Machine Learning (IN2064)

Lecture 12: Clustering

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Unsupervised learning

Main idea

- Given some unlabeled data $\{\boldsymbol{x}_i\}$ we want to discover latent structure in it.

Last week: Dimensionality reduction

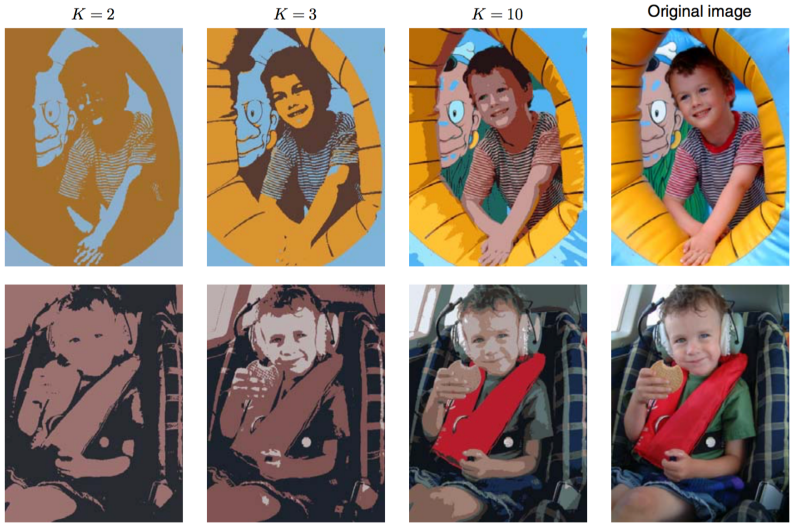
- Given high-dimensional data $\boldsymbol{x}_i \in \mathbb{R}^D$, find a continuous representation $\boldsymbol{z}_i \in \mathbb{R}^K$ with $K \ll D$, such that the structure is preserved.

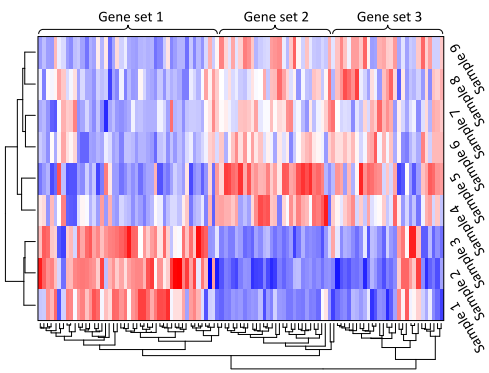
This week: Clustering

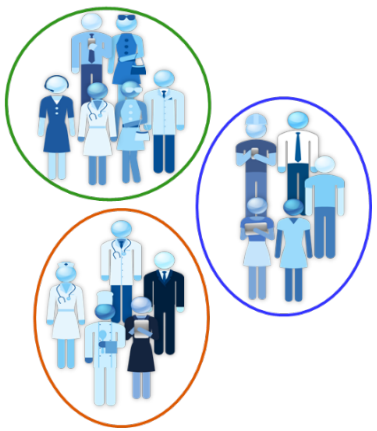
- Group objects $\boldsymbol{x}_i$ into K groups (clusters) based on their similarity.

Clustering: Examples

- Image segmentation
- User profiling
- Gene expression analysis
- Data compression
- Visualization
- ...







Sources: https://blogs.sas.com/content/subconsciousmusings/2016/05/26/data-mining-clustering/, https://en.wikipedia.org/wiki/Transcriptomics_technologies#/media/File:Transcriptomes_heatmap_example.svg, and C. Bishop - "Pattern Recognition and Machine Learning"

Problem definition

Given

- Collection of data points $\boldsymbol{X} = \{\boldsymbol{x}_1, ..., \boldsymbol{x}_N\} \subset \mathbb{X}$.

Goal

- For each object $\boldsymbol{x}_i$ find the corresponding assignment $z_i \in \{1, \ldots, K\}$ to one of the K groups (clusters), such that:
  - objects within the same group are similar to each other;
  - objects between different groups are dissimilar from each other;

Section 1

K-means Algorithm

Distance-based clustering

- If we want to group similar objects together, we need some notion of similarity to begin with.
- Typically defined as similarity function $s(\cdot, \cdot) : \mathbb{X} \times \mathbb{X} \to \mathbb{R}$.
- Alternatively: minimize dissimilarity, usually provided by a distance function $d(\cdot, \cdot)$.
- Typical distance functions include
  - Manhattan distance: $d(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sum_d |\boldsymbol{x}_{id} - \boldsymbol{x}_{jd}| = ||\boldsymbol{x}_i - \boldsymbol{x}_j||_1$
  - Euclidean distance: $d(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sqrt{\sum_d (\boldsymbol{x}_{id} - \boldsymbol{x}_{jd})^2} = ||\boldsymbol{x}_i - \boldsymbol{x}_j||_2$
  - Mahalanobis distance: $d(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sqrt{(\boldsymbol{x}_i - \boldsymbol{x}_j)^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x}_i - \boldsymbol{x}_j)}$

K-means

Model

- Consider the standard $\mathbb{R}^D$ space with Euclidean distance as metric.
- Each of K clusters is defined by its centroid $\boldsymbol{\mu}_k \in \mathbb{R}^D$.
- Cluster indicator $\boldsymbol{z}_i \in \{0,1\}^K$ with $\boldsymbol{z}_{ik} = 1 \iff \boldsymbol{x}_i$ belongs to cluster k (i.e. one-hot encoding).
- The K-means objective (also called distortion measure) is defined as

Sum of total distances by it's centroid

$$J(\boldsymbol{X}, \boldsymbol{Z}, \boldsymbol{\mu}) = \sum_{i=1}^{N} \sum_{k=1}^{K} \boldsymbol{z}_{ik} ||\boldsymbol{x}_i - \boldsymbol{\mu}_k||_2^2$$

Goal

- We need to find the "best" centroids $\boldsymbol{\mu}$ and cluster assignments $\boldsymbol{Z}$

$$\boldsymbol{Z}^*, \boldsymbol{\mu}^* = \arg\min_{\boldsymbol{Z}, \boldsymbol{\mu}} J(\boldsymbol{X}, \boldsymbol{Z}, \boldsymbol{\mu})$$

Minimizing the K-means objective

- The joint optimization problem is difficult to solve (discrete optim.; even if $\boldsymbol{Z}$ is assumed to be continuous it is non-convex)

$$\min_{\boldsymbol{Z},\boldsymbol{\mu}} J(\boldsymbol{X}, \boldsymbol{Z}, \boldsymbol{\mu}) = \min_{\boldsymbol{Z},\boldsymbol{\mu}} \sum_{i=1}^{N} \sum_{k=1}^{K} \boldsymbol{z}_{ik} ||\boldsymbol{x}_i - \boldsymbol{\mu}_k||_2^2$$

- However, the two subproblems

$$\min_{\boldsymbol{Z}} J(\boldsymbol{X}, \boldsymbol{Z}, \boldsymbol{\mu}) \qquad \text{and} \qquad \min_{\boldsymbol{\mu}} J(\boldsymbol{X}, \boldsymbol{Z}, \boldsymbol{\mu})$$

  have simple closed form solutions!

