Clustering algorithms

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Unit 5

– k-medoids clustering algorithms (PAM, CLARA, CLARANS)

– Probabilistic CFO clustering algorithms (EM)

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CFO hard clustering algorithms

Generalized Hard Algorithmic Scheme (GHAS)

k-Medoids Algorithms

- Each cluster is represented by a vector selected among the elements of X (medoid).

- A cluster contains
  - Its medoid
  - All vectors in X that
    - Are not used as medoids in other clusters
    - Lie closer to its medoid than the medoids representing other clusters.

In the k-medoids algorithms ONLY **point representatives** can be used to represent clusters

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k-Medoids Algorithms

Let

- Θ be the set of medoids of all clusters,
- I_{Θ} the set of indices of the points in X that constitute Θ and
- $I_{X\text{-}\Theta}$ the set of indices of the points that are not medoids.

Obtaining the set of medoids Θ that best represents the data set, X is equivalent to minimizing the following cost function

$$J(\Theta, U) = \sum_{i \in I_{X-\Theta}} \sum_{j \in I_{\Theta}} u_{ij} d(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

with

$$u_{ij} = \begin{cases} 1, & if\ d(x_i, x_j) = min_{q \in I_{\Theta}} d(x_i, x_q) \\ 0, & otherwise \end{cases}, \qquad i = 1, \ldots, N$$

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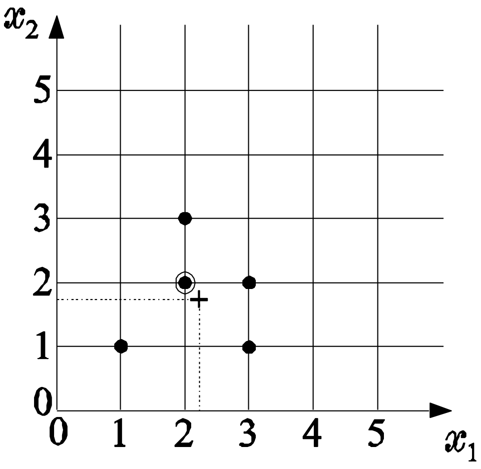
k-Medoids Algorithms

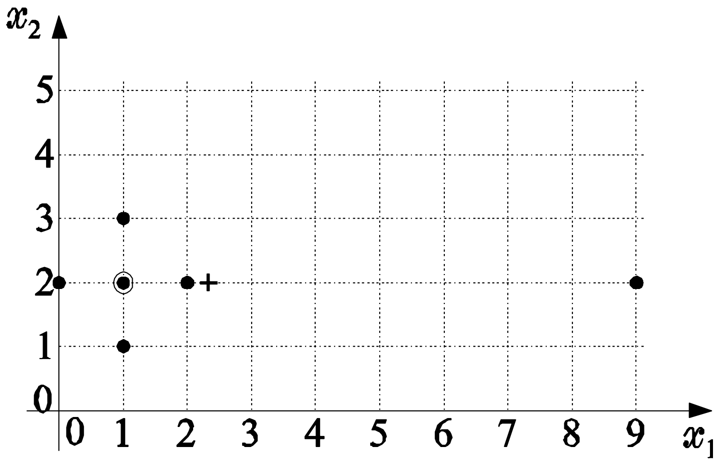
Example 3:

(a) The five-point two-dimensional set stems from the discrete domain $D = \{1,2,3,4, \ldots\} \times \{1,2,3,4, \ldots\}$. Its medoid is the circled point and its mean is the “$+$” point, which does not belong to D.

(b) In the six-point two-dimensional set , the point $(9,2)$ can be considered as an outlier. While the outlier affects significantly the mean of the set, it does not affect its medoid.



(a)



(b)

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Representing clusters with mean values **vs** representing clusters with medoids

Mean Values	Medoids
1. Suited only for continuous domains	**1. Suited for either cont. or discrete domains**
2. Algorithms using means are sensitive to outliers	**2. Algorithms using medoids are less sensitive to outliers**
3. The mean possess a clear geometrical and statistical meaning	3. The medoid has not a clear geometrical meaning
4. Algorithms using means are not computationally demanding	4. Algorithms using medoids are more computationally demanding

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k-Medoids Algorithms

Algorithms to be considered

- PAM (Partitioning Around Medoids)
- CLARA (Clustering LARge Applications)
- CLARANS (Clustering Large Applications based on RANdomized Search)

The PAM algorithm

- The number of clusters m is **required** *a priori*.

Definitions-preliminaries

- Two *sets* of medoids Θ and Θ', each one consisting of m elements, are called neighbors if they **share** $m-1$ elements.

- A set Θ of medoids with m elements can have $m(N-m)$ neighbors.

- Let Θ_{ij} denote the neighbor of Θ that results if $\boldsymbol{x}_j$, $j \in I_{X-\Theta}$ **replaces** $\boldsymbol{x}_i$, $i \in I_{\Theta}$.

- Let $\Delta J_{ij} = J(\Theta_{ij}, U_{ij}) - J(\Theta, U)$.

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The PAM algorithm

- *Determination of Θ that best represents the data*
  - Generate a set Θ of m medoids, randomly selected out of X.
  - (A) Determine the neighbor Θ_{qr}, $q \in I_\Theta$, $r \in I_{X-\Theta}$ among the $m(N-m)$ neighbors of Θ for which $\Delta J_{qr} = min_{i \in I_\Theta,\, j \in I_{X-\Theta}} \Delta J_{ij}$.
  - If $\Delta J_{qr} < 0$ then
    - Replace Θ by Θ_{qr}
    - Go to (A)
  - End

$$\Delta J_{qr} < 0 \Leftrightarrow J(\Theta_{qr}, U_{qr}) < J(\Theta, U)$$

- *Assignment of points to clusters*
  - Assign each $\boldsymbol{x} \in I_{X-\Theta}$ to the cluster represented by the closest to $\boldsymbol{x}$ medoid.

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Generalized Hard Algorithmic Scheme (GHAS)

The PAM algorithm

Computation of ΔJ_{ij}.

It is defined as:

$$\Delta J_{ij} = J(\Theta_{ij}, U_{ij}) - J(\Theta, U) = \sum_{s \in I_{X-\Theta_{ij}}} \sum_{t \in I_{\Theta_{ij}}} u_{st} d(\boldsymbol{x}_s, \boldsymbol{x}_t) - \sum_{s \in I_{X-\Theta}} \sum_{t \in I_{\Theta}} u_{st} d(\boldsymbol{x}_s, \boldsymbol{x}_t)$$

$$\equiv \sum_{h \in I_{X-\Theta}} C_{hij}$$

where C_{hij} is the *difference in J, resulting from the (possible) assignment of the vector $\boldsymbol{x}_h \in X - \Theta$ from the cluster it currently belongs to another, as a consequence of the replacement of $\boldsymbol{x}_i \in \Theta$ by $\boldsymbol{x}_j \in X - \Theta$*.

For the computation of C_{hij} associated with a specific each $\boldsymbol{x}_h \in X - \Theta$ it is required

- The **distance** of $\boldsymbol{x}_h$ from its **closest medoid** in Θ
- The **distance** of $\boldsymbol{x}_h$ from its **next to closest medoid** in Θ.
- The **distance** of $\boldsymbol{x}_h$ from the **newly inserted medoid** in Θ_{ij}.

