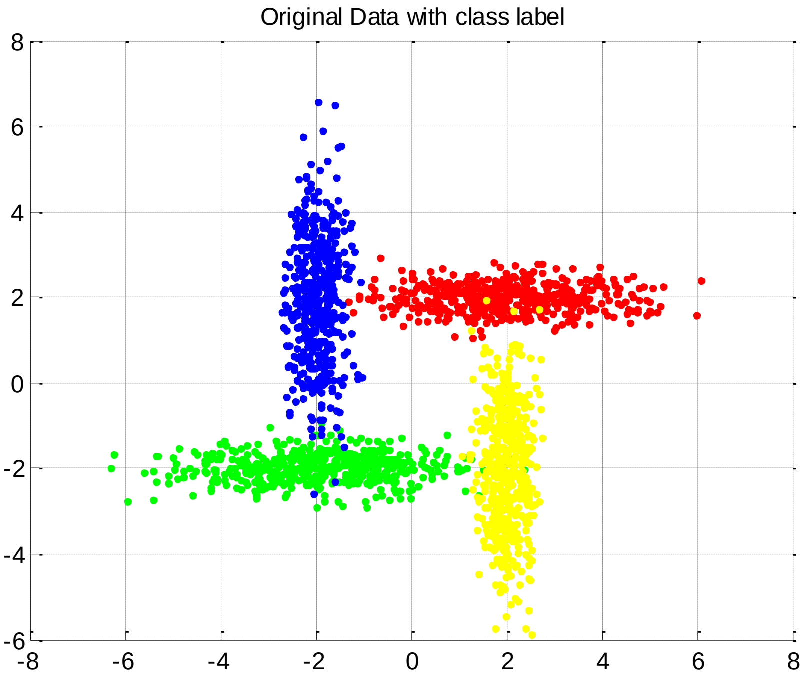
The limitation of K-means clustering

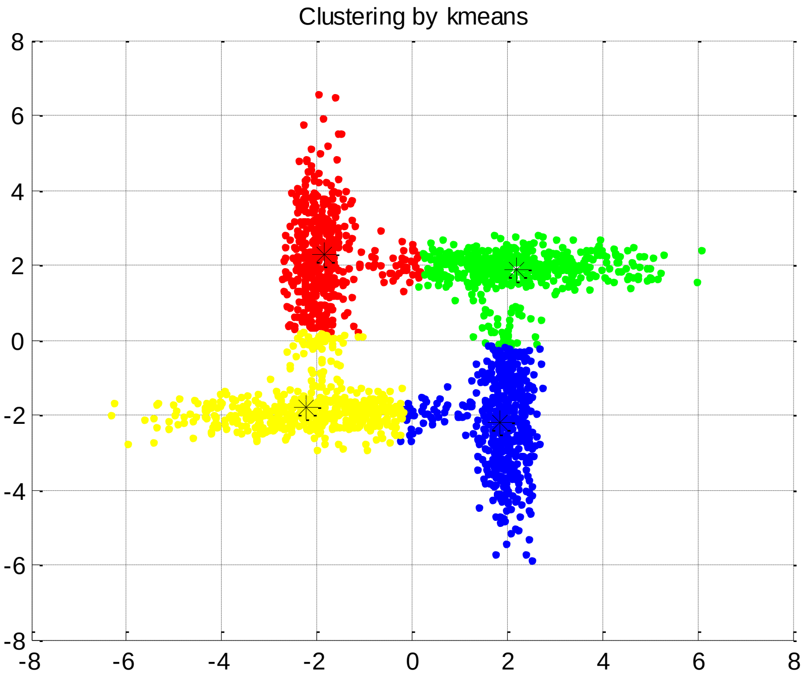
- The K-means algorithm often convergence to a local minimum.



The limitation of K-means clustering

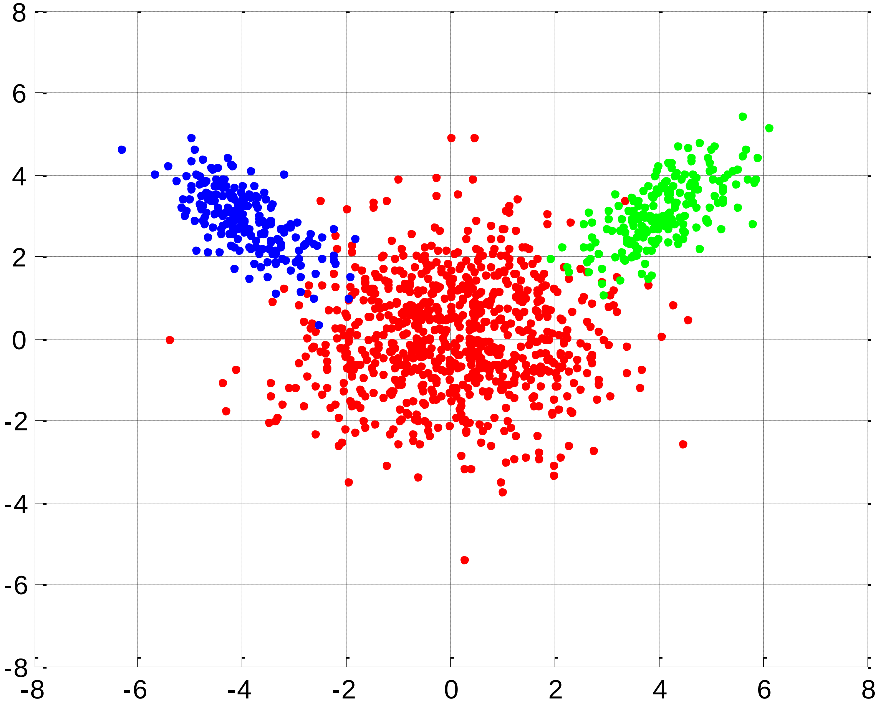
- The K-means algorithm adopts the hard assignment and doesn’t consider the data density and probabilistic distribution.

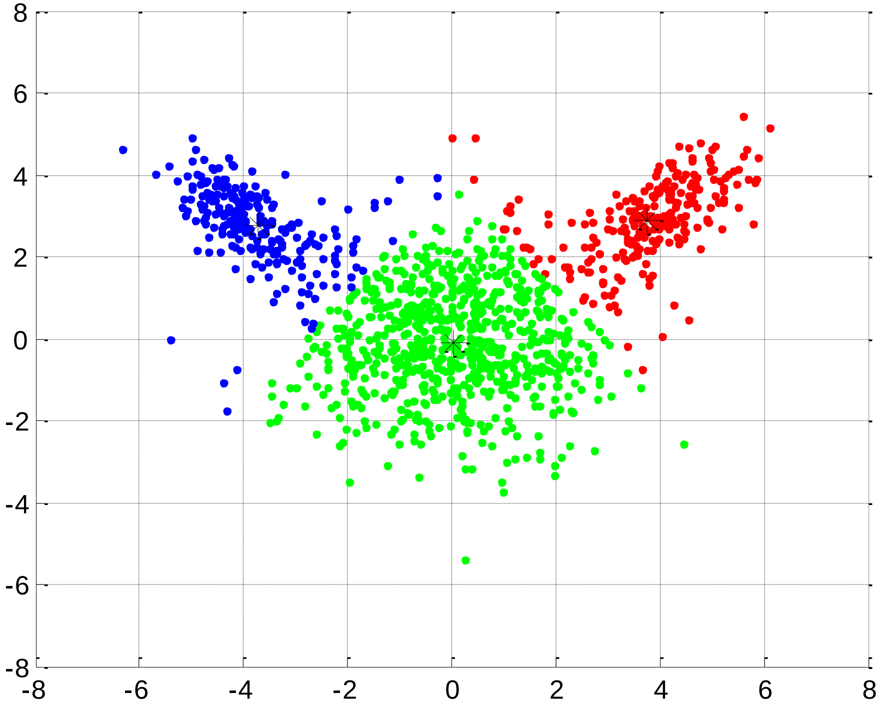




The limitation of K-means clustering

- The K-means algorithm adopts the hard assignment and doesn’t consider the data density and probabilistic distribution.


