PATTERN RECOGNITION AND MACHINE LEARNING

CHAPTER 9: MIXTURE MODELS AND EM

K-means Clustering

Suppose we have a data set $\{x_1, \ldots, x_N\}$ consisting of N observations of a random D-dimensional Euclidean variable x.

Our goal is to partition the data set into some number K of clusters

We can formalize this notion by first introducing a set of D-dimensional vectors μ_k, where $k = 1, \ldots, K$, in which μ_k is a prototype (center of clusters) associated with the kth cluster.

Our goal is then to find an assignment of data points to clusters, as well as a set of vectors $\{\mu_k\}$, such that the sum of the squares of the distances of each data point to its closest vector μ_k, is a minimum.

K-means Clustering

For each data point x_n, we introduce a corresponding set of binary indicator variables $r_{nk} \in \{0, 1\}$, where k = 1, . . . , K describing which of the K clusters the data point xn is assigned to, so that if data point x_n is assigned to cluster k then $r_{nk} = 1$, and $r_{nj} = 0$ for j not k.

We can then define an objective function, sometimes called a distortion measure, given by

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

Our goal is to find values for the $\{r_{nk}\}$ and the $\{\mu_k\}$ to minimize J.

First, we choose some initial values for the μ_k and we minimize J with respect to the r_{nk}, keeping the μ_k fixed.

In the second phase, we minimize J with respect to the μ_k, keeping r_{nk} fixed.

K-means Clustering

J is a linear function of r_{nk}, this optimization can be performed easily to give a closed form solution.

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

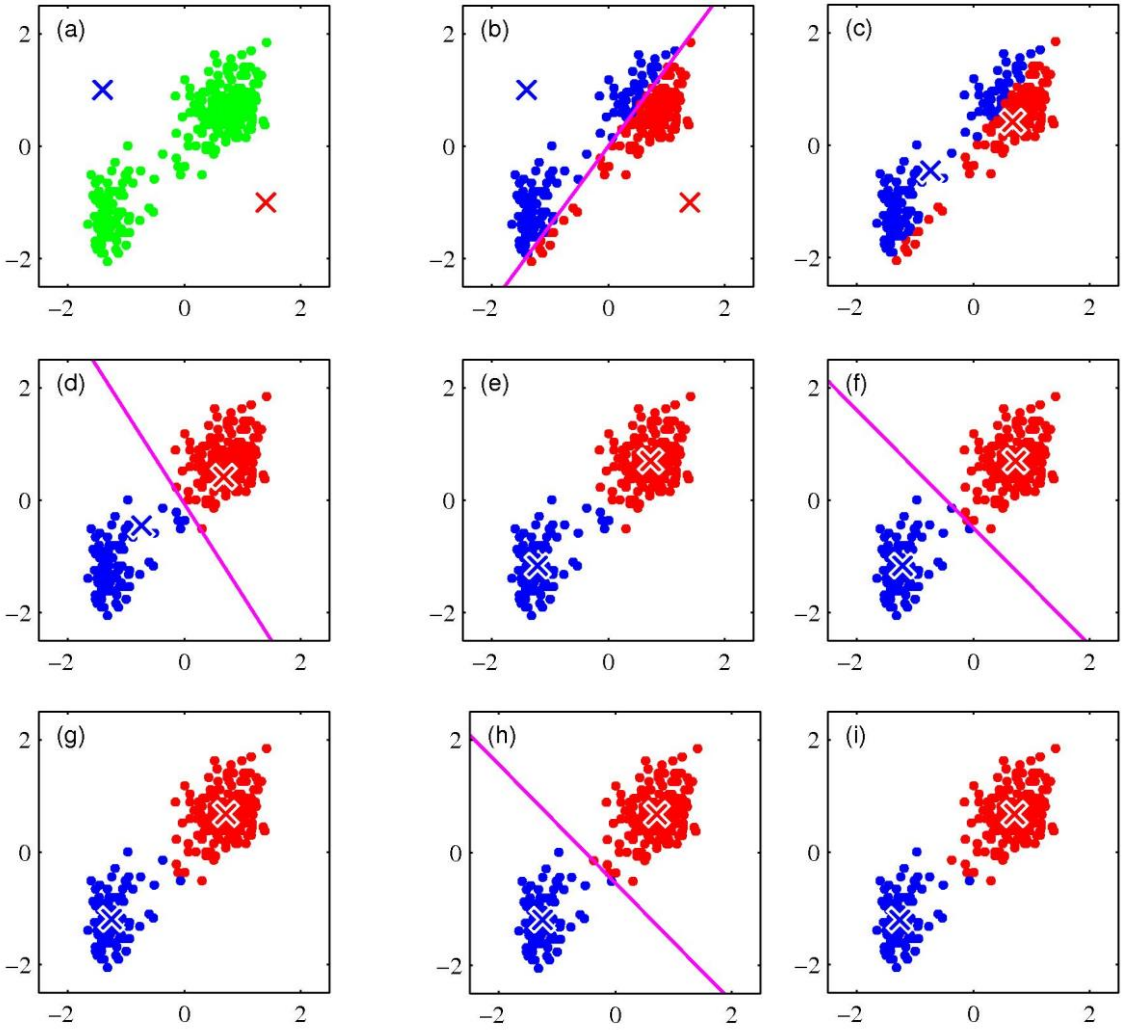
The objective function J is a quadratic function of μ_k, and it can be minimized by setting its derivative with respect to μ_k to zero:

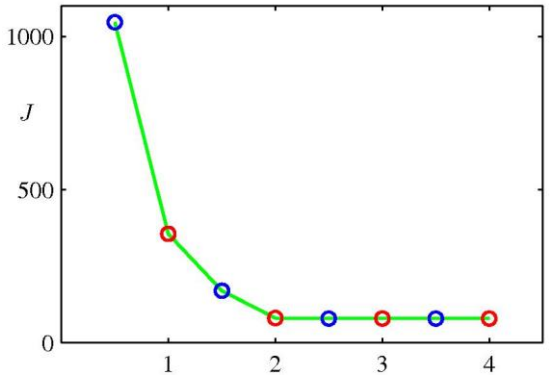
$$2\sum_{n=1}^{N} r_{nk}(\mathbf{x}_n - \boldsymbol{\mu}_k) = 0$$

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

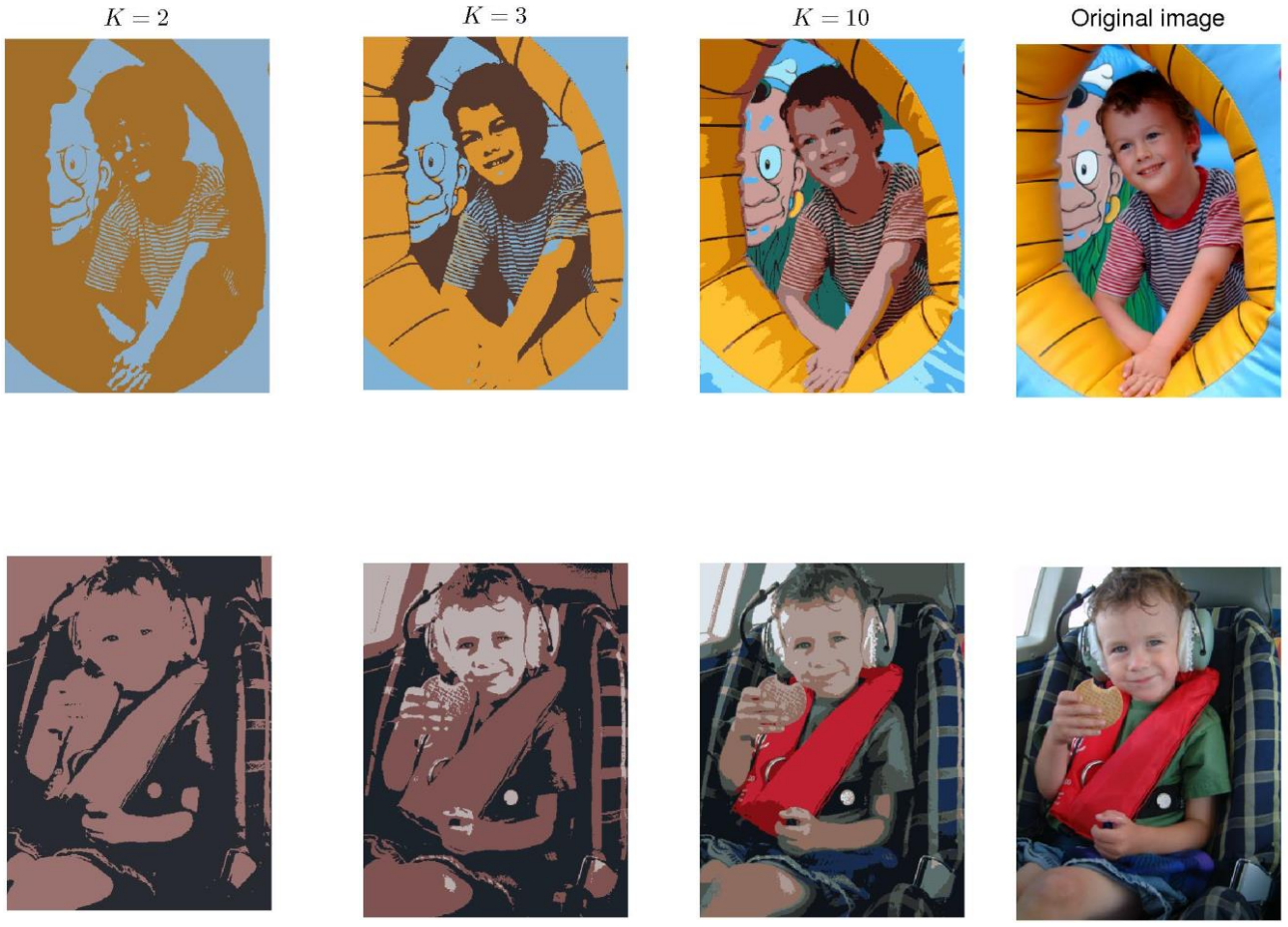
The denominator in this expression is equal to the number of points assigned to cluster k, and so this result has a simple interpretation, namely set μ_k equal to the mean of all of the data points x_n assigned to cluster k. For this reason, the procedure is known as the K-means algorithm.

K-means Clustering





K-means Clustering



Mixtures of Gaussians

A Gaussian mixture distribution can be written as a linear superposition of Gaussians in the form

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

Let us introduce a K-dimensional binary random variable z having a 1-of-K representation in which a particular element z_k is equal to 1 and all other elements are equal to 0.