- **Idea:** alternating optimization - update $\boldsymbol{Z}$ and $\boldsymbol{\mu}$ in turns!

- This method for solving K-means is called Lloyd's algorithm.

Lloyd's algorithm for K-means

1. Initialize the centroids $\boldsymbol{\mu} = \{\boldsymbol{\mu}_1, ..., \boldsymbol{\mu}_K\}$.
2. Update cluster indicators (solve $\min_{\boldsymbol{Z}} J(\boldsymbol{X}, \boldsymbol{Z}, \boldsymbol{\mu})$)

Solve this minimum

$$\boldsymbol{z}_{ik} = \begin{cases} 1 & \text{if } k = \arg\min_j ||\boldsymbol{x}_i - \boldsymbol{\mu}_j||^2, \\ 0 & \text{else.} \end{cases}$$

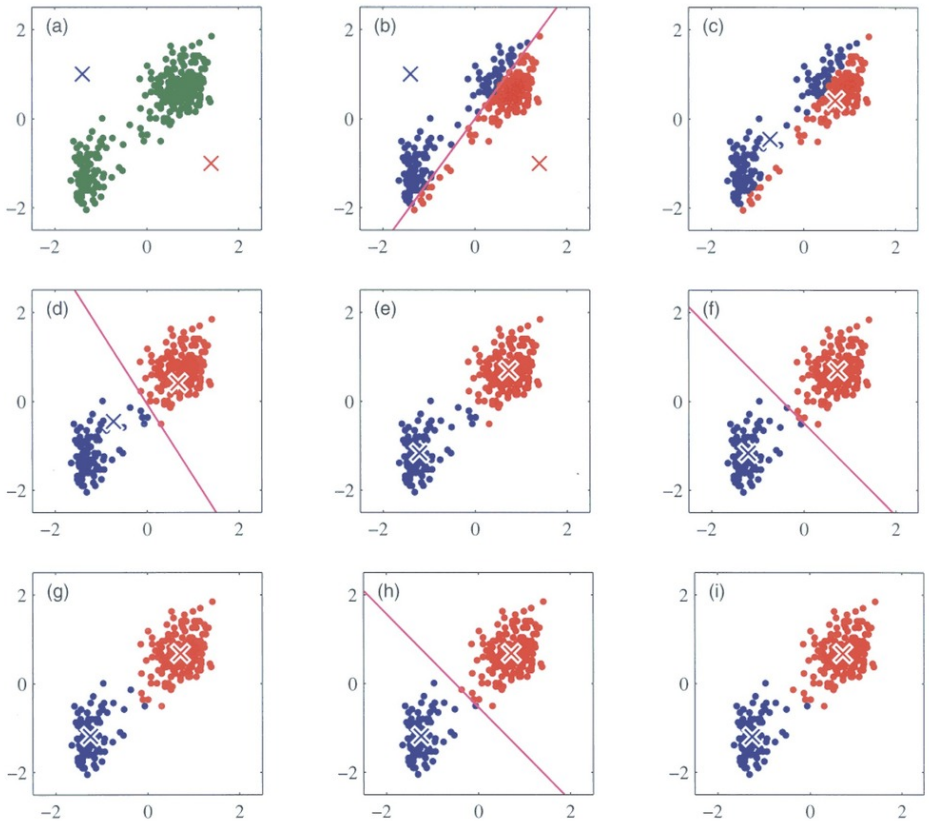
3. Update centroids (solve $\min_{\boldsymbol{\mu}} J(\boldsymbol{X}, \boldsymbol{Z}, \boldsymbol{\mu})$)

Update all the cenotrids as teh average of the points of that centroit

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{i=1}^{N} \boldsymbol{z}_{ik} \boldsymbol{x}_i \qquad \text{where } N_k = \sum_{i=1}^{N} \boldsymbol{z}_{ik}.$$

4. If objective $J(\boldsymbol{X}, \boldsymbol{Z}, \boldsymbol{\mu})$ has not converged, return to step 2.

K-means in action



An interactive demo is available at

- `https://user.ceng.metu.edu.tr/~akifakkus/courses/ceng574/k-means/`

Source: Bishop, Figure. 9.1

Initialization of the centroids

We saw in the interactive demo that the initial locations of the centroids $\boldsymbol{\mu}_k$ greatly affect the performance.

So, how do we initialize the centroids in a good way?

K-means++ algorithm

1. Choose the first centroid $\boldsymbol{\mu}_1$ uniformly at random among the data points. Chose centroid as a point of the data
2. For each point $\boldsymbol{x}_i$ compute the distance $D_i^2 = ||\boldsymbol{x}_i - \boldsymbol{\mu}_1||_2^2$. Compute all the distances
3. Sample the next centroid $\boldsymbol{\mu}_k$ from $\{\boldsymbol{x}_i\}$ with probability proportional to D_i^2. Sample from all points with a porbabilty function fo D
4. Recompute the distances $D_i^2 = \min\{||\boldsymbol{x}_i - \boldsymbol{\mu}_1||_2^2, ..., ||\boldsymbol{x}_i - \boldsymbol{\mu}_k||_2^2\}$.
5. Continue steps 3 and 4 until K initial centroids have been chosen.

Limitations of K-means

It is important to distinguish between the model (distortion $J(\boldsymbol{X}, \boldsymbol{Z}, \boldsymbol{\mu})$ in our case) and the algorithm used to fit it (here Lloyd's algorithm).

Modeling issues

- Underlying assumptions are not explicit
- Can't detect clusters with overlapping convex hulls
- Sensitivity to outliers
- No uncertainty measure

Algorithmic issues

- Extreme sensitivity to initialization

How can we address (some of) these issues?

Switch to the more principled probabilistic framework!

Section 2

Gaussian Mixture Model

Probabilistic unsupervised learning

- Goal: Design a probabilistic model for the data, $\mathrm{p}(\boldsymbol{x} \mid \boldsymbol{\theta})$, parametrized by $\boldsymbol{\theta}$ which we have to estimate.