Original Data with class label


Clustering by kmeans

Mixtures of Gaussians

Gaussian mixture distribution

- **Definition:** $\boxed{p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}$ $\quad \sum_{k=1}^{K} \pi_k = 1 \quad\quad 0 \leqslant \pi_k \leqslant 1$

- Introduce a K-dimensional binary random variable $\mathbf{z} = (z_1, z_2, \ldots, z_K)^{\mathrm{T}}$

$$z_k \in \{0, 1\} \qquad \textstyle\sum_k z_k = 1 \qquad p(z_k = 1) = \pi_k \quad \longrightarrow \quad p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k}$$

Latent variable

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

- Equivalent formulation of the Gaussian mixture:

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

$$= \sum_{j=1}^{K} \prod_{k=1}^{K} \left(\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right)^{I_{kj}} = \sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j) \qquad I_{kj} = \begin{cases} 1 & \text{if } k = j \\ 0 & \text{otherwise.} \end{cases}$$

$$\longrightarrow \quad \boxed{\gamma(z_k) \equiv p(z_k = 1|\mathbf{x}) = \frac{p(z_k = 1)p(\mathbf{x}|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(\mathbf{x}|z_j = 1)} = \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}}$$

responsibility

Gaussian mixture distribution

$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{x}|\mathbf{z})p(\mathbf{z}) = \sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$$

$$\gamma(z_k) \equiv p(z_k = 1|\mathbf{x}) = \frac{p(z_k = 1)p(\mathbf{x}|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(\mathbf{x}|z_j = 1)} = \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

responsibility

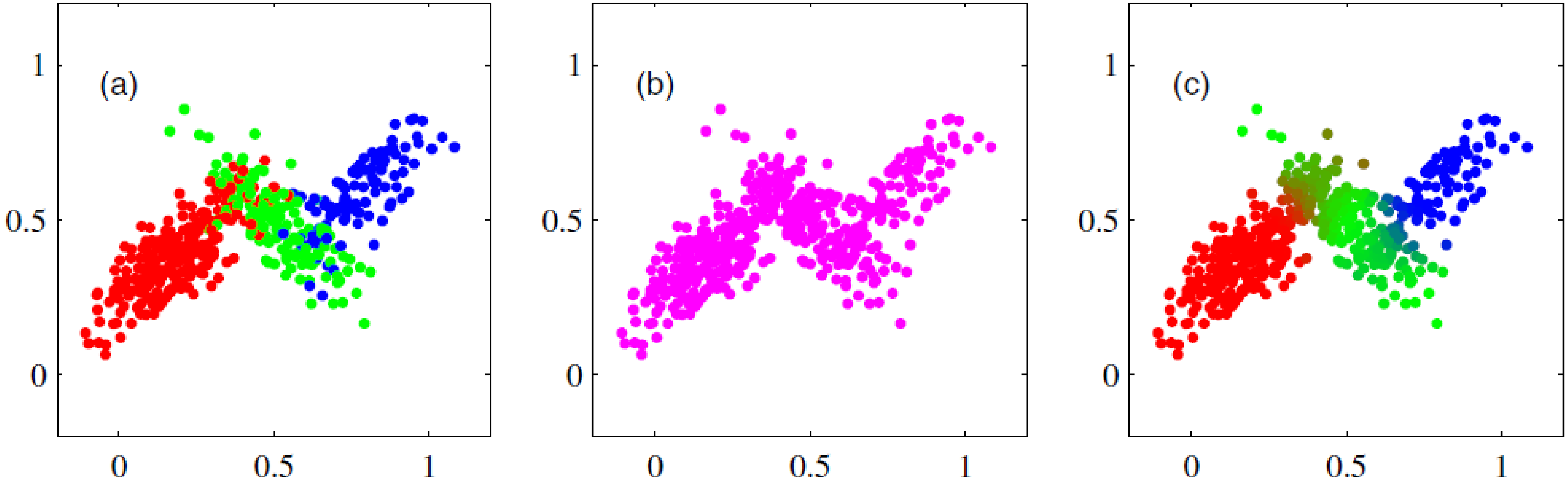


Figure 9.5 Example of 500 points drawn from the mixture of 3 Gaussians shown in Figure 2.23. (a) Samples from the joint distribution $p(\mathbf{z})p(\mathbf{x}|\mathbf{z})$ in which the three states of $\mathbf{z}$, corresponding to the three components of the mixture, are depicted in red, green, and blue, and (b) the corresponding samples from the marginal distribution $p(\mathbf{x})$, which is obtained by simply ignoring the values of $\mathbf{z}$ and just plotting the $\mathbf{x}$ values. The data set in (a) is said to be *complete*, whereas that in (b) is *incomplete*. (c) The same samples in which the colours represent the value of the responsibilities $\gamma(z_{nk})$ associated with data point $\mathbf{x}_n$, obtained by plotting the corresponding point using proportions of red, blue, and green ink given by $\gamma(z_{nk})$ for $k = 1, 2, 3$, respectively

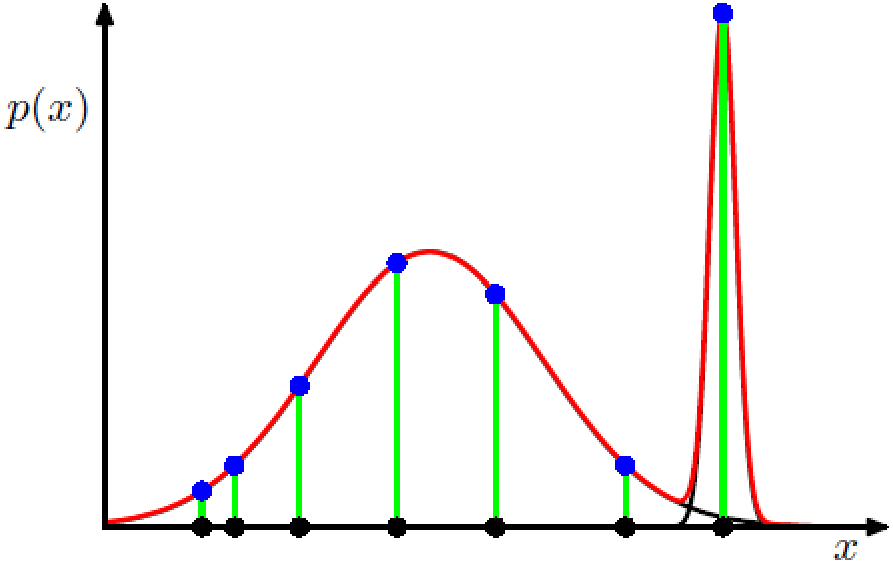
The difficulty of estimating parameters in GMM by ML

$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{x}|\mathbf{z})p(\mathbf{z}) = \sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)$$

- The log of the likelihood function of GMM:

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

- Issue #1: singularities
  - Collapses onto a specific data point



- Issue #2: identifiability
  - Total K! equivalent solutions
- Issue #3: no closed form solution
  - The derivatives of the log likelihood are complex.

