Data Science and Advanced Programming — Lecture 9

Unsupervised Machine Learning

Simon Scheidegger
Department of Economics, University of Lausanne, Switzerland

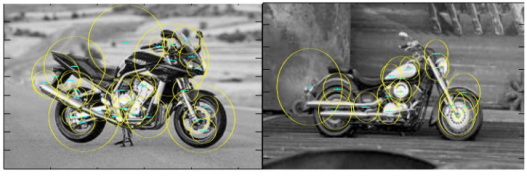
November 10th, 2025 | 12:30 - 16:00 | Internef 263

Today's Roadmap

1. k-Means
2. Evaluating Clusterings (read at home - here for completeness)
3. Gaussian Mixture Models
4. Principle Component Analysis (PCA)
5. Expectation Maximization (read at home - here for completeness)
6. Hierarchical Clustering
7. Density-based Clustering (cont'd)

Learning Parameters of Probability Distributions

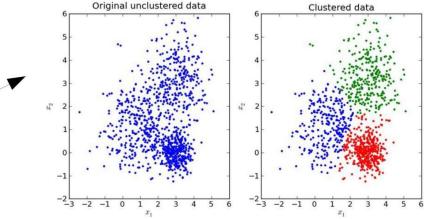
- In many settings not all variables are observed (labeled) in the training data $\boldsymbol{x}_i = (\boldsymbol{x}_i, \boldsymbol{h}_i)$
- e.g. Speech recognition: have speech signals, but not phoneme labels.
- e.g. **object recognition**: have object labels (car, bike), but **not part labels** (wheel, door, seat).
- Unobserved variables are called **LATENT VARIABLES**.



Recall — Unsupervised Learning

Learning "what normally happens".

- No output.
- Clustering: Grouping similar instances.
- Example applications:
  - Customer segmentation.
  - Image compression: Color quantization.
  - Bioinformatics: Learning motifs.

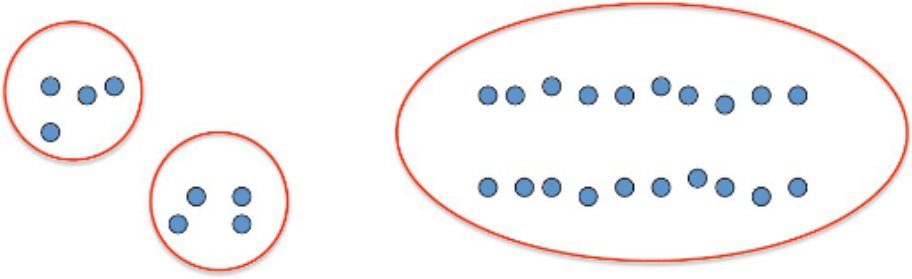


Motivation — Clustering

- Clustering, as a kind of **unsupervised learning**, aims at grouping data points into clusters.
- **Intuition**: Data points within
  - the same cluster should be close to each other
  - different clusters should be far apart from each other
- **Applications:**
  - segmentation of customers (e.g., for marketing campaigns)
  - organization/exploration of data (e.g., search results)
  - detection of outliers data points

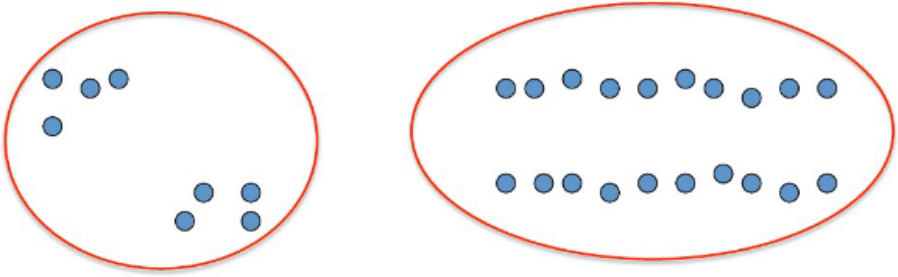
Clustering: Basic idea

- Basic idea: group together similar instances
- Example: 2D point patterns



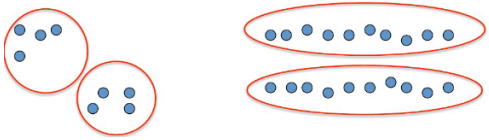
Clustering: Basic idea

- Basic idea: group together similar instances
- Example: 2D point patterns



Clustering: Basic idea

- Basic idea: group together similar instances
- Example: 2D point patterns

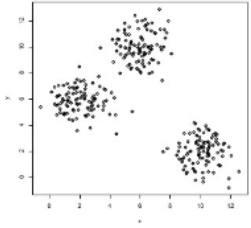


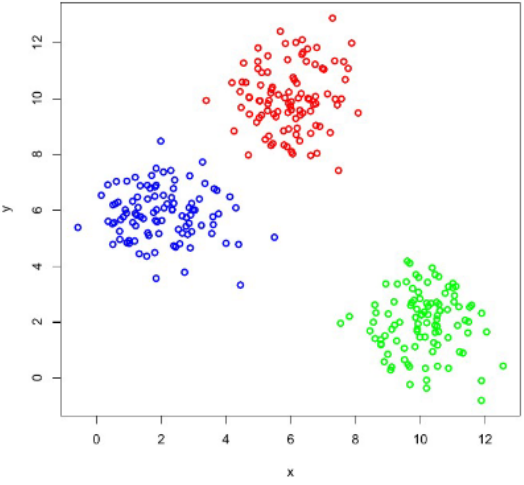
- **What could similar mean?**
- One option: small Euclidean distance (squared)

$$\text{dist}(\vec{x}, \vec{y}) = \|\vec{x} - \vec{y}\|_2^2$$

- **Clustering results are crucially dependent on the measure of similarity (or distance) between "points" to be clustered**

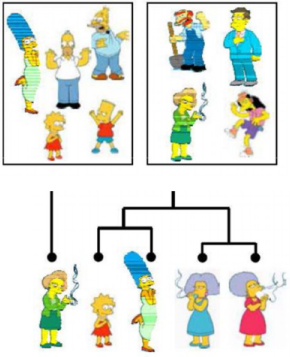
Clustering: Basic idea in color





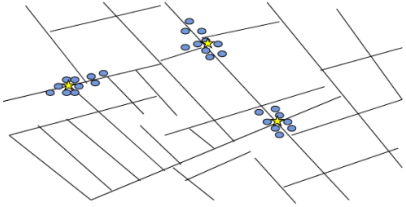
Clustering Algorithms

- Partition algorithms (Flat)
  - K-Means
  - Mixture of Gaussians
  - ...
- Hierarchical algorithms
  - Bottom-up - agglomerative
  - Top down - divisive



First (?) Application of Clustering

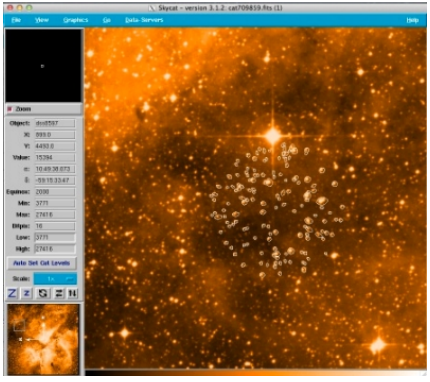
- John Snow, a London physician plotted the location of **cholera deaths** on a map during an outbreak in the 1850s.
- The locations indicated that cases were **clustered around certain intersections where there were polluted wells** — thus exposing both the problem and the solution.



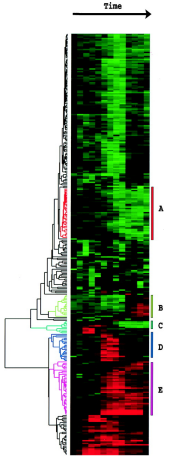
From: Nina Mishra HP Labs

Clustering Example: Astronomy

SkyCat (http://www.eso.org/sci/observing/tools/skycat.html): Clustered 2×10^9 sky objects into stars, galaxies, quasars, etc. based on radiation emitted in different spectrum bands



Another Clustering Example: Genetics

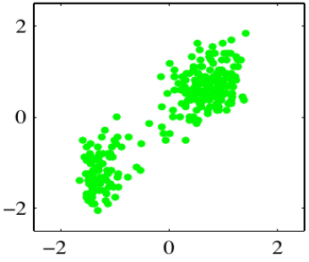


Eisen et al, PNAS 1998

1. k-Means – Unsupervised ML

Bishop, Chapter 9

- We will start with an unsupervised learning (clustering) problem:
- Given a dataset $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ each $\boldsymbol{x}_i \in \mathbb{R}^D$ partition the dataset into **K clusters** (e.g. healthy / sick patients).
- Intuitively, a cluster is a group of points, which are close together and far from others.



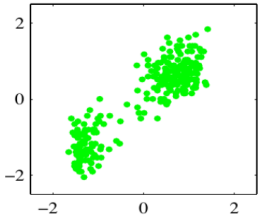
Distortion Measure

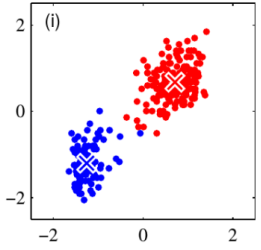
- Formally, introduce prototypes (or cluster centers) $\boldsymbol{\mu}_k \in \mathbb{R}^D$
- Use binary $r_{nk}, 1$ if point n is in cluster $k, 0$ otherwise (1-of- K coding scheme again)
- Find $\{\mu_k\}, \{r_{nk}\}$ to **minimize distortion measure**:

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|^2$$

e.g. two clusters $k = 1, 2$:

$$J = \sum_{x_n \in C_1} \|\boldsymbol{x}_n - \mu_1\|^2 + \sum_{x_n \in C_2} \|\boldsymbol{x}_n - \mu_2\|^2$$





Minimizing Distortion Measure

- Minimizing J directly is hard

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|^2$$

- However, two things are easy
  - If we know μ_k, minimizing J wrt r_{nk}
  - If we know r_{nk}, minimizing J wrt μ_k
- This suggests an **iterative procedure**
  - Start with initial guess for μ_k
  - Iteration of two steps:
    - Minimize J wrt r_{nk}
    - Minimize J wrt μ_k
  - Rinse and repeat until convergence

Determining Membership Variables

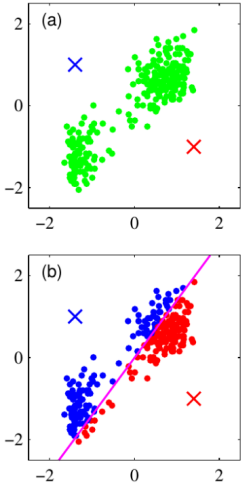
- Step 1 in an iteration of K-means is to minimize distortion measure J wrt. cluster membership variables r_{nk}

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|^2$$

- Terms for different data points x_n are independent, for each data point set r_{nk} to minimize

$$\sum_{k=1}^{K} r_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|^2$$

- Simply set $r_{nk} = 1$ for the cluster center μ_k with smallest distance.