What is the probability of x, with a distrivution wiht parameter alpha

- It's difficult to come up with a useful model $\mathrm{p}(\boldsymbol{x} \mid \boldsymbol{\theta})$ without making any assumptions about the data.

- When doing clustering, we implicitly assume that each point $\boldsymbol{x}$ belongs to some cluster (indicated by $\boldsymbol{z}$).
  $\Rightarrow$ Let's model $\mathrm{p}(\boldsymbol{x}, \boldsymbol{z} \mid \boldsymbol{\theta})$ instead!

All the data. given what is the porbability that I have a data x and that it belongs to z

- Let's recall what tools we developed during our discussion of supervised learning, and see if any of them can help us here.

- For this, assume for now, that we know the true cluster indicators $\boldsymbol{z}$, and are only interested in estimating $\boldsymbol{\theta}$.

Parameter estimation

How can we estimate the parameters $\boldsymbol{\theta}$ of a given model $\mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta})$?

Supervised learning

- Both $\boldsymbol{X} \in \mathbb{R}^{N \times D}$ and $\boldsymbol{Z} \in \{0, 1\}^{N \times K}$ are known.
- Simple solution - maximum likelihood estimation

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} | \boldsymbol{\theta})$$

MLE.I want that the probabilty of finding our data is maximum. Imagin that we know the data of X and Z. Once we have sigma.Then we have the distribution of x and Z

Unsupervised learning

- Only the data $\boldsymbol{X} \in \mathbb{R}^{N \times D}$ is given.
- Is there any way to estimate $\boldsymbol{\theta}$ in this case?

Latent variables

How can we estimate $\boldsymbol{\theta}$ when $\boldsymbol{Z}$ is unknown?

Since we chose to model $\mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta})$, we can compute the joint probability and obtain $\mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta})$ by marginalization

$$\mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta}) = \sum_{\boldsymbol{Z}} \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta}) = \sum_{\boldsymbol{Z}} \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{Z}, \boldsymbol{\theta}) \cdot \mathrm{p}(\boldsymbol{Z} \mid \boldsymbol{\theta})$$

Probability fo X is the sum of probabilities of all cases. Suppose p(x) = p(xy1) +p (xy2)

and optimize w.r.t $\boldsymbol{\theta}$

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta})$$

I want my data to be the most probable

Since the true $\boldsymbol{Z}$ are never observed and are only our abstraction used to simplify the model, they are called latent variables.[1]

[1] Sometimes also called hidden or explanatory variables.

Gaussian mixture model (GMM)

Assumption, P(X,Z|teta) = Product(p(xi,zi| teta). Multiplicatoin of all probabilities is the total probability

We decompose the joint probability $\mathrm{p}(\boldsymbol{x}, \boldsymbol{z} \mid \boldsymbol{\theta})$ using the product rule[2]

$$\mathrm{p}(\boldsymbol{x}, \boldsymbol{z} \mid \boldsymbol{\theta}) = \mathrm{p}(\boldsymbol{x} \mid \boldsymbol{z}, \boldsymbol{\theta}) \cdot \mathrm{p}(\boldsymbol{z} \mid \boldsymbol{\theta})$$

In Gaussian mixture model we assume:

- Cluster prior is categorical

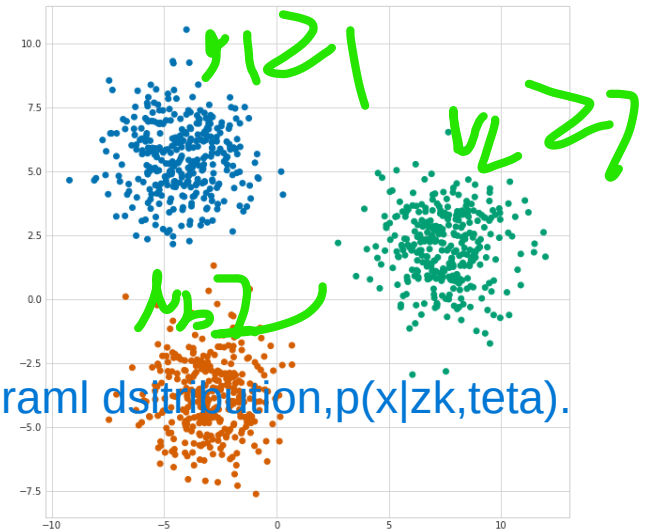
Categorical. z = 1,2,3. not continuious. Pi is a vetor like [0.2,0.4,0.4]

$$\mathrm{p}(\boldsymbol{z} \mid \boldsymbol{\theta}) = \mathrm{Cat}(\boldsymbol{\pi})$$

- Each cluster has its own multivariate normal distribution

We say that this follow a noraml dsitribution,p(x|zk,teta).

$$\mathrm{p}(\boldsymbol{x} \mid \boldsymbol{z}_k = 1, \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$



The parameters consist of the set of parameters of the prior and all conditional distributions $\boldsymbol{\theta} = \{\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}\}$.

Probaility of instance x having a 1 in xzk, is a gaussian. So for each xk we have a distributiof x. Given that we are in z=k, what is the probaiblity of x

[2] We assume that samples are drawn i.i.d., so consider only a single $(\boldsymbol{x}, \boldsymbol{z})$.

Generative process of GMM

We can draw samples from a GMM as follows.

Setup

We have K Gaussian components (clusters), each with known $\{\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}$, and known prior probabilities $\boldsymbol{\pi}_k$ for each cluster k.

Generative process

1. Draw a one-hot cluster indicator $\boldsymbol{z} \sim \mathrm{Cat}(\boldsymbol{\pi})$.

   $\boldsymbol{z}_k = 1 \iff$ current point belongs to cluster k.

2. Draw the sample $\boldsymbol{x} \sim \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ if $\boldsymbol{z}_k = 1$.

Draw a sample z,

if zk = 1, the x are around, with a mean of mk, and the vairance

Then creeatea sample x of the dsitribiution

We only observe the sample $\boldsymbol{x}$, and don't know which k it came from.

