Lecture 18: Cluster Analysis

Reading: Sections 8.5, 14.3

GU4241/GR5241 Statistical Machine Learning

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Clustering

We assign a class to each sample in the data matrix. However, the class *is not an output variable*; we only use input variables.

Clustering is an **unsupervised** procedure, whose goal is to find homogeneous subgroups among the observations. It has wide applications in practice. Image segmentation, handwritten digit identification, vector quantization

In this lecture, we will discuss 2 algorithms:

- Hierarchical clustering
- EM algorithm

We have discussed:

- K-means clustering
- K-medoids clustering

Handwritten digit identification

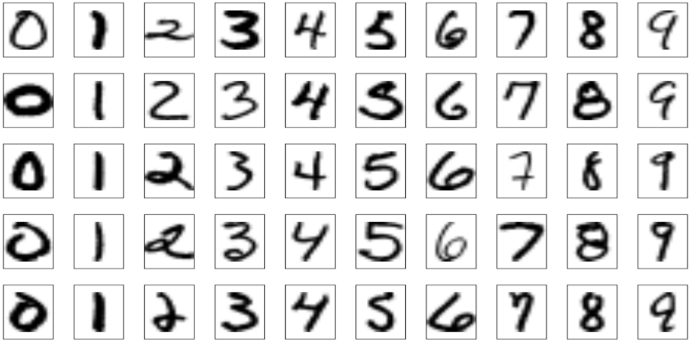
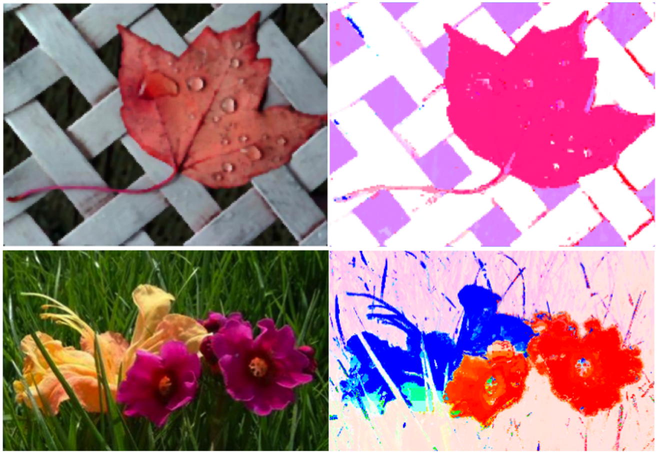


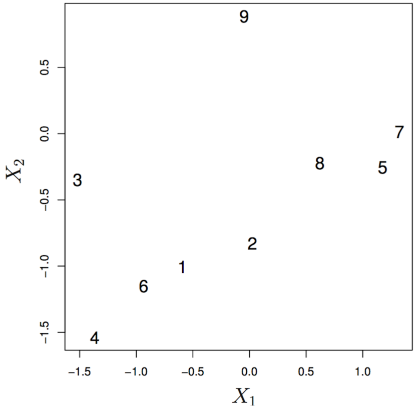
FIGURE 11.9. *Examples of training cases from ZIP code data. Each image is a* 16×16 8*-bit grayscale representation of a handwritten digit.*

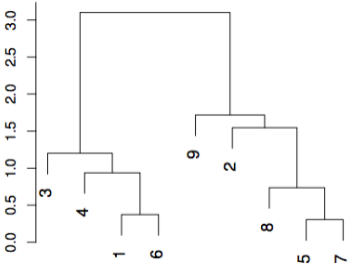
Image segmentation



Hierarchical clustering

Most algorithms for hierarchical clustering are *agglomerative*.





The output of the algorithm is a *dendogram*.