Determining Cluster Centers

- Step 2: fix r_{nk}, minimize J wrt the cluster centers μ_k

$$J = \sum_{k=1}^{K} \sum_{n=1}^{N} r_{nk} \|\boldsymbol{x}_n - \boldsymbol{\mu}_k\|^2 \quad \text{switch order of sums}$$

- So we can minimize wrt each μ_k separately
- Take derivative, set to zero:

$$2 \sum_{n=1}^{N} r_{nk} (\boldsymbol{x}_n - \boldsymbol{\mu}_k) = 0$$
$$\Leftrightarrow \boldsymbol{\mu}_k = \frac{\sum_n r_{nk} \boldsymbol{x}_n}{\sum_n r_{nk}}$$

i.e. mean of datapoints x_n assigned to cluster k ($\rightarrow$ "k-Means")

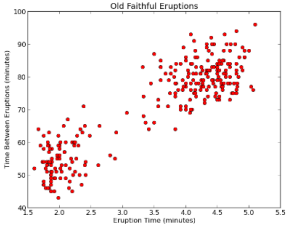
k-Means Algorithm

- Start with an initial guess for μ_k
- Iteration of two steps:
  1. Minimize J wrt $\mathrm{r_{nk}}$
     - Assign points to nearest cluster center
  2. Minimize J wrt μ_{k}
     - Set cluster center as average of points in cluster
- Rinse and repeat until convergence

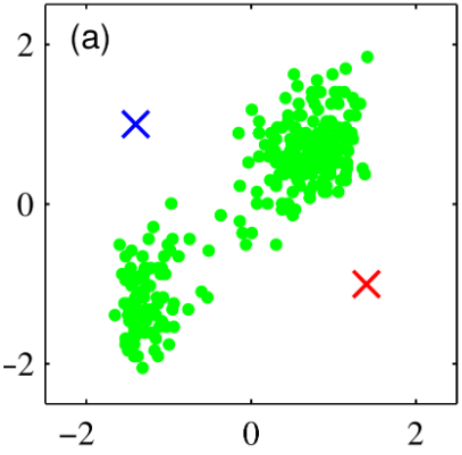
Old Faithful Dataset

https://www.stat.cmu.edu/~larry/all-of-statistics/=data/faithful.dat

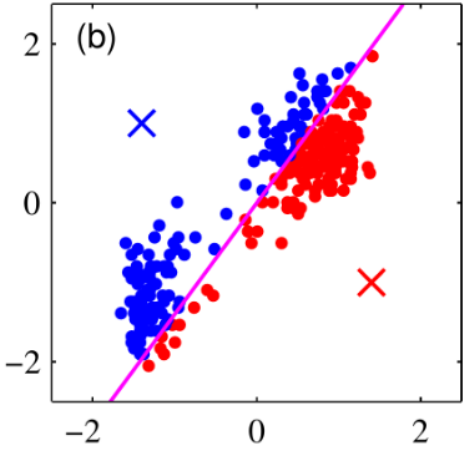
```
Description: (From R manual):

     Waiting time between eruptions and the duration of the eruption
     for the Old Faithful geyser in Yellowstone National Park, Wyoming,
     USA.

     A data frame with 272 observations on 2 variables.

eruptions  numeric  Eruption time in mins
waiting    numeric  Waiting time to next eruption
```



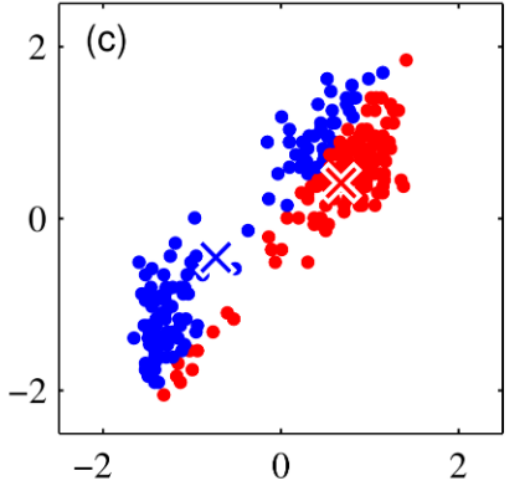
k-means example



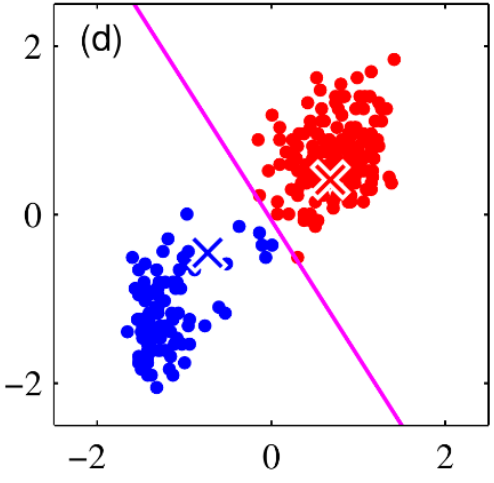
k-means example



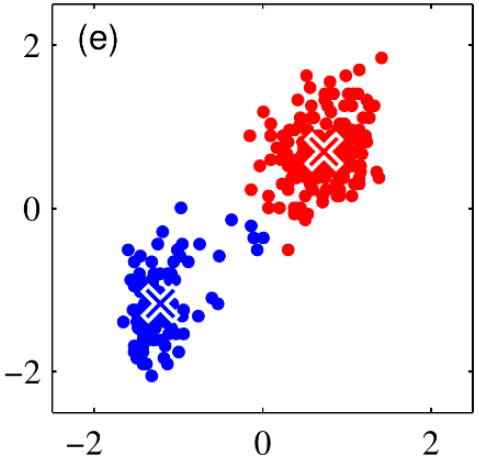
k-means example



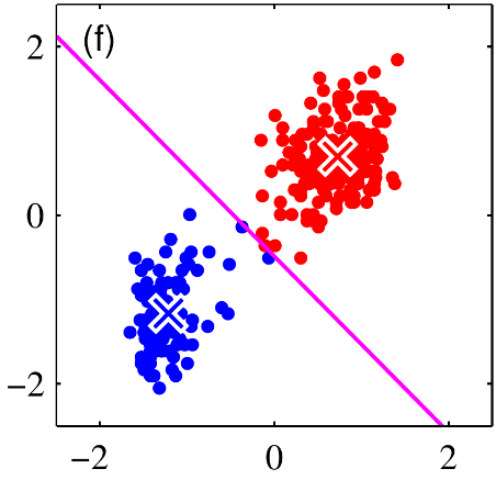
k-means example



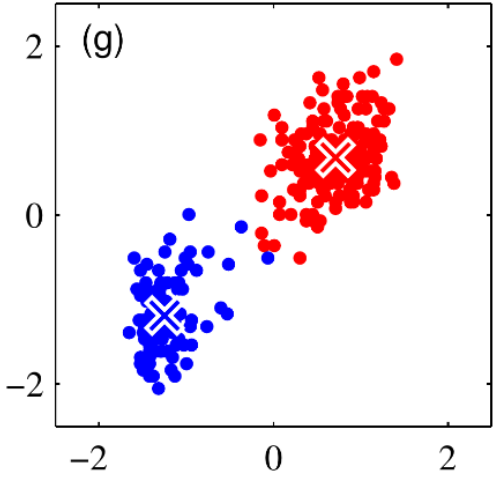
k-means example



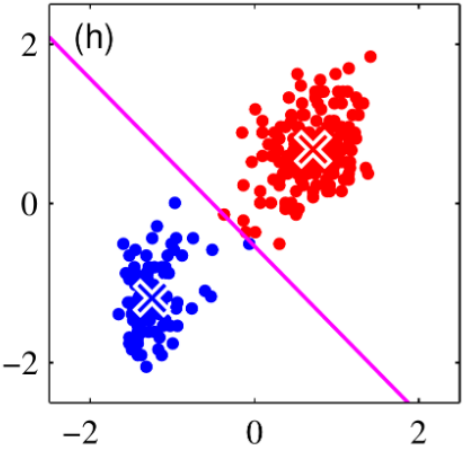
k-means example



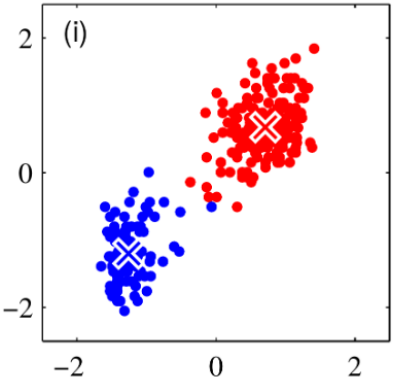
k-means example



k-means example

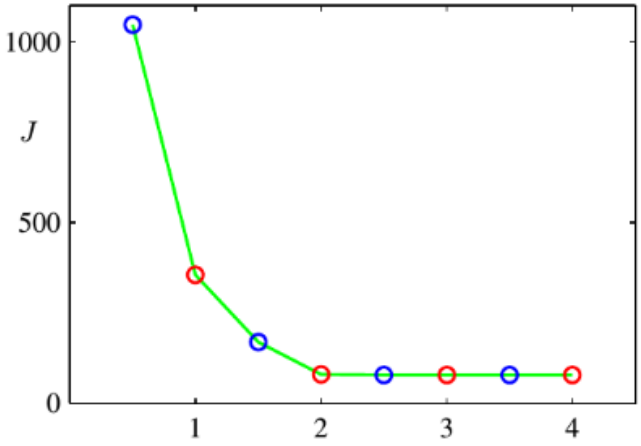


k-means example



Next step doesn't change membership — stop

Cost function J



k-means Convergence

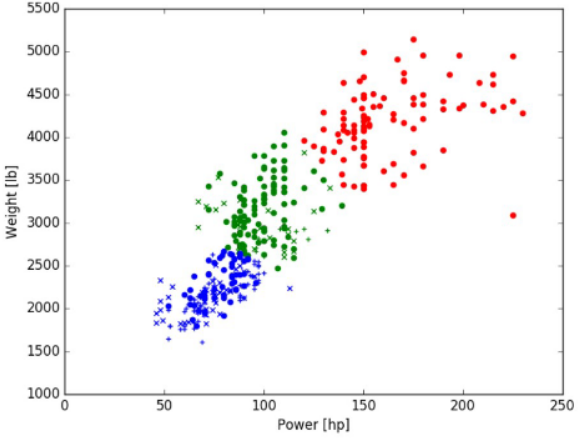
- **Repeat steps until no change in cluster assignments.**
- For each step, value of J either goes down, or we stop.
- Finite number of possible assignments of data points to clusters, so we are guaranteed to converge eventually.
- Note it may be a local maximum rather than a global maximum to which we converge.