GMM likelihood

Using marginalization over z, the probability of a single sample x under a Gaussian mixture model can be computed as

p(x|sigma, mu,other shit). Is the sum of all the probabilties p(zk=1,p(x,z))

$$\mathrm{p}(\boldsymbol{x} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{k=1}^{K} \mathrm{p}(\boldsymbol{z}_k = 1 \mid \boldsymbol{\pi}) \cdot \mathrm{p}(\boldsymbol{x} \mid \boldsymbol{z}_k = 1, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Normal distribution, seen above

p(x,z|given...)

$$= \sum_{k=1}^{K} \boldsymbol{\pi}_k \cdot \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

p(zk = 1|pi) is pi1,p12,

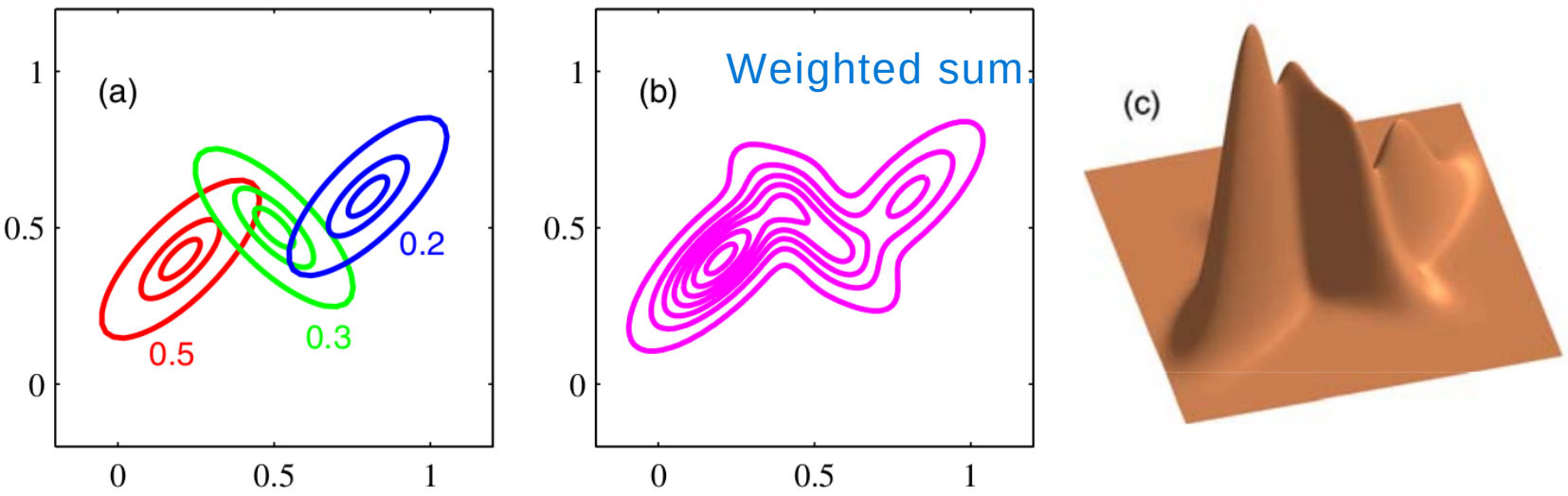
Hence, for the entire dataset $\boldsymbol{X} = \{\boldsymbol{x}_1, ..., \boldsymbol{x}_N\}$ the log-likelihood is

multiplication of everithing!

$$\log \mathrm{p}(\boldsymbol{X} | \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{i=1}^{N} \log \left(\sum_{k=1}^{K} \boldsymbol{\pi}_k \cdot \mathcal{N}(\boldsymbol{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right)$$

If I have n instances, I do teh sum over all instances. Sum beacuese we are in logarithim. We should make the multuplication. Becaus is p(X) = p(x1)*`(x29...

GMM density



(a) Isocontours of each component $\mathrm{p}(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ with respective mixing coefficients $\boldsymbol{\pi}_k$.

(b) Isocontours of the GMM distribution

$$\mathrm{p}(\boldsymbol{x} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{k=1}^{K} \boldsymbol{\pi}_k \cdot \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

(c) Surface plot of $\mathrm{p}(\boldsymbol{x} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$.

Source: Bishop, Figure. 2.23

Learning and inference in GMM

Remember, that we are interested in two things

Learning

- We want to determine the "optimal" values of the parameters (e.g., find values that maximize the log-likelihood)

$$\boldsymbol{\pi}^*, \boldsymbol{\mu}^*, \boldsymbol{\Sigma}^* = \arg\max_{\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}} \log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

Under the assumption of a Z, how likely is my data

We want the maximum of X, given the means of clusterring and everytihing. Is like saying waht is the porabbility of this dat given that I have 3 clusters of a mean and variance,

Inference

- Given the parameters $\{\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}\}$, we want to assign the points to clusters, i.e. compute the posterior distribution of cluster indicators

$$\mathrm{p}(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

(This is the actual goal of clustering.)

Given and X, what is teh porbability of being from z, once the parameters are known

Inference in GMM

By straightforward application of Bayes' rule, we obtain the posterior

$$\begin{aligned}\mathrm{p}(\boldsymbol{z}_{ik} = 1 \mid \boldsymbol{x}_i, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) &= \frac{\mathrm{p}(\boldsymbol{z}_{ik} = 1 \mid \boldsymbol{\pi})\ \mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{z}_{ik} = 1, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\mathrm{p}(\boldsymbol{x}_i \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})} \\ &= \frac{\boldsymbol{\pi}_k \mathcal{N}(\boldsymbol{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \boldsymbol{\pi}_j \mathcal{N}(\boldsymbol{x}_i \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}\end{aligned}$$

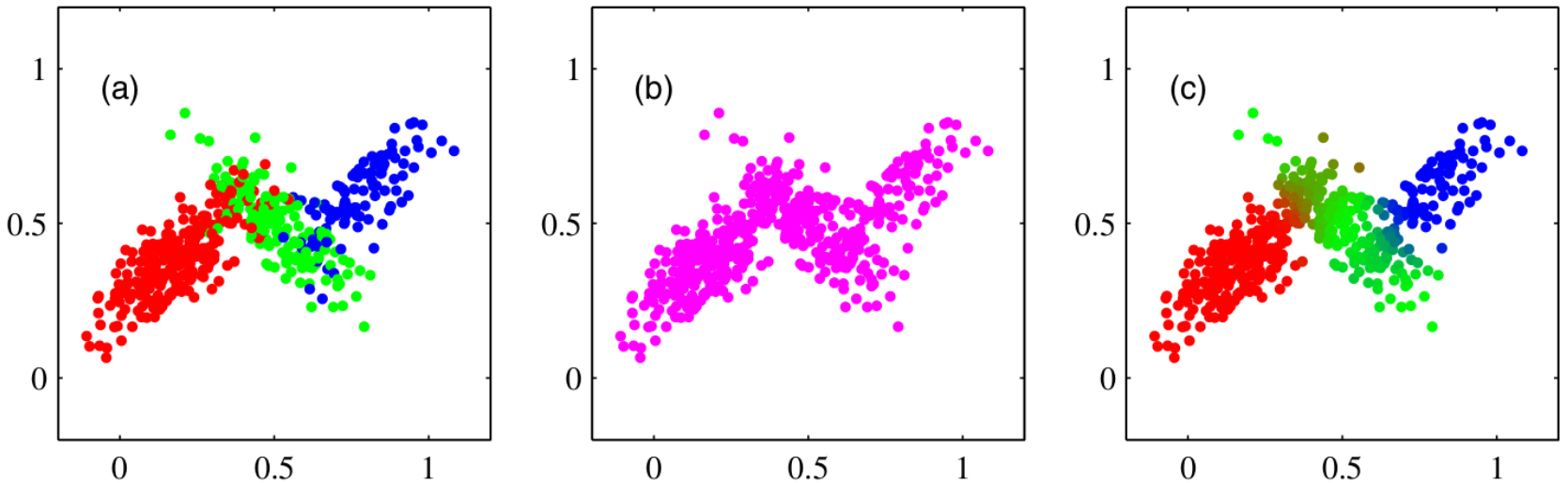
sum of all k gaussians, of all. if x is from z =1, if from z=2 and z=3

