Data Mining
Cluster Analysis: Basic Concepts and Algorithms

Lecture Notes for Chapter 7

Introduction to Data Mining, 2nd Edition

by

Tan, Steinbach, Karpatne, Kumar

Bisecting K-means

Bisecting K-means

Variant of K-means that can produce a hierarchical clustering

Algorithm 8.2 Bisecting K-means algorithm.

repeat
    Initialize the list of clusters to contain the cluster consisting of all points.

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repeat
    Remove a cluster from the list of clusters.
    {Perform several "trial" bisections of the chosen cluster.}
    for $i = 1$ to *number of trials* **do**
        Bisect the selected cluster using basic K-means.
    end for
    Select the two clusters from the bisection with the lowest total SSE.
    Add these two clusters to the list of clusters.
until Until the list of clusters contains K clusters.

Bisecting K-Means

- The algorithm is exhaustive terminating at singleton clusters (unless K is known)

- Terminating at singleton clusters
  - Is time consuming
  - Singleton clusters are meaningless
  - Intermediate clusters are more likely to correspond to real classes

- No criterion for stopping bisections before singleton clusters are reached.

Combining Bisecting K-means and K-means

- The resulting clusters can be refined by using their centroids as **the initial centroids for the basic K-means.**

- Why is this necessary?
  – K-means algorithm is guaranteed to find a clustering that represents a local minimum wrt the SSE
  – Bisecting K-means uses the K- means algorithm **locally** to bisect individual clusters.
  – **The final set of clusters does not represent a clustering that is a local minimum wrt the total SSE**

X-Means

- **X-Means** clustering algorithm is an **extended K-Means** which tries to automatically **determine the number of clusters** based on BIC scores.

- As Bisecting K-means starts with only one cluster

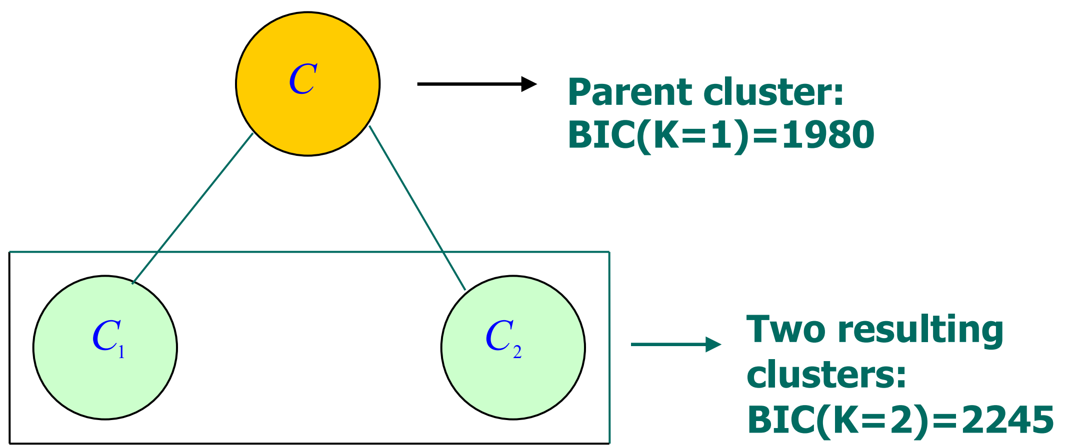
- The X-Means goes into action after each run of K-Means, **making local decisions** about which subset of the current centroids should split in order to better fit the data.

- The splitting decision is done by computing the **Bayesian Information Criterion** (BIC).

