CS 2750 Machine Learning
Lecture 18

Density estimation with hidden variables and missing values

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Project proposals

Due: **Wednesday, March 24, 2004**

- **1-2 pages long**

Proposal

- **Written proposal:**
  1. Outline of a learning problem, type of data you have available. Why is the problem important?
  2. Learning methods you plan to try and implement for the problem. References to previous work.
  3. How do you plan to test, compare learning approaches
  4. Schedule of work (approximate timeline of work)
- **A PPT (3 slide) summary of points 1-4**

Learning probability distribution

Basic learning settings:

- A set of random variables $\mathbf{X} = \{X_1, X_2, \ldots, X_n\}$
- **A model of the distribution** over variables in X with parameters Θ
- **Data** $D = \{D_1, D_2, .., D_N\}$

  s.t. $D_i = (x_1^i, x_2^i, \ldots x_n^i)$

Objective: find parameters $\hat{\Theta}$ that describe the data

Assumptions considered so far:

- Known parameterizations
- No hidden variables
- No-missing values

Hidden variables

Modeling assumption:

Variables $\mathbf{X} = \{X_1, X_2, \ldots, X_n\}$ are related through hidden variables

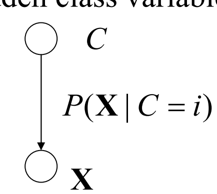
Why to add hidden variables?

- **More flexibility in describing the distribution** $P(\mathbf{X})$
- **Smaller parameterization of** $P(\mathbf{X})$
  - **New independences can be introduced via hidden variables**

Example:

- Latent variable models
  - hidden classes (categories)

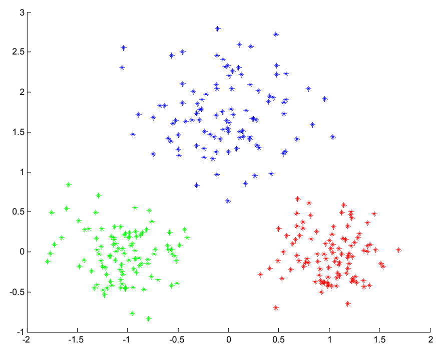
Hidden class variable



Hidden variable model. Example.

- We want to represent the probability model of a population in a two dimensional space $\mathbf{X} = \{X_1, X_2\}$

Observed data



Hidden variable model

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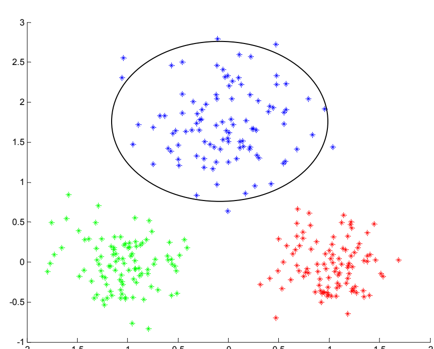

Hidden variable model

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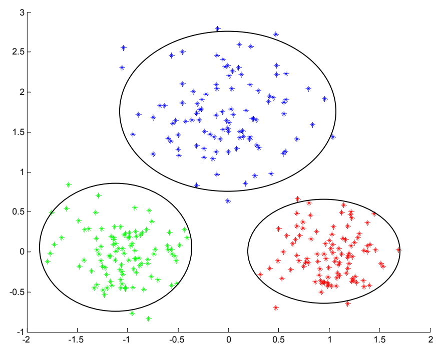

Hidden variable model

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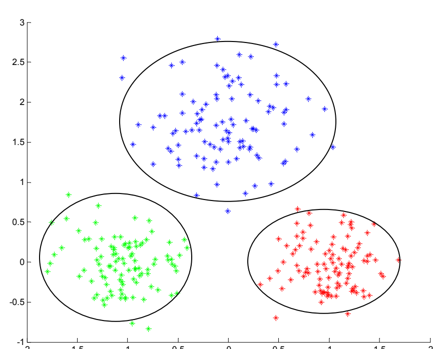
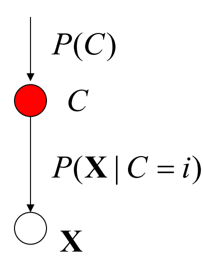


