Gaussian Mixture Models

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Motivation

K-means forces the clusters to be *spherical*, but sometimes it is desirable to have *elliptical* clusters. Another issue is that, in K-means, each example can only belong to one cluster, but this may not always be a good choice, e.g. for data points that are near the "border". Both of these problems are solved by using Gaussian Mixture Model.

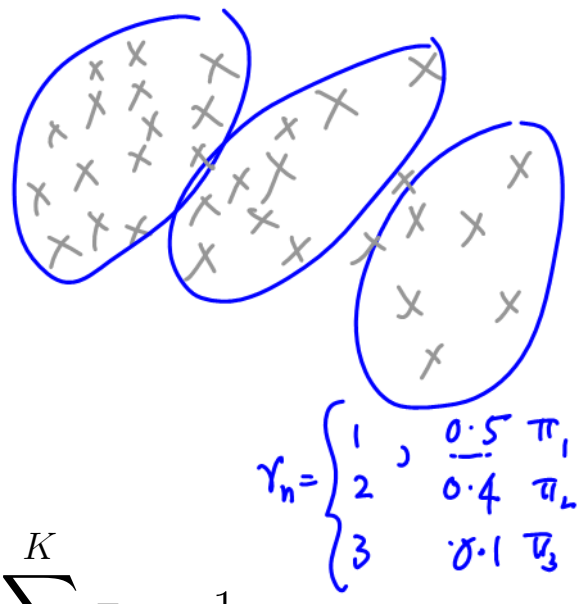
Clustering with Gaussians

The first issue is resolved by using full covariance matrices $\mathbf{\Sigma}_k$ instead of *isotropic* covariances.

$$p(\mathbf{X}|\boldsymbol{\mu}, \mathbf{\Sigma}, \mathbf{r}) = \prod_{n=1}^{N} \prod_{k=1}^{K} [\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \mathbf{\Sigma}_k)]^{r_{nk}}$$

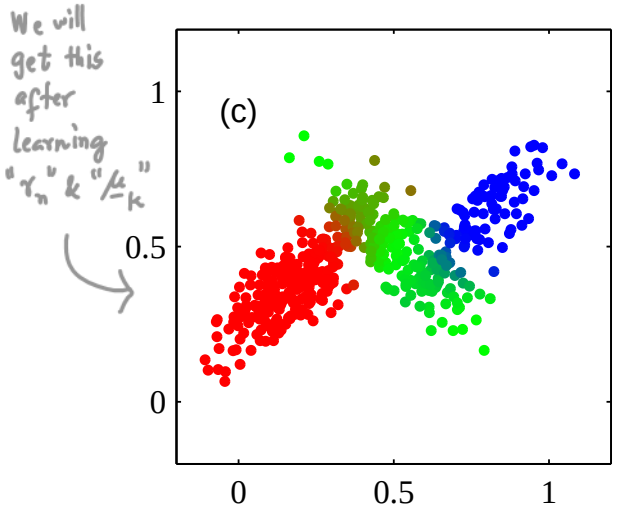
Soft-clustering

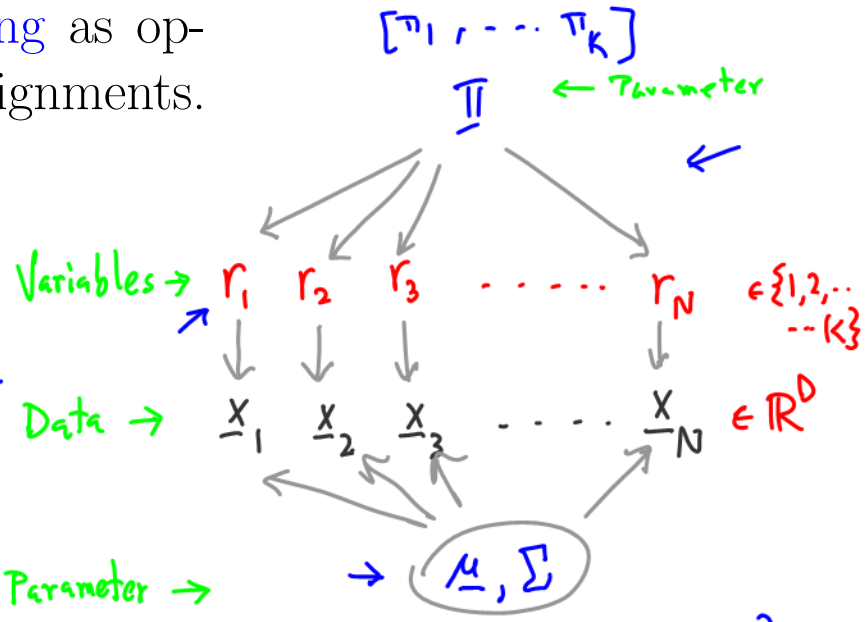
The second issue is resolved by defining r_n to be a random variable. Specifically, define $r_n \in \{1, 2, \ldots, K\}$ that follows a multinomial distribution.



$$p(r_n = k) = \pi_k \text{ where } \pi_k > 0, \forall k \text{ and } \sum_{k=1}^{K} \pi_k = 1$$

This leads to soft-clustering as opposed to having "hard" assignments.