Bayesian Information Criterion (BIC)

- A strategy to stop the Bisecting algorithm when meaningful clusters are reached to avoid **over-splitting**
- Using BIC as splitting criterion of a cluster in order to decide whether a cluster should split or no
- BIC measures the improvement of the cluster structure between a cluster and its two children clusters.
- Compute the BIC score of:
  - A cluster
  - Two children clusters
- BIC approximates the probability that the M_j is describing the real clusters in the data

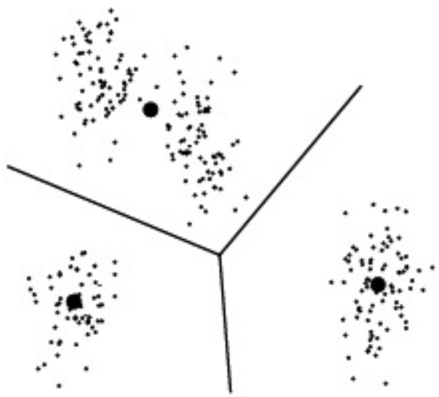
BIC based split



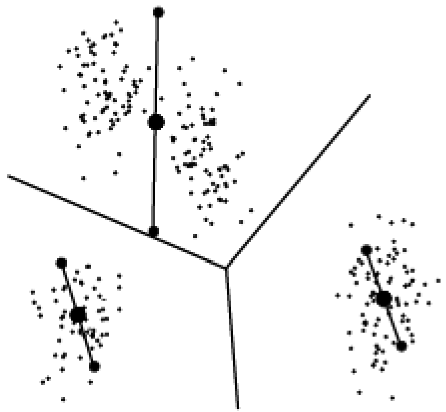
The BIC score of the parent cluster is less than BIC score of the generated cluster structure => we accept the bisection.

X-Means

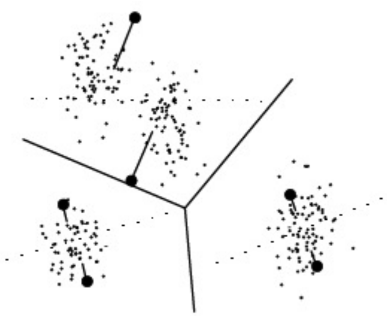
1. K-means with k=3



2. Split each centroid in 2 children moving a distance propotional to the region size in opposite direction (random)

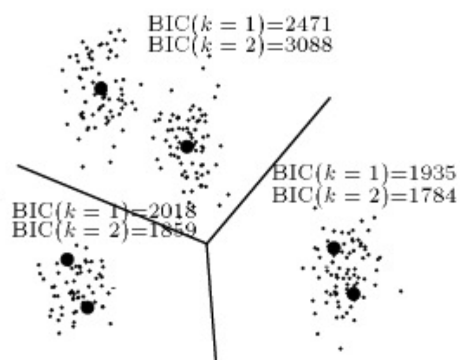


3. Run 2-means in each region locally



4. Compare BIC of parent and children

5. Only centroids with higher BIC survives



X-Means

- Forward search for the appropriate value of k in a given range $[r_1, r_{max}]$:
  - Recursively split each cluster and use BIC score to decide if we should keep each split

1. Run K-means with $k=r_1$
2. Improve structure
3. If $k > r_{max}$ Stop and return the best-scoring model

- Use local BIC score to decide on keeping a split
- Use global BIC score to decide which K to output at the end

Mixture Models and the EM Algorithm

Model-based clustering (probabilistic)

- In order to understand our data, we will assume that there is a generative process (a model) that creates/describes the data, and we will try to find the model that **best fits** the data.
  - Models of different complexity can be defined, but we will assume that our model is a distribution from which data points are sampled
  - **Example**: the data is the height of all people in **Greece**
- In most cases, a single distribution is not good enough to describe all data points: **different parts of the data follow a different distribution**
  - **Example**: the data is the height of all people in Greece and China
  - We need a mixture model
  - Different distributions correspond to different clusters in the data.

Algorithm 9.2 EM algorithm.

1: Select an initial set of model parameters.
   (As with K-means, this can be done randomly or in a variety of ways.)

2: **repeat**

3: **Expectation Step** For each object, calculate the probability that each object belongs to each distribution, i.e., calculate $prob(distribution\ j|\mathbf{x}_i, \Theta)$.

4: **Maximization Step** Given the probabilities from the expectation step, find the new estimates of the parameters that maximize the expected likelihood.

5: **until** The parameters do not change.
   (Alternatively, stop if the change in the parameters is below a specified threshold.)