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The PAM algorithm (cont.)

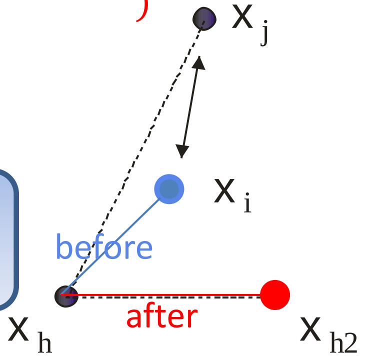
Computation of C_{hij}:

$\boldsymbol{x}_h$ **belongs** to the cluster represented by $\boldsymbol{x}_i$ ($\boldsymbol{x}_{h2}$ Θ denotes the second closest to $\boldsymbol{x}_h$ **representative**) **and** $d(\boldsymbol{x}_h, \boldsymbol{x}_j) \geq d(\boldsymbol{x}_h, \boldsymbol{x}_{h2})$. Then

$$C_{hi\,j} = d(\boldsymbol{x}_h, \boldsymbol{x}_{h2}) - d(\boldsymbol{x}_h, \boldsymbol{x}_i) \geq 0$$

Contribution of $\boldsymbol{x}_h$ to $J(\Theta_{ij}, U_{ij})$

Contribution of $\boldsymbol{x}_h$ to $J(\Theta, U)$

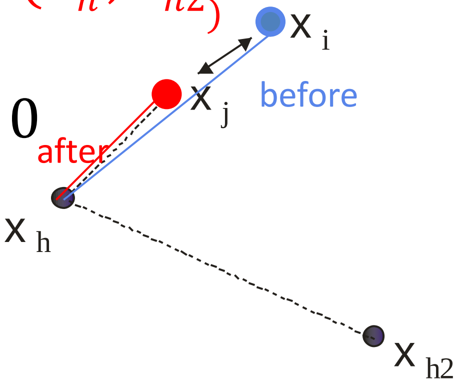


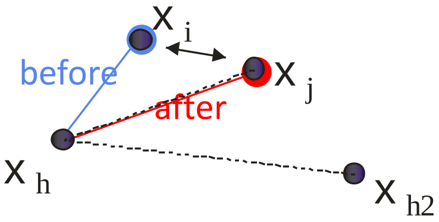
$\boldsymbol{x}_h$ **belongs** to the cluster represented by $\boldsymbol{x}_i$ ($\boldsymbol{x}_{h2}$ Θ denotes the second closest to $\boldsymbol{x}_h$ representative) **and** $d(\boldsymbol{x}_h, \boldsymbol{x}_j) \leq d(\boldsymbol{x}_h, \boldsymbol{x}_{h2})$. Then

$$C_{hij} = d(\boldsymbol{x}_h, \boldsymbol{x}_j) - d(\boldsymbol{x}_h, \boldsymbol{x}_i)\ (><)\ 0$$

Contribution of $\boldsymbol{x}_h$ to $J(\Theta_{ij}, U_{ij})$

Contribution of $\boldsymbol{x}_h$ to $J(\Theta, U)$





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The PAM algorithm (cont.)

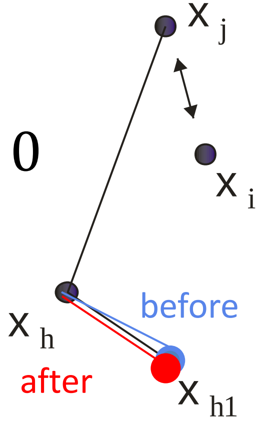
Computation of C_{hij} (cont.):

$\boldsymbol{x}_h$ is not represented by $\boldsymbol{x}_i$ ($\boldsymbol{x}_{h1}$ denotes the closest to $\boldsymbol{x}_h$ medoid) **and** $d(\boldsymbol{x}_h, \boldsymbol{x}_{h1_{)}} \leq d(\boldsymbol{x}_h, \boldsymbol{x}_j)$. Then

$$C_{hij} = d(\boldsymbol{x}_h, \boldsymbol{x}_j) - d(\boldsymbol{x}_h, \boldsymbol{x}_{h1}) = 0$$

Contribution of $\boldsymbol{x}_h$ to $J(\Theta_{ij}, U_{ij})$

Contribution of $\boldsymbol{x}_h$ to $J(\Theta, U)$



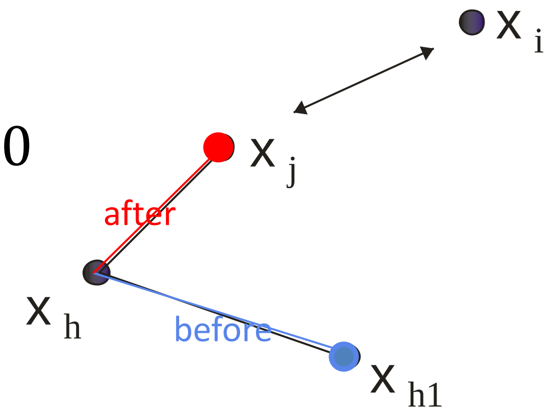
Most frequent scenario

$\boldsymbol{x}_h$ is not represented by $\boldsymbol{x}_i$ ($\boldsymbol{x}_{h1}$ denotes the closest to $\boldsymbol{x}_h$ medoid) **and** $d(\boldsymbol{x}_h, \boldsymbol{x}_{h1_{)}} > d(\boldsymbol{x}_h, \boldsymbol{x}_j)$. Then

$$C_{hij} = d(\boldsymbol{x}_h, \boldsymbol{x}_j) - d(\boldsymbol{x}_h, \boldsymbol{x}_{h1}) < 0$$

Contribution of $\boldsymbol{x}_h$ to $J(\Theta_{ij}, U_{ij})$

Contribution of $\boldsymbol{x}_h$ to $J(\Theta, U)$



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Generalized Hard Algorithmic Scheme (GHAS)

The PAM algorithm (cont.)

Remarks:

- Experimental results show the PAM works satisfactorily with small data sets.

- Its computational complexity is $O(m(N-m)^2)$. Unsuitable for large data sets.

