Lecture 7: Clustering (cont'd)

Felix Held, Mathematical Sciences

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CHALMERS
UNIVERSITY OF TECHNOLOGY | UNIVERSITY OF GOTHENBURG

Bottom-up approach to clustering

Two approaches to combinatorial clustering

Top-down approach

- Start with all observations in one group and split them into clusters
- Examples: k-means and k-medoids

Bottom-up approach

- Start with all observations individually and join them together to build clusters

A bottom-up approach

Let g_l^i be the set of samples in cluster l at iteration i.

Hierarchical clustering

1. **Initialization:** Let each observation $\mathbf{x}_l$ be in its own cluster g_l^0 for $l = 1, \ldots, n$
2. **Joining:** In step i, join the two clusters g_l^{i-1} and g_m^{i-1} that are closest to each other, resulting in $n - i$ clusters
3. After $n - 1$ steps all observations are in one big cluster

Questions

- How do we measure distance between clusters?
- How do we get a final clustering with a certain number of clusters?

Linkage

Cluster-cluster distance is called **linkage**

Distance between clusters g and h

Let $\mathbf{D} \in \mathbb{R}^{n \times n}$ be a distance matrix between samples.

1. **Average Linkage:**

$$d(g, h) = \frac{1}{|g| \cdot |h|} \sum_{\substack{\mathbf{x}_l \in g \\ \mathbf{x}_m \in h}} \mathbf{D}_{l,m}$$

2. **Single Linkage**

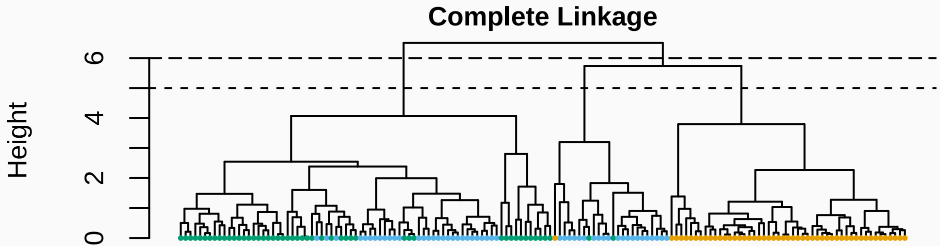
$$d(g, h) = \min_{\substack{\mathbf{x}_l \in g \\ \mathbf{x}_m \in h}} \mathbf{D}_{l,m}$$

3. **Complete Linkage**

$$d(g, h) = \max_{\substack{\mathbf{x}_l \in g \\ \mathbf{x}_m \in h}} \mathbf{D}_{l,m}$$

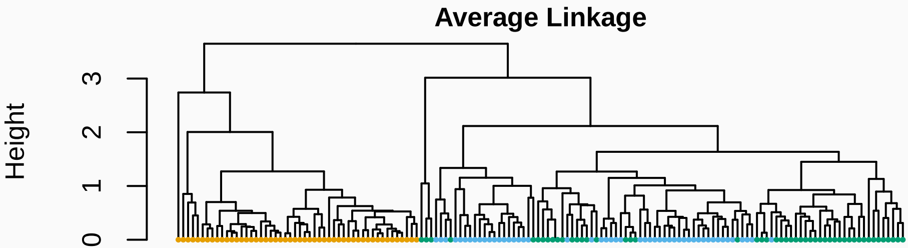
Dendrograms

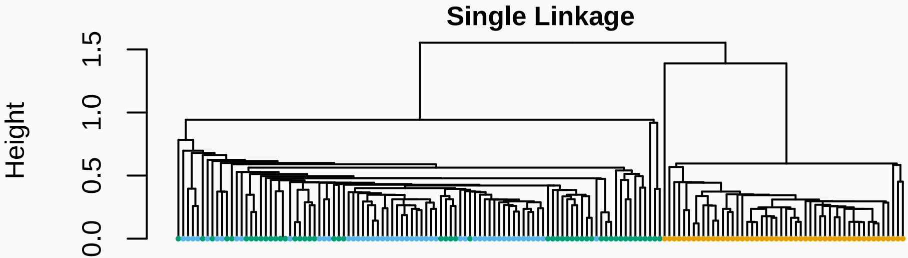
Hierarchical clustering applied to **iris dataset**