over the entries of $\boldsymbol{Z}$. We will call this quantity the responsibility of component k for the observation i.

We also introduce shorthand notation for it

$$\gamma(\boldsymbol{z}_{ik}) = \mathrm{p}(\boldsymbol{z}_{ik} = 1 \mid \boldsymbol{x}_i, \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$$

Inference: Example



(a) Data colored according to the true underlying $\boldsymbol{Z}$.

(b) Observed data $\boldsymbol{X}$.

(c) Data colored according to the inferred $\gamma(\boldsymbol{Z})$ (with $\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}$ known).

Source: Bishop, Figure. 9.5

Learning in GMM

Maximization of the log-likelihood w.r.t. the parameters appears to be more challenging. Recall that the log-likelihood is

$$\log \mathrm{p}(\boldsymbol{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{i=1}^{N} \log \left(\sum_{k=1}^{K} \boldsymbol{\pi}_k \cdot \mathcal{N}(\boldsymbol{x}_i \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right).$$

p(z)*p(x|z..) = P(x,z)

p(xi)

Due to the summation over k, the logarithm doesn't act directly on the Gaussian density.

log of a sum is bullshit, we can not optimize

This happens to be a serious problem, as this means that the derivatives w.r.t. the model parameters $\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}$ have no analytical roots.[3]

Can not be solverd

Is there anything that we can do in this case?

[3] i.e. we cannot obtain closed form expressions for the optimal values of $\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}$.

Learning in GMM

Recall from the Linear Classification lecture (Linear Discriminant Analysis) that parameter estimation is rather straightforward if $\boldsymbol{Z}$ is known.

That is, we know how to solve the "easy" problem

max of p(X,Z), the thing inside of the second sum

$$\boldsymbol{\pi}^*, \boldsymbol{\mu}^*, \boldsymbol{\Sigma}^* = \underset{\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}}{\arg\max} \log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) \qquad (*)$$

Too bad we don't know anything about $\boldsymbol{Z}$... Or do we?

Learning in GMM

Recall from the Linear Classification lecture (Linear Discriminant Analysis) that parameter estimation is rather straightforward if $\boldsymbol{Z}$ is known.

in LDA we know teh mus and everything

That is, we know how to solve the "easy" problem

$$\boldsymbol{\pi}^*, \boldsymbol{\mu}^*, \boldsymbol{\Sigma}^* = \arg\max_{\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}} \log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) \qquad (*)$$

Too bad we don't know anything about $\boldsymbol{Z}$... Or do we?

y us the probability of Z, given X

Idea: use our initial beliefs $\gamma_0(\boldsymbol{Z}) = \mathrm{p}(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\pi}^{(0)}, \boldsymbol{\mu}^{(0)}, \boldsymbol{\Sigma}^{(0)})$ and solve the easier problem (*).

Start with random Z, and usse y0. we compute gamma 0 as an aprox wiht some pi, mu and var

Learning in GMM: from $\mathrm{p}(\boldsymbol{X})$ to $\mathrm{p}(\boldsymbol{X}, \boldsymbol{Z})$

Instead of optimizing $\mathrm{p}(\boldsymbol{X})$ directly, we introduce the latent variables $\boldsymbol{Z}$ by taking their expectation and formulate the proxy objective

$$\mathop{\mathbb{E}}_{\boldsymbol{Z} \sim \gamma_t(\boldsymbol{Z})} \left[\log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) \right].$$

Expectation, We do not have the sum inside the log

Now the $\log$ acts directly on $\mathrm{p}(\boldsymbol{X}, \boldsymbol{Z})$ and we can optimize the whole expression. Note, that $\gamma_t(\boldsymbol{Z})$ and the optimizers $\boldsymbol{\pi}^*$, $\boldsymbol{\mu}^*$ and $\boldsymbol{\Sigma}^*$ recursively depend on each other.

This motivates the expectation maximization (EM) algorithm that iterates the following two steps until convergence:

1. Evaluate the posterior distribution $\gamma_t(\boldsymbol{Z})$ with respect to the current estimate of the parameters $\{\boldsymbol{\pi}^{(t)}, \boldsymbol{\mu}^{(t)}, \boldsymbol{\Sigma}^{(t)}\}$
2. Obtain the next iteration of the parameters by solving

$$\boldsymbol{\pi}^{(t+1)}, \boldsymbol{\mu}^{(t+1)}, \boldsymbol{\Sigma}^{(t+1)} = \mathop{\arg\max}_{\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}} \mathop{\mathbb{E}}_{\boldsymbol{Z} \sim \gamma_t(\boldsymbol{Z})} \left[\log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) \right]$$

with the given parameters, we can

EM algorithm for GMM

1. Initialize model parameters $\{\boldsymbol{\pi}^{(0)}, \boldsymbol{\mu}_1^{(0)}, ..., \boldsymbol{\mu}_K^{(0)}, \boldsymbol{\Sigma}_1^{(0)}, ..., \boldsymbol{\Sigma}_K^{(0)}\}$.
2. **E step**. Evaluate the responsibilities

$$\gamma_t(\boldsymbol{z}_{ik}) = \frac{\boldsymbol{\pi}_k^{(t)} \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)})}{\sum_{j=1}^{K} \boldsymbol{\pi}_j^{(t)} \mathcal{N}(\boldsymbol{x}_i | \boldsymbol{\mu}_j^{(t)}, \boldsymbol{\Sigma}_j^{(t)})}.$$

Then we compute the p (z|x,--)