Clustering Cars based on Power and Weight

demo/k_means_car.py

```
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler
from sklearn.cluster import KMeans
import matplotlib.pyplot as plt
# load data
cars = pd.read_csv('auto-mpg.data.txt',header=None, sep='\s+')
# extract power and weight as data matrix X
X = cars.iloc[:, [3,4]].values
# extract origin as target value y
y = cars.iloc[:, 7].values
# normalize data
min_max_scaler = MinMaxScaler()
min_max_scaler.fit(X) # determine min and max
X_normalized = min_max_scaler.transform(X)
# apply k-Means
km = KMeans(n_clusters=3, random_state=0).fit(X_normalized)
# plot cars
# U.S. : o / Europe: x / Japan : +
m = ['o' if o==1 else 'x' if o==2 else '+' for o in y]
# Cluster 1 : red / Cluster 2 : blue / Cluster 3 : green
c = ['red' if l==0 else 'blue' if l==1 else 'green' for l in km.labels_]
for i in range(0,len(X)):
    plt.scatter(X[i,0], X[i,1], color=c[i], marker=m[i])
plt.xlabel('Power [hp]')
plt.ylabel('Weight [lb]')
plt.show()
```

Clustering Cars based on Power and Weight: Plot



2. Evaluating Clustering: Some Notation

Read at home — here for completeness

- Consider a **set of data points** $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ $\quad \mathbf{x}_i \in \mathbb{R}^m$
- Objective: Determine clustering (also: grouping, partitioning)

$$\mathcal{C} = \{C_1, \ldots, C_k\} \quad \text{with} \quad C_i \subseteq \mathcal{D}$$

such that

- clusters are disjoint $\forall i \neq j : C_i \cap C_j = \emptyset$
- each data point is assigned to a cluster

$$\bigcup_{C_i \in \mathcal{C}} C_i = \mathcal{D}$$

Evaluating Clustering

- **How can we evaluate the quality of a clustering computed?**
- **External measures** assume that ideal clustering is known (e.g., class labels assigned to data points)

$$\mathcal{I} = \left\{I_1, \ldots, I_{|\mathcal{I}|}\right\} \quad \text{with} \quad I_i \subseteq \mathcal{D}$$

- **Internal measures** assume no knowledge of ideal clustering (i.e., we only know the data points and the clustering)

Purity

- Purity of a cluster is the fraction of data points therein that belongs to the dominant cluster from the ideal clustering

$$\text{purity}\,(C_i) = \frac{1}{|C_i|} \max_{I_j \in \mathcal{I}} |C_i \cap I_j|$$

- Purity of a clustering is then the weighted average of the purity values of its clusters

$$\text{purity}(\mathcal{C}) = \sum_{C_i \in \mathcal{C}} \frac{|C_i|}{n} \text{purity}\,(C_i)$$

Purity

C_1

C_2

C_3

$\text{purity}(C_1) = \frac{2}{3}$ $\text{purity}(C_2) = \frac{2}{4}$ $\text{purity}(C_3) = \frac{1}{2}$

$$\text{purity}(\mathcal{C}) = \frac{3}{9} \cdot \frac{2}{3} + \frac{4}{9} \cdot \frac{2}{4} + \frac{2}{9} \cdot \frac{1}{2} \approx 0.56$$

BetaCV

- **BetaCV**, as an internal measure, considers the ratio of average distances between pairs of points within the same or different clusters

$$\text{BetaCV}(\mathcal{C}) = \frac{W_{\text{in}} \,/ N_{\text{in}}}{W_{\text{out}} \,/ N_{\text{out}}}$$

- with N_{in} and N_{out} as pairs of data points within the same or within different clusters

$$N_{\text{in}} = \frac{1}{2} \sum_{C_i \in \mathcal{C}} |C_i| \left(|C_i| - 1\right) \quad N_{\text{out}} = \frac{1}{2} \sum_{C_i, C_j \in \mathcal{C}, C_i \neq C_j} |C_i| \, |C_j|$$

BetaCV

- **BetaCV**, as an internal measure, considers the ratio of average distances between pairs of points within the same or different clusters

$$\text{BetaCV}(\mathcal{C}) = \frac{W_{\text{in}} / N_{\text{in}}}{W_{\text{out}} / N_{\text{out}}}$$

- and W_{in} and W_{out} as the total distance of pairs of data points within the same or within different clusters

$$W_{\text{in}} = \frac{1}{2} \sum_{C_i \in \mathcal{C}} \sum_{\mathbf{x},\mathbf{y} \in C_i} d(\mathbf{x},\mathbf{y}) \quad W_{\text{out}} = \frac{1}{2} \sum_{C_i, C_j \in \mathcal{C}} \sum_{\mathbf{x} \in C_i} \sum_{\mathbf{y} \in C_j} d(\mathbf{x},\mathbf{y})$$

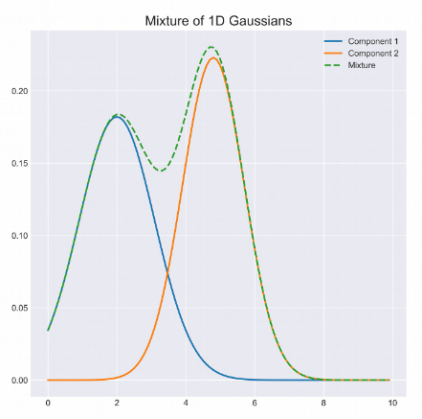
Dunn Index

- Dunn Index, as another **internal measure**, compares the minimal distance between any pair of data points from different clusters against the maximal distance between any pair of data points from the same cluster.

$$\text{DunnIndex}(\mathcal{C}) = \frac{\min\limits_{\mathbf{x}\in C_i, \mathbf{y}\in C_j, C_i \neq C_j} d(\mathbf{x}, \mathbf{y})}{\max\limits_{\mathbf{x}\in C_i, \mathbf{y}\in C_i} d(\mathbf{x}, \mathbf{y})}$$

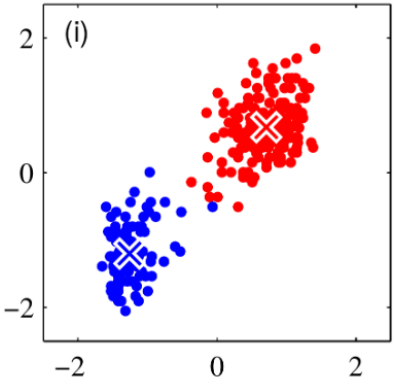
3. Gaussian Mixture Models

See Bishop (2006), Chapter 9; Murphy (2012), Chapter 11

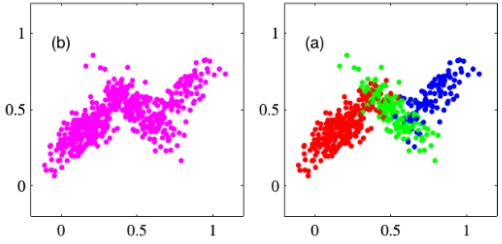


Hard Assignment versus Soft Assignment

- In the K-means algorithm, a hard assignment of points to clusters is made.
- However, for points near the decision boundary, this may not be such a good idea.
- Instead, we could think about making a **soft assignment** of points to clusters.



Gaussian Mixture Models

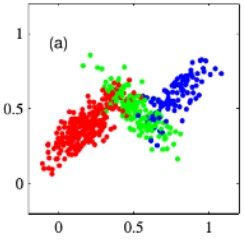


- The Gaussian mixture model (**or Mixture of Gaussians MoG**) models the data as a combination of Gaussians.
- Above shows a dataset generated by drawing samples from three different Gaussians.

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\mathbf{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right). \quad p\left(z_k = 1\right) = \pi_k$$

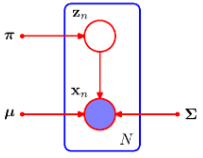
A Generative Model

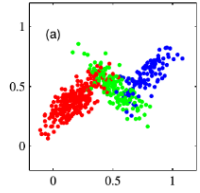
- The mixture of Gaussians is a generative model.
- To generate a data point x_n, we first generate a value for a - discrete variable $\mathrm{z_n} \in \{1, \ldots, \mathrm{K}\}$
- We then generate a value $\boldsymbol{x_n} \sim \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ for the corresponding Gaussian



A Graphical Model

- Note z_n is a latent variable, unobserved.
- Need to give conditional distributions $p(z_n)$ and $p(x_n \mid z_n)$
- The one-of-K representation is helpful here: $\mathrm{z_{nK}} \in \{0, 1\}$, $z_n = (z_{n1}, \ldots, z_{nK})$

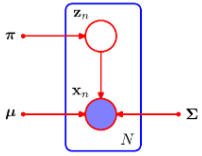


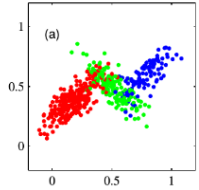


Graphical Model — Latent Component Variable

- Use a Bernoulli distribution for $p(z_n)$
  - i.e. $p(z_{nk} = 1) = \pi_k$
  - Parameters to this distribution $\{\pi_K\}$
- Must have $0 \leq \pi_k \leq 1$ and $\sum_{k=1}^{K} \pi_k = 1$
- $p(\boldsymbol{z}_n) = \prod_{k=1}^{K} \pi_k^{z_{nk}}$

Graphical Model – Observed Variable



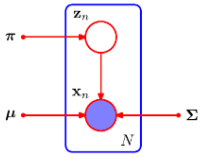


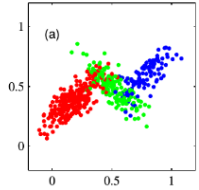
- Use a Gaussian distribution for $\mathrm{p}\left(\mathrm{x}_n \mid \mathrm{z}_n\right)$
- Parameters to this distribution $\{\mu_k, \Sigma_k\}$

$$p\left(\boldsymbol{x}_n \mid z_{nk}=1\right)=\mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)$$

$$p\left(\boldsymbol{x}_n \mid \boldsymbol{z}_n\right)=\prod_{k=1}^{K} \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)^{z_{nk}}$$

A Graphical Model – Joint Distribution





- The full **joint distribution** is given by:

$$p(\boldsymbol{x}, \boldsymbol{z}) = \prod_{n=1}^{N} p(\boldsymbol{z}_n)\, p(\boldsymbol{x}_n \mid \boldsymbol{z}_n)$$
$$= \prod_{n=1}^{N} \prod_{k=1}^{K} \pi_k^{z_{nk}} \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_{nk}}$$

Marginal over Observed (MoG) Variables

- The marginal distribution $p(x_n)$ for this model is:

$$p(\boldsymbol{x}_n) = \sum_{\boldsymbol{z}_n} p(\boldsymbol{x}_n, \boldsymbol{z}_n) = \sum_{z_n} p(\boldsymbol{z}_n)\, p(\boldsymbol{x}_n \mid \boldsymbol{z}_n)$$
$$= \sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

- A mixture of Gaussians

MoG Conditional over Latent Variable

- The conditional $p(z_{nk} = 1 \mid x_n)$ will play an important role for learning
- It is denoted by $\gamma(z_{nk})$ can be computed as:

$$\begin{aligned}\gamma(z_{nk}) \equiv p(z_{nk} = 1 \mid \boldsymbol{x}_n) &= \frac{p(z_{nk} = 1)\, p(\boldsymbol{x}_n \mid z_{nk} = 1)}{\sum_{j=1}^{K} p(z_{nj} = 1)\, p(\boldsymbol{x}_n \mid z_{nj} = 1)} \\ &= \frac{\pi_k \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}\end{aligned}$$