- Leaf colours represent iris type: setosa, versicolor and virginica
- **Height** is the distance between clusters
- The tree can be **cut** at a certain height to achieve a final clustering. Long branches mean large increase in within cluster scatter at join

Dendrograms for other linkages





Notes on hierarchical clustering and linkage

Linkage criteria

- Average linkage is most commonly used and encourages average similarity between all pairs in the two clusters.
- Single linkage tends to create clusters that are quite spread out since it only considers the closest observations between clusters
- Complete linkage tends to produce ‘tight’ clusters

New view on clustering

- Clusters are joined by closeness to each other, not by closeness to some centre
- e.g. single linkage hierarchical clustering can handle the circle around a disc example from last lecture

Model-based clustering

Model-based clustering

- All methods discussed so far were **non-parametric clustering methods** based on
  1. a distance/dissimilarity measure
  2. a construction algorithm
- Performance depended on **choices** such as the metric and how to select the cluster count
- Assuming an underlying theoretical model for the feature space worked well in classification (LDA, QDA, logistic regression).

  Is this transferable to clustering?

Remember QDA

In Quadratic Discriminant Analysis (QDA) we assumed

$$p(\mathbf{x}|i) = N\left(\mathbf{x}|\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i\right) \quad \text{and} \quad p(i) = \pi_i$$

This can be written as a **Gaussian Mixture Model (GMM)** for $\mathbf{x}$ where

$$p(\mathbf{x}) = \sum_{i=1}^{K} p(i)p(\mathbf{x}|i) = \sum_{i=1}^{K} \pi_i N\left(\mathbf{x}|\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i\right)$$

QDA used that the classes i_l and feature vectors $\mathbf{x}_l$ of the observations were known to calculate π_i, $\boldsymbol{\mu}_i$ and $\boldsymbol{\Sigma}_i$.

What if we only know the features $\mathbf{x}_l$?

Maximum Likelihood for GMMs?

The log-likelihood for the data $\mathbf{X} \in \mathbb{R}^{n \times p}$ and all unknowns

$$\theta = (\pi_1, \boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1, \dots, \pi_K, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_K)$$

is

$$\log p(\mathbf{X}|\theta) = \sum_{l=1}^{n} \log \left(\sum_{i=1}^{K} \pi_i N\left(\mathbf{x}_l | \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i\right) \right)$$

Taking the gradient (with chain-rule) and solving for $\boldsymbol{\mu}_i$ gives

$$\boldsymbol{\mu}_i = \frac{\sum_{l=1}^{n} \eta_{li} \mathbf{x}_l}{\sum_{l=1}^{n} \eta_{li}} \quad \text{where} \quad \eta_{li} = \frac{\pi_i N(\mathbf{x}_l | \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)}{\sum_{j=1}^{K} \pi_j N(\mathbf{x}_l | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

Note: There is a **non-linear cyclic dependence** between η_{li} and $\boldsymbol{\mu}_i$.

Expectation-Maximization for GMMs

Finding the MLE for parameters θ in GMMs results in an iterative process called **Expectation-Maximization (EM)**

1. Initialize θ
2. **E-Step:** Update

$$\eta_{li} = \frac{\pi_i N(\mathbf{x}_l | \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)}{\sum_{j=1}^{K} \pi_j N(\mathbf{x}_l | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

3. **M-Step:** Update

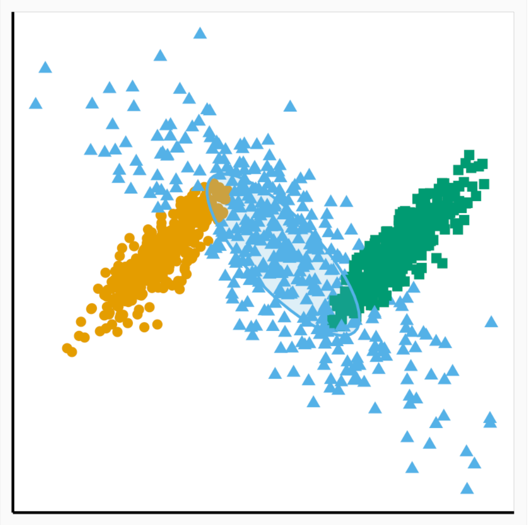
$$\boldsymbol{\mu}_i = \frac{\sum_{l=1}^{n} \eta_{li} \mathbf{x}_l}{\sum_{l=1}^{n} \eta_{li}} \qquad \pi_i = \frac{\sum_{l=1}^{n} \eta_{li}}{n}$$

$$\boldsymbol{\Sigma}_i = \frac{1}{\sum_{l=1}^{n} \eta_{li}} \sum_{l=1}^{n} \eta_{li} (\mathbf{x}_l - \boldsymbol{\mu}_i)(\mathbf{x}_l - \boldsymbol{\mu}_i)^\top$$