$\{\mu_1 \mu_2 \ldots \mu_K\} = \mu$

$\{\Sigma_1 \Sigma_2 \ldots \Sigma_K\} = \Sigma$

$\theta = \{\mu, \Sigma, \pi\}$

$p(x_1, x_2 \ldots, x_N, r_1, r_2, \ldots r_N / \theta)$

$= p(X, r / \theta)$

Gaussian mixture model

Together, the likelihood and the prior define the joint distribution of Gaussian mixture model (GMM):

Joint $p(\mathbf{X}, \cancel{r_n} r | \boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi})$. prior

$$= \prod_{n=1}^{N} p(\mathbf{x}_n | r_n, \boldsymbol{\mu}, \boldsymbol{\Sigma}) p(r_n | \boldsymbol{\pi})$$

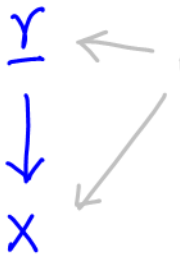
likelihood

$$= \prod_{n=1}^{N} \prod_{k=1}^{K} [\{\mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\}^{r_{nk}}] \prod_{k=1}^{K} [\pi_k]^{r_{nk}}$$

Joint = likelihood × Prior

$P_\theta(D, r) = P_\theta(D/r) P_\theta(r)$

Latent variable models



Here, $\mathbf{x}_n$ are observed data vectors, r_n are *latent* unobserved variables, and the unknown *parameters* are given by $\boldsymbol{\theta} := \{\boldsymbol{\mu}_1, \ldots, \mu_K, \boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_K, \boldsymbol{\pi}\}$.

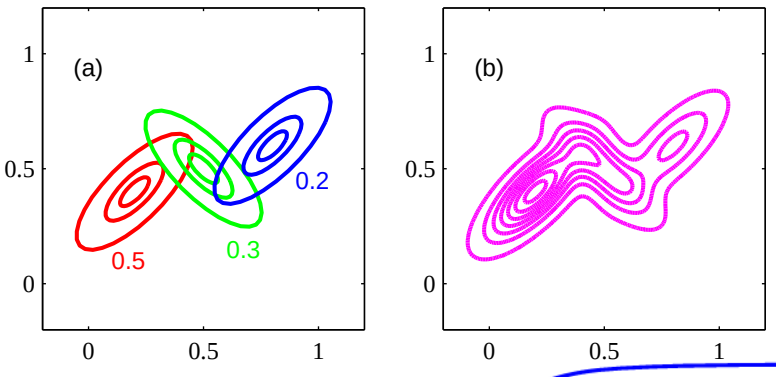
This is a generative model

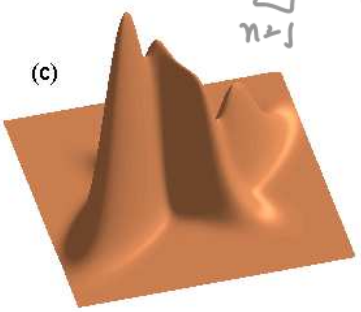
Marginal likelihood

GMM is a latent variable model with r_n being the unobserved (latent) variables. An advantage of treating r_n as latent variables instead of *parameters* is that we can *marginalize* them out to get a cost function that does not depend on r_n, i.e. as if r_n never existed.

Specifically, we get the following marginal likelihood by marginalizing r_n out from the likelihood:

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





Deriving cost functions this way, is good for *statistical efficiency*. Without a latent variable model, the number of parameters grow at rate $O(N)$. After marginalization, the growth is reduced to $O(D^2K)$ (assuming $D, K << N$).

Maximum likelihood

To get a maximum (marginal) likelihood estimate of $\boldsymbol{\theta}$, we maximize the following:

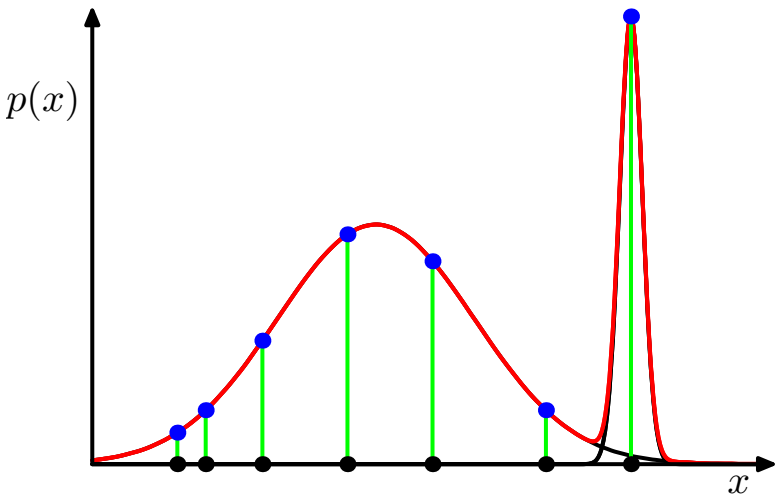
$$\max_{\boldsymbol{\theta}} \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

w.r.t. θ

Is this cost convex? Identifiable? Bounded?

$\theta^* = \max_{\theta} \log P_\theta(x)$

$\theta \rightarrow P_\theta(x)$ is one-to-one



To do

1. Understand K-means extension to GMM. Why do we need to treat r_n as a random variable? Identify the joint, likelihood, prior, and marginal distributions, respectively.
2. Understand identifiability and the difficulty with the maximum-likelihood estimation.