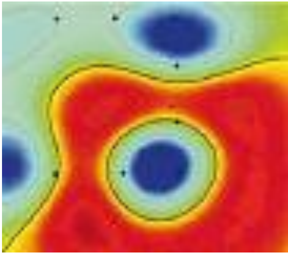
Technische Universität Berlin



Lecture 12

Expectation Maximization and Clustering

Hannah Marienwald

Lecture based on Bishop, C. (2006). Pattern Recognition and Machine Learning. Ch. 9.
Most Figures are also taken from there.

Recap

- Supervised Learning:
  Training data comprises of input data and their corresponding target label
  Goal: find mapping between input and label
  Examples: classification, regression, ...

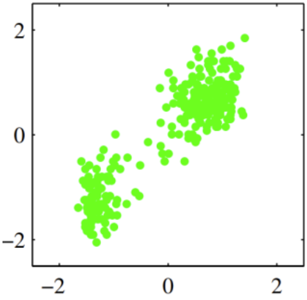
- Unsupervised Learning:
  Training data only consist of the input data without labels
  Goal: find structure in the data
  Examples: clustering, density estimation, PCA, ...

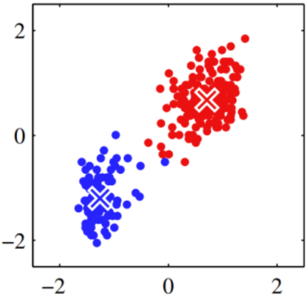
Outline

- K-means Clustering
- Gaussian Mixture Models (GMM)
- Expectation Maximization (EM)

Clustering

- **Input:** N data points in d-dimensions, $\{x_n\}_{n=1}^{N} \subseteq \mathbb{R}^d$
- **Goal:** partition the data into K *clusters* based on distances
- **Cluster:** set of data points whose inter-point distances are small compared to the distances to points outside of the cluster





K-Means

- **Input:** N data points in d-dimensions, $\{x_n\}_{n=1}^N \subseteq \mathbb{R}^d$
- **Goal:** partition the data into K clusters based on distances
- **Idea:** assign each data point to the cluster with the closest *cluster center* μ_k. Define the *assignments*

$$z_{n,k} = \begin{cases} 1, \text{if } x_n \text{ belongs to cluster } k \\ 0, \text{otherwise} \end{cases}$$

- **Objective:** minimize

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{n,k} \cdot \|x_n - \mu_k\|^2$$

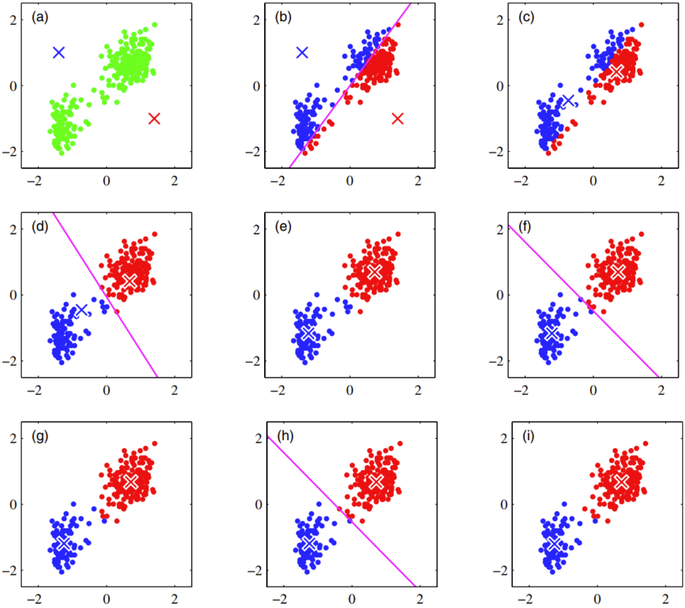
- K-Means finds $z_{n,k}$ and μ_k for all n, k by minimizing J