Expectation-Maximization algorithm for GMM

$$\ln p(\mathbf{X}|\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln\left\{\sum_{k=1}^{K}\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right\} \qquad \sum_{k=1}^{K} \pi_k = 1 \qquad 0 \leqslant \pi_k \leqslant 1$$

M Step

- Solve $\boldsymbol{\mu}_k$:

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

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

Weighting factor

- Solve Σ_k :

$$\frac{\partial \ln p(\mathbf{X}|\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Sigma})}{\partial \boldsymbol{\Sigma}_k} = 0 \Rightarrow \boldsymbol{\Sigma}_k = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

- Solve π_k :

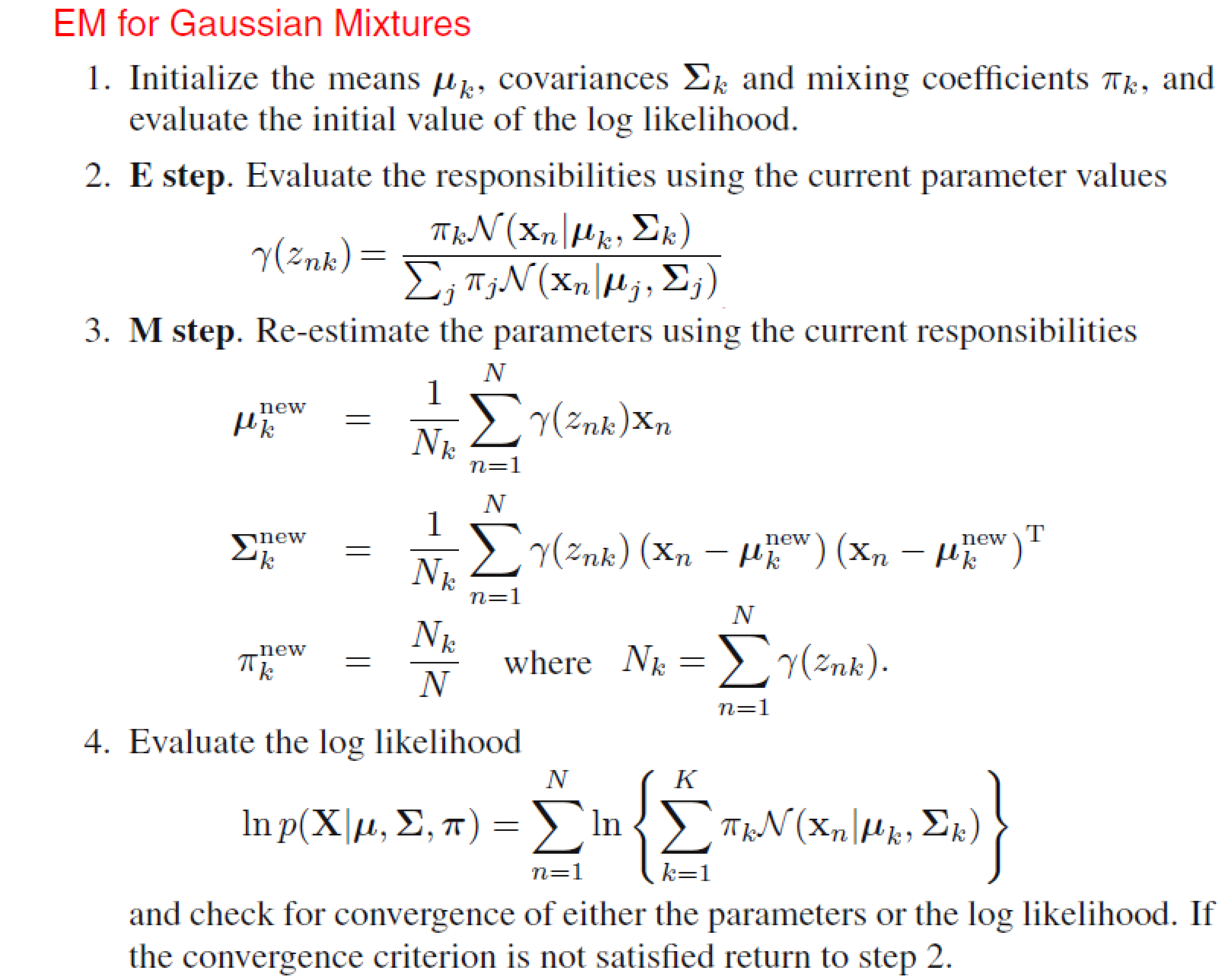
$$\frac{\partial}{\partial \pi_k}\left\{\ln p(\mathbf{X}|\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Sigma}) + \lambda\left(\sum_{k=1}^{K}\pi_k - 1\right)\right\} = 0 \Rightarrow 0 = \sum_{n=1}^{N}\frac{\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j,\boldsymbol{\Sigma}_j)} + \lambda \Rightarrow \pi_k = \frac{N_k}{N}$$

E Step

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

Each iteration will increase the log likelihood function.

Expectation-Maximization algorithm for GMM



EM for Gaussian Mixtures

1. Initialize the means $\boldsymbol{\mu}_k$, covariances $\boldsymbol{\Sigma}_k$ and mixing coefficients π_k, and evaluate the initial value of the log likelihood.

2. **E step**. Evaluate the responsibilities using the current parameter values

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

3. **M step**. Re-estimate the parameters using the current responsibilities

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

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

$$\pi_k^{\text{new}} = \frac{N_k}{N} \quad \text{where} \quad N_k = \sum_{n=1}^{N}\gamma(z_{nk}).$$

4. Evaluate the log likelihood

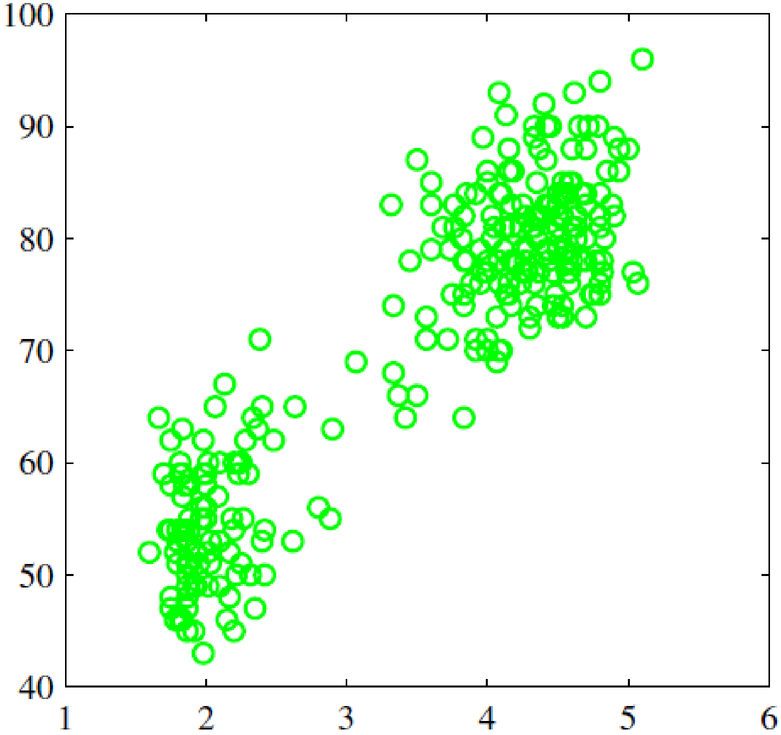
$$\ln p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) = \sum_{n=1}^{N}\ln\left\{\sum_{k=1}^{K}\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right\}$$

and check for convergence of either the parameters or the log likelihood. If the convergence criterion is not satisfied return to step 2.