EM (Expectation Maximization) Algorithm

- Initialize the values of the parameters in Θ to some random values
- Repeat until convergence
  - E-Step: Given the parameters Θ estimate the membership probabilities $P(G|x_i)$ and $P(C|x_i)$
  - M-Step: Compute the parameter values that (in expectation) maximize the data likelihood

E-Step: Assignment of points to clusters:
K-means: hard assignment,
EM: soft assignment

M-Step:
K-means: Computation of centroids
EM: Computation of the new model parameters

Gaussian Distribution

- Example: the data is the height of all people in Greece
  - Experience has shown that this data follows a Gaussian (Normal) distribution
  - Reminder: Normal distribution:

$$P(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

  - μ = mean, σ = standard deviation

Gaussian Model

- What is a model?
  - A Gaussian distribution is fully defined by the mean μ and the standard deviation σ
  - We define our model as the pair of parameters $\theta = (\mu, \sigma)$

- This is a general principle: a model is defined as a vector of parameters θ

Fitting the model

- We want to find the normal distribution that best fits our data
  - Find the best values for μ and σ
  - But what does best fit mean?

Maximum Likelihood Estimation (MLE)

- Suppose that we have a vector $X = (x_1, \dots, x_n)$ of values
- And we want to fit a Gaussian $N(\mu, \sigma)$ model to the data
- Probability of observing point x_i:

$$P(x_i) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- Probability of observing all points (assume independence)

$$P(X) = \prod_{i=1}^{n} P(x_i) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- We want to find the parameters $\theta = (\mu, \sigma)$ that maximize the probability $P(X|\theta)$

Maximum Likelihood Estimation (MLE)

- The probability $P(X|\theta)$ as a function of θ is called the Likelihood function

$$L(\theta) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- It is usually easier to work with the Log-Likelihood function

$$LL(\theta) = -\sum_{i=1}^{n} \frac{(x_i - \mu)^2}{2\sigma^2} - \frac{1}{2} n \log 2\pi - n \log \sigma$$

- Maximum Likelihood Estimation
  - Find parameters μ, σ that maximize $LL(\theta)$

$$\mu = \frac{1}{n}\sum_{i=1}^{n} x_i = \mu_X$$

Sample Mean

$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2 = \sigma_X^2$$

Sample Variance

MLE

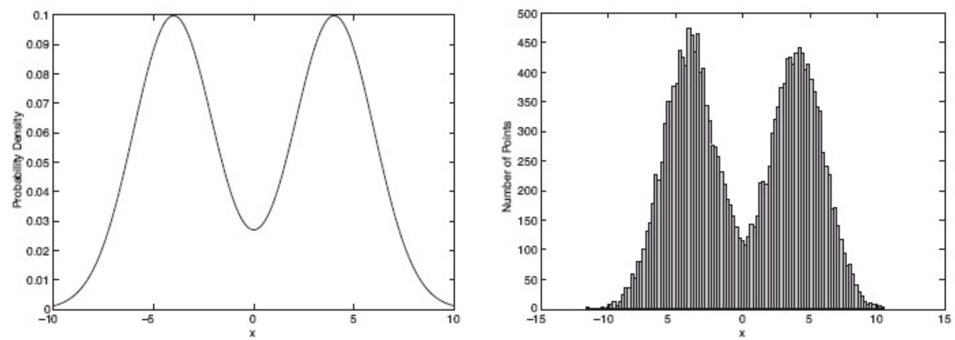
- Note: these are also the most likely parameters given the data

$$P(\theta|X) = \frac{P(X|\theta)P(\theta)}{P(X)}$$

- If we have no prior information about θ, or X, then maximizing $P(X|\theta)$ is the same as maximizing $P(\theta|X)$

Mixture of Gaussians

- Suppose that you have the heights of people from Greece and China and the distribution looks like the figure below