3. **M step**. Re-estimate the parameters

Maximization of the expectande

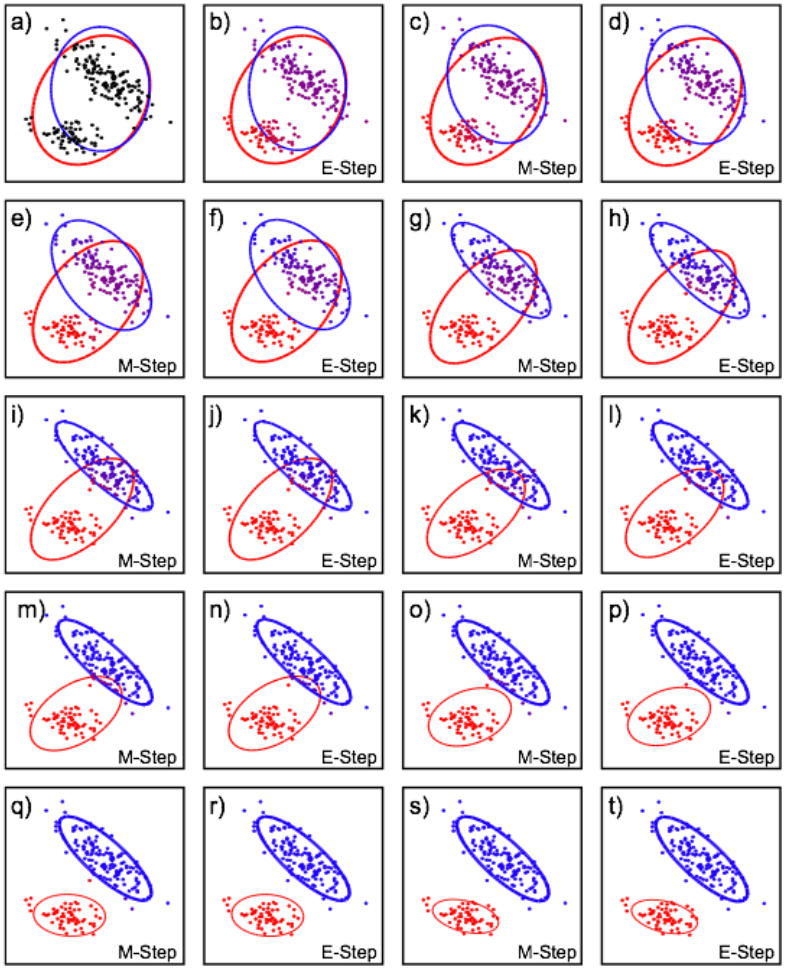
$$\boldsymbol{\mu}_k^{(t+1)} = \frac{1}{N_k} \sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_{ik}) \boldsymbol{x}_i$$

$$\boldsymbol{\Sigma}_k^{(t+1)} = \frac{1}{N_k} \sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_{ik}) (\boldsymbol{x}_i - \boldsymbol{\mu}_k^{(t+1)})(\boldsymbol{x}_i - \boldsymbol{\mu}_k^{(t+1)})^T$$

$$\boldsymbol{\pi}_k^{(t+1)} = \frac{N_k}{N} \qquad \text{where } N_k = \sum_{i=1}^{N} \gamma_t(\boldsymbol{z}_{ik}).$$

4. Iterate steps 2 & 3 until $\mathbb{E}_{\boldsymbol{Z} \sim \gamma_t(\boldsymbol{Z})} \left[\log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\pi}^{(t)}, \boldsymbol{\mu}^{(t)}, \boldsymbol{\Sigma}^{(t)}) \right]$ converges

EM algorithm for GMM: Demo



Gif: `https://upload.wikimedia.org/wikipedia/commons/6/69/EM_Clustering_of_Old_Faithful_data.gif`

Source: Computer Vision: Models, Learning, and Inference - S.J.Prince

EM algorithm in general

The Expectation-Maximization algorithm (EM) is applicable to more models than just GMMs.

In its most general form, the two steps are

- **E step** - evaluate the posterior $\gamma_t(\boldsymbol{Z}) = \mathrm{p}(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}^{(t)})$.
- **M step** - maximize the expected joint log-likelihood $\log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta})$ w.r.t. $\boldsymbol{\theta}$ under the current beliefs $\gamma_t(\boldsymbol{Z})$

$$\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} \mathop{\mathbb{E}}_{\boldsymbol{Z} \sim \gamma_t(\boldsymbol{Z})} [\log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta})]$$

Note: we do **not** get a closed form solution neither for $\gamma(\boldsymbol{Z})$, nor for the parameters, as $\gamma(\boldsymbol{Z})$ and $\boldsymbol{\theta}$ recursively depend on each other.

Therefore, we have to iterate between these two steps until the objective $\mathbb{E}_{\boldsymbol{Z} \sim \gamma(\boldsymbol{Z})} [\log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta})]$ converges.

EM algorithm: A justification

Let $\mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta})$ be a parametric probabilistic model with latent variables $\boldsymbol{Z}$ and $\mathrm{q}(\boldsymbol{Z})$ any probability distribution. Then we have

$$\log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta}) = \sum_{\boldsymbol{Z}} \mathrm{q}(\boldsymbol{Z}) \log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta})$$

sum(q(Z)) goes to 1, this is nto marginalization

$$= \sum_{\boldsymbol{Z}} \mathrm{q}(\boldsymbol{Z}) \log \frac{\mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta})}{\mathrm{p}(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta})}$$

Use product rle: p(X,Z|teta) = P(Z|X, teata)*P (X|teat)

$$= \sum_{\boldsymbol{Z}} \mathrm{q}(\boldsymbol{Z}) \log \frac{\mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta})}{\mathrm{p}(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta})} \cdot \frac{\mathrm{q}(\boldsymbol{Z})}{\mathrm{q}(\boldsymbol{Z})}$$

$$= \sum_{\boldsymbol{Z}} \mathrm{q}(\boldsymbol{Z}) \log \frac{\mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta})}{\mathrm{q}(\boldsymbol{Z})} - \sum_{\boldsymbol{Z}} \mathrm{q}(Z) \log \frac{\mathrm{p}(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta})}{\mathrm{q}(\boldsymbol{Z})}$$

$$= \underbrace{\mathop{\mathbb{E}}_{\boldsymbol{Z} \sim \mathrm{q}} \left[\log \frac{\mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta})}{\mathrm{q}(\boldsymbol{Z})} \right]}_{\mathcal{L}(\mathrm{q}, \boldsymbol{\theta})} + \mathbb{KL} \left(\mathrm{q} \,||\, \mathrm{p}(\cdot \mid \boldsymbol{X}, \boldsymbol{\theta}) \right).$$

Expectation of something

Keodivergence, adn always non-neagative. The expectaition si a lower bound

$\mathcal{L}(\mathrm{q}, \boldsymbol{\theta})$ is a lower-bound on $\log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta})$ for *any* q.