EM algorithm for GMM: experiment

- The Old Faithful data set:

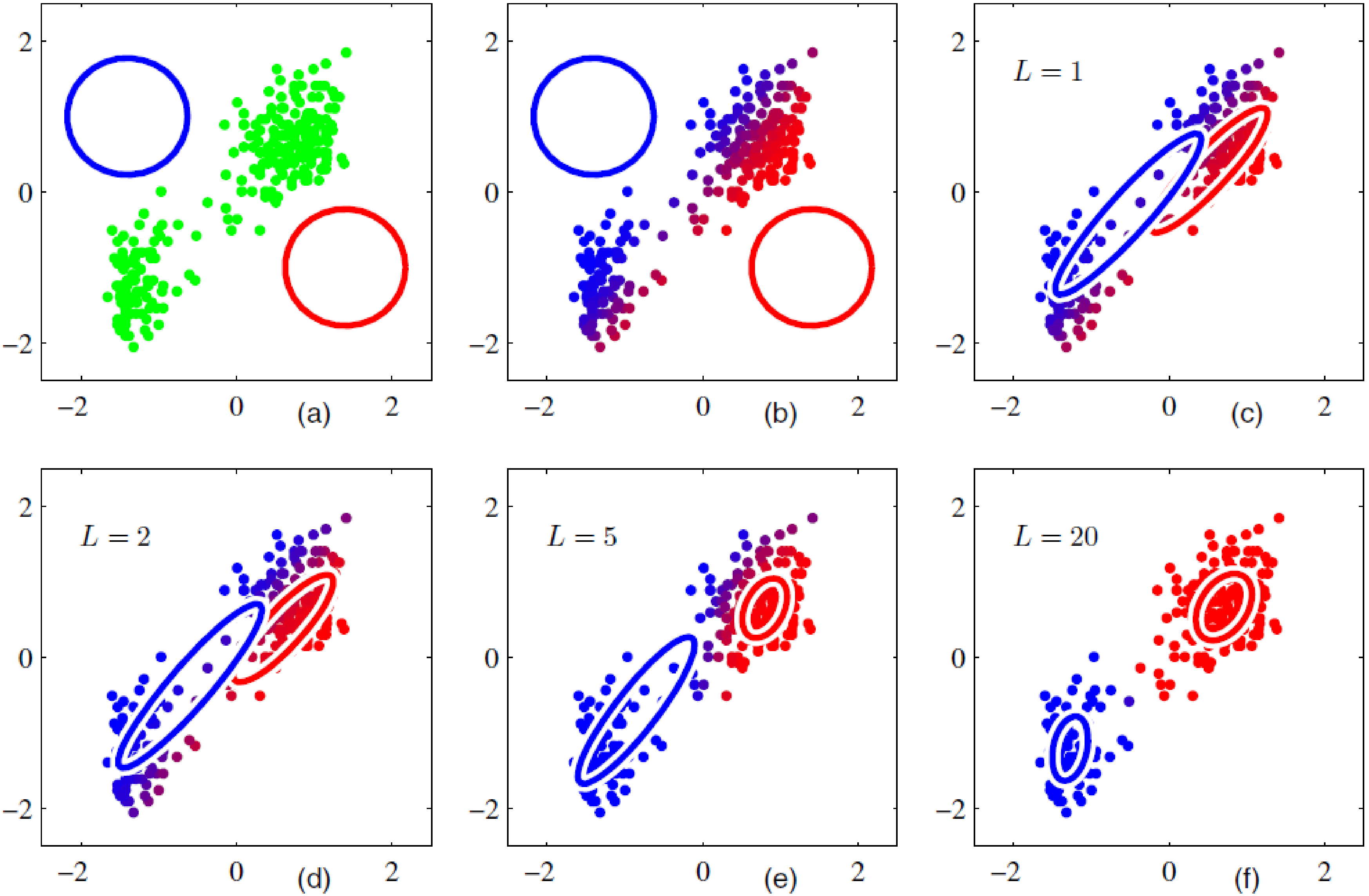
The Old Faithful geyser in Yellowstone National Park. ©Bruce T. Gourley www.brucegourley.com.



Plot of the time to the next eruption in minutes (vertical axis) versus the duration of the eruption in minutes (horizontal axis) for the Old Faithful data set.

EM algorithm for GMM: experiment

- The Old Faithful data set:



An Alternative View of EM

The general EM algorithm

- The log likelihood of a discrete latent variables model:

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

Direct optimization of this log likelihood function is difficult!

- *The goal of EM algorithm is to find maximum likelihood solution for models having latent variables.*

- For the complete data set $\{\mathbf{X}, \mathbf{Z}\}$, the log likelihood function:

$$\ln p(\mathbf{X}|\boldsymbol{\theta}) \Longrightarrow \ln p(\mathbf{X},\mathbf{Z}|\boldsymbol{\theta})$$

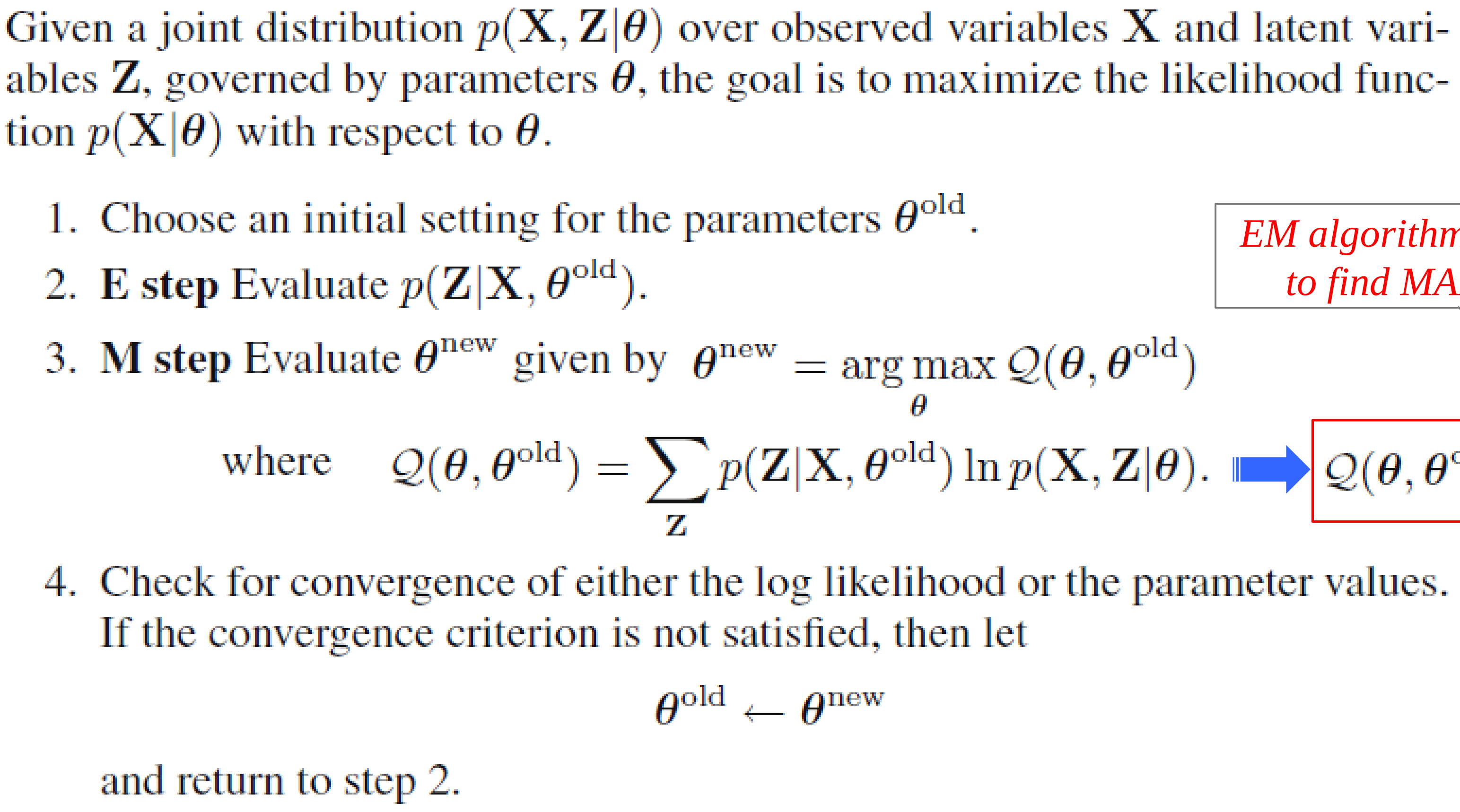
Suppose that maximization of this complete-data log likelihood function is very easier!