K-Means

Input: data points $\{x_n\}_{n=1}^{N}$, number of clusters K
Returns: cluster center $\{\mu_k\}_{k=1}^{K}$, cluster assignments $\{z_{n,k}\}_{n,k=1}^{N,K}$

1. Randomly initialize μ_k for all $k \in \{1, \dots, K\}$
2. Loop until convergence:
   2.1. Minimize J wrt. $z_{n,k}$ and keep μ_k fixed:
   assign x_n to the closest center
   $$z_{n,k} = \begin{cases} 1, \text{if } k = \underset{j}{\operatorname{argmin}} \left\| x_n - \mu_j \right\|^2 \\ 0, \text{otherwise} \end{cases}$$
   2.2. Minimize J wrt. μ_k and keep $z_{n,k}$ fixed:
   update the cluster centers $\mu_k = \frac{\sum_{n=1}^{N} z_{n,k} \cdot x_n}{\sum_{n=1}^{N} z_{n,k}}$

K-Means



How to determine K?

- By prior knowledge otherwise:
- Heuristic 1:
  Plot J for different values of K. In general, $J \to 0$ as $K \to N$ but there might be a dip which indicates a good value.
  倾斜
- Heuristic 2:
  For a suitable K the cluster centers and assignments are stable across different runs (started from different random initializations). Rerun K-means several times for different values of K and choose the one for which the results change the least.

根据已有知识（如有）：

- **启发式方法1**：绘制不同 K 值下的 J。通常情况下，随着 $K \to N$，$J \to 0$，但可能会出现一个“倾斜”点（即拐点），提示了一个较优的 K 值。
- **启发式方法2**：对于合适的 K，聚类中心和分配在不同运行中保持稳定（从不同的随机初始化开始）。针对不同的 K 多次运行 K-Means 算法，选择结果变化最小的 K 值。

K-Means

每次迭代都会减少J 的值。
保证收敛。
可能只找到局部最小值而非全局最小值。
可以扩展为适用于一般相异性测量。
硬分配：每个数据点只能严格属于一个聚类。

- Each iteration reduces value of J
- Guaranteed convergence
- Might only find local instead of global minimum
- Extension to general dissimilarity measures possible
- Hard assignment (every data points belongs to exactly one cluster)

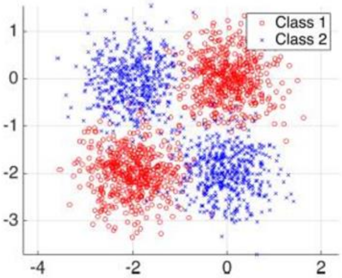
Gaussian Mixture Models (GMM)

Density Estimation

- Multivariate Gaussian distribution

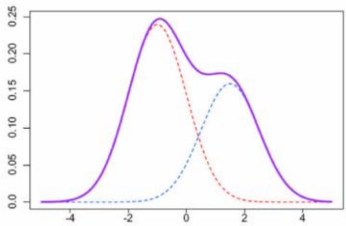
$$\mathcal{N}(x|\mu,\Sigma) = p(x|\mu,\Sigma)$$
$$= \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \cdot \exp\left[-\frac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)\right]$$

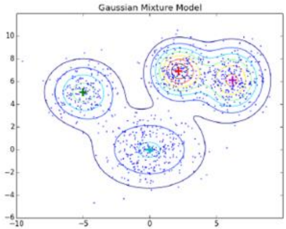
- Single Gaussian might not always be a good fit



Mixture of Gaussians

- Linear superposition of K Gaussians
  $p(x|\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{k=1}^{K} \tau_k \cdot \mathcal{N}(x|\mu_k, \Sigma_k)$
- with prior probabilities
  $0 \leq \tau_k \leq 1$ and $\sum_{k=1}^{K} \tau_k = 1$





Figures from Eugene Weinstein, Yu Zhu

Maximum Likelihood for GMMs

- Find maximum likelihood estimators for $\theta = (\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$ for data set $X = (x_1, \dots, x_N)$?