Model : 3 Gaussians with a hidden class variable



Mixture of Gaussians

Probability of the occurrence of a data point $\boldsymbol{x}$ is modeled as

$$p(\mathbf{x}) = \sum_{i=1}^{k} p(C = i)\, p(\mathbf{x} \mid C = i)$$

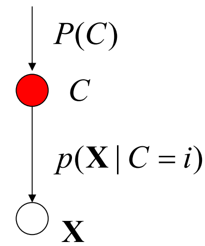
where

$p(C = i)$

= probability of a data point coming from class $C=i$

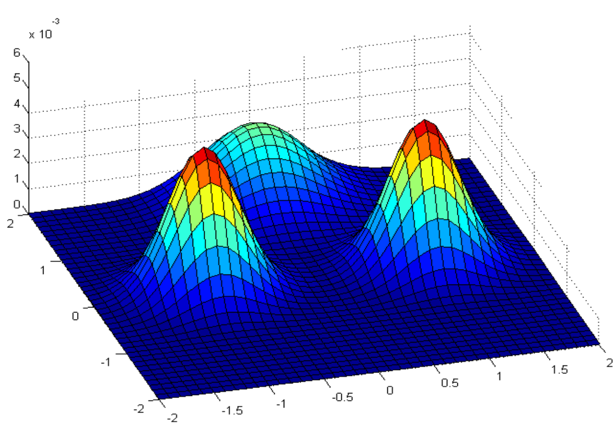
$p(\mathbf{x} \mid C = i) \approx N(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$

= class-conditional density (modeled as Gaussian) for class i



Mixture of Gaussians

- Density function for the Mixture of Gaussians model

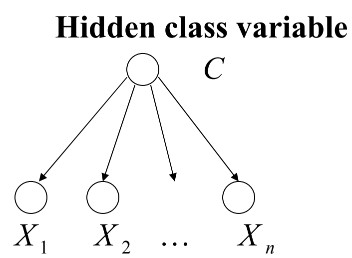


Naïve Bayes with a hidden class variable

Introduction of a hidden variable can reduce the number of parameters defining $P(\mathbf{X})$

Example:

- Naïve Bayes model with a hidden class variable



Attributes are independent given the class

- **Useful in customer profiles**
  - Class value = type of customers

Missing values

A set of random variables $\mathbf{X} = \{X_1, X_2, \ldots, X_n\}$

- **Data** $D = \{D_1, D_2, .., D_N\}$
- **But some values are missing**

$D_i = (x_1^i, x_3^i, \ldots x_n^i)$

Missing value of x_2^i

$D_{i+1} = (x_3^i, \ldots x_n^i)$

Missing values of x_1^i, x_2^i

Etc.

- **Example:** **medical records**
- **We still want to estimate parameters of** $P(\mathbf{X})$

Density estimation

Goal: Find the set of parameters $\hat{\Theta}$

Estimation criteria:

- **ML** $\max_{\Theta} p(D \mid \mathbf{\Theta}, \xi)$
- **Bayesian** $p(\mathbf{\Theta} \mid D, \xi)$

Possible optimization methods for the ML: gradient-ascent, conjugate gradient, Newton-Rhapson, etc.

- **Problem:** No or very small advantage from the structure of the corresponding belief network

Expectation-maximization (EM) method

- An alternative optimization method
- Suitable when there are missing or hidden values
- **Takes advantage of the structure of the belief network**

General EM

The key idea of a method:

Compute the parameter estimates iteratively by performing the following two steps:

Two steps of the EM:

1. **Expectation step**. Complete the values for all hidden and missing variables with expectations for the current set of parameters $\mathbf{\Theta}'$
2. **Maximization step**. Compute the new estimates of $\mathbf{\Theta}$ for the 'completed' data

Stop when no improvement possible

EM

Let H – be a set of all variables with hidden or missing values

Derivation

$$P(H, D \mid \Theta, \xi) = P(H \mid D, \Theta, \xi) P(D \mid \Theta, \xi)$$

$$\log P(H, D \mid \Theta, \xi) = \log P(H \mid D, \Theta, \xi) + \log P(D \mid \Theta, \xi)$$

$$\underline{\log P(D \mid \Theta, \xi)} = \log P(H, D \mid \Theta, \xi) - \log P(H \mid D, \Theta, \xi)$$