- $\gamma(z_{nk})$ is the responsibility of component k for datapoint n

MoG Learning

- Given a set of observations $\{x_1, \ldots, x_N\}$, without the latent
- variables z_n, how can we learn the parameters?
- Model parameters are $\theta = \{\pi_k, \mu_k, \Sigma_k\}$
- **Answer will be similar to k-means:**
  - If we know the latent variables z_n, fitting the Gaussians is easy
  - If we know the Gaussians μ_k, Σ_k, finding the latent variables is easy
- Rather than latent variables, we will use responsibilities $\gamma(z_{nk})$

MoG Maximum Likelihood Learning

- Given a set of observations $\{x_1, \ldots, x_N\}$, without the latent variables z_n, how can we learn the parameters?
- Model parameters are $\theta = \{\pi_k, \mu_k, \Sigma_k\}$
- We can use the maximum likelihood criterion:

$$\begin{aligned}\boldsymbol{\theta}_{ML} &= \arg\max_{\boldsymbol{\theta}} \prod_{n=1}^{N} \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right) \\ &= \arg\max_{\boldsymbol{\theta}} \sum_{n=1}^{N} \log \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right) \right\}\end{aligned}$$

- Unfortunately, closed-form solution not possible this time - log of sum rather than log of product

MoG Maximum Likelihood Learning - Problem

- Maximum likelihood criterion, 1-D:

$$\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} \sum_{n=1}^{N} \log \left\{ \sum_{k=1}^{K} \pi_k \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{ -\left(x_n - \mu_k\right)^2 / \left(2\sigma^2\right) \right\} \right.$$

- Suppose we set $\mu_k = x_n$ for some k and n, then we have one term in the sum:

$$\begin{aligned} & \pi_k \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left\{ -\left(x_n - \mu_k\right)^2 / \left(2\sigma^2\right) \right\} \\ = & \pi_k \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left\{ -(0)^2 / \left(2\sigma^2\right) \right\} \end{aligned}$$

- In the limit as $\sigma_k \to 0$, this goes to ∞
- So ML solution is to set some $\mu_k = x_n$, and $\sigma_k = 0$!

ML for Mixture of Gaussians

- Keeping this problem in mind, we will develop an algorithm for ML estimation of the parameters for a MoG model
- Search for a local optimum.
- Consider the log-likelihood function

$$\ell(\boldsymbol{\theta}) = \sum_{n=1}^{N} \log \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right) \right\}$$

- We can try taking derivatives and setting to zero, even though no closed form solution exists.

Maximizing Log-Likelihood - Means

$$\ell(\boldsymbol{\theta}) = \sum_{n=1}^{N} \log \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right) \right\}$$

$$\frac{\partial}{\partial \mu_k} \ell(\boldsymbol{\theta}) = \sum_{n=1}^{N} \frac{\pi_k \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right)}{\sum_j \pi_j \mathcal{N}\left(\boldsymbol{x}_n \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j\right)} \boldsymbol{\Sigma}_k^{-1}\left(\boldsymbol{x}_n - \boldsymbol{\mu}_k\right)$$

$$= \sum_{n=1}^{N} \gamma\left(z_{nk}\right) \boldsymbol{\Sigma}_k^{-1}\left(\boldsymbol{x}_n - \boldsymbol{\mu}_k\right)$$

- Setting derivative to 0 , and multiply by Σ_k

$$\sum_{n=1}^{N} \gamma\left(z_{nk}\right) \boldsymbol{\mu}_k = \sum_{n=1}^{N} \gamma\left(z_{nk}\right) \boldsymbol{x}_n$$

$$\Leftrightarrow \boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma\left(z_{nk}\right) \boldsymbol{x}_n \text{ where } N_k = \sum_{n=1}^{N} \gamma\left(z_{nk}\right)$$

Maximizing Log-Likelihood: Means and Covariances

- Note that the mean μ_k is a weighted combination of points x_n, using the responsibilities $\mathrm{y}\left(\mathrm{z_{nk}}\right)$ for the cluster k

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma\left(z_{nk}\right) \boldsymbol{x}_n$$

- $N_k = \sum_{n=1}^{N} \gamma\left(z_{nk}\right)$ is the effective number of points in the cluster
- A similar result comes from taking derivatives wrt. the covariance matrices Σ_k :

$$\boldsymbol{\Sigma}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma\left(z_{nk}\right) \left(\boldsymbol{x}_n - \boldsymbol{\mu}_k\right) \left(\boldsymbol{x}_n - \boldsymbol{\mu}_k\right)^T$$

Maximizing Log-Likelihood: Mixing Coefficients

- We can also maximize wrt. the mixing coefficients π_k
- Note there is a constraint that $\sum_k \pi_k = 1$
- Use Lagrange multipliers
- End up with: $\pi_k = \frac{N_k}{N}$ average responsibility that component k takes.

Three Parameter Types and Three Equations

- These three equations a solution does not make

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma\left(z_{nk}\right) \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma\left(z_{nk}\right) \left(\boldsymbol{x}_n - \boldsymbol{\mu}_k\right) \left(\boldsymbol{x}_n - \boldsymbol{\mu}_k\right)^T$$

$$\pi_k = \frac{N_k}{N}$$

- **All depend on $\gamma(z_{nk})$, which depends on all 3 !**
- **But an iterative scheme can be used**

EM for Mixtures of Gaussians

- Initialize parameters, then iterate:
  - **E step**: Calculate responsibilities using current parameters

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\boldsymbol{x}_n \mid \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}$$

  - **M step**: Re-estimate parameters using these $y(z_{nk})$

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \boldsymbol{x}_n$$

$$\boldsymbol{\Sigma}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) (\boldsymbol{x}_n - \boldsymbol{\mu}_k)(\boldsymbol{x}_n - \boldsymbol{\mu}_k)^T$$

$$\pi_k = \frac{N_k}{N}$$

  - This algorithm is known as the expectation-maximization algorithm (EM)
    - Next we describe its general form, why it works, and why it's called EM (but first an example)

The Likelihood

- The form of the Gaussian mixture distribution is governed by the parameters $\boldsymbol{\pi}, \boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$, where we have used the notation $\boldsymbol{\pi} \equiv \{\pi_1, \ldots, \pi_k\}, \boldsymbol{\mu} \equiv \{\mu_1, \ldots, \mu_k\}, \boldsymbol{\Sigma} \equiv \{\Sigma_1, \ldots \Sigma_k\}$.
- One way to set the values of these parameters is to use **maximum likelihood.**
- The log of the likelihood function is given by

$$\ln p(\mathbf{X} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right) \right\}$$

where $X = \{x_1, \ldots, x_N\}$.

Problems with optimizing the likelihood

- The situation is now much more complex than with a single Gaussian, due to the presence of the summation over k inside the logarithm.
- As a result,the maximum likelihood solution for the parameters no longer has a closed-form analytical solution.
- One approach to maximizing the likelihood function is to use iterative numerical optimization techniques.
- Gradient methods could be used but are painful to implement. $\Longrightarrow$ Non-convex optimization problem! (multiple optima possible)

Example in one dimension

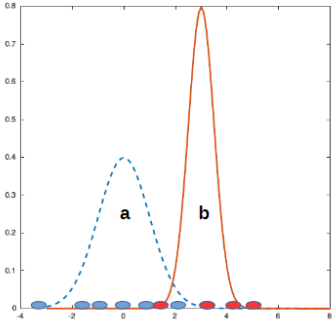
- Observations $x_1 \dots x_n$
- $K = 2$ Gaussians with unknown μ, σ^2
- Estimation trivial if we know the source of each observation

$$\mu_b = \frac{x_1 + x_2 + \dots + x_{n_b}}{n_b}$$
$$\sigma_b^2 = \frac{(x_1 - \mu_1)^2 + \dots + (x_n - \mu_n)^2}{n_b}$$

Example in one dimension

- Observations $x_1 \dots x_n$
- $K = 2$ Gaussians with unknown μ, σ^2
- Estimation trivial if we know the source of each observation

$$\mu_b = \frac{x_1 + x_2 + \dots + x_{n_b}}{n_b}$$
$$\sigma_b^2 = \frac{(x_1 - \mu_1)^2 + \dots + (x_n - \mu_n)^2}{n_b}$$



Example: Expectation Maximization in 1d (II)

- What if we don't know the source?
- If we knew parameters of the Gaussians (μ, σ^2)

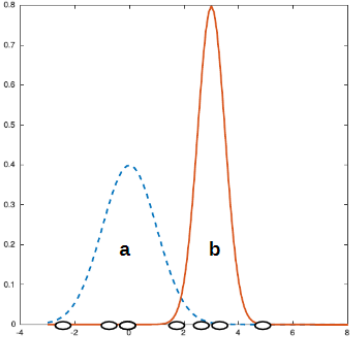
Example: Expectation Maximization in 1d (II)

- What if we don't know the source?
- If we knew parameters of the Gaussians (μ, σ^2)

$\rightarrow$ can guess whether point is more likely to be *a* or *b*.

$$P(b \mid x_i) = \frac{P(x_i \mid b)\, P(b)}{P(x_i \mid b)\, P(b) + P(x_i \mid a)\, P(a)}$$

$$P(x_i \mid b) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left(-\frac{(x_i - \mu_b)^2}{2\sigma_b^2}\right)$$



EM Algorithm (in 1d)

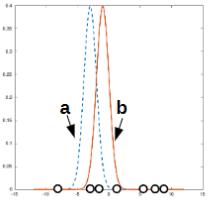
A fundamental problem:

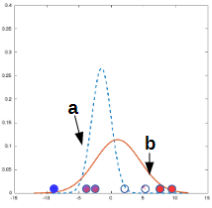
- we need (μ_a, σ_a^2) and (μ_b, σ_b^2) to guess the source of the points.
- we need to know the source to estimate (μ_a, σ_a^2) and (μ_b, σ_b^2).