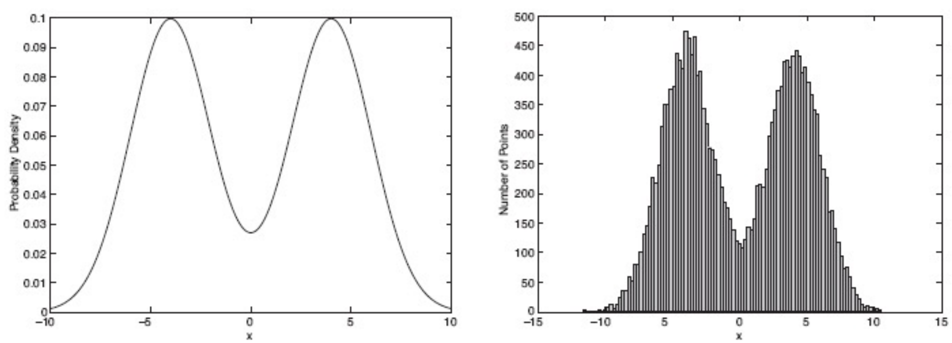
(a) Probability density function for the mixture model.

(b) 20,000 points generated from the mixture model.

Figure 9.2. Mixture model consisting of two normal distributions with means of -4 and 4, respectively. Both distributions have a standard deviation of 2.

Mixture of Gaussians

- In this case the data is the result of the mixture of two Gaussians
  - One for Greek people, and one for Chinese people
  - Identifying for each value which Gaussian is most likely to have generated it will give us a clustering.



(a) Probability density function for the mixture model.

(b) 20,000 points generated from the mixture model.

Figure 9.2. Mixture model consisting of two normal distributions with means of -4 and 4, respectively. Both distributions have a standard deviation of 2.

Mixture Model

- A value x_i is generated according to the following process:
  - First select the nationality
    - With probability π_G select Greek, with probability π_C select China ($\pi_G + \pi_C = 1$)

  - Given the nationality, generate the point from the corresponding Gaussian
    - $P(x_i|\theta_G) \sim N(\mu_G, \sigma_G)$ if Greece
    - $P(x_i|\theta_C) \sim N(\mu_C, \sigma_C)$ if China

Mixture Models

- Our model has the following parameters

$$\Theta = (\pi_G, \pi_C, \mu_G, \mu_C, \sigma_G, \sigma_C)$$

Mixture probabilities | Distribution Parameters

- For value x_i, we have:

$$P(x_i|\Theta) = \pi_G P(x_i|\theta_G) + \pi_C P(x_i|\theta_C)$$

- For all values $X = (x_1, \ldots, x_n)$

$$P(X|\Theta) = \prod_{i=1}^{n} P(x_i|\Theta)$$

- We want to estimate the parameters that maximize the Likelihood of the data

Mixture Models

- Once we have the parameters $\Theta = (\pi_G, \pi_C, \mu_G, \mu_C, \sigma_G, \sigma_C)$ we can estimate the membership probabilities $P(G|x_i)$ and $P(C|x_i)$ for each point x_i:
  - This is the probability that point x_i belongs to the Greek or the Chinese population (cluster)

$$P(G|x_i) = \frac{P(x_i|G)P(G)}{P(x_i|G)P(G) + P(x_i|C)P(C)}$$
$$= \frac{P(x_i|G)\pi_G}{P(x_i|G)\pi_G + P(x_i|C)\pi_C}$$

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$$\pi_G = \frac{1}{n}\sum_{i=1}^{n} P(G|x_i) \qquad \pi_C = \frac{1}{n}\sum_{i=1}^{n} P(C|x_i)$$

Fraction of population in G,C

$$\mu_C = \sum_{i=1}^{n} \frac{P(C|x_i)}{n * \pi_C} x_i \qquad \mu_G = \sum_{i=1}^{n} \frac{P(G|x_i)}{n * \pi_G} x_i$$

MLE Estimates if π's were fixed

$$\sigma_C^2 = \sum_{i=1}^{n} \frac{P(C|x_i)}{n * \pi_C} (x_i - \mu_C)^2 \qquad \sigma_G^2 = \sum_{i=1}^{n} \frac{P(G|x_i)}{n * \pi_G} (x_i - \mu_G)^2$$

Advantages & Disadvantages

- Disadvantages of EM:
  - It can be slow thus it’s not suitable fot large dimensionality
  - It does not work in case of few data points
  - It has difficulty in case of noise and outliers

- Advantages of EM:
  - More geneal wrt K-means because it can use different types f distributions
  - It can find cluster with different size and shape