4. Repeat steps 2 and 3 until convergence

GMM clustering example

- Yellow and green clusters share a covariance matrix
- The blue cluster has a different one
- GMM clustering on only the data points without knowledge of the class labels recovers the covariance structures and clusters



Why does Expectation-Maximization work?

Likelihood of the complete data

- **Assume** that the **classes i_l are known** and code them as $z_{lj} = 1$ if $i_l = j$ and $z_{lj} = 0$ otherwise. Collect them in $\mathbf{Z} \in \mathbb{R}^{n \times K}$.
- $(\mathbf{X}, \mathbf{Z})$ are called the **complete data**, and **incomplete data** when only $\mathbf{X}$ is observed
- The class assignments $\mathbf{Z}$ are called **latent variables**
- **Complete data likelihood**

$$\log p(\mathbf{X}, \mathbf{Z} | \theta) = \sum_{l=1}^{n} \sum_{i=1}^{K} z_{li} \left(\log(\pi_i) + \log(N(\mathbf{x}_l | \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i))\right)$$

  and the parameters in θ are easy to estimate (QDA).
- **Incomplete data likelihood**

$$\log p(\mathbf{X} | \theta) = \sum_{l=1}^{n} \log \left(\sum_{i=1}^{K} \pi_i N\left(\mathbf{x}_l | \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i\right) \right)$$

Decomposing the incomplete data likelihood

- **For known $\mathbf{Z}$**

$$p(\mathbf{X}|\theta) = \frac{p(\mathbf{X},\mathbf{Z}|\theta)}{p(\mathbf{Z}|\mathbf{X},\theta)}, \quad \text{i.e.}$$

$$\log p(\mathbf{X}|\theta) = \log p(\mathbf{X},\mathbf{Z}|\theta) - \log p(\mathbf{Z}|\mathbf{X},\theta)$$

  is a **decomposition** of the log-likelihood for $\mathbf{X}$ given θ

- For any density $q(\mathbf{Z})$ it holds that

$$\log p(\mathbf{X}|\theta) = \log \frac{p(\mathbf{X},\mathbf{Z}|\theta)}{q(\mathbf{Z})} - \log \frac{p(\mathbf{Z}|\mathbf{X},\theta)}{q(\mathbf{Z})}$$

- **Average** over $\mathbf{Z}$ according to the density $q(\mathbf{Z})$

$$\log(p(\mathbf{X}|\theta)) = \mathbb{E}_{q(\mathbf{Z})}\left[\log \frac{p(\mathbf{X},\mathbf{Z}|\theta)}{q(\mathbf{Z})}\right] - \mathbb{E}_{q(\mathbf{Z})}\left[\log \frac{p(\mathbf{Z}|\mathbf{X},\theta)}{q(\mathbf{Z})}\right]$$

$$=: F(q,\theta) + \mathrm{KL}(q||p(\cdot|\mathbf{X},\theta))$$

  where $\mathrm{KL}(q||p(\cdot|\mathbf{X},\theta))$ is called the **Kullback-Leibler (KL) divergence** of $q(\mathbf{Z})$ and $p(\cdot|\mathbf{X},\theta)$.

Decomposing the incomplete data likelihood (II)

It can be shown (using **Jensen's inequality**) that

$$\mathrm{KL}(q||p(\cdot|\mathbf{X},\theta)) = -\mathbb{E}_{q(\mathbf{Z})}\left[\log \frac{p(\mathbf{Z}|\mathbf{X},\theta)}{q(\mathbf{Z})}\right] \geq 0$$

with equality if $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X},\theta)$.

This implies that

$$\log p(\mathbf{X}|\theta) \geq F(q,\theta)$$

is a **lower bound** which is tight (i.e. equality holds) if $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X},\theta)$.

This gives us a **recipe** on how to choose $q(\mathbf{Z})$.