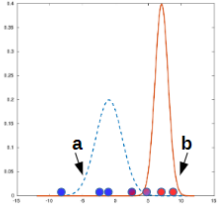
EM algorithm:

1. **Start** with two randomly placed Gaussians $(\mu_a, {\sigma_a}^2)$ and $(\mu_b, {\sigma_b}^2)$.
2. **E(xpectation) step:**
   - for each point: $P(b \mid x_i) =$ does it look like it came from b ?
3. **M(aximization)-step:**
   - adjust (μ_a, σ_a^2) and (μ_b, σ_b^2) to fit points assigned to them.
4. **Iterate until convergence.**

EM in 1d







$$P(x_i \mid b) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left(-\frac{(x_i - \mu_b)^2}{2\sigma_b^2}\right)$$

$$b_i = P(b \mid x_i) = \frac{P(x_i \mid b)\, P(b)}{P(x_i \mid b)\, P(b) + P(x_i \mid a)\, P(a)}$$

$$a_i = P(a \mid x_i) = 1 - b_i$$

$$\mu_b = \frac{b_1 x_1 + b_2 x_2 + \ldots + b_n x_{n_h}}{b_1 + b_2 + \ldots + b_n}$$

$$\sigma_b^2 = \frac{b_1 (x_1 - \mu_1)^2 + \ldots + b_n (x_n - \mu_n)^2}{b_1 + b_2 + \ldots + b_n}$$

$$\mu_a = \frac{a_1 x_1 + a_2 x_2 + \ldots + a_n x_{n_n}}{a_1 + a_2 + \ldots + a_n}$$

$$\sigma_a^2 = \frac{a_1 (x_1 - \mu_1)^2 + \ldots + a_n (x_n - \mu_n)^2}{a_1 + a_2 + \ldots + a_n}$$

→ We could also estimate priors:

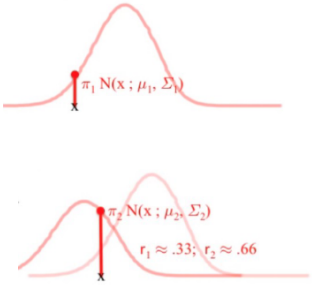
$$P(b) = (b_1 + b_2 + \ldots b_n)/n$$
$$P(a) = 1 - P(b)$$

EM in the multidimensional case

- Start with parameters describing each cluster
- Mean μ_c, Covariance Σ_c, "size" π_c
- **E-step ("Expectation"):**
  - For **each observation/point** x_i
  - Compute "r_{ic}", the probability that it belongs to cluster c.
    - Compute its probability under model c.
    - Normalize to sum to one (over clusters c).

$$r_{ic} = \frac{\pi_c \mathcal{N}(x_i; \mu_c, \Sigma_c)}{\sum_{c'} \pi_{c'} \mathcal{N}(x_i; \mu_{c'}, \Sigma_{c'})}$$

  - If x_i is very likely under the c-th Gaussian, it gets high weight.
  - Denominator just makes r's sum to one.



EM in the multidimensional case

- **M-step ("Maximization step"):**
  - For each cluster (Gaussian) $z = c$
  - Update its parameters using the (weighted) data points

$$N_c = \sum_i r_{ic}$$ Total responsibility allocated to cluster c

$$\pi_c = \frac{N_c}{N}$$ Fraction of total assigned to cluster c

$$\underbrace{\mu_c = \frac{1}{N_c} \sum_i r_{ic} x_i}_{\text{Weighted mean of assigned data}} \qquad \underbrace{\Sigma_c = \frac{1}{N_c} \sum_i r_{ic} (x_i - \mu_c)^T (x_i - \mu_c)}_{\text{weighted covariance of assigned data (use new weighted means here)}}$$

Expectation-Maximization: Summary

- Likelihood of the data

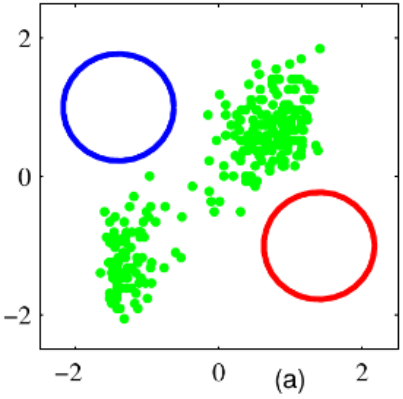
$$P(x_1, \ldots, x_N) = \Pi_{i=1}^{N} \sum_{k=1}^{K} P(x_i \mid k)\, P(k)$$

- Each step increases the log-likelihood of our model

$$\ln p(\mathbf{X} \mid \boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

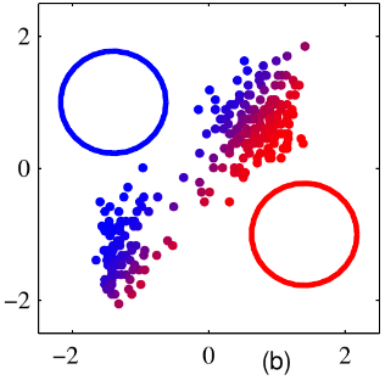
- Iterate until convergence
  - Convergence guaranteed — another ascent method.
- Cannot discover k.

MoG EM — Example



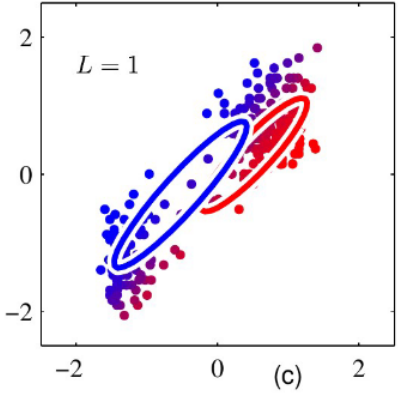
- Same initialization as with K-means before
- Often, K-means is actually used to initialize EM

MoG EM — Example



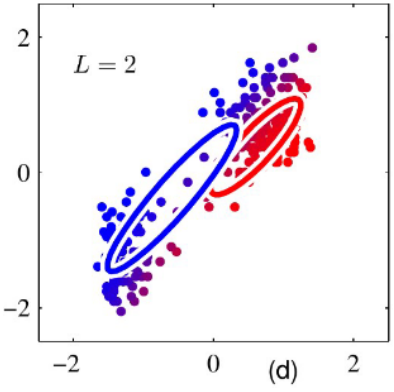
Calculate responsibilities $\gamma(z_{nk})$

MoG EM — Example



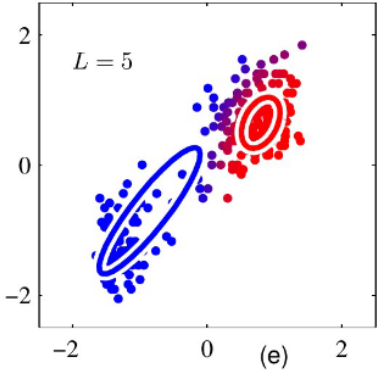
Calculate model parameters $\{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}$ using these responsibilities

MoG EM — Example



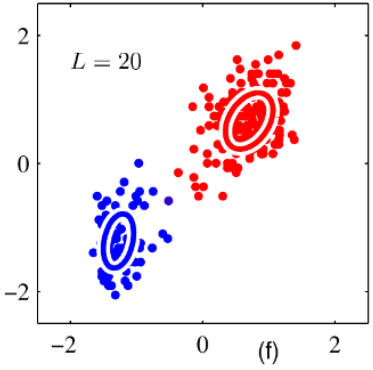
Iteration 2

MoG EM — Example



Iteration 5

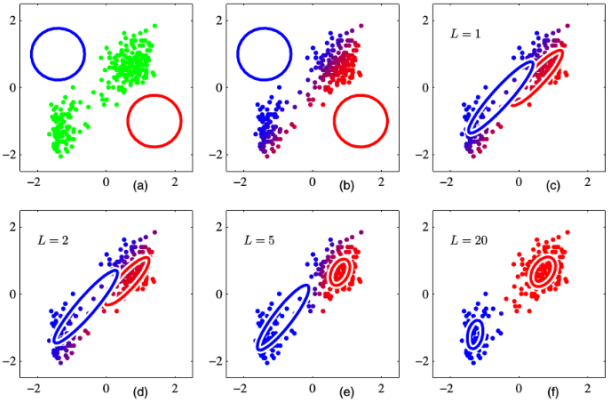
MoG EM — Example



Interation 20 — converged

Gaussian mixture models:d>1

See Bishop (2006) for details



Bayesian Information Criterion (BIC)

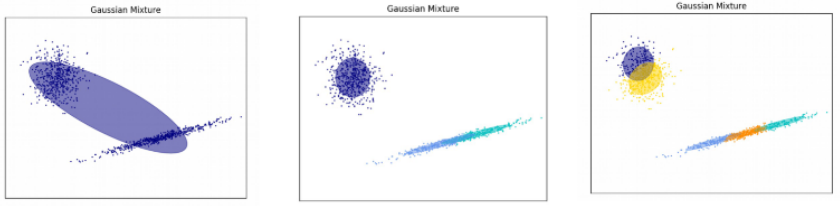
- How to pick k?
- Probabilistic model:
  $\mathrm{L} = \ln p(\mathbf{X} \mid \pi, \mu, \Sigma) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}\left(\mathbf{x}_n \mid \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\right) \right\}$
  - Tries to "fit" the data (maximize likelihood)
- Choose K that makes L as large as possible?
  - $\mathrm{K} = \mathrm{n}$: each data point has its own "source"
  - may not work well for new data points
- Split points into training set **T** and validation set **V**
  - for each k : fit parameters of **T**
  - measure likelihood of V
  - sometimes still best when $\mathrm{k} = \mathrm{n}$
- "Occam's razor":
  - Pick the "simplest" of all models that fits the data.
  - Assess, e.g., via Bayes Information Criterion (BIC): $\max_p\{L - 1/2p * \log(n)\}$
  - L: Likelihood; p: # Parameters in the model - how simple is the model.

Hands-on example

https://scikit-learn.org/stable/modules/mixture.html

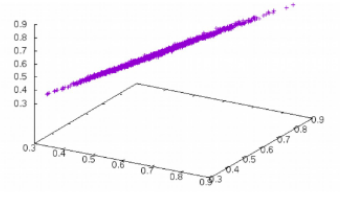
demo/GMM_scikit_example.py

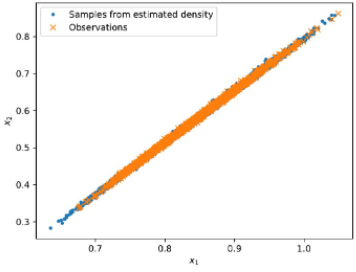
- Plot the confidence ellipsoids of a mixture of two Gaussians obtained with Expectation Maximization (GaussianMixture class)
- The model has access to 1,3 , and 5 components with which to fit the data. Note that the Expectation Maximization model will necessarily use ALL components
- In the 5-component example, we can see that the Expectation Maximization model splits some components arbitrarily, because it is trying to fit too many components.