- Log-likelihood

$$
\begin{aligned}
L(\theta) &= \log p(X|\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) \\
&= \log \left[\prod_{n=1}^{N} \sum_{k=1}^{K} \tau_k \cdot \mathcal{N}(x_n|\mu_k, \Sigma_k) \right] \\
&= \sum_{n=1}^{N} \log \left[\sum_{k=1}^{K} \tau_k \cdot \mathcal{N}(x_n|\mu_k, \Sigma_k) \right] \\
&= \sum_{n=1}^{N} \log \left[\sum_{k=1}^{K} \tau_k \cdot \left(\frac{(2\pi)^{-\frac{d}{2}}}{|\Sigma_\mathrm{k}|^{\frac{1}{2}}} \cdot \exp\left[-\frac{1}{2} (x_n - \mu_k)^T \Sigma_\mathrm{k}^{-1} (x_n - \mu_k) \right] \right) \right]
\end{aligned}
$$

- Difficult to optimize and no analytic solution.

GMMs with Latent Variables

潜在的

隐藏

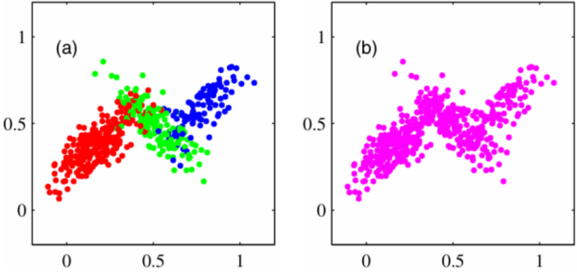
- **Trick:** introduce auxiliary variables indicating from which Gaussian each data point was sampled

$$z_{n,k} = \begin{cases} 1, \text{if } x_n \text{ belongs to Gaussian } k \\ 0, \text{otherwise} \end{cases}$$

$$p(z_{n,k} = 1) = \tau_k$$

$$p(x_n | z_{n,k} = 1) = \mathcal{N}(x_n | \mu_k, \Sigma_k)$$

- The assignments $z_{n,k}$ are *latent*, i.e., not observed



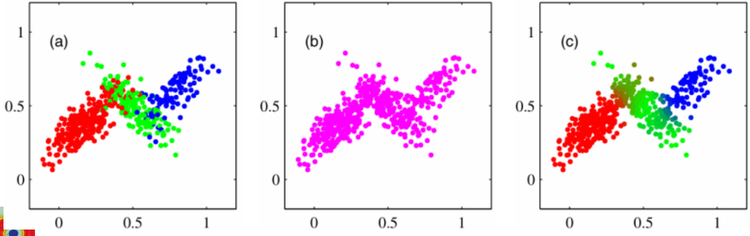
GMMs with Latent Variables

- Latent assignments

$$z_{n,k} = \begin{cases} 1, x_n \text{ belongs to } k \\ 0, \text{otherwise} \end{cases}, \qquad p(z_{n,k} = 1) = \tau_k, \qquad p(x_n | z_{n,k} = 1) = \mathcal{N}(x_n | \mu_k, \Sigma_k)$$

- Using Bayes rule

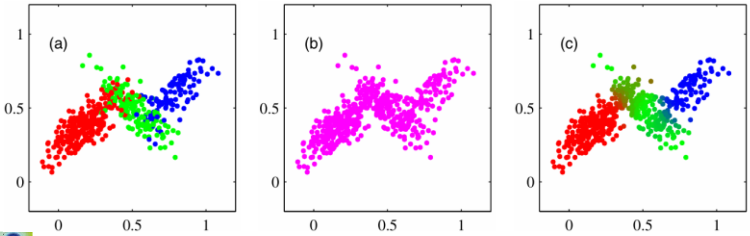
$$p(z_{n,k} = 1 | x_n) = \frac{p(z_{n,k} = 1) \cdot p(x_n | z_{n,k} = 1)}{\sum_{j=1}^{K} p(z_{n,j} = 1) \cdot p(x_n | z_{n,j} = 1)} = \frac{\tau_k \mathcal{N}(x_n | \mu_k, \Sigma_k)}{\sum_j \tau_j \mathcal{N}(x_n | \mu_j, \Sigma_j)}$$