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Generalized Hard Algorithmic Scheme (GHAS)

The PAM algorithm (Example)

Data set: $X = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4, \boldsymbol{x}_5, \boldsymbol{x}_6\}$, with

$\boldsymbol{x}_1 = [0{,}3]^T, \boldsymbol{x}_2 = [1{,}3]^T, \boldsymbol{x}_3 = [2{,}3]^T, \boldsymbol{x}_4 = [0{,}0]^T, \boldsymbol{x}_5 = [1{,}0]^T, \boldsymbol{x}_1 = [2{,}0]^T.$

Set of medoids: $\Theta = \{\boldsymbol{x}_4, \boldsymbol{x}_5\}$

Computation of $J(\Theta, U)$ (**Squared Euclidean distance** is considered):

$$\boldsymbol{x}_1 \longrightarrow d(\boldsymbol{x}_1, \boldsymbol{x}_4) = 9 < 10 = d(\boldsymbol{x}_1, \boldsymbol{x}_5) \longrightarrow u_{14} = 1, u_{15} = 0$$

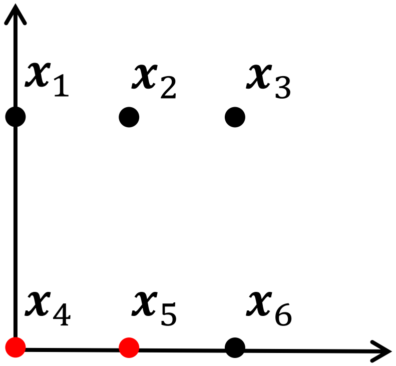
$$\boldsymbol{x}_2 \longrightarrow d(\boldsymbol{x}_2, \boldsymbol{x}_4) = 10 > 9 = d(\boldsymbol{x}_2, \boldsymbol{x}_5) \longrightarrow u_{24} = 0, u_{25} = 1$$

$$\boldsymbol{x}_3 \longrightarrow d(\boldsymbol{x}_3, \boldsymbol{x}_4) = 13 > 10 = d(\boldsymbol{x}_3, \boldsymbol{x}_5) \longrightarrow u_{34} = 0, u_{35} = 1$$

$$\boldsymbol{x}_4 \longrightarrow d(\boldsymbol{x}_4, \boldsymbol{x}_4) = 0 < 1 = d(\boldsymbol{x}_4, \boldsymbol{x}_5) \longrightarrow u_{44} = 1, u_{45} = 0$$

$$\boldsymbol{x}_5 \longrightarrow d(\boldsymbol{x}_5, \boldsymbol{x}_4) = 1 > 0 = d(\boldsymbol{x}_5, \boldsymbol{x}_5) \longrightarrow u_{54} = 0, u_{55} = 1$$

$$\boldsymbol{x}_6 \longrightarrow d(\boldsymbol{x}_6, \boldsymbol{x}_4) = 2 > 1 = d(\boldsymbol{x}_6, \boldsymbol{x}_5) \longrightarrow u_{64} = 0, u_{65} = 1$$



$$J(\Theta, U) = \begin{array}{ll} u_{14} d(\boldsymbol{x}_1, \boldsymbol{x}_4) + & u_{15} d(\boldsymbol{x}_1, \boldsymbol{x}_5) + \\ u_{24} d(\boldsymbol{x}_1, \boldsymbol{x}_4) + & u_{25} d(\boldsymbol{x}_1, \boldsymbol{x}_5) + \\ u_{34} d(\boldsymbol{x}_1, \boldsymbol{x}_4) + & u_{35} d(\boldsymbol{x}_1, \boldsymbol{x}_5) + \\ u_{44} d(\boldsymbol{x}_1, \boldsymbol{x}_4) + & u_{45} d(\boldsymbol{x}_1, \boldsymbol{x}_5) + \\ u_{54} d(\boldsymbol{x}_1, \boldsymbol{x}_4) + & u_{55} d(\boldsymbol{x}_1, \boldsymbol{x}_5) + \\ u_{64} d(\boldsymbol{x}_1, \boldsymbol{x}_4) + & u_{65} d(\boldsymbol{x}_1, \boldsymbol{x}_5) \end{array} = \begin{array}{ll} 1 \cdot 9 + & 0 \cdot 10 + \\ 0 \cdot 10 + & 1 \cdot 9 + \\ 0 \cdot 13 + & 1 \cdot 10 + \\ 1 \cdot 0 + & 0 \cdot 1 + \\ 0 \cdot 1 + & 1 \cdot 0 + \\ 0 \cdot 2 + & 1 \cdot 1 \end{array} = \mathbf{29}$$

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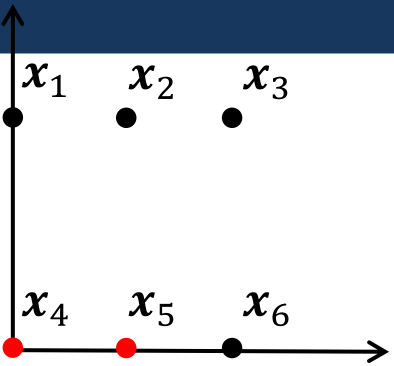
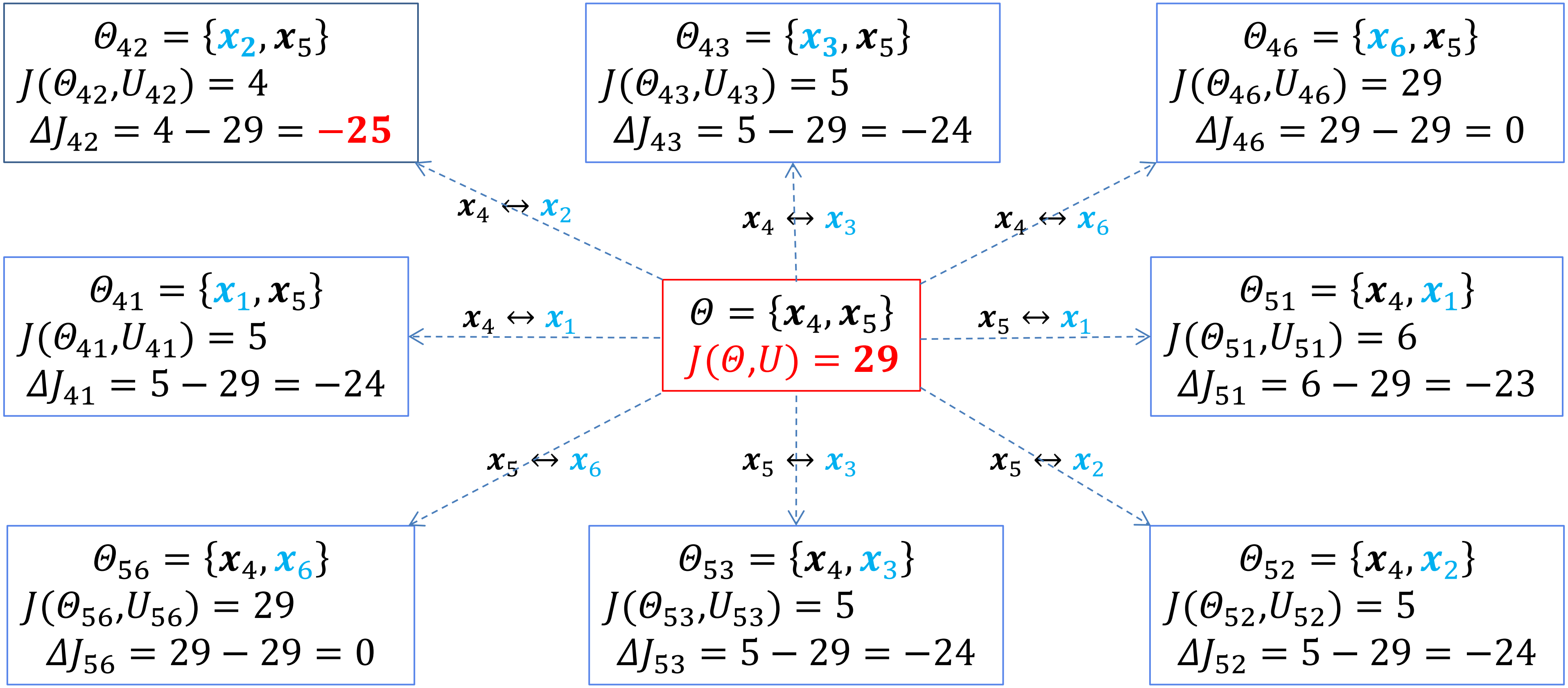
Generalized Hard Algorithmic Scheme (GHAS)