Hands-on example 2

- We simulate a bunch of data (e.g., an ergodic set). — it is in a text file (ergodic_data.txt - 3 dimensions)
- We apply GMM (build_density.py)
- We can sample data from the fitted GMM model (sample.py)





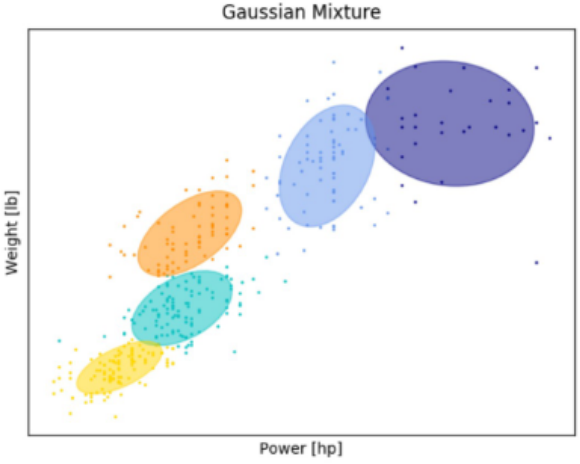
GMM — Cars based on Power and Weight

```
import itertools
import numpy as np
from scipy import linalg
import matplotlib.pyplot as plt
import matplotlib as mpl
from sklearn import mixture
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler
import matplotlib.pyplot as plt

color_iter = itertools.cycle(['navy', 'c', 'cornflowerblue', 'gold','darkorange'])

# load data
cars = pd.read_csv('auto-mpg.data.txt',header=None, sep='\s+')
# extract power and weight as data matrix X
X = cars.iloc[:, [3,4]].values
# extract origin as target value y
y = cars.iloc[:, 7].values

# normalize data
min_max_scaler = MinMaxScaler()
min_max_scaler.fit(X) # determine min and max
X_normalized = min_max_scaler.transform(X)
## Fit a Gaussian mixture with EM using five components
gmm = mixture.GaussianMixture(n_components=5, covariance_type='full').fit(X_normalized)
plot_results(X_normalized, gmm.predict(X_normalized), gmm.means_, gmm.covariances_, 0,
             'Gaussian Mixture')
plt.show()
```

Cont.

```
def plot_results(X, Y_, means, covariances, index, title):
splot = plt.subplot(1, 1, 1 + index)
for i, (mean, covar, color) in enumerate(zip(
        means, covariances, color_iter)):
    v, w = linalg.eigh(covar)
    v = 2. * np.sqrt(2.) * np.sqrt(v)
    u = w[0] / linalg.norm(w[0])
    # as the DP will not use every component it has access to
    # unless it needs it, we shouldn't plot the redundant
    # components.
    if not np.any(Y_ == i):
        continue
    plt.scatter(X[Y_ == i, 0], X[Y_ == i, 1], .8, color=color)

    # Plot an ellipse to show the Gaussian component
    angle = np.arctan(u[1] / u[0])
    angle = 180. * angle / np.pi  # convert to degrees
    ell = mpl.patches.Ellipse(mean, v[0], v[1], 180. + angle, color=color)
    ell.set_clip_box(splot.bbox)
    ell.set_alpha(0.5)
    splot.add_artist(ell)

plt.xticks(())
plt.yticks(())
plt.xlabel('Power [hp]')
plt.ylabel('Weight [lb]')
plt.title(title)
```

GMM — Cars based on Power and Weight



4. Expectation Maximization: A General Version of EM

- In general, we are interested in maximizing the likelihood

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

  where $\mathbf{X}$ denotes all observed variables, and $\mathbf{Z}$ denotes all latent (hidden, unobserved) variables
- Assume that maximizing $p(X \mid \boldsymbol{\theta})$ is difficult (e.g. mixture of Gaussians)
- But maximizing $p(X, Z \mid \theta)$ is tractable (everything observed)
  - $p(X, Z \mid \theta)$ is referred to as the complete-data likelihood function, which we don't have

A Lower Bound

- The strategy for optimization will be to introduce a lower bound on the likelihood
  - This lower bound will be based on the complete-data likelihood, which is easy to optimize
- Iteratively increase this lower bound
- Make sure we're increasing the likelihood while doing so

A Decomposition Trick

- To obtain the lower bound, we use a decomposition:

$$\ln p(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta}) = \ln p(\boldsymbol{X} \mid \boldsymbol{\theta}) + \ln p(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}) \text{ product rule}$$

$$\ln p(\boldsymbol{X} \mid \boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + KL(q \| p)$$

$$\mathcal{L}(q, \boldsymbol{\theta}) \equiv \sum_{\boldsymbol{Z}} q(\boldsymbol{Z}) \ln \left\{ \frac{p(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta})}{q(\boldsymbol{Z})} \right\}$$

$$KL(q \| p) \equiv -\sum_{\boldsymbol{Z}} q(\boldsymbol{Z}) \ln \left\{ \frac{p(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta})}{q(\boldsymbol{Z})} \right\}$$

- $\mathrm{KL}(q \| \mathrm{l})$ is known as the Kullback-Leibler divergence (KL-divergence), and is ≥ 0 (next slide) $\longrightarrow$ Hence $\ln p(\boldsymbol{X} \mid \boldsymbol{\theta}) \geq \mathcal{L}(q, \boldsymbol{\theta})$

TODO colors

Kullback-Leibler Divergence

- $KL(p(x)\|q(x))$ is a measure of the difference between distributions $p(x)$ and $q(x)$:

$$KL(p(x)\|q(x)) = -\sum_x p(x) \log \frac{q(x)}{p(x)}$$

- Motivation: average additional amount of information required to encode x using code assuming distribution $q(x)$ when x actually comes from $p(x)$
- Note it is not symmetric: $KL(q(x)\|p(x)) \neq KL(p(x)\|q(x))$ in general
- It is non-negative:
  - Jensen's inequality: $\quad -\ln\left(\sum_x x p(x)\right) \leq -\sum_x p(x) \ln x$
  - Apply to KL:

$$KL(p\|q) = -\sum_x p(x) \log \frac{q(x)}{p(x)} \geq -\ln\left(\sum_x \frac{q(x)}{p(x)} p(x)\right) = -\ln \sum_x q(x) = 0$$

Increasing the Lower Bound — E-step

- EM is an iterative optimization technique which tries to maximize this lower bound: $\ln p(\boldsymbol{X} \mid \boldsymbol{\theta}) \geq \mathcal{L}(q, \boldsymbol{\theta})$

E step: Fix $\boldsymbol{\theta}^{old}$, maximize $\mathcal{L}(q, \boldsymbol{\theta}^{old})$ wrt q

i.e. Choose distribution q to maximize $\mathcal{L}$

Reordering bound:

$$\mathcal{L}(q, \boldsymbol{\theta}^{old}) = \ln p(\boldsymbol{X}|\boldsymbol{\theta}^{old}) - KL(q||p)$$

$\ln p(\boldsymbol{X}|\boldsymbol{\theta}^{old})$ does not depend on q

Maximum is obtained when $KL(q||p)$ is as small as possible

Occurs when $q = p$, i.e. $q(\boldsymbol{Z}) = p(\boldsymbol{Z}|\boldsymbol{X}, \boldsymbol{\theta})$

This is the posterior over $\boldsymbol{Z}$, recall these are the responsibilities from MoG model

Increasing the Lower Bound — M-step

M step: Fix q, maximize $\mathcal{L}(q, \boldsymbol{\theta})$ wrt $\boldsymbol{\theta}$
The maximization problem is on

$$\begin{aligned} \mathcal{L}(q, \boldsymbol{\theta}) &= \sum_{\boldsymbol{Z}} q(\boldsymbol{Z}) \ln p(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta}) - \sum_{\boldsymbol{Z}} q(\boldsymbol{Z}) \ln q(\boldsymbol{Z}) \\ &= \sum_{\boldsymbol{Z}} p\left(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}^{\text{old}}\right) \ln p(\boldsymbol{X}, \boldsymbol{Z} \mid \boldsymbol{\theta}) - \sum_{\boldsymbol{Z}} p\left(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}^{\text{old}}\right) \ln p\left(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}^{\text{old}}\right) \end{aligned}$$

Second term is constant with respect to $\boldsymbol{\theta}$
First term is ln of complete data likelihood, which is assumed easy to optimize
Expected complete log likelihood - what we think complete data likelihood will be

Why does EM work?

- In the M-step we changed from θ^{old} to θ^{new}
- This increased the lower bound L, unless we were at a maximum (so we would have stopped)
- This must have caused the log likelihood to increase
- The E-step set q to make the KL-divergence 0:

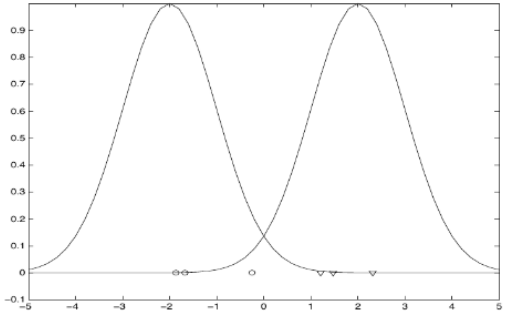
$$\ln p\left(\boldsymbol{X} \mid \boldsymbol{\theta}^{\text{old}}\right) = \mathcal{L}\left(q, \boldsymbol{\theta}^{\text{old}}\right) + KL(q\|p) = \mathcal{L}\left(q, \boldsymbol{\theta}^{\text{old}}\right)$$

- Since the lower bound L increased when we moved from θ^{old} to θ^{new}

$$\begin{aligned}\ln p\left(\boldsymbol{X} \mid \boldsymbol{\theta}^{\text{old}}\right) = \mathcal{L}\left(q, \boldsymbol{\theta}^{\text{old}}\right) &< \mathcal{L}\left(q, \boldsymbol{\theta}^{\text{new}}\right) \\ &= \ln p\left(\boldsymbol{X} \mid \boldsymbol{\theta}^{\text{new}}\right) - KL\left(q\|p^{\text{new}}\right)\end{aligned}$$

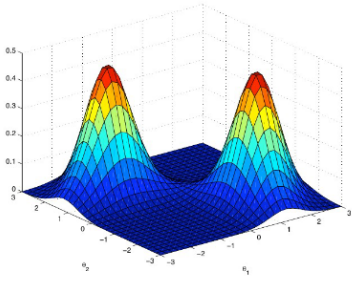
- So the log-likelihood has increased going from θ^{old} to θ^{new}

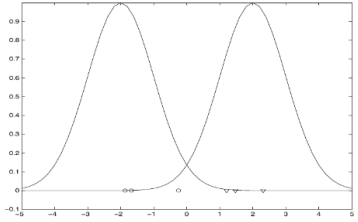
Bounding Example



Consider 2 component 1-D MoG with known variances.