Expectation-Maximization

1. **Expectation step:** For given parameters $\theta^{(m)}$ the density $q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \theta^{(m)})$ ensures that $F(q, \theta^{(m)}) = \log p(\mathbf{X}|\theta^{(m)})$. Note that then

$$F(q, \theta) = \mathbb{E}_{p(\mathbf{Z}|\mathbf{X}, \theta^{(m)})}[\log p(\mathbf{X}, \mathbf{Z}|\theta)] - \mathbb{E}_{p(\mathbf{Z}|\mathbf{X}, \theta^{(m)})}\left[\log p(\mathbf{Z}|\mathbf{X}, \theta^{(m)})\right]$$
$$=: Q(\theta, \theta^{(m)}) + \text{constant}$$

2. **Maximization step:** Maximize $F(q, \theta)$ through

$$\theta^{(m+1)} = \arg\max_{\theta} Q(\theta, \theta^{(m)})$$

The incomplete data likelihood increases in each step until convergence to a **local maximum**.

How to use the EM algorithm?

Two step procedure

1. Compute for given $\theta^{(m)}$
$$q(\mathbf{Z}) = p(\mathbf{Z}|\mathbf{X}, \theta^{(m)}).$$
2. Maximize in θ
$$Q(\theta, \theta^{(m)}) = \mathbb{E}_{p(\mathbf{Z}|\mathbf{X},\theta^{(m)})}\left[\log p(\mathbf{X}, \mathbf{Z}|\theta)\right]$$

Applying EM to the GMM clustering problem (I)

Expectation step

Given $\mathbf{X}$ and $\theta^{(m)}$

$$p(\mathbf{Z}|\mathbf{X}, \theta^{(m)}) = \frac{p(\mathbf{X}, \mathbf{Z}|\theta^{(m)})}{p(\mathbf{X}|\theta^{(m)})} = \prod_{l=1}^{n} \frac{\prod_{i=1}^{K}(\pi_i N(\mathbf{x}_l|\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i))^{z_{li}}}{\sum_{j=1}^{K} \pi_j N\left(\mathbf{x}_l|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\right)}$$

and recall that

$$\log p(\mathbf{X}, \mathbf{Z}|\theta) = \sum_{l=1}^{n}\sum_{i=1}^{K} z_{li}\left(\log(\pi_i) + \log(N(\mathbf{x}_l|\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i))\right).$$

To compute $Q(\theta, \theta^{(m)})$ we only need to compute

$$\mathbb{E}_{p(\mathbf{Z}|\mathbf{X}, \theta^{(m)})}[z_{li}] = \frac{\pi_i N(\mathbf{x}_l|\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)}{\sum_{j=1}^{K} \pi_j N(\mathbf{x}_l|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)} = \eta_{li}$$

the so-called **responsibility** of class i for having generated the observation $\mathbf{x}_l$.

Applying EM to the GMM clustering problem (II)

Maximization step

This results in

$$Q(\theta, \theta^{(m)}) = \sum_{l=1}^{n} \sum_{i=1}^{K} \eta_{li} \left(\log(\pi_i) + \log(N(\mathbf{x}_l | \boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i))\right)$$

which is maximized by the MLE estimates

$$\boldsymbol{\mu}_i = \frac{\sum_{l=1}^{n} \eta_{li} \mathbf{x}_l}{\sum_{l=1}^{n} \eta_{li}} \qquad \pi_i = \frac{\sum_{l=1}^{n} \eta_{li}}{n}$$

$$\boldsymbol{\Sigma}_i = \frac{1}{\sum_{l=1}^{n} \eta_{li}} \sum_{l=1}^{n} \eta_{li} (\mathbf{x}_l - \boldsymbol{\mu}_i)(\mathbf{x}_l - \boldsymbol{\mu}_i)^\top$$

Cluster selection

A **final clustering** can be selected with

$$C(\mathbf{x}_l) = \arg\max_i \eta_{li}$$

or responsibilities can be used as a **soft clustering**

Cluster count selection

Model selection criteria for MLE can be used, e.g. minimal **Bayesian Information Criterion (BIC)**

$$\begin{aligned} \mathrm{BIC}(K) = & -2\log(p(\mathbf{X}|\theta, K)) \\ & + \log(n) \cdot \underbrace{[(K-1) + K \cdot p + K \cdot \frac{p(p+1)}{2}]}_{\text{number of model parameters}} \end{aligned}$$

which is valid for large n.