The PAM algorithm (Example)



Data set: $X = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4, \boldsymbol{x}_5, \boldsymbol{x}_6\}$, with
$\boldsymbol{x}_1 = [0,3]^T, \boldsymbol{x}_2 = [1,3]^T, \boldsymbol{x}_3 = [2,3]^T, \boldsymbol{x}_4 = [0,0]^T, \boldsymbol{x}_5 = [1,0]^T, \boldsymbol{x}_1 = [2,0]^T.$
Set of medoids: $\Theta = \{\boldsymbol{x}_4, \boldsymbol{x}_5\}$



$\Theta_{42} = \{\boldsymbol{x}_2, \boldsymbol{x}_5\}$
$J(\Theta_{42}, U_{42}) = 4$
$\Delta J_{42} = 4 - 29 = \mathbf{-25}$

$\Theta_{43} = \{\boldsymbol{x}_3, \boldsymbol{x}_5\}$
$J(\Theta_{43}, U_{43}) = 5$
$\Delta J_{43} = 5 - 29 = -24$

$\Theta_{46} = \{\boldsymbol{x}_6, \boldsymbol{x}_5\}$
$J(\Theta_{46}, U_{46}) = 29$
$\Delta J_{46} = 29 - 29 = 0$

$\boldsymbol{x}_4 \leftrightarrow \boldsymbol{x}_2$

$\boldsymbol{x}_4 \leftrightarrow \boldsymbol{x}_3$

$\boldsymbol{x}_4 \leftrightarrow \boldsymbol{x}_6$

$\Theta_{41} = \{\boldsymbol{x}_1, \boldsymbol{x}_5\}$
$J(\Theta_{41}, U_{41}) = 5$
$\Delta J_{41} = 5 - 29 = -24$

$\boldsymbol{x}_4 \leftrightarrow \boldsymbol{x}_1$

$\Theta = \{\boldsymbol{x}_4, \boldsymbol{x}_5\}$
$J(\Theta, U) = \mathbf{29}$

$\boldsymbol{x}_5 \leftrightarrow \boldsymbol{x}_1$

$\Theta_{51} = \{\boldsymbol{x}_4, \boldsymbol{x}_1\}$
$J(\Theta_{51}, U_{51}) = 6$
$\Delta J_{51} = 6 - 29 = -23$

$\boldsymbol{x}_5 \leftrightarrow \boldsymbol{x}_6$

$\boldsymbol{x}_5 \leftrightarrow \boldsymbol{x}_3$

$\boldsymbol{x}_5 \leftrightarrow \boldsymbol{x}_2$

$\Theta_{56} = \{\boldsymbol{x}_4, \boldsymbol{x}_6\}$
$J(\Theta_{56}, U_{56}) = 29$
$\Delta J_{56} = 29 - 29 = 0$

$\Theta_{53} = \{\boldsymbol{x}_4, \boldsymbol{x}_3\}$
$J(\Theta_{53}, U_{53}) = 5$
$\Delta J_{53} = 5 - 29 = -24$

$\Theta_{52} = \{\boldsymbol{x}_4, \boldsymbol{x}_2\}$
$J(\Theta_{52}, U_{52}) = 5$
$\Delta J_{52} = 5 - 29 = -24$

It is $\Delta J_{42} = min_{i \in I_{\Theta},\, j \in I_{X-\Theta}} \Delta J_{ij} = -25 < 0$
Thus, according to **PAM**, Θ will be **replaced** by Θ_{42}.

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Generalized Hard Algorithmic Scheme (GHAS)

The CLARA algorithm

- It is more suitable for large data sets.
- The strategy:
  - **Draw** randomly a sample X' of size N' from the entire data set.
  - **Run** the PAM algorithm to **determine** Θ' that best represents X'.
  - Use Θ' in the place of Θ to represent the entire data set X.
- The rationale:
  - Assuming that X' has been selected in a way representative of the statistical distribution of the data points in X, Θ' is expected to be a good approximation of Θ, which would have been produced if PAM were run on the entire X.
- The algorithm:
  - Draw s sample subsets of size N' from X, denoted by $X'_1, \dots, X'_s$ (typically $s = 5, N' = 40 + 2m$).
  - Run PAM on each one of them and identify $\Theta'_1, \dots, \Theta'_s$.
  - Choose the set Θ'_j that minimizes

$$J(\Theta, U) = \sum_{i \in I_{X-\Theta'}} \sum_{j \in I_{\Theta'}} u_{ij} d(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

based on the entire data set X.

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Generalized Hard Algorithmic Scheme (GHAS)

The CLARANS algorithm

- It is more suitable for large data sets.
- It follows the philosophy of PAM with the difference that only a randomly selected fraction $q(< m(N-m))$ of the neighbors of the current medoid set is considered.
- It performs several runs (s) starting from different initial choices for Θ.

The algorithm:

```
– For $i = 1$ to $s$
    o **Initialize** randomly $\Theta$.
    o (A) **Select** randomly $q$ neighbors of $\Theta$.
    o For $j = 1$ to $q$
       * **If** the present neighbor of $\Theta$ is **better** than $\Theta$ (in terms of $J(\Theta, U)$) then
          -- **Set** $\Theta$ equal to its neighbor
          -- Go to (A)
       * End If
    o End For
    o Set $\Theta^i = \Theta$
– End For
– **Select** the best $\Theta^i$ with respect to $J(\Theta, U)$.
– Based on $\Theta^i$, assign each $\boldsymbol{x} \in X - \Theta$ to the cluster whose representative is closest to $\boldsymbol{x}$
```

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Generalized Hard Algorithmic Scheme (GHAS)

The CLARANS algorithm (cont.)

Remarks:

- CLARANS **depends** on q and s. Typically, $s = 2$ and
  $$q = \max(0.125m(N-m), 250)$$
- As q approaches $m(N-m)$ CLARANS approaches PAM and the complexity increases.
- CLARANS can also be described in terms of graph theory concepts.
- CLARANS unravels better quality clusters than CLARA.
- In some cases, CLARA is significantly faster than CLARANS.
- CLARANS retains its quadratic computational nature and thus it is not appropriate for very large data sets.

Probability and statistics: a brief review

Random variable (RV): It models the output of an experiment.