- For the incomplete data set $\{\mathbf{X}\}$, we adopt the following steps to find maximum likelihood solution:

Expectation of this complete-data log likelihood function

$$\begin{tikzcd}
\boxed{\boldsymbol{\theta}^{\text{old}}} \arrow[d] & \boldsymbol{\theta}^{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta},\boldsymbol{\theta}^{\text{old}}) \arrow[l] \\
p(\mathbf{Z}|\mathbf{X},\boldsymbol{\theta}^{\text{old}}) \arrow[r] & \boxed{\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X},\mathbf{Z}|\boldsymbol{\theta})] = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X},\boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{X},\mathbf{Z}|\boldsymbol{\theta}) = \mathcal{Q}(\boldsymbol{\theta},\boldsymbol{\theta}^{\text{old}})} \arrow[u]
\end{tikzcd}$$

The general EM algorithm



The General EM Algorithm

Given a joint distribution $p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})$ over observed variables $\mathbf{X}$ and latent variables $\mathbf{Z}$, governed by parameters $\boldsymbol{\theta}$, the goal is to maximize the likelihood function $p(\mathbf{X}|\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$.

1. Choose an initial setting for the parameters $\boldsymbol{\theta}^{\text{old}}$.
2. **E step** Evaluate $p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}})$.
3. **M step** Evaluate $\boldsymbol{\theta}^{\text{new}}$ given by $\boldsymbol{\theta}^{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}})$

   where $$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}). \Rightarrow \boxed{\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) + \ln p(\boldsymbol{\theta})}$$

EM algorithm can be used to find MAP solution

4. Check for convergence of either the log likelihood or the parameter values. If the convergence criterion is not satisfied, then let
$$\boldsymbol{\theta}^{\text{old}} \leftarrow \boldsymbol{\theta}^{\text{new}}$$
and return to step 2.

Gaussian mixtures revisited

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

- *For the complete data set* {**X**, **Z**}, *the log likelihood function:*

$$p(\mathbf{X},\mathbf{Z}|\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\pi}) = \prod_{n=1}^{N}\prod_{k=1}^{K}\pi_k^{z_{nk}}\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)^{z_{nk}} \qquad \sum_{k=1}^{K}\pi_k = 1 \qquad 0 \leqslant \pi_k \leqslant 1$$

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

➡ $$\frac{\partial}{\partial\pi_k}\left\{\ln p(\mathbf{X},\mathbf{Z}|\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\pi}) + \lambda\left(\sum_{k=1}^{K}\pi_k - 1\right)\right\} = 0$$ ➡ $$\pi_k = \frac{1}{N}\sum_{n=1}^{N} z_{nk}$$

Gaussian mixtures revisited

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

- *For the incomplete data set $\{\mathbf{X}\}$, the posterior distribution of the latent variables:*

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

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

- *Expectation:*

$$\Rightarrow \mathbb{E}[z_{nk}] = \frac{\sum_{\mathbf{z}_n} z_{nk}\prod_{k'}\left[\pi_{k'}\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_{k'},\boldsymbol{\Sigma}_{k'})\right]^{z_{nk'}}}{\sum_{\mathbf{z}_n}\prod_{j}\left[\pi_j\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j,\boldsymbol{\Sigma}_j)\right]^{z_{nj}}} = \frac{\pi_k\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K}\pi_j\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j,\boldsymbol{\Sigma}_j)} = \gamma(z_{nk})$$

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

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

$$\boldsymbol{\mu}^{\text{old}}, \boldsymbol{\Sigma}^{\text{old}} \text{ and } \boldsymbol{\pi}^{\text{old}} \Rightarrow \gamma(z_{nk}) \Rightarrow \underset{\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\pi}}{\arg\max}\,\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X},\mathbf{Z}|\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\pi})] \Rightarrow \boldsymbol{\mu}^{\text{new}}, \boldsymbol{\Sigma}^{\text{new}} \text{ and } \boldsymbol{\pi}^{\text{new}}$$

Relation to K-means

- Consider a Gaussian mixture model in which the covariance matrices of the mixture components are given by $\epsilon\mathbf{I}$, where ϵ is a variance parameter that is shared by all of the components, and $\mathbf{I}$ is the identity matrix, so that

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

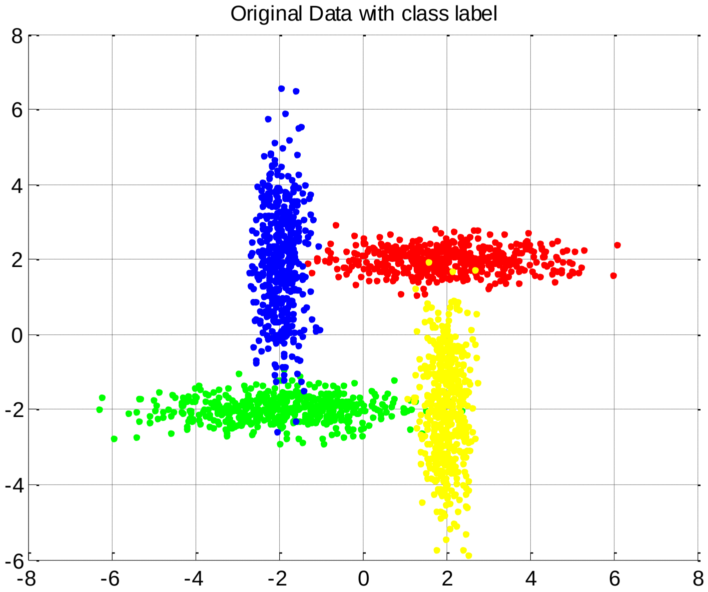
$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} \xrightarrow[\text{fixed constant}]{\text{treat } \epsilon \text{ as a}} \gamma(z_{nk}) = \frac{\pi_k \exp\left\{-\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2/2\epsilon\right\}}{\sum_j \pi_j \exp\left\{-\|\mathbf{x}_n - \boldsymbol{\mu}_j\|^2/2\epsilon\right\}}$$

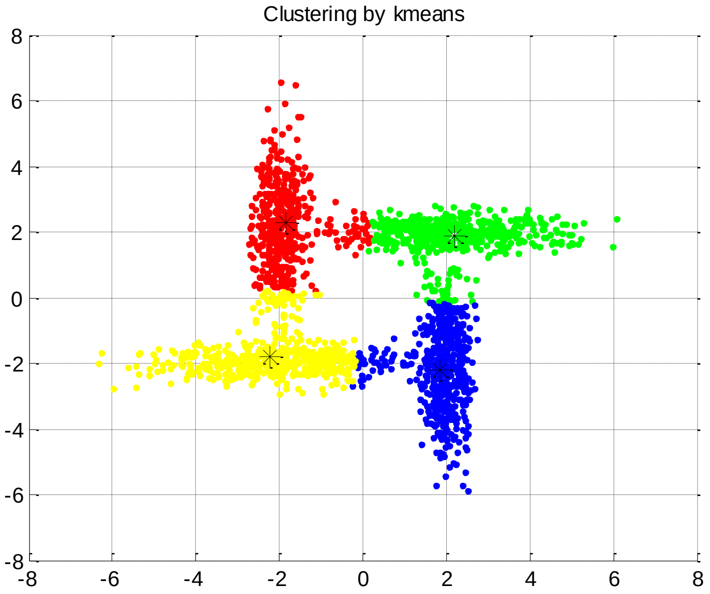
- If we consider the limit $\epsilon \to 0$, we see that in the denominator the term for which $\|\mathbf{x}_n - \boldsymbol{\mu}_j\|^2$ is smallest will go to zero most slowly, and hence the responsibilities $\gamma(z_{nk})$ for the data point $\mathbf{x}_n$ all go to zero except for term j, for which the responsibility $\gamma(z_{nj})$ will go to unity.