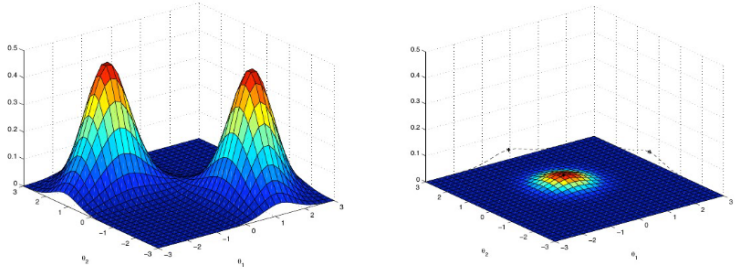
Bounding Example





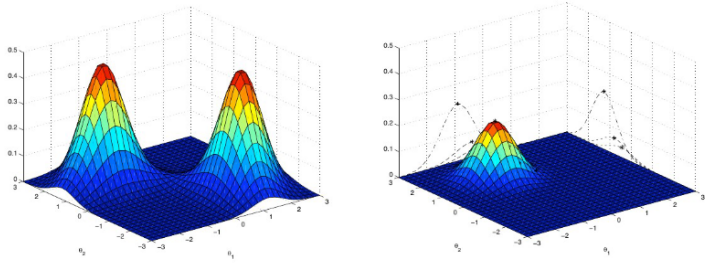
True likelihood function
Recall we're fitting means θ_1, θ_2

Bounding Peaks



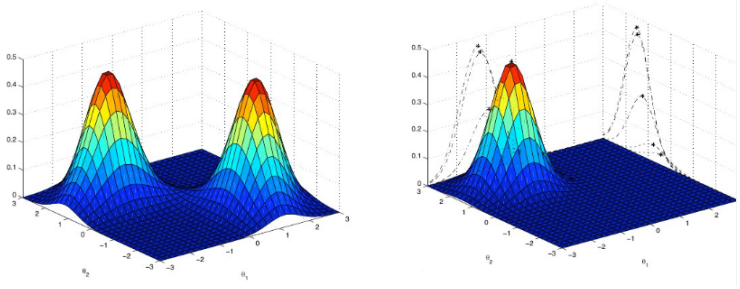
- Lower bound the likelihood function using averaging distribution $q(Z)$
  - $\ln p(\boldsymbol{X} \mid \boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + KL(q(\boldsymbol{Z}) \| p(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}))$
  - Since $q(\boldsymbol{Z}) = p\left(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}^{\text{old}}\right)$, bound is tight (equal to actual likelihood) at $\boldsymbol{\theta} = \boldsymbol{\theta}^{\text{old}}$

Bounding Peaks



- Lower bound the likelihood function using averaging distribution $q(Z)$
  - $\ln p(\boldsymbol{X} \mid \boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + KL(q(\boldsymbol{Z}) \| p(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}))$
  - Since $q(\boldsymbol{Z}) = p\left(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}^{\text{old}}\right)$, bound is tight (equal to actual likelihood) at $\boldsymbol{\theta} = \boldsymbol{\theta}^{\text{old}}$

Bounding Peaks



- Lower bound the likelihood function using averaging distribution $q(Z)$
  - $\ln p(\boldsymbol{X} \mid \boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + KL(q(\boldsymbol{Z}) \| p(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}))$
  - Since $q(\boldsymbol{Z}) = p\left(\boldsymbol{Z} \mid \boldsymbol{X}, \boldsymbol{\theta}^{\text{old}}\right)$, bound is tight (equal to actual likelihood) at $\boldsymbol{\theta} = \boldsymbol{\theta}^{\text{old}}$

Recall About the EM Algorithm

Some good things about EM:

- no learning rate (step-size) parameter.
- automatically enforces parameter constraints.
- very fast for low dimensions.
- each iteration guaranteed to improve likelihood.

Some bad things about EM:

- can get stuck in local minima.
- can be slower than conjugate gradient (especially near convergence).
- requires expensive inference step.
- is a maximum likelihood/MAP (maximum a posterior) method.

EM — Summary

- EM finds local maximum to likelihood

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

- Iterates two steps:
  - E step "fills" in the missing variables Z (calculates their distribution)
  - M step maximizes expected complete log likelihood (expectation wrt E step distribution)
- This works because these two steps are performing a coordinatewise hill-climbing on a lower bound on the likelihood $p(\boldsymbol{X} \mid \boldsymbol{\theta})$

5. Hierarchical Clustering

- k-Means determines a flat clustering of data points; there is no relationship between the clusters
- Hierarchical clustering determines a sequence of increasingly fine-grained clusterings

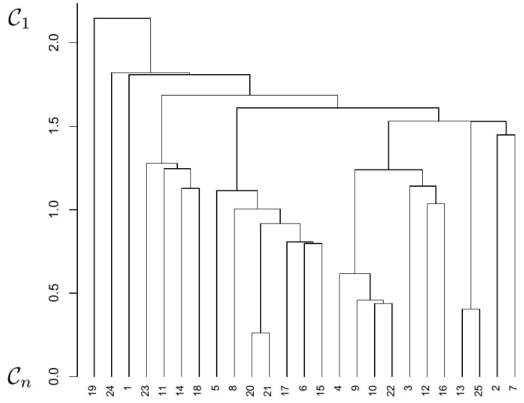
$$\mathcal{C}_1, \ldots, \mathcal{C}_n$$

- $\mathcal{C}_1 = \{\mathcal{D}\}$ contains all data points in a single cluster
- $\mathcal{C}_n = \{\{\mathbf{x}_i\} : \mathbf{x}_i \in \mathcal{D}\}$ contains one cluster per data point
- Clustering $\mathrm{C_i}$ is contained in clustering $\mathcal{C}_{i-1}$

$$\forall C_j \in \mathcal{C}_i : \exists C_l \in \mathcal{C}_{i-1} : C_j \subseteq C_l$$

Dendrogram

Sequence of clusterings can be visualized in a dendrogram



Hierarchical Agglomerative vs. Divisive Clustering

- Hierarchical Agglomerative Clustering (HAC)
  - starts with the most fine-grained clustering $\mathcal{C}_n$
  - proceeds bottom-up and merges the two closest clusters in $\mathcal{C}_i$ to obtain the more coarse-grained clustering $\mathcal{C}_{i-1}$
- Hierarchical Divisive Clustering (HDC)
  - starts with the most coarse-grained clustering $\mathcal{C}_1$
  - proceeds top-down and splits one of the clusters in $\mathcal{C}_{i-1}$ to obtain the more fine-grained clustering $\mathcal{C}_1$

Hierarchical Agglomerative vs. Divisive Clustering

- Hierarchical Agglomerative Clustering (HAC)
  - starts with the most fine-grained clustering $\mathcal{C}_n$
  - proceeds bottom-up and merges the two closest clusters in $\mathcal{C}_i$ to obtain the more coarse-grained clustering $\mathcal{C}_{i-1}$
- So far, we can only measure distance between data points, but we need a measure of distance between clusters

Linkage Criteria

Linkage criteria measure distance between two clusters based on the distance between data points therein

Single-Link

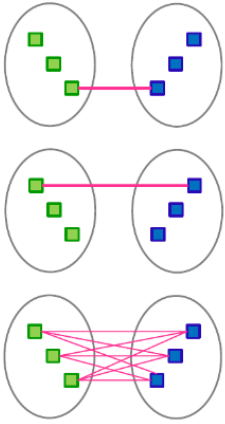
$$\delta(C_i, C_j) = \min\{d(\mathbf{x}, \mathbf{y}) \mid \mathbf{x} \in C_i, \mathbf{y} \in C_j\}$$

Complete-Link

$$\delta(C_i, C_j) = \max\{d(\mathbf{x}, \mathbf{y}) \mid \mathbf{x} \in C_i, \mathbf{y} \in C_j\}$$

Average-Link

$$\delta(C_i, C_j) = \frac{1}{|C_i|\,|C_j|} \sum_{\mathbf{x} \in C_i} \sum_{\mathbf{y} \in C_j} d(\mathbf{x}, \mathbf{y})$$



Pseudocode: Hierarchical Agglomerative Clustering

```
// Start with each data point in a separate cluster
C_n = {{x_i} : x_i ∈ D};

for(int t = n; t > 1; t--) {
  // Determine the two clusters closest to each other
  C_i^*, C_j^* = argmin_{C_i, C_j ∈ C_t : C_i ≠ C_j} δ(C_i, C_j);

  // Merge the two clusters
  C_{t-1} = (C_t \ {C_i^*, C_j^*}) ∪ {C_i^* ∪ C_j^*};
}
```

HAC Example

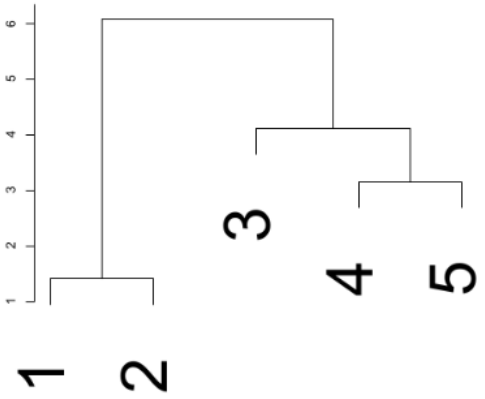
- Consider the following data points in $\mathbb{R}^2$

$$\begin{aligned} \mathbf{x_1} &= (1,0) \\ \mathbf{x_2} &= (2,1) \\ \mathbf{x_3} &= (8,0) \\ \mathbf{x_4} &= (12,1) \\ \mathbf{x_5} &= (15,1) \end{aligned} \qquad \mathbf{d} = \begin{bmatrix} 0.00 & 1.41 & 7.00 & 11.05 & 14.04 \\ & 0.00 & 6.08 & 10.00 & 13.04 \\ & & 0.00 & 4.12 & 7.07 \\ & & & 0.00 & 3.00 \\ & & & & 0.00 \end{bmatrix}$$

- With distance matrix d

HAC with Single-Link Example

HAC with single-link based on distance matrix d

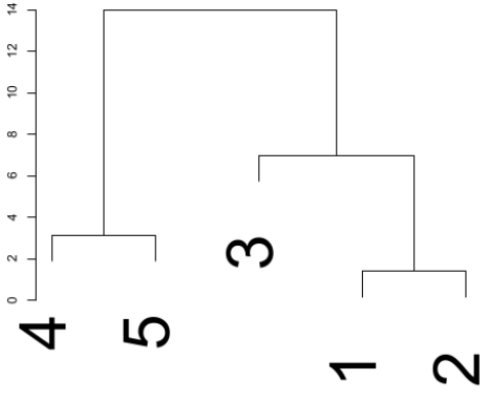


$$\mathcal{C}_1 = \{\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5\}\}$$
$$\mathcal{C}_2 = \{\{\mathbf{x}_1, \mathbf{x}_2\}, \{\mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5\}\}$$
$$\mathcal{C}_3 = \{\{\mathbf{x}_1, \mathbf{x}_2\}, \{\mathbf{x}_3\}, \{\mathbf{x}_4, \mathbf{x}_5\}\}$$
$$\mathcal{C}_4 = \{\{\mathbf{x}_1, \mathbf{x}_2\}, \{\mathbf{x}_3\}, \{\mathbf{x}_4\}, \{\mathbf{x}_5\}\}$$
$$\mathcal{C}_5 = \{\{\mathbf{x}_1\}, \{\mathbf{x}_2\}, \{\mathbf{x}_3\}, \{\mathbf{x}_4\}, \{\mathbf{x}_5\}\}$$

$$\mathbf{d} = \begin{bmatrix} 0.00 & 1.41 & 7.00 & 11.05 & 14.04 \\ & 0.00 & 6.08 & 10.00 & 13.04 \\ & & 0.00 & 4.12 & 7.07 \\ & & & 0.00 & 3.00 \\ & & & & 0.00 \end{bmatrix}$$