RV types:

- Discrete
- continuous

Discrete random variables:

- A **discrete RV** *x* can take any value *x* from a finite or countably infinite set *X.*
- *X*: sample space or state space.
- **Event:** Any subset of *X.*
- **Elementary** or **simple event**: A single element subset of *X*.
- **Example:** Consider the die roll experiment. X={1,2,3,4,5,6}
- Events: “Odd number”, “number>3”, “2”, “5”

Elementary events

Probability and statistics: a brief review

Discrete random variables (cont.)**:**

•**Notation:** Probability of the event $x\!=\!x \in X$: $P(x\!=\!x) \equiv P(x)$

•*P*(.):A function called probability mass function (pmf) satisfying

- ✓ $P(x) \geq 0, \forall x \in X$
- ✓ $\sum_{x \in X} P(x) = 1$

Probability and statistics: a brief review

Discrete random variables (cont.):

The case of more than one random variables: Definitions

Discrete RV	x	y
Sample space	$X=\{x_1,\ldots,x_{nx}\}$	$Y=\{y_1,\ldots,y_{ny}\}$

Joint probability: $P(x_i, y_j) \equiv P(x=x_i \text{ AND } y=y_j)$

- It corresponds to the case where x takes the value x_i **AND** y takes the value y_j, **simultaneously**.

Marginal probabilities: $P(x_i) \equiv P(x=x_i)$, $P(y_j) = P(y=y_j)$

- This terminology is used only when more than one rvs are involved.

Conditional probability: $P(x_i | y_j) \equiv P(x=x_i \mid y=y_j) = P(x_i,y_j) / P(y_j)$

- It corresponds to the case where x takes the value x_i **given that** y takes the value y_j.

Probability and statistics: a brief review

Discrete random variables (cont.):

The case of more than one variables: Properties

Discrete RV	x	y
Sample space	$X=\{x_1,\ldots,x_{nx}\}$	$Y=\{y_1,\ldots,y_{ny}\}$

Sum rule: $P(x)=\sum_{y\in Y}P(x,y), \quad \forall x\in X$

Product rule: $P(x,y)=P(x\,|\,y)P(y)$

Statistical independence: $P(x,y)=P(x)P(y)$

A consequence: $P(x\,|\,y)=P(x) \quad P(y\,|\,x)=P(y)$

Bayes rule: $$P(y\,|\,x)=\frac{P(x\,|\,y)P(y)}{P(x)}$$

It plays a key role in ML.

or $$P(y\,|\,x)=\frac{P(x\,|\,y)P(y)}{\sum_{y\in Y}P(x\,|\,y)P(y)}$$

Probability and statistics: a brief review

Continuous random variables:

•A **continuous RV** x can take any value $x \in R$.

•Sample space or state space: R

Corresponds to the probability mass function from the discrete case.

•**Events:** $\{x \le x\}$, $\{x_1 < x \le x_2\}$, $\{x \ge x\}$

•**Cumulative distribution function** (**cdf**): $F_x(x) = P(x \le x)$

It assigns “mass” to events.

•It is $F_x(\infty) = P(x < \infty) = 1$

•**Probability of events** in terms of **cdf**:

- $P(x \le x) = F_x(x)$
- $P(x_1 < x \le x_2) = P(x \le x_2) - P(x \le x_1) = F_x(x_2) - F_x(x_1)$
- $P(x \ge x) = = P(x \le \infty) - P(x \le x) = 1 - P(x \le x) = 1 - F_x(x)$

Probability and statistics: a brief review

Continuous random variables (cont.)**:**

- **Assumption:** $F_x(x)$ is *continuous* and *differentiable*.

- **Probability density function (pdf)**:

$$p_x(x) = \frac{dF_x(x)}{dx}$$

It assigns “mass” to values.

- **cdf** in terms of **pdf:**

$$F_x(x) = \int_{-\infty}^{x} p_x(z)dz$$

- **Probability of events** in terms of **pdf**:

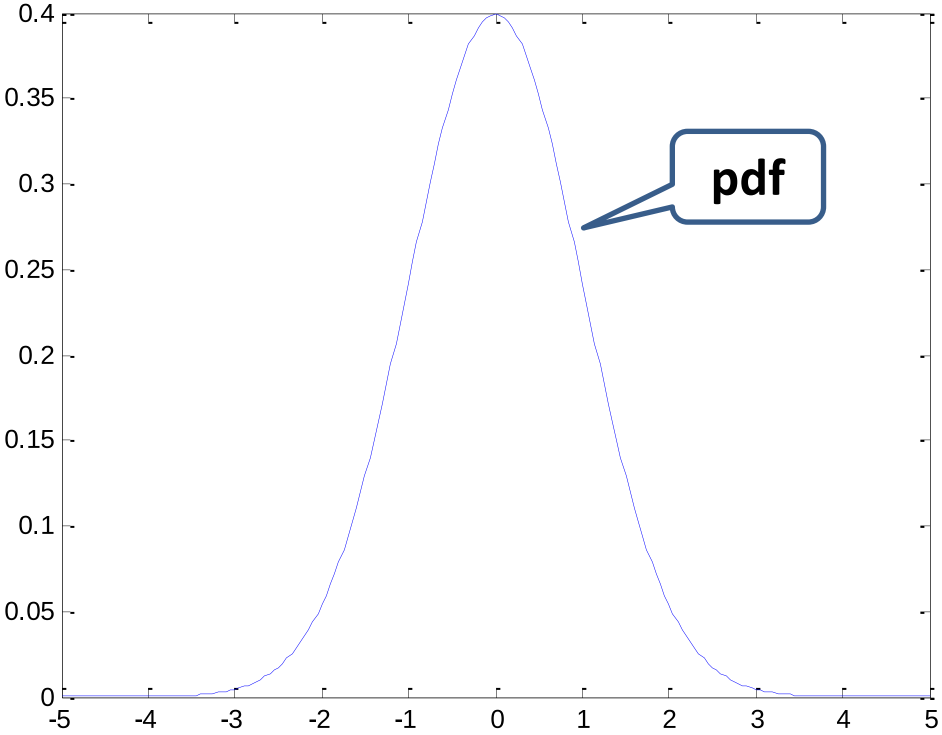
➢ $P(x \le x) = F_x(x) = \int_{-\infty}^{x} p_x(z)dz$

➢ $P(x_1 < x \le x_2) = P(x \le x_2) - P(x \le x_1) = F_x(x_2) - F_x(x_1) = \int_{x_1}^{x_2} p_x(x)dx$