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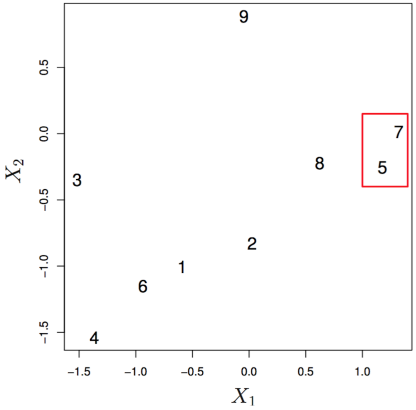

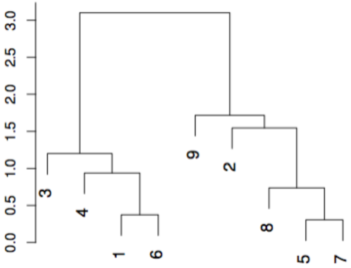

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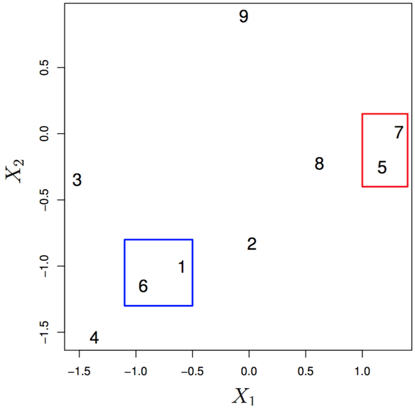

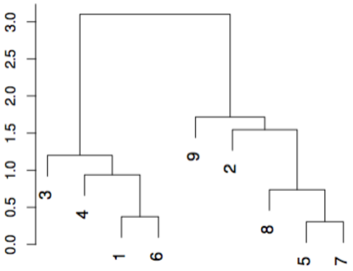

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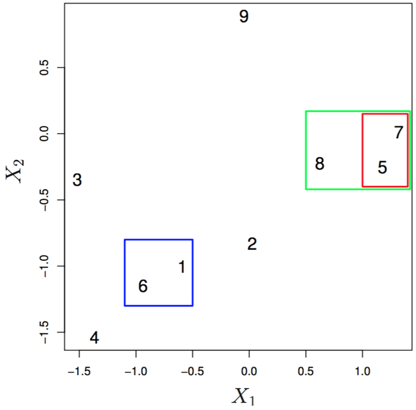

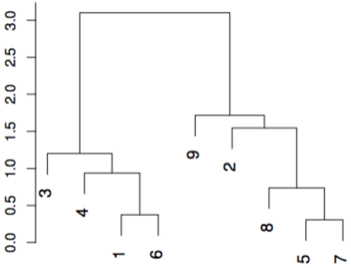

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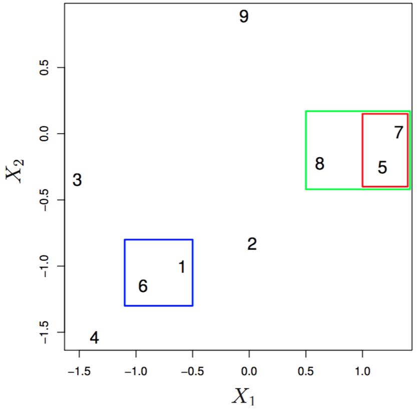
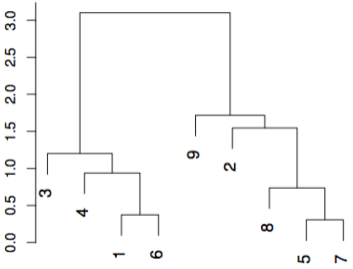
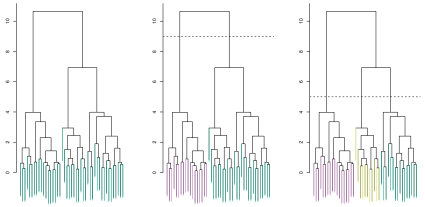




We must be careful about how we interpret the dendogram.

Hierarchical clustering



ISL Figure 10.9

- The number of clusters is not fixed.
- Hierarchical clustering is not always appropriate.

  e.g. Market segmentation for consumers of 3 different nationalities.
  - Natural 2 clusters: gender
  - Natural 3 clusters: nationality

  These clusterings are not nested or hierarchical.

Notion of distance between clusters

At each step, we link the 2 clusters that are "closest" to each other.

Hierarchical clustering algorithms are classified according to the notion of distance between clusters.

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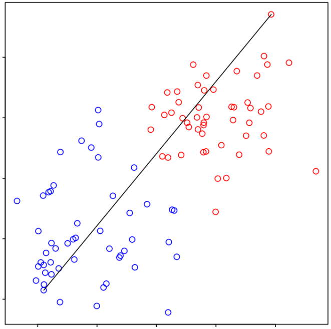

Complete linkage:
The distance between 2 clusters is the *maximum* distance between any pair of samples, one in each cluster.