GMMs for Clustering

- GMMs can be used to find clustering
- $p\left(z_{n,k} = 1 \middle| x_n\right)$ is *soft-assignment* to cluster k
- For clustering, we need to determine optimal values of $\theta = (\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$ and $p\left(z_{n,k} = 1 \middle| x_n\right)$
- Maximum (log) likelihood hard to optimize

$$\log p(X|\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \log\left[\sum_{k=1}^{K} \tau_k \cdot \mathcal{N}(x_n|\mu_k, \Sigma_k)\right]$$



EM for GMMs

- No closed form for maximum (log) likelihood solution, because optimal $(\tau_k, \mu_k, \Sigma_k)$ depend on $p(z_{n,k} = 1 | x_n)$ which in turn depends on $(\tau_k, \mu_k, \Sigma_k)$
- **Expectation Maximization**: finds maximum likelihood solutions for models with latent variables
- Each iteration is guaranteed to increase the log likelihood
- Not guaranteed to find global optimum only local

- **最大（对数）似然解没有闭合形式**，因为最优的 $(\tau_k, \mu_k, \Sigma_k)$ 依赖于 $p(z_{n,k} = 1 | x_n)$，而它反过来又依赖于 $(\tau_k, \mu_k, \Sigma_k)$。
- **期望最大化（Expectation Maximization）**：用于具有潜在变量的模型，找到最大似然解。
- 每次迭代都**保证增加对数似然值**。
- **不保证找到全局最优解**，仅能找到局部最优解。

EM for GMMs

Input: data points $\{x_n\}_{n=1}^{N}$, number of clusters K
Returns: GMM parameters $(\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$, soft assignments $\{p(z_{n,k} = 1 | x_n)\}_{n,k=1}^{N,K}$

1. Randomly initialize $(\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$ for all $k \in \{1, \dots, K\}$
2. Loop until convergence:
   - 2.1. Update $p(z_{n,k} = 1 | x_n)$ and keep $(\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$ fixed. ← E-step
   - 2.2. Update $(\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$ and keep $p(z_{n,k} = 1 | x_n)$ fixed. ← M-step

(formulas on next slide)

EM for GMMs

- Recall

$$p(z_{n,k} = 1 | x_n) = \frac{\tau_k \mathcal{N}(x_n | \mu_k, \Sigma_k)}{\sum_j \tau_j \mathcal{N}(x_n | \mu_j, \Sigma_j)}$$

  and set

$$N_k = \sum_{n=1}^{N} p(z_{n,k} = 1 | x_n)$$

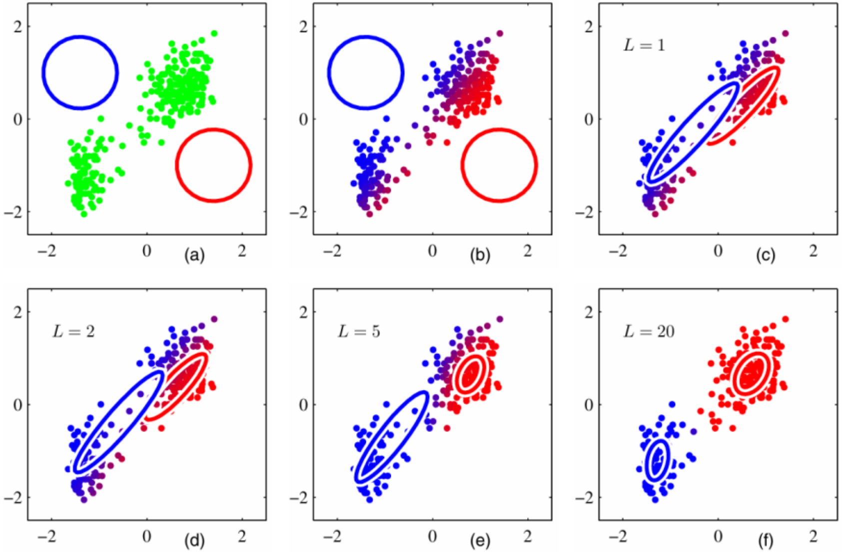
- Update formulas are obtained by setting the derivative of $\log p(X | \boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$ to 0:

$$\mu_k = \frac{1}{N_k} \sum_{n=1}^{N} p(z_{n,k} = 1 | x_n) \cdot x_n$$

$$\Sigma_k = \frac{1}{N_k} \sum_{n=1}^{N} p(z_{n,k} = 1 | x_n) \cdot (x_n - \mu_k)(x_n - \mu_k)^T$$

$$\tau_k = \frac{N_k}{N} \quad \text{(constrained optimization)}$$

EM for GMMs



K-Means

- K-means is a limit of Gaussian mixture models with EM where for all k, $\Sigma_k = \sigma^2 I$ are fixed (not optimized) and $\sigma^2 \to 0$. This yields *hard* assignments and K-means.

Input: data points $\{x_n\}_{n=1}^{N}$, number of clusters K

Returns: cluster center $\{\mu_k\}_{k=1}^{K}$, cluster assignments $\{z_{n,k}\}_{n,k=1}^{N,K}$

1. Randomly initialize μ_k for all $k \in \{1, \dots, K\}$
2. Loop until convergence:

   2.1. Minimize J wrt. $z_{n,k}$ and keep μ_k fixed:
   assign x_n to the closest center

   E-step

$$z_{n,k} = \begin{cases} 1, \text{if } k = \underset{j}{\operatorname{argmin}} \left\| x_n - \mu_j \right\|^2 \\ 0, \text{otherwise} \end{cases}$$

   2.2. Minimize J wrt. μ_k and keep $z_{n,k}$ fixed:

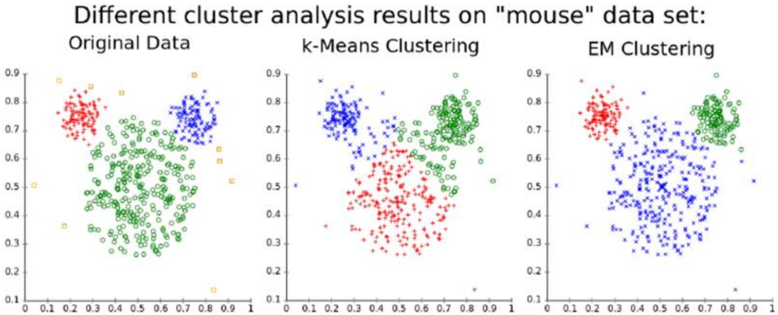
   M-step

   update the cluster centers $\mu_k = \frac{\sum_{n=1}^{N} z_{n,k} \cdot x_n}{\sum_{n=1}^{N} z_{n,k}}$

Comparison

In contrast to K-means, GMM allows for

- unequal cluster variances
- unequal cluster probabilities
- non-spherical clusters 非球型
- soft cluster



(Figure taken from Wikipedia)

Expectation Maximization (EM)

Expectation Maximization

- **Goal**: find maximum likelihood solutions for models having latent variables
- **Notation**:
  X: observed variables
  Z: latent variables
  θ: model parameters
  $\{X, Z\}$: complete data set
  $\{X\}$: incomplete data set
- **Difficulty**: optimizing the incomplete-data log likelihood $\log p(X|\theta) = \log[\sum_Z p(X, Z|\theta)]$ is hard because of sum inside the log, but maximizing the complete-data log likelihood $\log p(X, Z|\theta)$ is straightforward
- Only information we have about Z is through its posterior distribution $p(Z|X, \theta)$
- **Idea**: consider instead the expectation of $\log p(X, Z|\theta)$ under posterior $p(Z|X, \theta)$

Expectation Maximization

- **Goal:** find maximum likelihood solutions for models having latent variables
- **Notation:**
  X: observed variables
  Z: latent variables
  θ: model parameters
  $\{X, Z\}$: complete data set
  $\{X\}$: incomplete data set
- **Idea:** consider instead the expectation of $\log p(X, Z|\theta)$ under posterior $p(Z|X, \theta)$