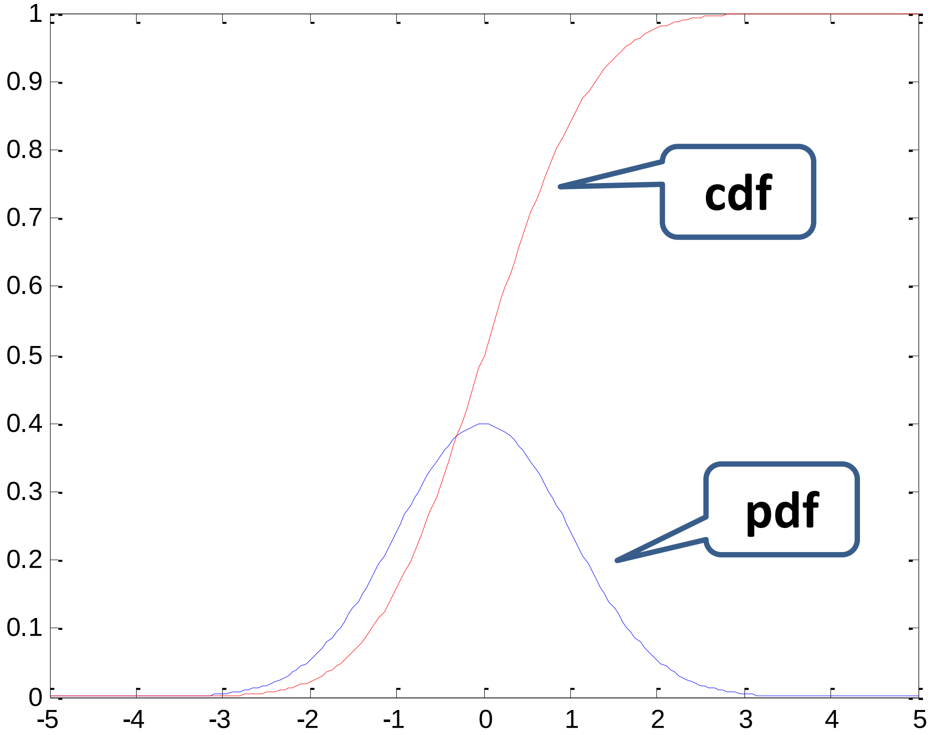
➢ $P(x \ge x) = = P(x \le \infty) - P(x \le x) = 1 - P(x \le x) = 1 - F_x(x) = \int_{-\infty}^{x} p_x(z)dz$

Probability and statistics: a brief review

Continuous random variables (cont.):



pdf



cdf

pdf

Probability and statistics: a brief review

Continuous random variables (cont.):

- Since $P(-\infty<\mathrm{x}<+\infty)=1$ it is: $\int_{-\infty}^{+\infty} p_{\mathrm{x}}(x)dx=1$

- It is $P(x<\mathrm{x}\leq x+\Delta x)=\int_{x}^{x+\Delta x} p_{\mathrm{x}}(z)dz \approx p_{\mathrm{x}}(x)\Delta x$

As $\Delta x \to 0$, $P(x<\mathrm{x}<x+\Delta x)=P(\mathrm{x}=x)=0$.

The probability of a continuous rv to take a single value is zero.

The case of more than one variables:

Continuous RV	x	y
Sample space	R	R

NOTE: All rules stated for the probability mass function in the discrete case are stated for the pdf in the continuous case.

Product rule

$$p(x,y)=p(x\,|\,y)\,p(y)$$

We drop the name of rv from the subscript of *p*.

Sum rule

$$p(x)=\int_{-\infty}^{+\infty} p(x,y)dy$$

Probability and statistics: a brief review

Useful quantities related to (continuous) rvs:

For **discrete** rv's, the integrals become summations.

- **Mean** (**expected**) **value** of a **rv** *x*: $\mathrm{E}[\mathrm{x}] = \int_{-\infty}^{+\infty} xp(x)dx$

- **Variance** of a **rv** *x* : $\sigma_{\mathrm{x}}^2 = \int_{-\infty}^{+\infty} (x - \mathrm{E}[\mathrm{x}])^2 p(x)dx = \mathrm{E}[(\mathrm{x} - \mathrm{E}(\mathrm{x}))^2]$

- **Mean** (**expected**) **value** of a **function** of an **rv** *x* : $\mathrm{E}[f(\mathrm{x})] = \int_{-\infty}^{+\infty} f(x)p(x)dx$

- **Mean** of a **function** of two **rv's** ***x*, *y***: $\mathrm{E}_{\mathrm{x,y}}[f(\mathrm{x, y})] = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(x,y)p(x,y)dxdy$

- **Conditional mean** of an rv *y* given *x = x*: $\mathrm{E}[\mathrm{y} \mid x] = \int_{-\infty}^{+\infty} yp(y \mid x)dy$

- It is $\mathrm{E}_{\mathrm{x,y}}[f(\mathrm{x, y})] = E_{\mathrm{x}}[E_{\mathrm{y|x}}[f(\mathrm{x, y})]]$

- **Covariance** between two **rvs** *x* and *y*: $\mathrm{cov}(\mathrm{x, y}) = \mathrm{E}[(\mathrm{x} - \mathrm{E}[\mathrm{x}])(\mathrm{y} - \mathrm{E}[\mathrm{y}])]$

- **Correlation** between two **rv's** *x* and *y*: $r_{\mathrm{xy}} \equiv \mathrm{E}(\mathrm{xy}) = \mathrm{cov}(x, y) + \mathrm{E}[\mathrm{x}]\mathrm{E}[\mathrm{y}]$

- **Correlation coefficient** $r_{xy} = \frac{E[x-E[x])(y-E[y])]}{\sigma_x\sigma_y}$

Probability and statistics: a brief review

Random vectors

- A **collection** of **rvs:** $\boldsymbol{x}=[x_1,x_2,\ldots x_l]^T$

- **Probability density function** (**pdf**) of $\boldsymbol{x}$: The joint pdf of $x_1,x_2,\ldots x_l$.

  $p(\boldsymbol{x})=p(x_1,x_2,\ldots x_l)$

- **Covariance matrix** of $\boldsymbol{x}$:

$$\mathrm{cov}(\mathbf{x}) = \mathrm{E}[(\mathbf{x}-\mathrm{E}[\mathbf{x}])(\mathbf{x}-\mathrm{E}[\mathbf{x}])^{\mathrm{T}}] = \begin{bmatrix} \mathrm{cov}(\mathrm{x}_1,\mathrm{x}_1) & \cdots & \mathrm{cov}(\mathrm{x}_1,\mathrm{x}_l) \\ \vdots & \ddots & \vdots \\ \mathrm{cov}(\mathrm{x}_l,\mathrm{x}_1) & \cdots & \mathrm{cov}(\mathrm{x}_l,\mathrm{x}_l) \end{bmatrix}$$

- **Correlation matrix** of $\boldsymbol{x}$: $R_{\mathbf{x}} = \mathrm{E}[\mathbf{x}\mathbf{x}^{\mathrm{T}}] = \begin{bmatrix} \mathrm{E}(\mathrm{x}_1\mathrm{x}_1) & \cdots & \mathrm{E}(\mathrm{x}_1\mathrm{x}_l) \\ \vdots & \ddots & \vdots \\ \mathrm{E}(\mathrm{x}_l\mathrm{x}_1) & \cdots & \mathrm{E}(\mathrm{x}_l\mathrm{x}_l) \end{bmatrix}$

- It is $R_{\mathbf{x}} \equiv \mathrm{E}[\mathbf{x}\mathbf{x}^{\mathrm{T}}] = \mathrm{cov}(\mathbf{x}) + \mathrm{E}[\mathbf{x}]\mathrm{E}[\mathbf{x}^{\mathrm{T}}]$

Exercise: Prove this identity

Probability and statistics: a brief review

Random vectors (cont.)