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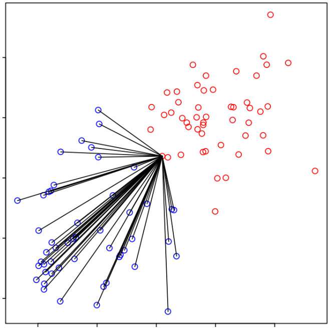

Average linkage:
The distance between 2 clusters is the average of all pairwise distances.

Notion of distance between clusters

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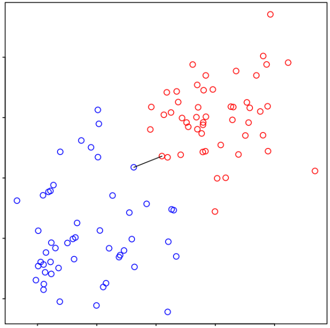

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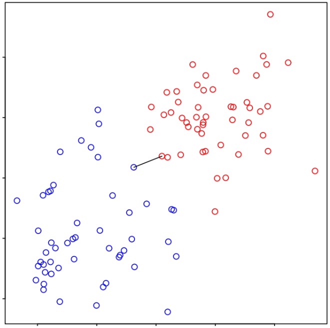
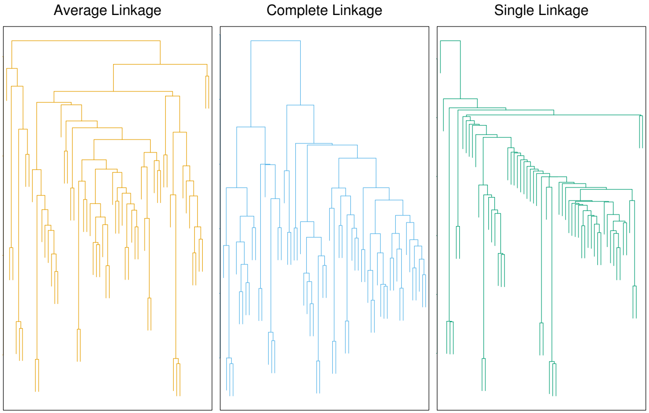


Single linkage:
The distance between 2 clusters is the *minimum* distance between any pair of samples, one in each cluster.

Suffers from the *chaining phenomenon*

Example



ESL Figure 14.13

Mixture Models

Mixture

For a parametric model $p(x|\theta)$ and a probability density q, a distribution of the form

$$\pi(x) = \int_{\mathcal{T}} p(x|\theta)q(\theta)d\theta$$

is called a **mixture model**. The distribution given by q is called the **mixing distribution**.

Interpretation

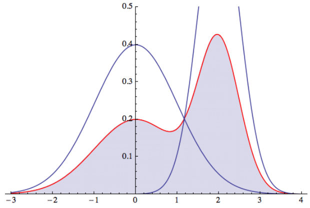
Mixtures describe two-stage sampling procedures. We can generate samples from π as follows:

1. Sample $\theta_i \sim q$.
2. Sample $X_i \sim p(\,.\,|\theta_i)$.

The distribution of a sample $x_1, \dots, x_n$ generated in this manner has density π.

Illustration

Mixture of two Gaussians

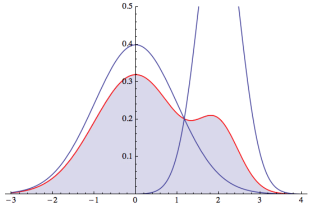


The curve outlined in red is the mixture

$$\pi(x) = 0.5g(x|0,1) + 0.5g(x|2,0.5) \ ,$$

where g is the Gaussian density. The blue curves are the component densities.

Influence of the weights



Here, the weights $c_1 = c_2 = 0.5$ above have been changed to $c_1 = 0.8$ and $c_2 = 0.2$. The component distributions are the same as above.

Example: Continuous Mixture

Example

We are mostly interested *discrete* mixing distributions, but θ can be continuous variable, as in the following example.