Log-likelihood of data

Average both sides with $P(H \mid D, \Theta', \xi)$ for Θ'

$$E_{H|D,\Theta'} \log P(D \mid \Theta, \xi) = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi) - E_{H|D,\Theta'} \log P(H \mid \Theta, \xi)$$

$$\underbrace{\log P(D \mid \Theta, \xi)}_{\text{Log-likelihood of data}} = Q(\Theta \mid \Theta') + H(\Theta \mid \Theta')$$

EM algorithm

Algorithm (general formulation)

Initialize parameters Θ

Repeat

Set $\Theta' = \Theta$

1. **Expectation step**

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

2. **Maximization step**

$$\Theta = \arg\max_{\Theta} Q(\Theta \mid \Theta')$$

until no or small improvement in Θ $(\Theta = \Theta')$

Questions: Why this leads to the ML estimate ?

What is the advantage of the algorithm?

EM algorithm

- Why is the EM algorithm correct?
- **Claim: maximizing Q improves the log-likelihood**

$$l(\Theta) = Q(\Theta \mid \Theta') + H(\Theta \mid \Theta')$$

Difference in log-likelihoods (current and next step)

$$l(\Theta) - l(\Theta') = Q(\Theta \mid \Theta') - Q(\Theta' \mid \Theta') + H(\Theta \mid \Theta') - H(\Theta' \mid \Theta')$$

Subexpression $H(\Theta \mid \Theta') - H(\Theta' \mid \Theta') \geq 0$

Kullback-Leibler (KL) divergence (distance between 2 distributions)

$$KL(P \mid R) = \sum_i P_i \log \frac{P_i}{R_i} \geq 0$$ Is always positive !!!

$$H(\Theta \mid \Theta') = -E_{H|D,\Theta'} \log P(H \mid \Theta, \xi) = -\sum_i p(H \mid D, \Theta') \log P(H \mid \Theta, \xi)$$

$$H(\Theta \mid \Theta') - H(\Theta' \mid \Theta') = \sum_i P(H \mid D, \Theta') \log \frac{P(H \mid \Theta', \xi)}{P(H \mid \Theta, \xi)} \geq 0$$

EM algorithm

Difference in log-likelihoods

$$l(\Theta) - l(\Theta') = Q(\Theta \mid \Theta') - Q(\Theta' \mid \Theta') + H(\Theta \mid \Theta') - H(\Theta' \mid \Theta')$$

$$l(\Theta) - l(\Theta') \geq Q(\Theta \mid \Theta') - Q(\Theta' \mid \Theta')$$

Thus

by **maximizing Q we maximize the log-likelihood**

$$l(\Theta) = Q(\Theta \mid \Theta') + H(\Theta \mid \Theta')$$

EM is a first-order optimization procedure

- **Climbs the gradient**
- **Automatic learning rate**

No need to adjust the learning rate !!!!

EM advantages

Key advantages:

- In many problems (e.g. Bayesian belief networks)

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

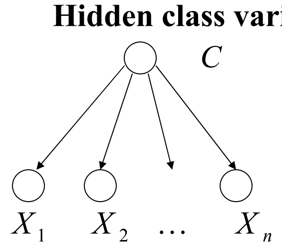
  - has a nice form and the maximization of Q can be carried in the closed form
- No need to compute Q before maximizing
- We directly optimize
  - use quantities corresponding to expected counts

Naïve Bayes with a hidden class and missing values

Assume:

- $P(\mathbf{X})$ is modeled using a Naïve Bayes model with hidden class variable
- Missing entries (values) for attributes in the dataset D

Hidden class variable



Attributes are independent given the class

EM for the Naïve Bayes

- **We can use EM to learn the parameters**

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

- **Parameters:**

π_j prior on class j

θ_{ijk} probability of an attribute i having value k given class j

- **Indicator variables:**

δ_j^l for example l, the class is j ; if true (=1) else false (=0)

δ_{ijk}^l for example l, the class is j and the value of attrib i is k

because the class is hidden and some attributes are missing, the values (0,1) of indicator variables are not known; they are hidden