Caveat with MLE for GMMs

- Centering one mixture component on an observation (i.e. $\boldsymbol{\mu}_i = \mathbf{x}_l$ for some i and l) and letting its variance go to zero can drive the likelihood to infinity
  - 'Outside of scope'-solution:
    Bayesian framework and Inverse-Wishart prior on $\boldsymbol{\Sigma}_i$
  - Initialize $\boldsymbol{\Sigma}_i$ with large enough variances and potentially restart if bad convergence
- Like k-means, this algorithm is sensitive to starting values

GMMs and EM for classification

GMM for classification

In QDA $p(\mathbf{x}|i) = N(\mathbf{x}|\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$ capture classes with **elliptic shape**.

Assume features are described by a GMM, i.e.

$$p(\mathbf{x}|i) = \sum_{m=1}^{M_i} \pi_{im} N(\mathbf{x}|\boldsymbol{\mu}_{im}, \boldsymbol{\Sigma})$$

where

- M_i components for class i
- π_{im} is the probability of mixture component m for class i
- Covariance matrix $\boldsymbol{\Sigma}$ is assumed to be constant across mixture components and classes

Component membership z_{lm} is a latent variable for the observation $(\mathbf{x}_l, i_l)$ with $z_{lm} = 1$ if $\mathbf{x}_l$ is in component $m \in \{1, \ldots, M_{i_l}\}$ and $z_{lm} = 0$ otherwise

Mixture DA

Finding the MLE for the mixture DA parameters can be achieved through **Expectation-Maximization (EM)**

1. Initialize θ
2. **E-Step:** Update

$$\eta_{lm} = \frac{\pi_{i_l m} N(\mathbf{x}_l | \boldsymbol{\mu}_{i_l m}, \boldsymbol{\Sigma})}{\sum_{j=1}^{M_{i_l}} \pi_{i_l j} N(\mathbf{x}_l | \boldsymbol{\mu}_{i_l j}, \boldsymbol{\Sigma})}$$

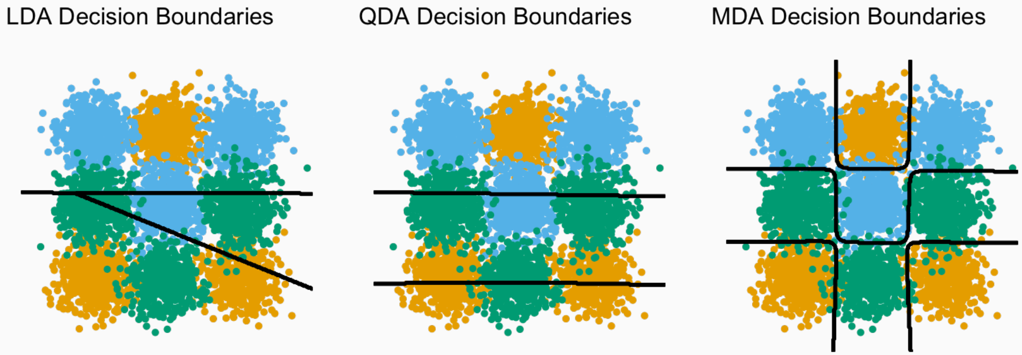
3. **M-Step:** Update

$$\boldsymbol{\mu}_{im} = \frac{\sum_{i_l = i} \eta_{lm} \mathbf{x}_l}{\sum_{i_l = i} \eta_{lm}} \qquad \pi_{im} = \frac{\sum_{i_l = i} \eta_{lm}}{n_i}$$

$$\boldsymbol{\Sigma} = \frac{1}{n} \sum_{i=1}^{K} \sum_{i_l = i} \sum_{m=1}^{M_i} \eta_{lm} (\mathbf{x}_l - \boldsymbol{\mu}_{im})(\mathbf{x}_l - \boldsymbol{\mu}_{im})^\top$$

4. Repeat steps 2 and 3 until convergence

MDA example


LDA Decision Boundaries
QDA Decision Boundaries
MDA Decision Boundaries

Take-home message

- Hierarchical clustering and its linkage-methods allow for a different non-parametric approach with visual output (dendrogram)
- Expectation-Maximization allows us to perform model-based clustering
- Both clustering and classification methods profit from using Gaussian Mixture Models