Mixture components

1. Sample $\theta \sim \text{Gamma}(\alpha, \beta)$.
2. Regard θ as an inverse variance $\frac{1}{\sigma^2} := \theta$ and sample

$$X \sim \text{Normal}(0, \sigma)$$

Mixture distribution

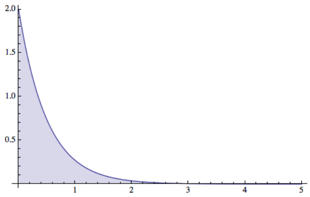
The distribution of X is the mixture with density

$$\pi(x|0, \nu := \frac{\alpha}{\beta}, \tau := 2\alpha) = \int_{\mathbb{R}_+} p_{\text{Normal}}(x|0, 1/\theta) q_{\text{Gamma}}(\theta|\alpha, \beta) d\theta$$

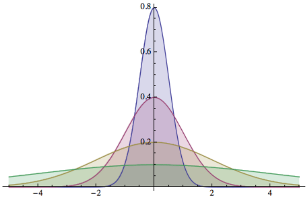
This is **Student's t-distribution** with parameters 0 (the mean of the normal), ν, τ.

Example: Continuous Mixture

Mixture components

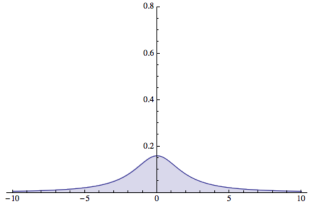


Gamma distribution

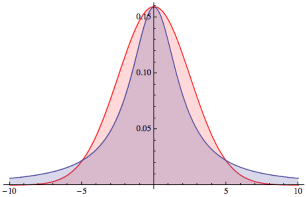


Normal distribution, different variances

Mixture distribution



The mixture is a Student distribution. Mixing over different variances results in "heavy tails".



Comparison: Normal distribution (red) vs Student distribution (blue)

Finite Mixtures

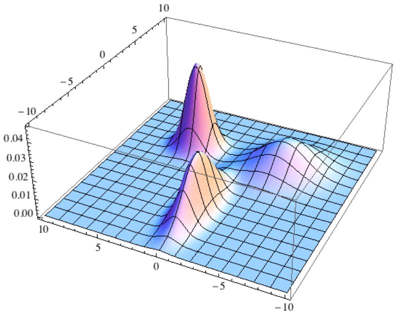
Finite Mixture Model

A **finite mixture model** is a distribution with density of the form

$$\pi(x) = \sum_{k=1}^{K} c_k p(x|\theta_k) \ ,$$

where $\sum_k c_k = 1$ and $c_k \geq 0$.

Example: Finite mixture of Gaussians



Finite Mixtures

Interpretation as mixture

A mixture is of the form

$$\pi(x) = \int_{\mathcal{T}} p(x|\theta) q(\theta) d\theta \ .$$

We choose q as

$$q = \sum_{k=1}^{K} c_k \delta_{\theta_k}$$

for K fixed values $\theta_k \in \mathcal{T}$. Recall that integration against the Dirac distribution δ_θ "picks out" the function value at θ.

The mixture with mixing distribution q is therefore

$$\begin{aligned}\pi(x) &= \int_{\mathcal{T}} p(x|\theta) \Big(\sum_{k=1}^{K} c_k \delta_{\theta_k} \Big) d\theta = \sum_{k=1}^{K} c_k \int_{\mathcal{T}} p(x|\theta) \delta_{\theta_k} d\theta \\ &= \sum_{k=1}^{K} c_k p(x|\theta_k) \ .\end{aligned}$$

Sampling

Sampling from a finite mixture

For a finite mixture with fixed parameters c_k and θ_k, the two-step sampling procedure is:

1. Choose a mixture component at random. Each component k is selected with probability c_k.
2. Sample x_i from $p(x|\theta_k)$.

Note: We always repeat both steps, i.e. for x_{i+1}, we choose again choose a (possibly different) component at random.