H – a collection of all indicator variables

EM for the Naïve Bayes model

- We can use EM to do the learning of parameters

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

$$\log P(H, D \mid \Theta, \xi) = \log \prod_{l=1}^{N} \prod_{j} \pi_j^{\delta_j^l} \prod_{i} \prod_{k} \theta_{ijk}^{\delta_{ijk}^l}$$

$$= \sum_{l=1}^{N} \sum_{j} (\delta_j^l \log \pi_j + \sum_{i} \sum_{k} \delta_{ijk}^l \log \theta_{ijk})$$

$$E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi) = \sum_{l=1}^{N} \sum_{j} (E_{H|D,\Theta'}(\delta_j^l) \log \pi_j + \sum_{i} \sum_{k} E_{H|D,\Theta'}(\delta_{ijk}^l) \log \theta_{ijk})$$

$$E_{H|D,\Theta'}(\delta_j^l) = p(C_l = j \mid D_l, \Theta')$$

$$E_{H|D,\Theta'}(\delta_{ijk}^l) = p(X_{il} = k, C_l = j \mid D_l, \Theta')$$

Substitutes 0,1 with expected value

EM for Naïve Bayes model

- Computing derivatives of $\boldsymbol{Q}$ for parameters and setting it to 0 we get:

$$\pi_j = \frac{\tilde{N}_j}{N} \qquad \theta_{ijk} = \frac{\tilde{N}_{ijk}}{\sum_{k=1}^{r_i} \tilde{N}_{ijk}}$$

$$\tilde{N}_j = \sum_{l=1}^{N} E_{H|D,\Theta'}(\delta_j^l) = \sum_{l=1}^{N} p(C_l = j \mid D_l, \Theta')$$

$$\tilde{N}_{ijk} = \sum_{l=1}^{N} E_{H|D,\Theta'}(\delta_{ijk}^l) = \sum_{l=1}^{N} p(X_{il} = k, C_l = j \mid D_l, \Theta')$$

- **Important:**
  - **Use expected counts instead of counts !!!**
    - Re-estimate the parameters using expected counts

EM for BBNs

- The same result applies to learning of parameters of **any Bayesian belief network** with discrete-valued variables

$$Q(\Theta \mid \Theta') = E_{H|D,\Theta'} \log P(H, D \mid \Theta, \xi)$$

$$\theta_{ijk} = \frac{\tilde{N}_{ijk}}{\sum_{k=1}^{r_i} \tilde{N}_{ijk}} \longleftarrow \text{Parameter value maximizing } \boldsymbol{Q}$$

$$\tilde{N}_{ijk} = \sum_{l=1}^{N} p(x_i^{\,l} = k, pa_i^{\,l} = j \mid D^l, \Theta')$$

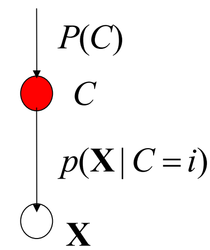
may require inference

- **Again:**
  - Use expected counts instead of counts

Gaussian mixture model

Probability of occurrence of a data point $\boldsymbol{x}$ is modeled as

$$p(\mathbf{x}) = \sum_{i=1}^{k} p(C = i)\, p(\mathbf{x} \mid C = i)$$



where

$p(C = i)$

= probability of a data point coming from class $C=i$

$p(\mathbf{x} \mid C = i) \approx N(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$

= class conditional density (modeled as a Gaussian) for class I

<u>Remember:</u> *C* is hidden !!!!

Generative Naïve Bayes classifier model

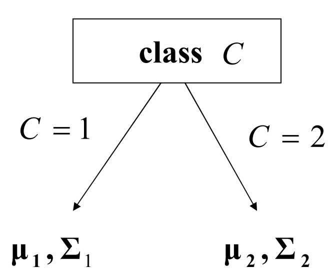
- Generative classifier model based on the Naïve Bayes
- Assume the class labels are known. The ML estimate is

$$N_i = \sum_{j: C_l = i} 1$$

$$\tilde{\pi}_i = \frac{N_i}{N}$$

$$\tilde{\boldsymbol{\mu}}_i = \frac{1}{N_i} \sum_{j: C_l = i} \mathbf{x}_j$$

$$\tilde{\boldsymbol{\Sigma}}_i = \frac{1}{N_i} \sum_{j: C_l = i} (\mathbf{x}_j - \boldsymbol{\mu}_i)(\mathbf{x}_j - \boldsymbol{\mu}_i)^T$$