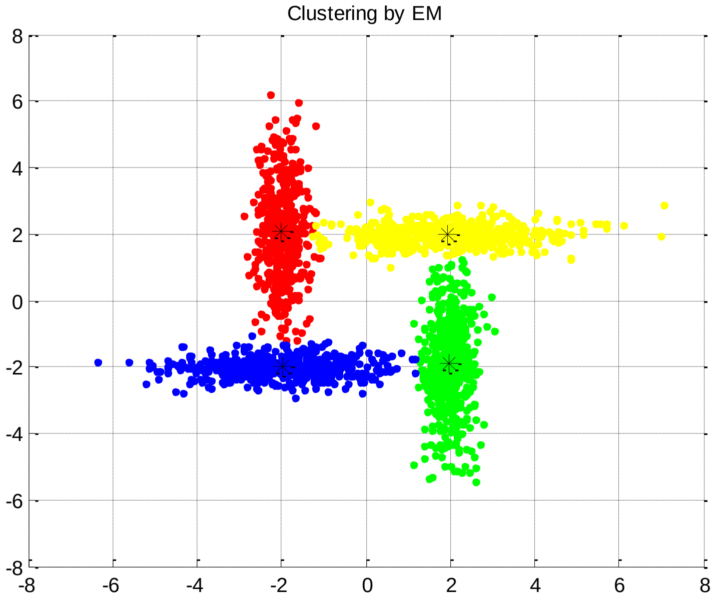
$$\mathbb{E}_{\mathbf{Z}}[\ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi})] \to -\frac{1}{2}\sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2 + \text{const}$$

$$J = \sum_{n=1}^{N}\sum_{k=1}^{K} r_{nk}\|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2 \qquad r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\mathbf{x}_n - \boldsymbol{\mu}_j\|^2 \\ 0 & \text{otherwise.} \end{cases}$$