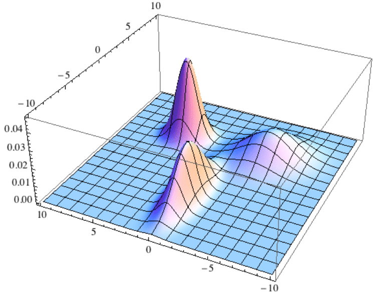
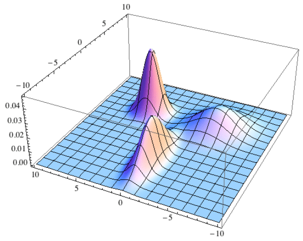
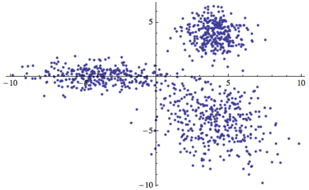


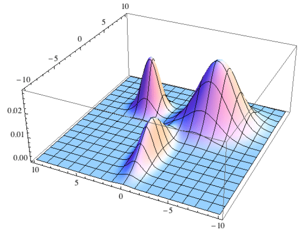
Illustration: Mixture of Gaussian in 2D



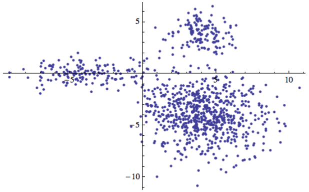
Plot of the mixture density.



A sample of size 1000.



Same components as above, with weight of one component increased.



A sample of 1000 points. Note how the relative size of one cluster has increased.

Finite Mixtures and Clustering

Clustering with finite mixtures

For a clustering problem with K clusters,

$$p(x|\theta_k) = \text{model of cluster } k$$

The weight c_k is the relative cluster size.

Estimation problem

If K is fixed and given, the unknown parameters of a mixture model are the weights c_k and the cluster parameters θ_k. The parameters of finite mixtures are estimated using a method known as the *EM algorithm*.

Mixture Estimation

Maximum likelihood for finite mixtures

Writing down the maximum likelihood problem is straightforward:

$$(\hat{\mathbf{c}}, \hat{\boldsymbol{\theta}}) := (\hat{c}_1, \dots, \hat{c}_K, \hat{\theta}_1, \dots, \hat{\theta}_K) = \arg\max_{\mathbf{c}, \boldsymbol{\theta}} \prod_{i=1}^{n} \Big(\sum_{k=1}^{K} c_k p(x_i | \theta_k) \Big)$$

The maximality equation for the logarithmic likelihood is

$$\frac{\partial}{\partial(\mathbf{c}, \boldsymbol{\theta})} \sum_{i=1}^{n} \log \Big(\sum_{k=1}^{K} c_k p(x_i | \theta_k) \Big) = 0$$

The component equation for each θ_k is:

$$\sum_{i=1}^{n} \frac{c_k \frac{\partial}{\partial \theta_k} p(x_i | \theta_k)}{\sum_{k=1}^{K} c_k p(x_i | \theta_k)} = 0$$

Solving this problem is analytically infeasible (note that we cannot multiply out the denominator, because of the sum over i). Even numerical solution is often difficult.

Latent Variables

Problems with ML estimation

- Solving the ML problem is difficult.
- For clustering, the maximum likelihood solution does not tell us *which* cluster generated each x_i.

Cluster assignments

- The mixture assumption implies that each x_i was generated from one component.
- For each x_i, we again use an **assignment variable** $m_i \in \{1, \dots, K\}$ which encodes which cluster x_i was sampled from.

Latent Variables

Since we do not know which component each x_i was generated by, the values of the assignment variables are *unobserved*. Such variables whose values are not observed are called **latent variables** or **hidden variables**.

Estimation With Latent Variables

Latent variables as auxiliary information

If we knew the correct assignments m_i, we could:

- Estimate each component distribution $p(x|\theta_k)$ separately, using only the data assigned to cluster k.
- Estimate the cluster proportions c_k as $\hat{c}_k := \frac{\#\text{points in cluster } k}{n}$.

EM algorithm: Idea

The EM algorithm estimates values of the latent variables to simplify the estimation problem. EM altnernates between two steps:

1. Estimate assignments m_i given current estimates of the parameters c_k and θ_k ("E-step").
2. Estimate parameters c_i and θ_k given current estimates of the assignments ("M-step").

These two steps are iterated repeatedly.