Exercise: Prove these statements

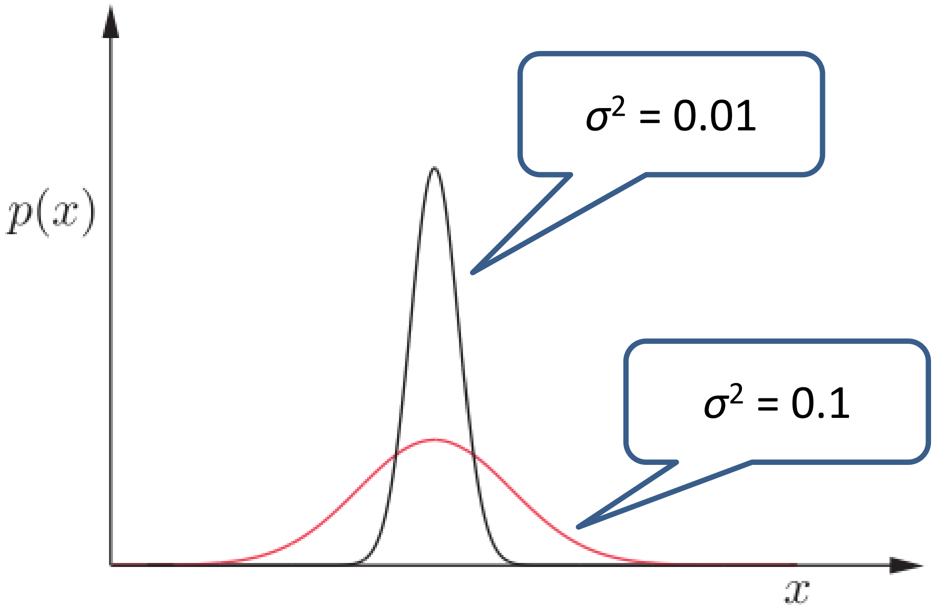
- **Remark:** Both $R_{\boldsymbol{x}}$ and cov($\boldsymbol{x}$) are symmetric and positive definite lxl matrices.

A square matrix A is symmetric iff $A^{\mathrm{T}}=A$.

A square matrix A is positive definite iff $\boldsymbol{z}^{\mathrm{T}}A\boldsymbol{z}>0,\ \forall \boldsymbol{z}\in \mathrm{R}^{l}$.

Probability and statistics: a brief review

- **One dim. normal (Gaussian) distribution** $x \sim N(\mu,\sigma^2)$ **or** $N(x|\mu,\sigma^2)$ **:**
  - Sample space: R
  - It is
    - $$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{(x-\mu)^2}{2\sigma^2})$$
    - $E[x]=\mu$
    - $\sigma_x^2 = \sigma^2$.



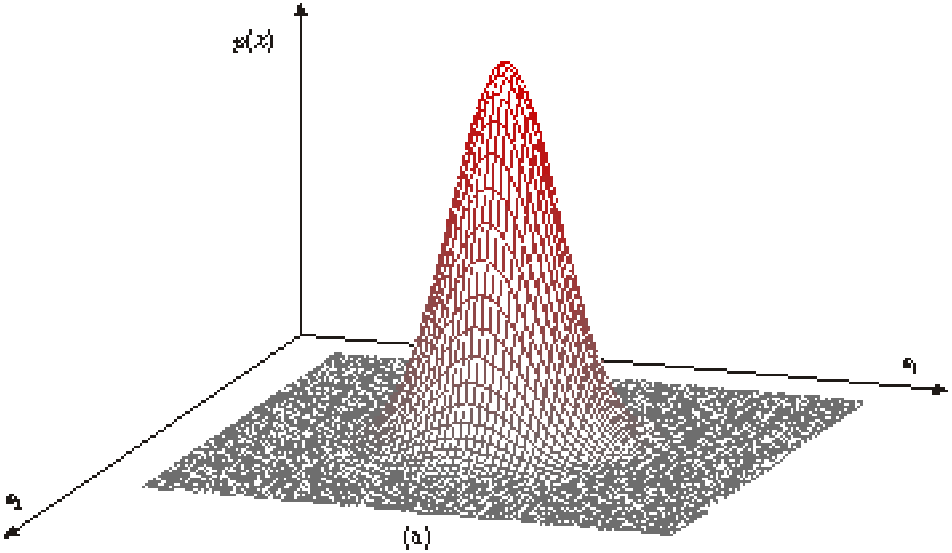
Probability and statistics: a brief review

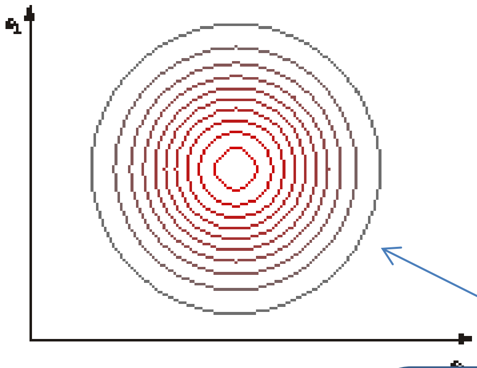
- **Multi dim. normal (Gaussian) distribution $\boldsymbol{x}\sim N(\boldsymbol{\mu},\boldsymbol{\Sigma})$ or $N(\boldsymbol{x}|\ \boldsymbol{\mu},\boldsymbol{\Sigma})$:**

  - Sample space: R^l
  - It is
    - $p(\boldsymbol{x}) = \dfrac{1}{(2\pi)^{l/2}\,|\Sigma|^{1/2}}\exp\left(-\dfrac{(\boldsymbol{x}-\boldsymbol{\mu})^{\mathrm{T}}\Sigma^{-1}(\boldsymbol{x}-\boldsymbol{\mu})}{2}\right)$
    - E[**x**]=$\boldsymbol{\mu}$
    - *cov*(**x**) = *Σ*.

Probability and statistics: a brief review

- **Multi dim. normal (Gaussian) distribution $\boldsymbol{x} \sim N(\boldsymbol{\mu},\boldsymbol{\Sigma})$ or $N(\boldsymbol{x}|\ \boldsymbol{\mu},\boldsymbol{\Sigma})$:**