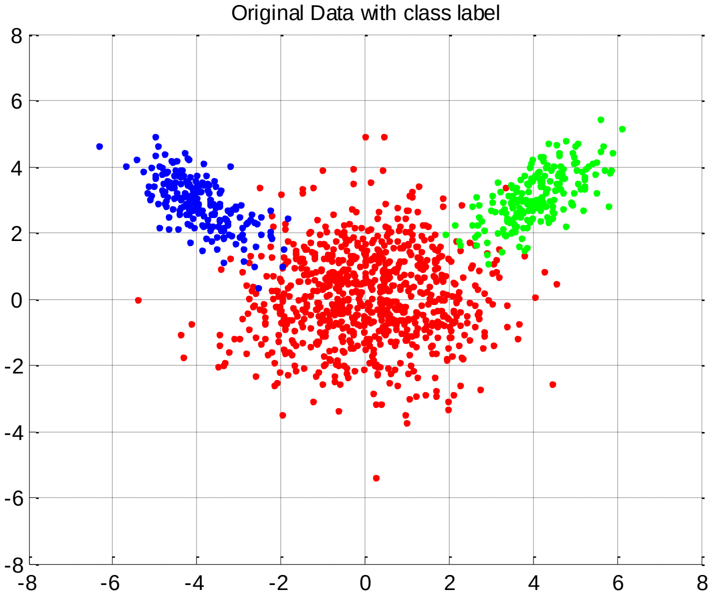
EM for GMM vs. K-means

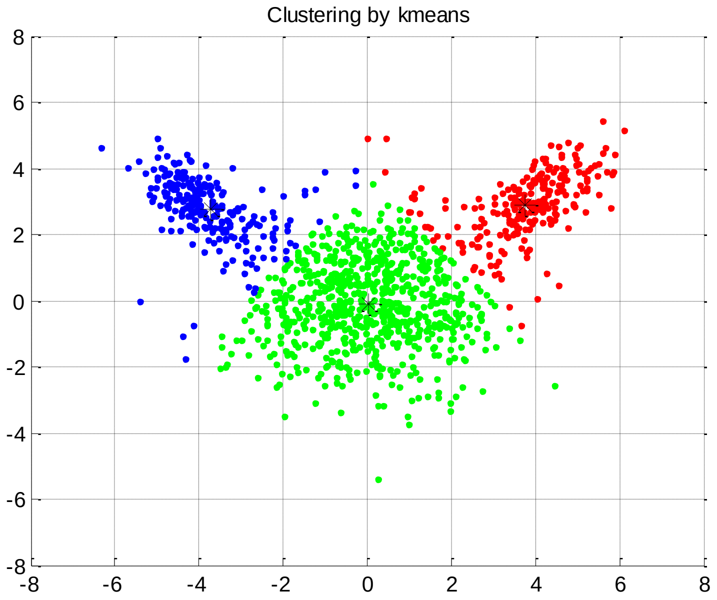

Original Data with class label

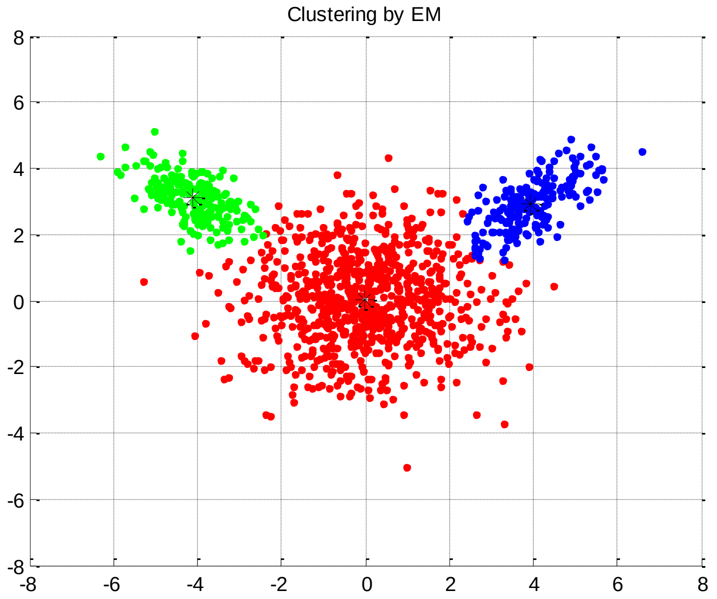

Clustering by kmeans


Clustering by EM

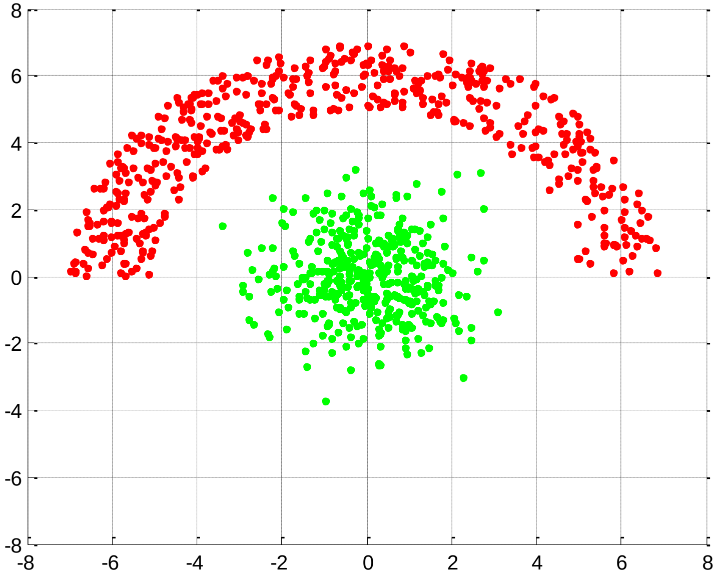
EM for GMM vs. K-means



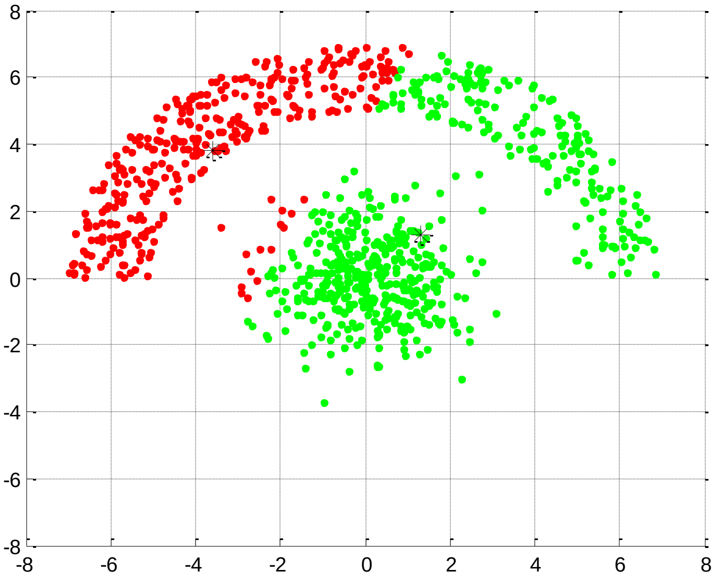




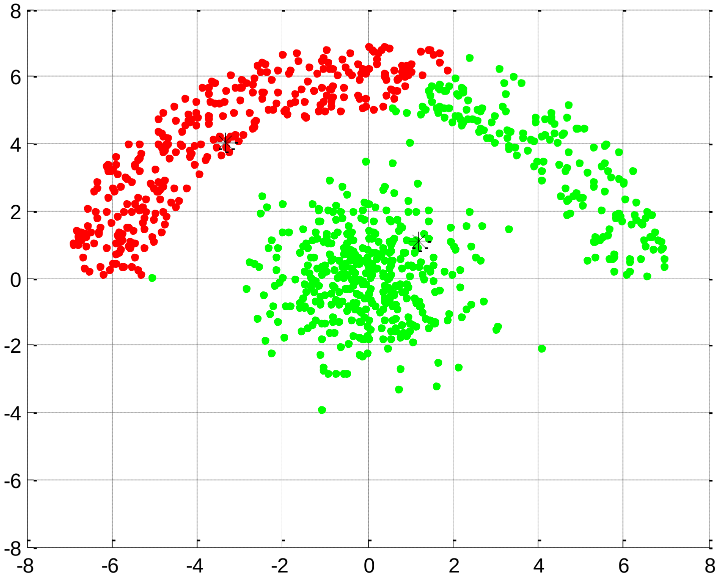
EM for GMM vs. K-means



Original Data with class label

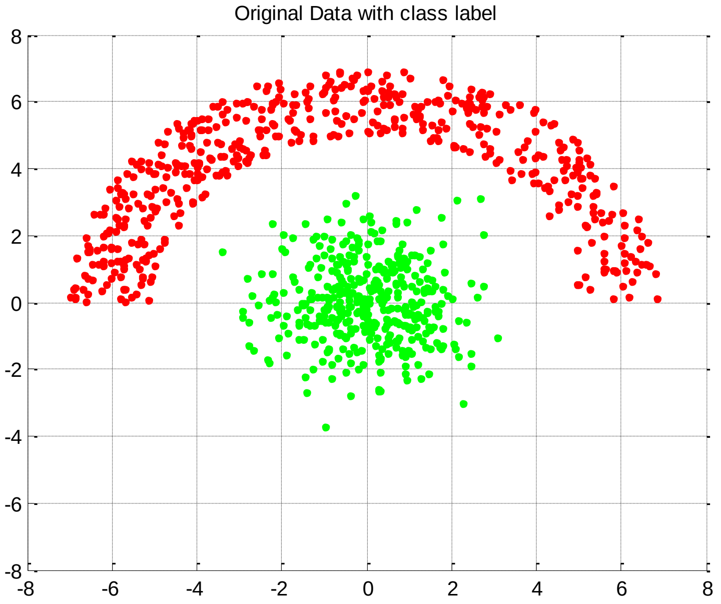


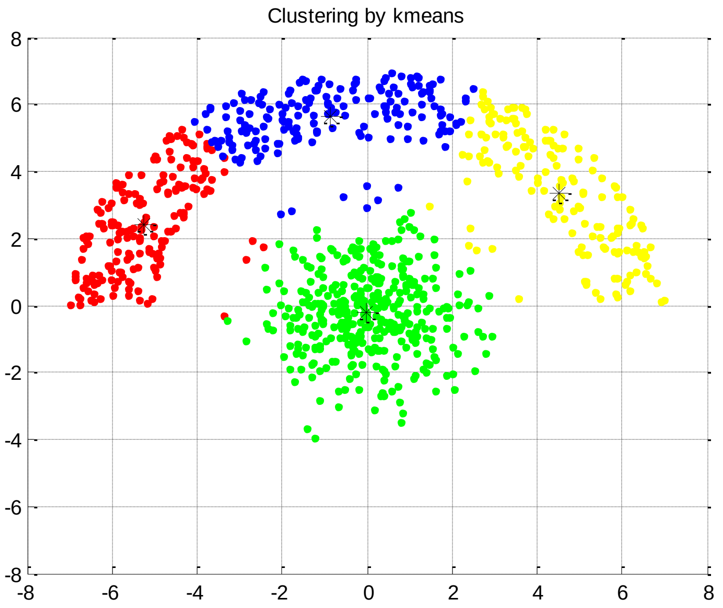
Clustering by kmeans

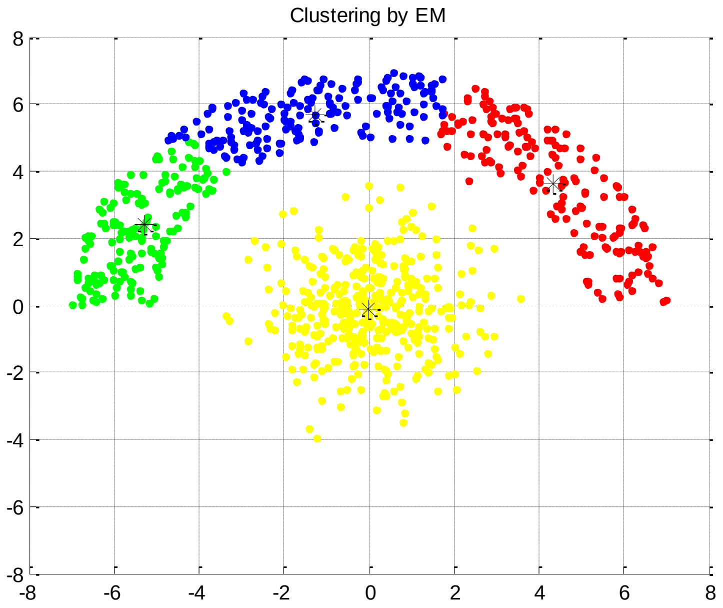


Clustering by EM

EM for GMM vs. K-means


Original Data with class label


Clustering by kmeans


Clustering by EM

The EM Algorithm in General

The EM algorithm is a general technique for finding maximum likelihood solutions for probabilistic models having latent variables.