EM algorithm: The E-step

keodivergeg is 0 if teh distribution of q = distribition of p

$$\log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta}) = \mathcal{L}(\mathrm{q}, \boldsymbol{\theta}) + \mathbb{KL}\left(\mathrm{q} \,||\, \mathrm{p}(\cdot \mid \boldsymbol{X}, \boldsymbol{\theta})\right)$$

The lefthand side is constant with respect to q and the $\mathbb{KL}$ divergence is non-negative. Therefore $\mathcal{L}(\mathrm{q}, \boldsymbol{\theta})$ is maximal when the $\mathbb{KL}$ divergence is 0 which happens when $\mathrm{q}(\boldsymbol{Z}) = \gamma(\boldsymbol{Z}) = \mathrm{p}(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta})$.

the maximum l(1,sigma)/lowe bound, is when q(z) = y(Z) = p (Z,X,sigma).

This constitutes the E-step and ensures that the lower bound $\mathcal{L}(\mathrm{q}, \boldsymbol{\theta})$ is tight, i.e.

$$\log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta}) = \mathcal{L}(\mathrm{q}, \boldsymbol{\theta}).$$

Note that

aprox

$$\mathcal{L}(\mathrm{q}, \boldsymbol{\theta}) = \mathop{\mathbb{E}}_{\boldsymbol{Z} \sim \mathrm{q}} \left[\log \frac{\mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta})}{\mathrm{q}(\boldsymbol{Z})} \right] = \underbrace{\mathop{\mathbb{E}}_{\boldsymbol{Z} \sim \mathrm{q}} \left[\log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta}) \right]}_{\text{our proxy from GMMs}} + \underbrace{\mathbb{H}[\mathrm{q}(\cdot)]}_{\text{independent of } \boldsymbol{\theta}}.$$

EM algorithm: The M-step

$$\log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta}) = \mathcal{L}(\mathrm{q}, \boldsymbol{\theta}) + \mathbb{KL}\left(\mathrm{q} \,||\, \mathrm{p}(\cdot \mid \boldsymbol{X}, \boldsymbol{\theta})\right)$$

After the E-step we have $\log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta}) = \mathcal{L}(\mathrm{q}, \boldsymbol{\theta})$. So if we now perform the M-step and maximize $\mathcal{L}(\mathrm{q}, \boldsymbol{\theta})$ with respect to $\boldsymbol{\theta}$, either

- $\mathcal{L}(\mathrm{q}, \boldsymbol{\theta})$ does not change, we are at a local maximum of $\log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta})$ and EM converges
- or $\mathcal{L}(\mathrm{q}, \boldsymbol{\theta})$ "pushes" up against $\log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta})$.

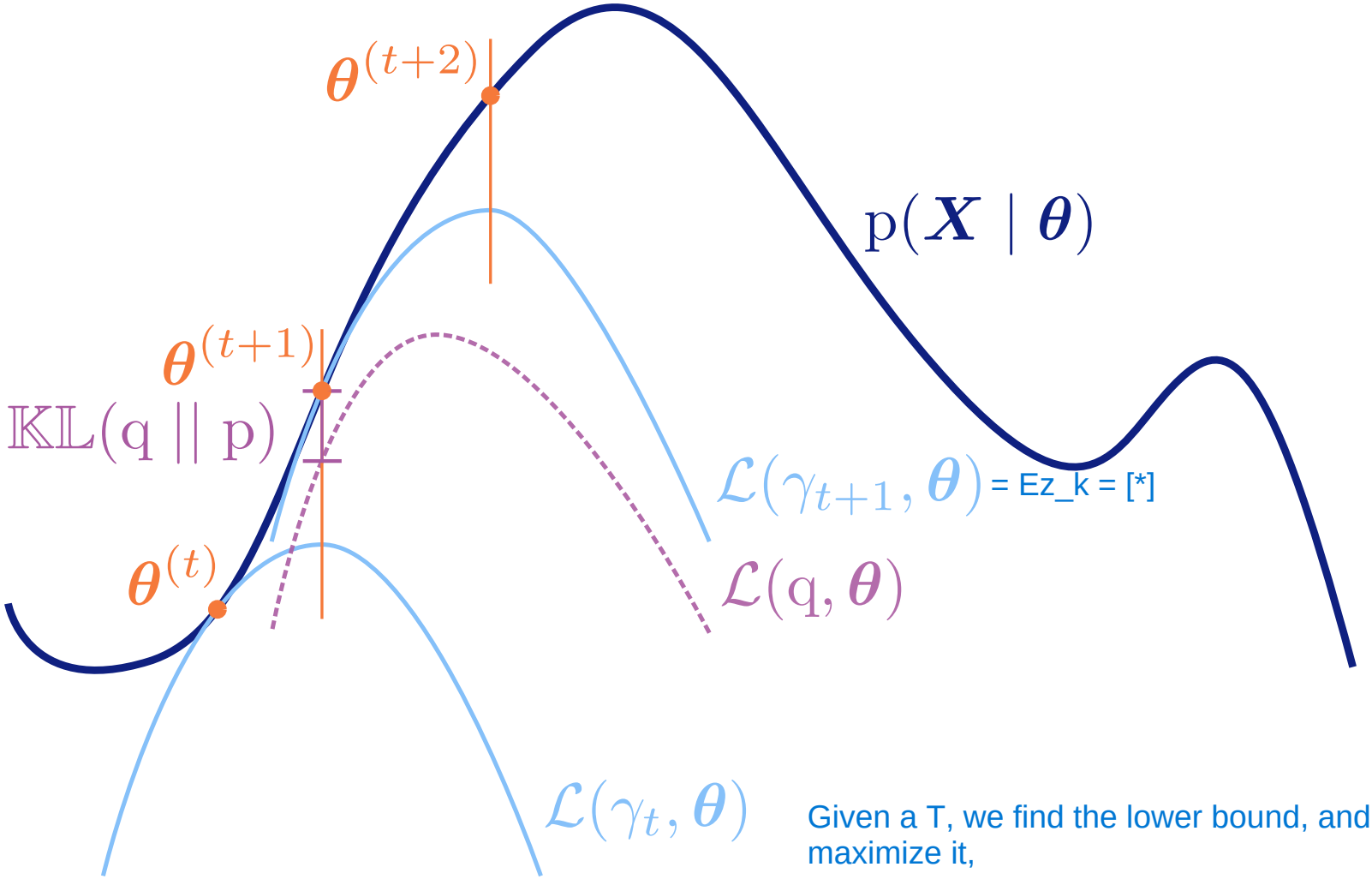
In the latter case, we receive parameters $\boldsymbol{\theta}'$ that have a higher data log-likelihood. Furthermore, the same equation that we started with holds again

$$\log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta}') = \mathcal{L}(\mathrm{q}, \boldsymbol{\theta}') + \mathbb{KL}\left(\mathrm{q} \,||\, \mathrm{p}(\cdot \mid \boldsymbol{X}, \boldsymbol{\theta}')\right)$$

and we can perform another iteration.