E-step: Calculate *expectation* of $\log p(X, Z|\theta)$ under $p(Z|X, \theta)$

M-step: *Maximize* this expectation for model parameters θ

General EM Algorithm

Input: joint distribution $p(X, Z|\theta)$

Returns: maximum likelihood estimations for θ

1. Initialize θ^{old}
2. Loop until convergence*:
   - 2.1. Evaluate $p\left(Z \middle| X, \theta^{\text{old}}\right)$. ← E-step
   - 2.2. Update θ^{new} as ← M-step

     $$\theta^{\text{new}} = \underset{\theta}{\operatorname{argmax}}\left\{\sum_Z p\left(Z \middle| X, \theta^{\text{old}}\right) \log p(X, Z|\theta)\right\}$$
   - 2.3. $\theta^{\text{old}} \leftarrow \theta^{\text{new}}$

* for convergence check either the log likelihood or model parameters for changes

Gaussian Mixtures Revisited

- Incomplete-data log likelihood

$\log p(X|\theta) = \log[\sum_Z p(X, Z|\theta)]$ ← general EM

$\log p\,(X|\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_n \log[\sum_k \tau_k \mathcal{N}(x_n|\mu_k, \Sigma_k)]$ ← EM for GMM

- Complete-data log likelihood

$\log p(X, Z|\theta)$

$\log p(X, Z|\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$

$= \log \prod_n \prod_k \tau_k^{z_{n,k}} \cdot \mathcal{N}(x_n|\mu_k, \Sigma_k)^{z_{n,k}}$

$= \sum_n \sum_k z_{n,k} \cdot (\log \tau_k + \log \mathcal{N}(x_n|\mu_k, \Sigma_k))$

- Posterior

$p(Z|X, \theta)$

$p(Z|X, \boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) \propto \prod_n \prod_k \tau_k^{z_{n,k}} \cdot \mathcal{N}(x_n|\mu_k, \Sigma_k)^{z_{n,k}}$

- Expectation of complete-data log likelihood under posterior

$\mathbb{E}_{Z\sim p(Z|X,\theta)}\,[\log p(X, Z|\theta)]$

$\mathbb{E}_{Z\sim p(Z|X, \boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma})}[\log p(X, Z|\boldsymbol{\tau}, \boldsymbol{\mu}, \boldsymbol{\Sigma})]$

$= \sum_n \sum_k p(z_{n,k}|x_n, \mu_k, \Sigma_k) \cdot (\log \tau_k + \log \mathcal{N}(x_n|\mu_k, \Sigma_k))$

$= \sum_n \sum_k \frac{\tau_k \mathcal{N}(x_n|\mu_k, \Sigma_k)}{\sum_j \tau_j \mathcal{N}(x_n|\mu_j, \Sigma_j)} \cdot (\log \tau_k + \log \mathcal{N}(x_n|\mu_k, \Sigma_k))$

EM increases Likelihood

Why does every iteration of EM cause an increase in the (log) likelihood?

- **Goal**: find maximum likelihood solutions for models having latent variables
- **Notation**:

  X: observed variables $\{X, Z\}$: complete data set

  Z: latent variables $\{X\}$: incomplete data set

  θ: model parameters
- $q(Z)$: any distribution over Z

$$\log p(X|\theta) = \underbrace{\sum_Z q(Z) \log \left[\frac{p(X,Z|\theta)}{q(Z)}\right]}_{=: \mathcal{L}(q,\theta)} + \underbrace{\sum_Z q(Z) \log \left[\frac{q(Z)}{p(Z|X,\theta)}\right]}_{= KL\left(q(z) \parallel p(Z|X,\theta)\right)}$$

(for decomposition see slide 32)

(this is further explained on slides 33-35)