Gaussian mixture model

- In the Gaussian mixture Gaussians are not labeled
- We can apply **EM algorithm**:
  - re-estimation based on the class posterior

$$h_{il} = p(C_l = i \mid \mathbf{x}_l, \Theta') = \frac{p(C_l = i \mid \Theta')\, p(x_l \mid C_l = i, \Theta')}{\sum_{u=1}^{m} p(C_l = u \mid \Theta')\, p(x_l \mid C_l = u, \Theta')}$$

$$N_i = \sum_l h_{il}$$

Count replaced with the expected count

$$\tilde{\pi}_i = \frac{N_i}{N}$$

$$\tilde{\boldsymbol{\mu}}_i = \frac{1}{N_i} \sum_l h_{il} \mathbf{x}_j$$

$$\tilde{\boldsymbol{\Sigma}}_i = \frac{1}{N_i} \sum_l h_{il} (\mathbf{x}_j - \boldsymbol{\mu}_i)(\mathbf{x}_j - \boldsymbol{\mu}_i)^T$$

Gaussian mixture algorithm

- **Special case:** fixed covariance matrix for all hidden groups (classes) and uniform prior on classes
- **Algorithm**:

  Initialize means $\boldsymbol{\mu}_i$ for all classes i

  Repeat two steps until no change in the means:

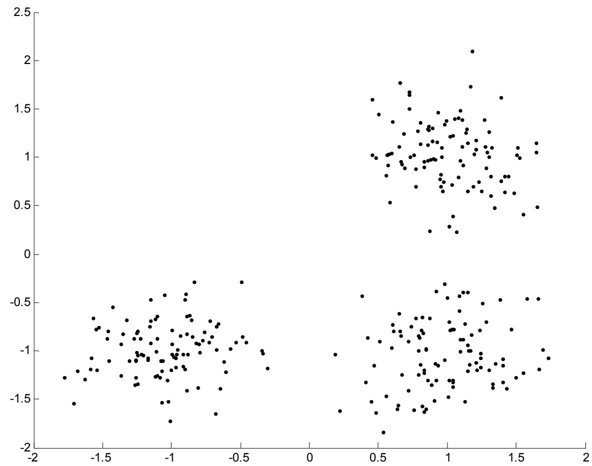
  1. Compute the class posterior for each Gaussian and each point (a kind of responsibility for a Gaussian for a point)

     Responsibility: $$h_{il} = \frac{p(C_l = i \mid \Theta')\, p(x_l \mid C_l = i, \Theta')}{\sum_{u=1}^{m} p(C_l = u \mid \Theta')\, p(x_l \mid C_l = u, \Theta')}$$

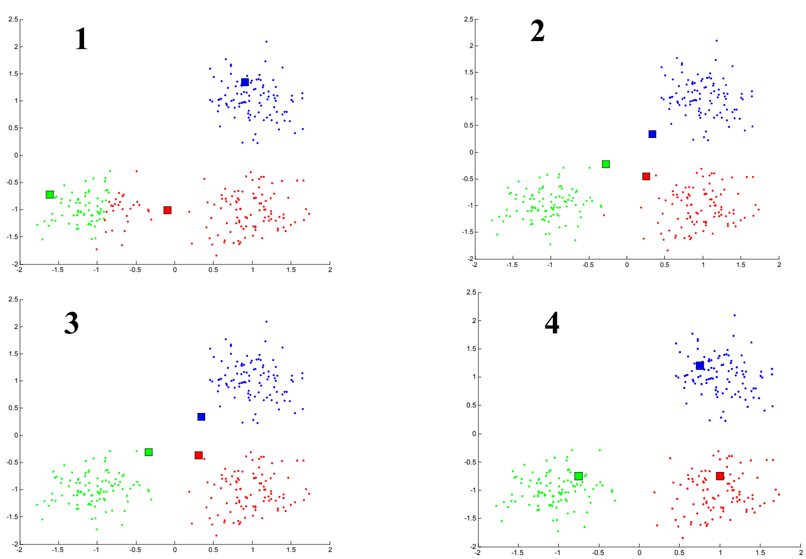
  2. Move the means of the Gaussians to the center of the data, weighted by the responsibilities

     New mean: $$\boldsymbol{\mu}_i = \frac{\sum_{l=1}^{N} h_{il} \mathbf{x}_l}{\sum_{l=1}^{N} h_{il}}$$

Gaussian mixture model - example



Gaussian mixture example

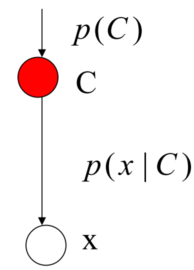


Gaussian mixture model. Gradient ascent.