Representation of Assignments

We re-write the assignments as vectors of length K:

$$\mathbf{x}_i \text{ in cluster } k \qquad \text{as} \qquad M_i := \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \longleftarrow k\text{th entry}$$

so $M_{ik} = 1$ if x_i in cluster k, and $M_{ik} = 0$ otherwise.
We collect the vectors into a matrix

$$\mathbf{M} = \begin{pmatrix} M_{11} & \dots & M_{1K} \\ \vdots & & \vdots \\ M_{n1} & \dots & M_{nK} \end{pmatrix}$$

Note: Rows = observations, columns = clusters
Row sums = 1, column sums = cluster sizes.

E-Step

Hard vs soft assignments

- The vectors M_i are "hard assignments" with values in $\{0,1\}$.
- EM computes "soft assignments" a_{ik} with values in $[0,1]$.
- Once the algorithm terminates, each point is assigned to a cluster by setting

  $$m_i := \operatorname*{argmax}_k a_{ik}$$

  The vectors M_i are the latent variables in the EM algorithm. The a_{ik} are there current estimates.

Assignment probabilities

The soft assignments are computed as

$$a_{ik} := \frac{c_k p(x_i|\theta_k)}{\sum_{l=1}^{K} c_l p(x_i|\theta_l)} \,.$$

They can be interpreted as

$$a_{ik} := \mathbb{E}[M_{ik}|x_i, \mathbf{c}, \boldsymbol{\theta}] = \text{Pr}\{x_i \text{ generated by component } k \,|\, \mathbf{c}, \boldsymbol{\theta}\}$$

M-Step (1)

Objective

The M-Step re-estimates $\mathbf{c}$ and $\boldsymbol{\theta}$. In principle, we use maximum likelihood within each cluster, but we have to combine it with the use of weights a_{ik} instead "switch variables" M_{ik}.

Cluster sizes

If we know which points belong to which cluster, we can estimate the cluster proportions c_k by counting point:

$$\hat{c}_k = \frac{\#\text{ points in cluster } k}{n} = \frac{\sum_{i=1}^{n} M_{ik}}{n}$$

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$$\hat{c}_k = \frac{\#\text{ points in cluster } k}{n} = \frac{\sum_{i=1}^{n} M_{ik}}{n}$$

Since we do not know M_{ik}, we substitute our current best guess, which are the expectations a_{ik}:

$$\hat{c}_k := \frac{\sum_{i=1}^{n} a_{ik}}{n}$$

M-Step (2)

Gaussian special case

The estimation of the component parameters θ depends on which distribution we choose for p. For now, we assume a Gaussian.

Component parameters

We use maximum likelihood to estimate $\theta = (\mu, \Sigma)$. We can write the MLE of μ_k as

$$\hat{\mu}_k := \frac{1}{\#\text{ points in cluster } k} \sum_{i:\ x_i \text{ in } k} x_i = \frac{\sum_{i=1}^{n} M_{ik} x_i}{\sum_{i=1}^{n} M_{ik}}$$

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By substituting current best guesses (=a_{ik}) again, we get:

$$\hat{\mu}_k := \frac{\sum_{i=1}^n a_{ik} x_i}{\sum_{i=1}^n a_{ik}}$$

For the covariance matrices:

$$\hat{\Sigma}_k := \frac{\sum_{i=1}^n a_{ik} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^t}{\sum_{i=1}^n a_{ik}}$$

Notation Summary

Assignment probabilities

$$\mathbf{a} = \begin{pmatrix} a_{11} & \dots & a_{1K} \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nK} \end{pmatrix} = \mathbb{E}\left[\begin{pmatrix} M_{11} & \dots & M_{1K} \\ \vdots & & \vdots \\ M_{n1} & \dots & M_{nK} \end{pmatrix}\right] = \begin{pmatrix} \mathbb{E}[M_{11}] & \dots & \mathbb{E}[M_{1K}] \\ \vdots & & \vdots \\ \mathbb{E}[M_{n1}] & \dots & \mathbb{E}[M_{nK}] \end{pmatrix}$$

Rows = observations, columns = clusters.