The values of z_k therefore satisfy $z_k \in \{0, 1\}$ and $\sum z_k = 1$, and we see that there are K possible states for the vector z according to which element is nonzero.

We shall define the joint distribution p(x, z) in terms of a marginal distribution p(z) and a conditional distribution p(x|z),

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

Mixtures of Gaussians

Another quantity that will play an important role is the conditional probability of z given x.
We shall use $\gamma(z_k)$ to denote $p(z_k = 1|x)$, whose value can be found using Bayes' theorem

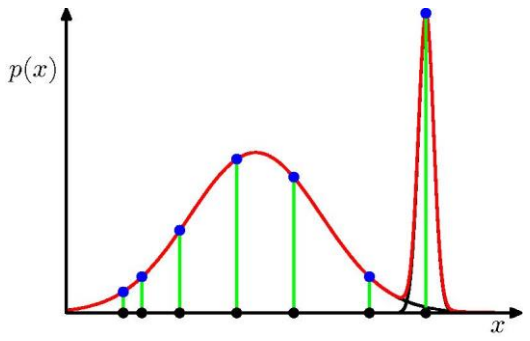
$$\gamma(z_k) \equiv p(z_k = 1|\mathbf{x}) = \frac{p(z_k = 1)p(\mathbf{x}|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(\mathbf{x}|z_j = 1)} = \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}.$$

Mixtures of Gaussians

Suppose we have a data set of observations $\{x_1, \ldots, x_N\}$, and we wish to model this data using a mixture of Gaussians.