- A set of parameters

$$\Theta = \{\pi_1, \pi_2, ..\pi_m, \mu_1, \mu_2, ...\mu_m\}$$

Assume unit variance terms and fixed priors



$$P(\mathbf{x} \mid C = i) = (2\pi)^{-1/2} \exp\left\{-\frac{1}{2}\|x - \mu_i\|^2\right\}$$

$$P(D \mid \Theta) = \prod_{l=1}^{N} \sum_{i=1}^{m} \pi_i (2\pi)^{-1/2} \exp\left\{-\frac{1}{2}\|x_l - \mu_i\|^2\right\}$$

$$l(\Theta) = \sum_{l=1}^{N} \log \sum_{i=1}^{m} \pi_i (2\pi)^{-1/2} \exp\left\{-\frac{1}{2}\|x_l - \mu_i\|^2\right\}$$

$$\frac{\partial l(\Theta)}{\partial \mu_i} = \sum_{l=1}^{N} h_{il}(x_l - \mu_i)$$

- very easy on-line update

EM versus gradient ascent

Gradient ascent

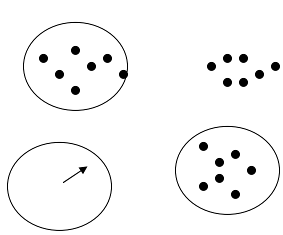
$$\mu_i \leftarrow \mu_i + \alpha \sum_{l=1}^{N} h_{il}(x_l - \mu_i)$$

Learning rate

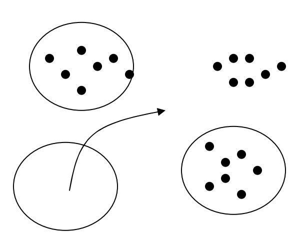
EM

$$\mu_i \leftarrow \frac{\sum_{l=1}^{N} h_{il} \mathbf{x}_l}{\sum_{l=1}^{N} h_{il}}$$

No learning rate



Small pull towards distant uncovered data



Renormalized – big jump in the first step

K-means approximation to EM

Expectation-Maximization:

- posterior measures the responsibility of a Gaussian for every point

$$h_{il} = \frac{p(C_l = i \mid \Theta')\, p(x_l \mid C_l = i, \Theta')}{\sum_{u=1}^{m} p(C_l = u \mid \Theta')\, p(x_l \mid C_l = u, \Theta')}$$

K- Means

- Only the closest Gaussian is made responsible for a point

$h_{il} = 1$ If i is the closest Gaussian

$h_{il} = 0$ Otherwise

Re-estimation of means

$$\boldsymbol{\mu}_i = \frac{\sum_{l=1}^{N} h_{il}\, \mathbf{x}_l}{\sum_{l=1}^{N} h_{il}}$$

- Results in moving the means of Gaussians to the center of the data points it covered in the previous step

K-means algorithm

Useful for clustering data:

- Assume we want to distribute data into *k* different groups
  - Similarity between data points is measured in terms of the distance
  - Groups are defined in terms of centers (also called means)

K-Means algorithm:

Initialize k values of means (centers)

Repeat two steps until no change in the means:

- Partition the data according to the current means (using the similarity measure)
- Move the means to the center of the data in the current partition

K-means algorithm

- **Properties**
  - converges to centers minimizing the sum of center-point distances (local optima)
  - The result may be sensitive to the initial means' values

- **Advantages:**
  - Simplicity
  - Generality – can work for an arbitrary distance measure

- **Drawbacks:**
  - Can perform poorly on overlapping regions
  - Lack of robustness to outliers (outliers are not covered)