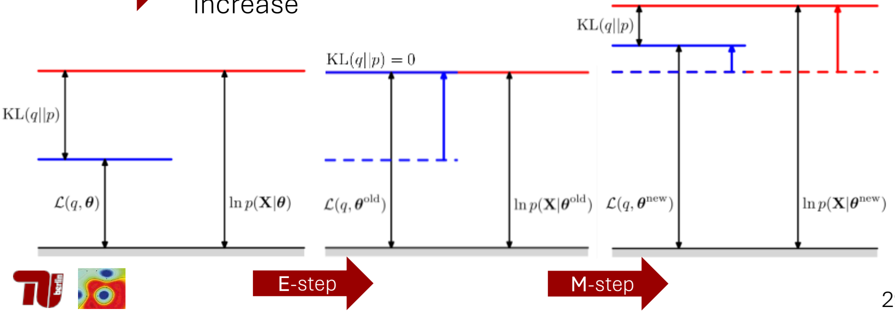
EM increases Likelihood

$$\log p(X|\theta) = \mathcal{L}(q,\theta) + KL\big(q(z) \parallel p(Z|X,\theta)\big)$$

- Because the $KL \geq 0$, $\mathcal{L}(q,\theta)$ is a lower bound on $\log p(X|\theta)$

E-step: Fixes θ, and maximizes the lower bound $\mathcal{L}(q,\theta)$ wrt. $q(Z)$ which causes $KL\big(q(z) \parallel p(Z|X,\theta)\big) = 0$

M-step: Fixes $q(Z)$, and maximizes the lower bound $\mathcal{L}(q,\theta)$ wrt. θ which causes $\mathcal{L}(q,\theta)$, correspondingly $\log p(X|\theta)$, to increase



Summary

- Clustering is an unsupervised learning problem with the goal to partition the data set into similar groups (clusters).
- K-means is a simple algorithm which provides a clustering solution, and is guaranteed to converge to a (local) optimum
- Gaussian Mixture Models are a powerful tool to model complex data distributions. They provide a soft-clustering as a byproduct. Their solution can be found by EM.
- Expectation Maximization finds maximum likelihood solutions for models with latent variables and has a wide application range (not just GMMs).

Additional Slides

Decomposition of $\log p(X|\theta)$

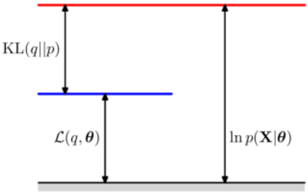
$$\log p(X|\theta) = \underbrace{\sum_Z q(Z) \log \left[\frac{p(X,Z|\theta)}{q(Z)}\right]}_{=:\mathcal{L}(q,\theta)} + \underbrace{\sum_Z q(Z) \log \left[\frac{q(Z)}{p(Z|X,\theta)}\right]}_{=KL\left(q(z) \parallel p(Z|X,\theta)\right)}$$

$$\begin{aligned}
&\sum_Z q(Z) \log \left[\frac{p(X,Z|\theta)}{q(Z)}\right] + \sum_Z q(Z) \log \left[\frac{q(Z)}{p(Z|X,\theta)}\right] \\
&= \sum_z q(Z) \log p(X,Z|\theta) - \cancel{q(Z) \log q(Z)} + \cancel{q(Z) \log q(Z)} - q(Z) \log p(Z|X,\theta) \\
&= \sum_Z q(Z) \cdot (\log p(X,Z|\theta) - \log p(Z|X,\theta)) \\
&\overset{*}{=} \sum_Z q(Z) \log p(X|\theta) = \log p(X|\theta) \cdot \sum_Z q(Z) = \log p(X|\theta)
\end{aligned}$$

*(product rule with logarithm: $\log p(X|\theta) = \log p(X,Z|\theta) - \log p(Z|X,\theta)$)

EM increases Likelihood

▶ $\log p(X|\theta)$ can be decomposed into two non-negative terms (for derivation see slide 31):
$\log p(X|\theta) = \mathcal{L}(q,\theta) + KL\big(q(z) \parallel p(Z|X,\theta)\big)$
▶ $KL\big(q(z) \parallel p(Z|X,\theta)\big) \geq 0$ measures the divergence between $q(z)$ and $p(Z|X,\theta)$ with
$KL\big(q(z) \parallel p(Z|X,\theta)\big) = 0 \;\Leftrightarrow q(z) = p(Z|X,\theta)$.
▶ Because $\log p(X|\theta) = \mathcal{L}(q,\theta) + KL(q \parallel p)$ and $KL(q \parallel p) \geq 0$, it follows that $\mathcal{L}(q,\theta) \leq \log p(X|\theta)$. $\mathcal{L}(q,\theta)$ is a lower bound on $\log p(X|\theta)$.