If we assume that the data points are drawn independently from the distribution, then we can express the Gaussian mixture model for this i.i.d. data set and the log of the likelihood function is given by

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



A further issue in finding maximum likelihood solutions arises from the fact that for any given maximum likelihood solution, a K-component mixture will have a total of K! equivalent solutions corresponding to the K! ways of assigning K sets of parameters to K components.

Mixtures of Gaussians

An elegant and powerful method for finding maximum likelihood solutions for models with latent variables is called the expectation-maximization algorithm, or EM algorithm

EM for Gaussian Mixtures

Given a Gaussian mixture model, the goal is to maximize the likelihood function with respect to the parameters (comprising the means and covariances of the components and the mixing coefficients).

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

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}. \tag{9.23}$$

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

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\mathbf{x}_n \tag{9.24}$$

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right)\left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right)^{\mathrm{T}} \tag{9.25}$$

$$\pi_k^{\text{new}} = \frac{N_k}{N} \tag{9.26}$$

where

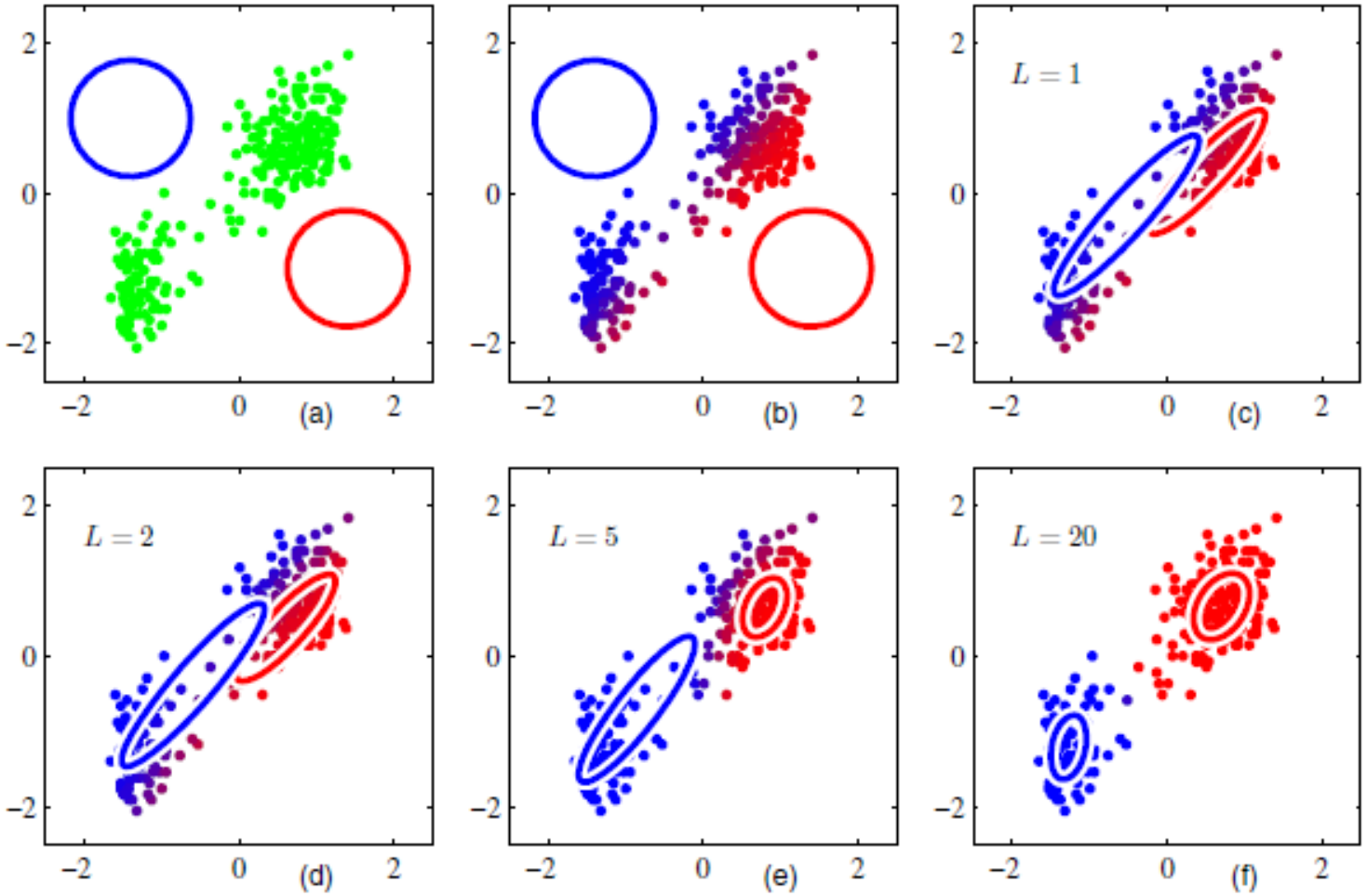
$$N_k = \sum_{n=1}^{N}\gamma(z_{nk}). \tag{9.27}$$