The EM Algorithm in General

- *We have known, for the incomplete data set* $\{\mathbf{X}\}$, *direct optimization of the log likelihood function is difficult:*

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

- *Introduce a distribution q(**Z**) defined over the latent variables, and we observe that, for any choice of q(**Z**), the following decomposition holds:*

*Functional of the distribution q(**Z**)*

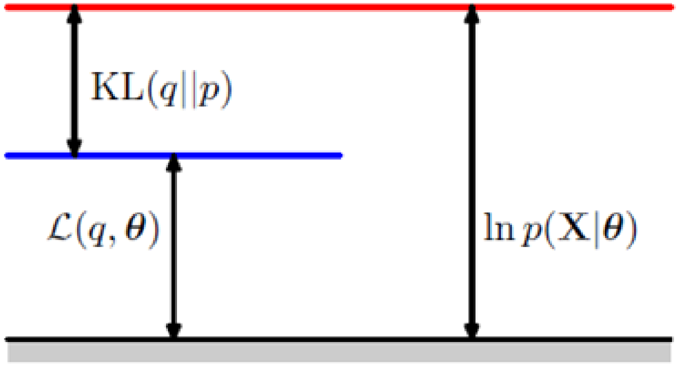
$$\ln p(\mathbf{X}|\boldsymbol{\theta}) = \mathcal{L}(q,\boldsymbol{\theta}) + \mathrm{KL}(q\|p)$$

Kullback-Leibler divergence

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

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

- *Proof:*


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

The EM Algorithm in General

- *The connection between the decomposition and EM algorithm:*

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

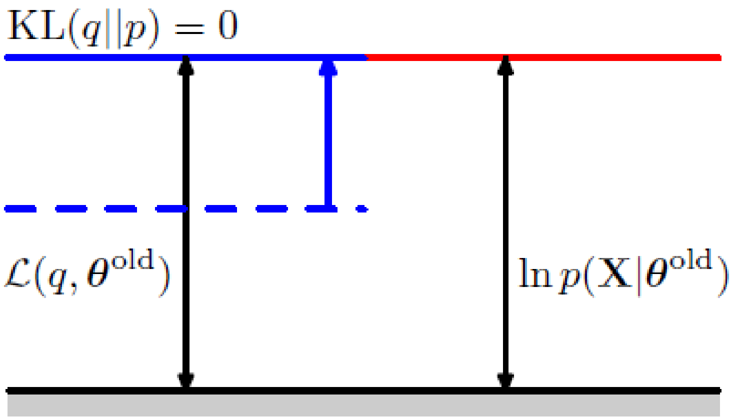
$$\mathcal{L}(q, \boldsymbol{\theta}) = \sum_{\mathbf{Z}} q(\mathbf{Z}) \ln \left\{ \frac{p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})}{q(\mathbf{Z})} \right\}$$

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

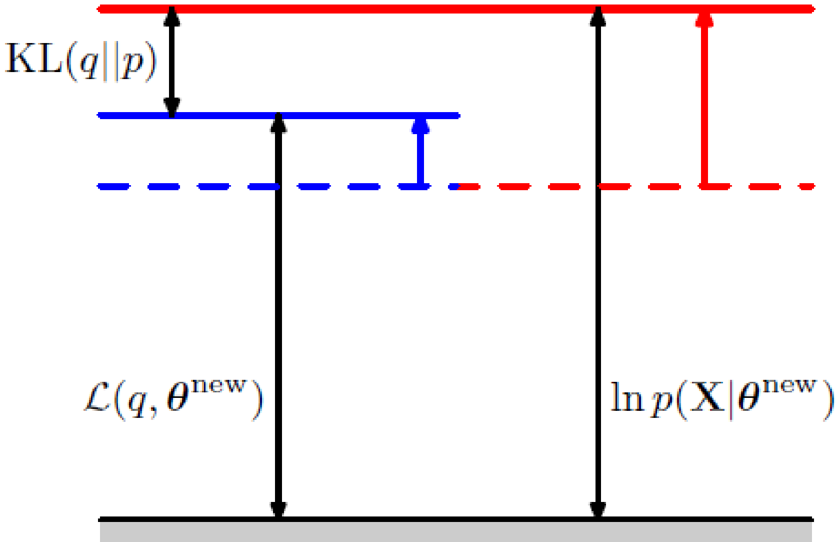
$$\begin{aligned} \mathcal{L}(q, \boldsymbol{\theta}) &= \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}) \\ &\quad - \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{Z}|\mathbf{X},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

E step

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

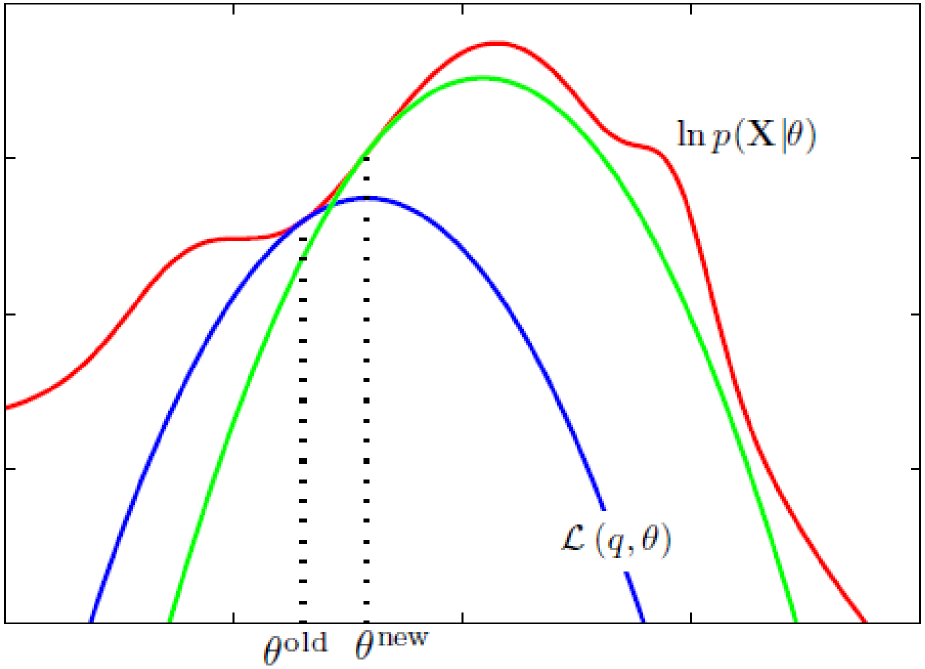

$\mathrm{KL}(q\|p) = 0$
$\mathcal{L}(q, \boldsymbol{\theta}^{\text{old}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\text{old}})$

M step


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

The EM Algorithm in General

- *The operation of the EM algorithm in the space of parameters:*



- *Extension of EM*
  - *The generalized EM (GEM)*
  - *Online EM*

Next: PCA and Eigenface