Mixture parameters

$\boldsymbol{\tau} = (\mathbf{c}, \boldsymbol{\theta})$ $\quad$ $\mathbf{c} =$ cluster proportions $\quad$ $\boldsymbol{\theta} =$ component parameters

Iterations

$\theta^{(\mathsf{j})}$, $\mathbf{a}^{(\mathsf{j})}$ etc = values in jth iteration

Summary: EM for Gaussian Mixture

Gaussian special case

$\theta = (\mu, \Sigma)$ (mean & covariance) $p(x|\theta) = g(x|\mu, \Sigma)$ (Gaussian density)

Algorithm

The EM algorithm for a finite mixture of Gaussians looks like this:

- **Initialize:** Choose random values $c_k^{(0)}$ and $\theta_k^{(0)}$.
- **E-Step:** Recompute the assignment weight matrix as

$$a_{ik}^{(j+1)} := \frac{c_k^{(j)} g(x_i|\theta_k^{(j)})}{\sum_{l=1}^{K} c_l^{(j)} g(x_i|\theta_l^{(j)})} .$$

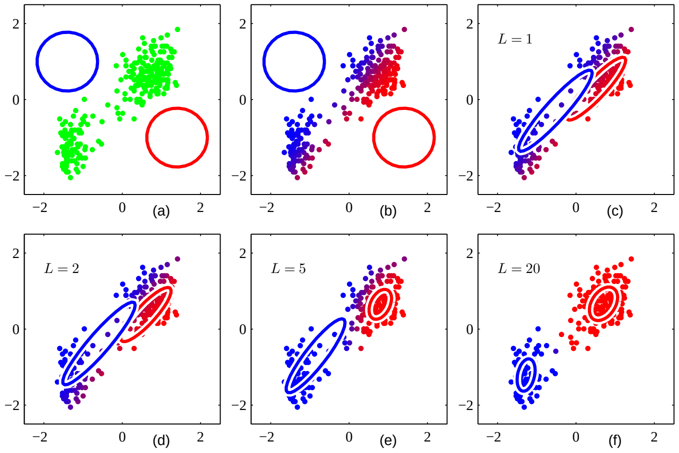
- **M-Step:** Recompute the proportions c_k and parameters $\theta_k = (\mu_k, \Sigma_k)$ as

$$\mu_k^{(j+1)} := \frac{\sum_{i=1}^{n} a_{ik}^{(j+1)} x_i}{\sum_{i=1}^{n} a_{ik}^{(j+1)}}, \quad \Sigma_k^{(j+1)} := \frac{\sum_{i=1}^{n} a_{ik}^{(j+1)} (x_i - \mu_k^{(j+1)})(x_i - \mu_k^{(j+1)})^t}{\sum_{i=1}^{n} a_{ik}^{(j+1)}}$$

The E-Step and M-Step are repeated alternatingly until convergence criterion (e.g. threshold) satisfied.

EM: Illustration

EM for a mixture of two Gaussians



The algorithm fits both the mean and the covariance parameter.

Convergence Properties

Log-likelihood

- It can be shown that the likelihood

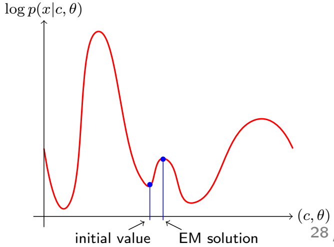
$$\prod_{i=1}^{n} \pi(x_i|\mathbf{c},\boldsymbol{\theta})$$

  always increases from each step to the next, unless $(\mathbf{c},\boldsymbol{\theta})$ is already a stationary point.

- The theory guarantees only that the algorithm terminates at a stationary point. That point can be a saddle point rather than a maximum (very rare problem).

The real problem: Local maxima

- EM is effectively a gradient method.
- The maxima it finds are **local maxima of the log-likelihood**.



EM in Practice

Comparing solutions

- If $(\mathbf{c}, \boldsymbol{\theta})$ and $(\mathbf{c}', \boldsymbol{\theta}')$ are two different EM solutions, we can always compute the log-likelihoods

  $$\sum_i \log \pi(x_i|\mathbf{c}, \boldsymbol{\theta}) \quad \text{and} \quad \sum_i \log \pi(x_i|\mathbf{c}', \boldsymbol{\theta}')$$

  (no approximations or complications!).
- The solution with the higher likelihood is better.
- This is a very convenient feature of EM: Different solutions are comparable.

Random restarts

In practice, the best way to use EM is often:

- Restart EM repeatedly with randomly chosen initial values.
- Compute the log-likelihoods of all solutions and compare them.
- Choose the solution achieving maximal log-likelihood.