4. Evaluate the log likelihood

$$\ln p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) = \sum_{n=1}^{N}\ln\left\{\sum_{k=1}^{K}\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right\} \tag{9.28}$$

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

Mixtures of Gaussians



Mixtures of Gaussians

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

$$\boldsymbol{\theta}^{\text{new}} = \arg\max_{\boldsymbol{\theta}} \mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) \tag{9.32}$$

where

$$\mathcal{Q}(\boldsymbol{\theta}, \boldsymbol{\theta}^{\text{old}}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \boldsymbol{\theta}^{\text{old}}) \ln p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}). \tag{9.33}$$

4. Check for convergence of either the log likelihood or the parameter values. If the convergence criterion is not satisfied, then let

$$\boldsymbol{\theta}^{\text{old}} \leftarrow \boldsymbol{\theta}^{\text{new}} \tag{9.34}$$

and return to step 2.

Comparison of the K-means algorithm with the EM algorithm for Gaussian mixtures shows that there is a close similarity.

Whereas the K-means algorithm performs a hard assignment of data points to clusters, in which each data point is associated uniquely with one cluster, the EM algorithm makes a soft assignment based on the posterior probabilities.

The EM Algorithm in General

Consider a probabilistic model in which we collectively denote all of the observed variables by X and all of the hidden variables by Z. The joint distribution p(X,Z|θ) is governed by a set of parameters denoted θ.

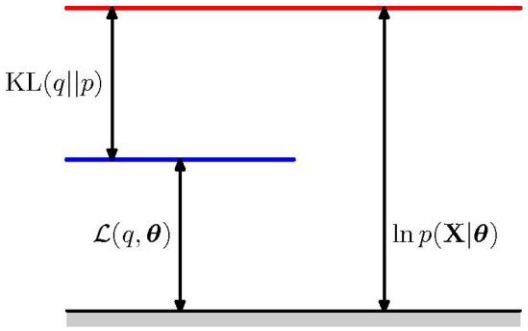
$$p(\mathbf{X}|\boldsymbol{\theta}) = \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}).$$

Next, we introduce a distribution q(Z) defined over the latent variables, and we observe that, for any choice of q(Z), the following decomposition holds

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

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

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



The Kullback-Leibler divergence ≥ 0.
L(q,Θ) = a lower bound