HAC with Single-Link Example

HAC with complete-link based on distance matrix d



$$\mathcal{C}_1 = \{\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_5\}\}$$
$$\mathcal{C}_2 = \{\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}, \{\mathbf{x}_4, \mathbf{x}_5\}\}$$
$$\mathcal{C}_3 = \{\{\mathbf{x}_1, \mathbf{x}_2\}, \{\mathbf{x}_3\}, \{\mathbf{x}_4, \mathbf{x}_5\}\}$$
$$\mathcal{C}_4 = \{\{\mathbf{x}_1, \mathbf{x}_2\}, \{\mathbf{x}_3\}, \{\mathbf{x}_4\}, \{\mathbf{x}_5\}\}$$
$$\mathcal{C}_5 = \{\{\mathbf{x}_1\}, \{\mathbf{x}_2\}, \{\mathbf{x}_3\}, \{\mathbf{x}_4\}, \{\mathbf{x}_5\}\}$$

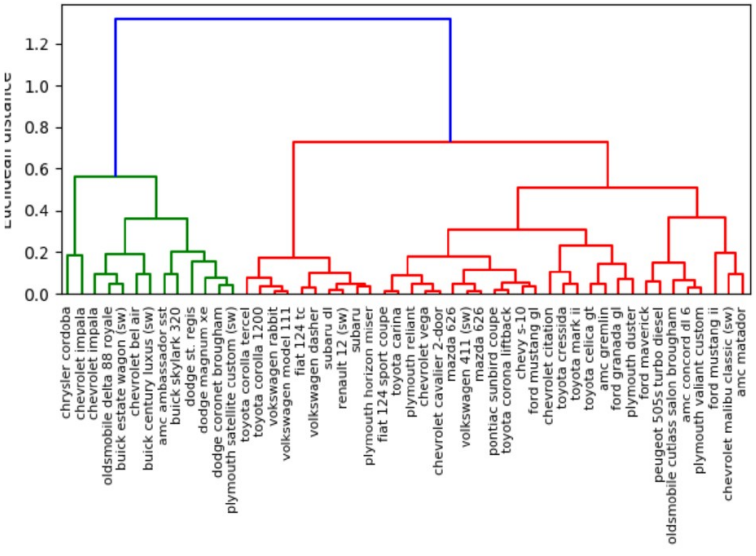
$$\mathbf{d} = \begin{bmatrix} 0.00 & 1.41 & 7.00 & 11.05 & 14.04 \\ & 0.00 & 6.08 & 10.00 & 13.04 \\ & & 0.00 & 4.12 & 7.07 \\ & & & 0.00 & 3.00 \\ & & & & 0.00 \end{bmatrix}$$

Clustering Cars based on Power and Weight

demo/HAC_example.py

```
import numpy as np
import pandas as pd
from sklearn.preprocessing import MinMaxScaler
from scipy.cluster.hierarchy import linkage
from scipy.cluster.hierarchy import dendrogram
import matplotlib.pyplot as plt

# load data
cars = pd.read_csv('auto-mpg.data.txt',header=None, sep='\s+')

# keep a sample of 50 cars
cars = cars.sample(50, random_state=0)
# extract labels
labels = cars.iloc[:,8].values
# extract power and weight as data matrix X
X = cars.iloc[:, [3,4]].values

# normalize data
min_max_scaler = MinMaxScaler()
min_max_scaler.fit(X) # determine min and max
X_normalized = min_max_scaler.transform(X)

# perform hierarchical agglomerative clustering using complete linkage
clusters = linkage(X_normalized, method='complete', metric='euclidean')

# plot dendrogram
dendrogram = dendrogram(clusters, labels=labels)
plt.tight_layout()
plt.ylabel('Euclidean distance')
plt.show()
```

Clustering Cars based on Power and Weight



6. Density-based Clustering

- k-Means as a representative-based clustering method can only find convey clusters and must assign every data point to a cluster.
- Density-based clustering methods determine clusters as regions having consistently high density and label isolated data points as noise
- Density-Based Spatial Clustering of Applications with Noise (DBSCAN)

Density-Based Clustering

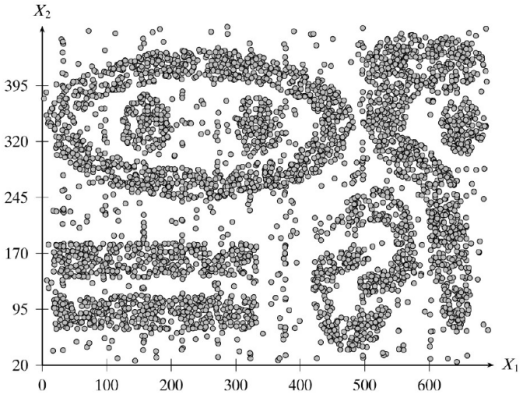


Fig. From Zaki and Meira (2014)

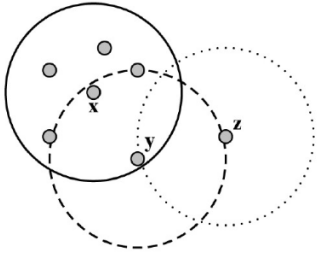
DBSCAN — the idea

- Epsilon Neighborhood of a data point x

$$N_\epsilon(\mathbf{x}) = \{\mathbf{y} \mid d(\mathbf{x}, \mathbf{y}) \leq \epsilon\}$$

  contains all points having distance less than or equal to ε
- Data point x is called a core to ε its epsilon neighborhood contains at least `minpts` data points (including x)
- Data point x is called a border point, if it is not a core, but belongs to the epsilon neighborhood of a core
- All other data points are considered noise

Core, Border, and Noise



$minpts = 6$

- Data point x is a core
- Data point y is a border point
- Data point z is noise

Reachability

- Data point x is directly reachable from data point y, if y is a core and x belongs to the epsilon neighborhood of y, i.e.

$$\mathbf{x} \in N_\epsilon(\mathbf{y})$$

- Data point x is (density) reachable from data point y,
- if there is a chain of data points $x_0, \ldots, x_1$, so that

$$x_0 = x \wedge x_l = y$$

  $\forall 1 \leq i \leq l$: x_i is directly reachable from x_{i-1}
- Reachability is not symmetric, since the data point y could be a core, but the data point x is not

Connectedness and Density-Based Clusters

- Two data points x and y are called connected, if there is a core z, so that both x and y are reachable from z
- Density-based cluster is a maximal subset of connected data points, i.e., there are no data points that could be added

DBSCAN

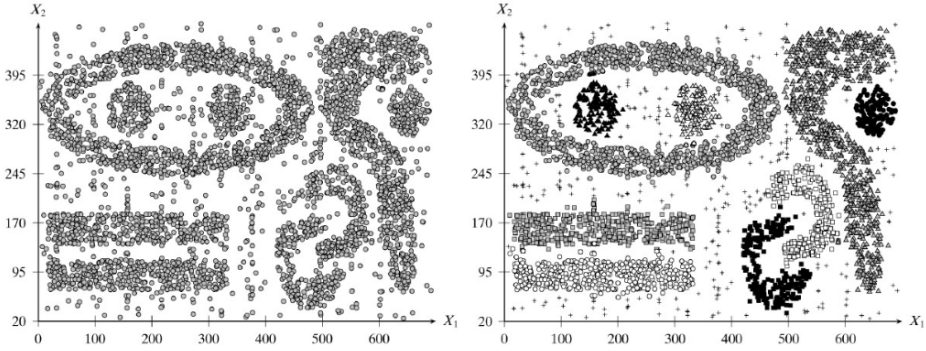
- Intuition:
  - Compute epsilon neighborhoods for all data points
  - Determine all cores
  - Determine noise
  - Grow a new density-based cluster from each data point that does not yet belong to an already-determined cluster
- Note that DBSCAN is not deterministic, since the assignment of data point to clusters depends on the order in which data points are considered

Pseudo-code DBSCAN

```
dbScan(D, ε, minpts) {
  // Cores
  Cores = ∅;

  for(x ∈ D) {
    // Compute epsilon neighborhoods
    N_ε(x) = computeNeighborhood(x, ε);

    // Initialize cluster id
    id(x) = ∅;

    // Check whether data point is a core
    if (N_ε(x) ≥ minpts) Cores = Cores ∪ {x};
  }

  // Grow density-based cluster from each core
  k = 0;
  for(x ∈ Cores) {
    if(id(x) == ∅) {
      k++;
      id(x) = k;
      densityConnected(x,k);
    }
  }

  // Determine clustering, border points, and noise
  C = ∅;
  for(i = 1...k) C = C ∪ {{x ∈ D : id(x) = k}};

  Noise = {x ∈ D : id(x) = ∅};
  Border = D \ {Cores ∪ Noise};
```

```
densityConnected(x, k) {
  for(y ∈ N_ε(x)) {
    id(y) = k;
    if (y ∈ Cores) densityConnected(y, k);
  }
}
```

DBSCAN in Action

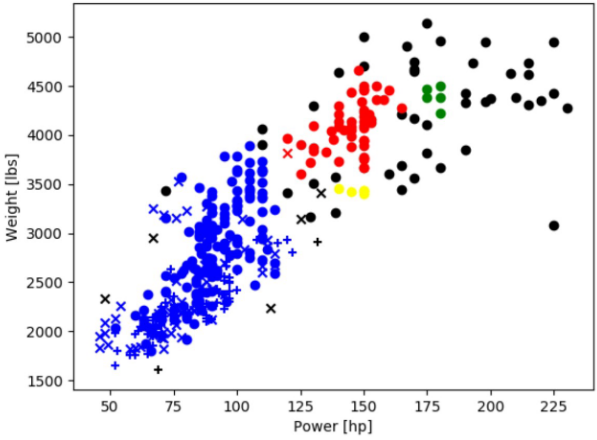


Clustering Cars based on Power and Weight

demo/DBSCAN_example.py

```
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler
from sklearn.cluster import DBSCAN
from matplotlib.backends.backend_pdf import PdfPages
import matplotlib.pyplot as plt
# load data
cars = pd.read_csv('auto-mpg.data.txt',header=None, sep='\s+')
# extract power and weight as data matrix X
X = cars.iloc[:, [3,4]].values
# extract origin as target value y
y = cars.iloc[:, 7].values
# normalize data
min_max_scaler = MinMaxScaler()
min_max_scaler.fit(X) # determine min and max
X_normalized = min_max_scaler.transform(X)
# DBSCAN
db = DBSCAN(eps=0.05,min_samples=5,metric='euclidean')
db.fit_predict(X_normalized)
# plot cars
# U.S. : o / Europe: x / Japan : +
m = ['o' if o==1 else 'x' if o==2 else '+' for o in y]
# Noise : black / Cluster 1 : red / Cluster 2 : blue /
# Cluster 3 : green / Cluster 4 : yellow
c = ['black' if l==-1 else 'red' if l==0 else 'blue' if l==1
else 'green' if l==2 else 'yellow' for l in db.labels_]
for i in range(0,len(X)):
    plt.scatter(X[i,0], X[i,1], color=c[i], marker=m[i])
plt.xlabel('Power [hp]')
plt.ylabel('Weight [lbs]')
plt.show()
```

Clustering Cars based on Power and Weight



Summary

- Hierarchical clustering determines a sequence of clusterings that can be visualized in a dendrogram
- DBSCAN as a density-based clustering method can find non-convex clusters and is able to label data points as noise
- DBSCAN comes with two hyper parameters ε and minpts that need to be carefully tuned based on the data