EM algorithm: Illustration

We maximize the lower boudn



Given a T, we find the lower bound, and then we maximize it,

EM algorithm: Summary

When should we use EM?

- Intractable to optimize the log-likelihood due to latent variables $\boldsymbol{Z}$

$$\log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{\theta}) = \log \left(\sum_{\boldsymbol{Z}} \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{Z}, \boldsymbol{\theta}) \, \mathrm{p}(\boldsymbol{Z} \mid \boldsymbol{\theta}) \right)$$

- Easy to optimize the joint probability

$$\log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta}) = \log \mathrm{p}(\boldsymbol{Z} \mid \boldsymbol{\theta}) + \log \mathrm{p}(\boldsymbol{X} \mid \boldsymbol{Z}, \boldsymbol{\theta})$$

The main idea of EM

- Use our current beliefs $\mathrm{p}(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}^{(t)})$ to "pretend" that we know $\boldsymbol{Z}$.
- E step - update the responsibilities $\gamma_t(\boldsymbol{Z}) = \mathrm{p}(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}^{(t)})$.
- M step - update parameters

$$\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} \mathop{\mathbb{E}}_{\boldsymbol{Z} \sim \gamma_t(\boldsymbol{Z})} \left[\log \mathrm{p}(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta}) \right]$$

Choosing number of clusters K: Heuristic methods

- Elbow/knee heuristic:
  Plot within-cluster sum of squared distances for varying K. Look for a bent (knee/elbow).
- Gap statistic:
  Compare within-cluster variation to uniform data. Choose smallest K such that gap statistic is within one std. dev. of gap at $K + 1$.
- Silhouette:
  Per point difference of mean distance within cluster to points in closest other cluster. Maximize mean of all points.

Don't forget cross-validation to prevent overfitting!

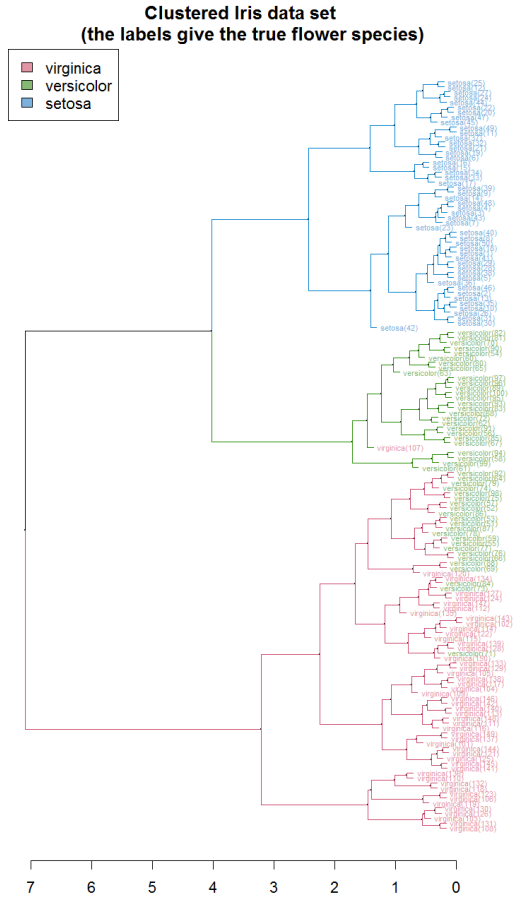
Choosing number of clusters K: Probabilistic methods

Needs generative model that defines the data likelihood $\hat{L} = \mathrm{p}(\boldsymbol{X} \mid \hat{\boldsymbol{Z}}, \hat{\boldsymbol{\theta}})$ (with optimal parameters $\hat{\boldsymbol{Z}}$, $\hat{\boldsymbol{\theta}}$).

- Bayesian information criterion (BIC):
  Approximate model likelihood $\mathrm{p}(\boldsymbol{X} \mid \text{model})$. Balances number of parameters vs. likelihood, $\mathrm{BIC} = M \log N - 2 \log \hat{L}$.
- Akaike information criterion (AIC):
  Estimate information lost by given model, $\mathrm{AIC} = 2M - 2 \log \hat{L}$
- Here M is the number of free parameters (e.g $K \cdot (D + D^2 + 1)$ for GMM) and N is the number of samples

Hierarchical clustering

- Agglomerative: Bottom-up, merge cluster pairs iteratively
- Divisive: Top-down, split data recursively



From `https://en.wikipedia.org/wiki/File:Iris_dendrogram.png`

Agglomorative clustering: How to choose pairs?

Cluster pairs are chosen by minimum cluster distance.

Linkage criterion defines cluster distance from sample distance:

- Complete-linkage clustering: Maximum sample distance
- Single-linkage clustering: Minimum sample distance
- Unweighted average linkage clustering (UPGMA): Mean sample distance
- Centroid linkage clustering (UPGMC): Centroid distance
- Weighted average linkage clustering (WPGMA): Distance defined recursively as average of distances in previous level (before merging)

Summary

- Clustering: Group objects into K groups
- K-means: Alternatingly (1) group objects by the closest centroids and (2) set the centroids to the group means

  Note: K-means update equivalent to isotropic GMM with $\sigma \to 0$! (exercise)
- GMM: Fit set of Gaussians to the data (via EM), group is the Gaussian with highest probability
- EM for GMM: Alternatingly update (1) responsibilities based on parameters and (2) parameters based on responsibilities.
- EM in general: Alternatingly (1) evaluate the expected posterior $\gamma_t(\boldsymbol{Z})$ (E-step) and (2) update parameters by maximizing $\mathcal{L}(\gamma_t, \boldsymbol{\theta})$ (M-step).
- Agglomorative clustering: Merge clusters recursively

Reading material

Reading material

- Bishop: chapters 9.1, 9.2, 9.3.0, 9.3.1
- Murphy: chapter 11.4.1, 11.4.2, 11.4.7 (optional)