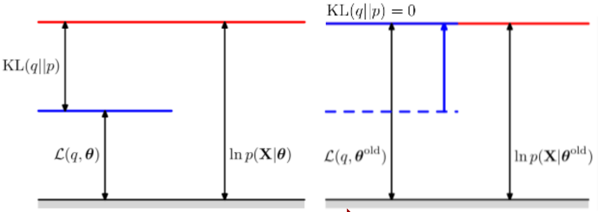


EM increases Likelihood

E-step

Fixes θ, and maximizes the lower bound $\mathcal{L}(q,\theta)$ wrt. $q(Z)$ which causes $KL\big(q(z) \parallel p(Z|X,\theta)\big) = 0$

- Maximization of $\mathcal{L}(q,\theta)$ wrt. $q(Z)$ causes $q(Z)$, and correspondingly $\mathcal{L}(q,\theta) = \sum_Z q(Z) \log\left[\frac{p(X,Z|\theta)}{q(Z)}\right]$ to change. A change in $q(Z)$ does not affect $\log p(X|\theta)$ because it does not depend on $q(Z)$.
- Because $\mathcal{L}(q,\theta) \leq \log p(X|\theta)$, its maximal value is obtained when $\mathcal{L}(q,\theta) = \log p(X|\theta)$. Because $\log p(X|\theta) = \mathcal{L}(q,\theta) + KL(q \parallel p)$ this implies $KL(q \parallel p) = 0$ at the maximum.
- In other words, the E-step causes $q(Z) = p(X,Z|\theta)$.

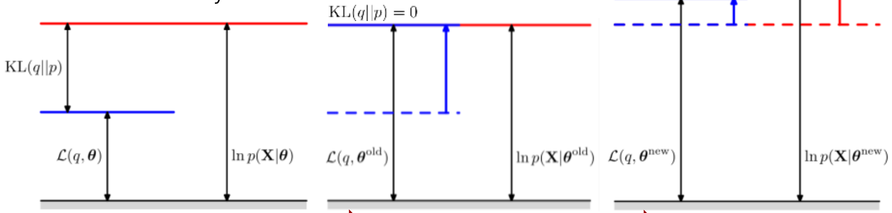


E-step

EM increases Likelihood

M-step Fixes $q(Z)$, and maximizes $\mathcal{L}(q,\theta)$ wrt. θ which causes $\mathcal{L}(q,\theta)$, correspondingly $\log p(X|\theta)$, to increase

- Maximization of $\mathcal{L}(q,\theta)$ wrt. θ gives new model parameters θ^{new}.
- Because the posterior $p(Z|X,\theta)$ also depends on θ, it will change too so that $q(Z) \neq p(X,Z|\theta^{\text{new}})$ and $KL(q \parallel p) > 0$.
- Because $\log p(X|\theta)$ depends on θ, it will change as well. Because $\log p(X|\theta^{\text{new}}) = \mathcal{L}(q,\theta^{\text{new}}) + KL\big(q(z) \parallel p(Z|X,\theta^{\text{new}})\big)$ with $\mathcal{L}(q,\theta^{\text{new}}) \geq \mathcal{L}\big(q,\theta^{\text{old}}\big)$ and $KL\big(q(z) \parallel p(Z|X,\theta^{\text{new}})\big) > 0$, it follows that $\log p(X|\theta^{\text{new}}) \geq \log p\big(X|\theta^{\text{old}}\big)$.
- In other words, EM causes the likelihood to increase in every iteration.



E-step M-step