K-means clustering algorithm

1. Assign each sample to a cluster from 1 to K arbitrarily, e.g. at random.
2. Iterate these two steps until the clustering is constant:
   - Find the *centroid* of each cluster ℓ; i.e. the average $\overline{x}_{\ell,:}$ of all the samples in the cluster:
     $$\overline{x}_{\ell,j} = \frac{1}{|\{i : C(i) = \ell\}|} \sum_{i:C(i)=\ell} x_{i,j} \quad \text{for } j = 1, \ldots, p.$$
   - Reassign each sample to the nearest centroid.

K-means: Gaussian Interpretation

K Gaussians

Consider the following algorithm:

- Suppose each μ_k is the expected value of a Gaussian density $p(x|\mu_k, \mathbb{I})$ with unit covariance.
- Start with K randomly chose means and iterate:
  1. Assign each x_i to the Gaussian under which it has the highest probability of occurence (more precisely: highest density value).
  2. Given the assignments, fit $p(x|\mu_k, \mathbb{I})$ by maximum likelihood estimation of μ_k from all points assigned to cluster k.

K-means: Gaussian Interpretation

Comparison to K-means

- Since the Gaussians are spherical with identical covariance, the density $p(x_i|\mu_k, \mathbb{I})$ is largest for the mean μ_k which is closest to x_i in Euclidean distance.
- The maximum likelihood estimator of μ_k is

$$\hat{\mu}_k := \frac{1}{\left|\{i : C(i) = k\}\right|} \sum_{i:C(i)=k} x_i$$

This is precisely the K-means algorithm!

Clustering is riddled with questions and choices

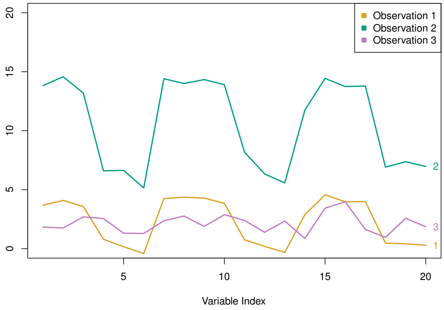
- Is clustering appropriate? i.e. Could a sample belong to more than one cluster?
    - Mixture models, soft clustering, topic models.
- Are the clusters robust?
    - Run the clustering on different random subsets of the data. Is the structure preserved?
    - Try different clustering algorithms. Are the conclusions consistent?
    - Most important: temper your conclusions.
- Should we scale the variables before doing the clustering.
    - Variables with larger variance have a larger effect on the Euclidean distance between two samples.

Clustering is riddled with questions and choices

- Does Euclidean distance capture dissimilarity between samples?

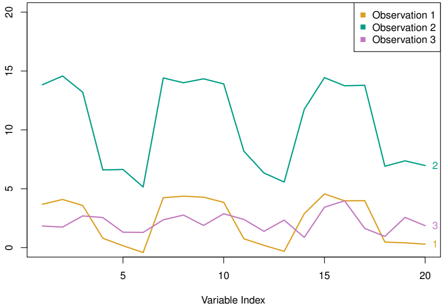
  Example: Suppose that we want to cluster customers at a store for market segmentation.

  - Samples are customers
  - Each variable corresponds to a specific product and measures the number of items bought by the customer during a year.



Correlation distance

- Euclidean distance would cluster all customers who purchase few things (orange and purple).
- Perhaps we want to cluster customers who purchase *similar* things (orange and teal).
- Then, the **correlation distance** may be a more appropriate measure of dissimilarity between samples.



Fact of correlation distance

Correlation is defined by

$$\rho(x_i, x_{i'}) = \frac{\sum_j (x_{ij} - \bar{x}_i)(x_{i'j} - \bar{x}_{i'})}{\sqrt{\sum_j (x_{ij} - \bar{x}_i)^2 \sum_j (x_{i'j} - \bar{x}_{i'})^2}},$$

where $\bar{x}_i$ = mean of obeservation i.

If observations are standardized:

$$x_{ij} \leftarrow \frac{x_{ij} - \bar{x}_i}{\sqrt{\sum_j (x_{ij} - \bar{x}_i)^2}},$$

then $2(1 - \rho(x_i, x_{i'})) = \sum_j (x_{ij} - x_{i'j}))^2$.