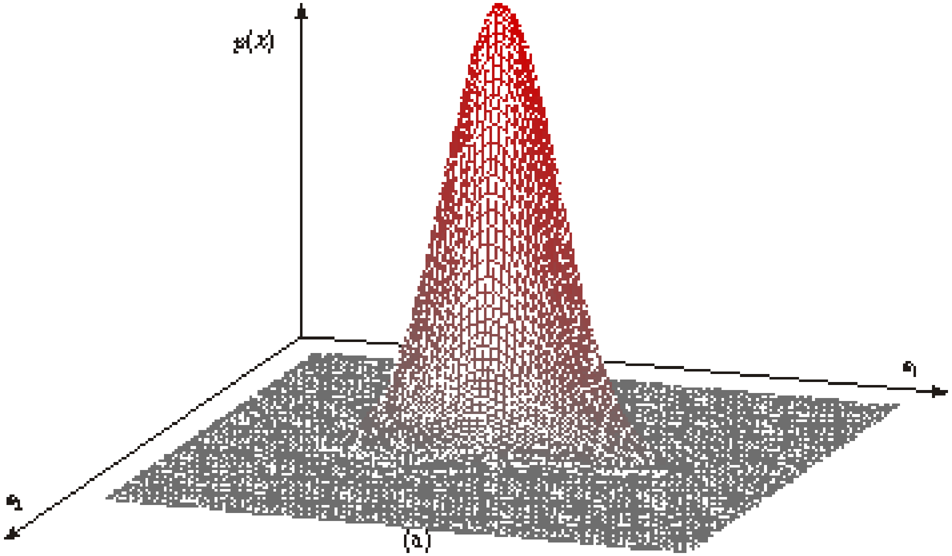


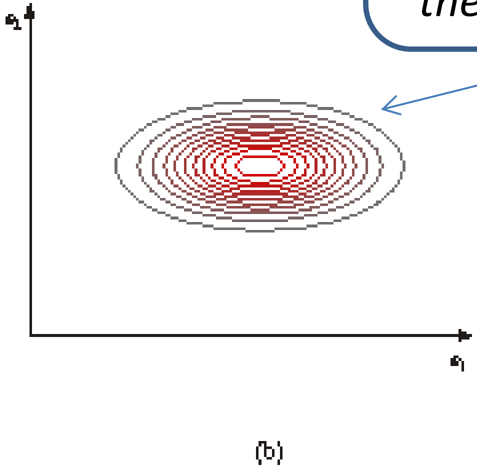


Σ: diagonal with equal diagonal entries

Isovalued curves:

- $(\boldsymbol{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\boldsymbol{x}-\mu)=const.$
- *All points on it share the value $p(\boldsymbol{x})$*

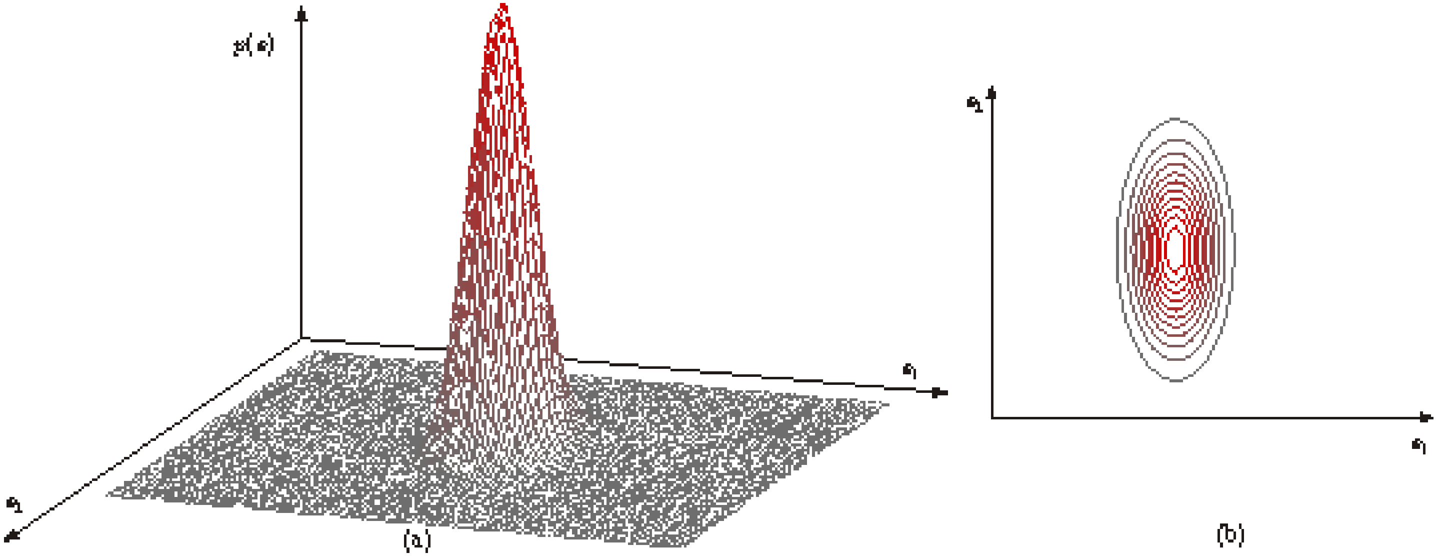




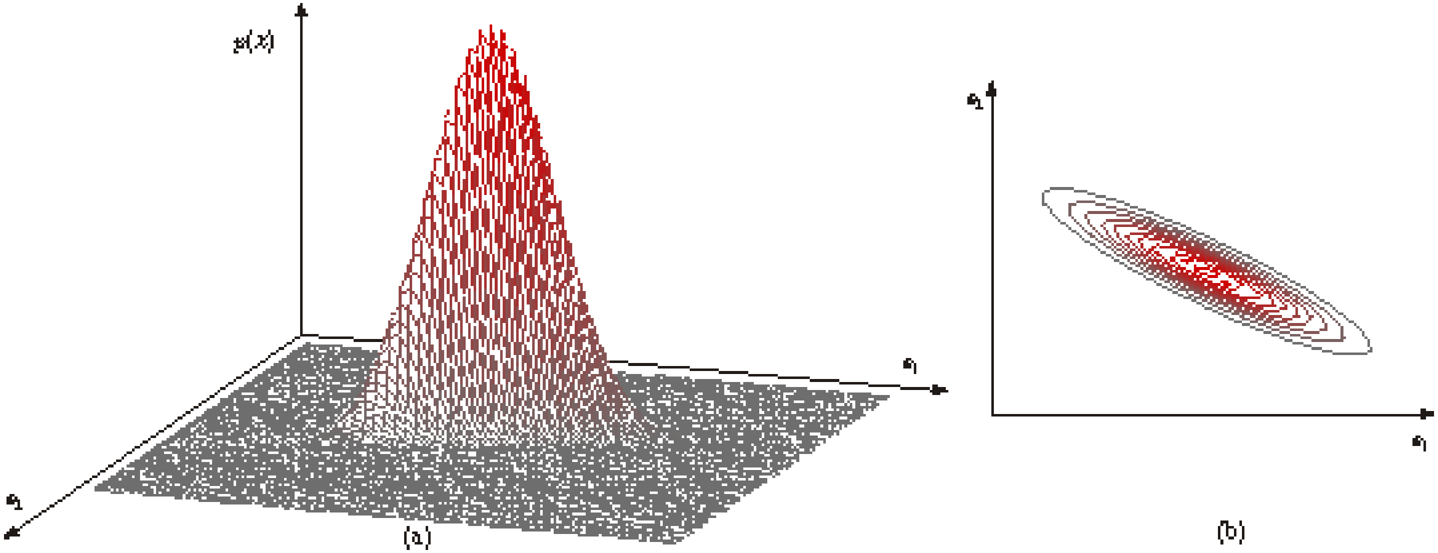
Σ: diagonal with $\sigma_1^2 >> \sigma_2^2$

Probability and statistics: a brief review

- **Multi dim. normal (Gaussian) distribution $\boldsymbol{x} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ or $N(\boldsymbol{x} | \boldsymbol{\mu}, \boldsymbol{\Sigma})$:**

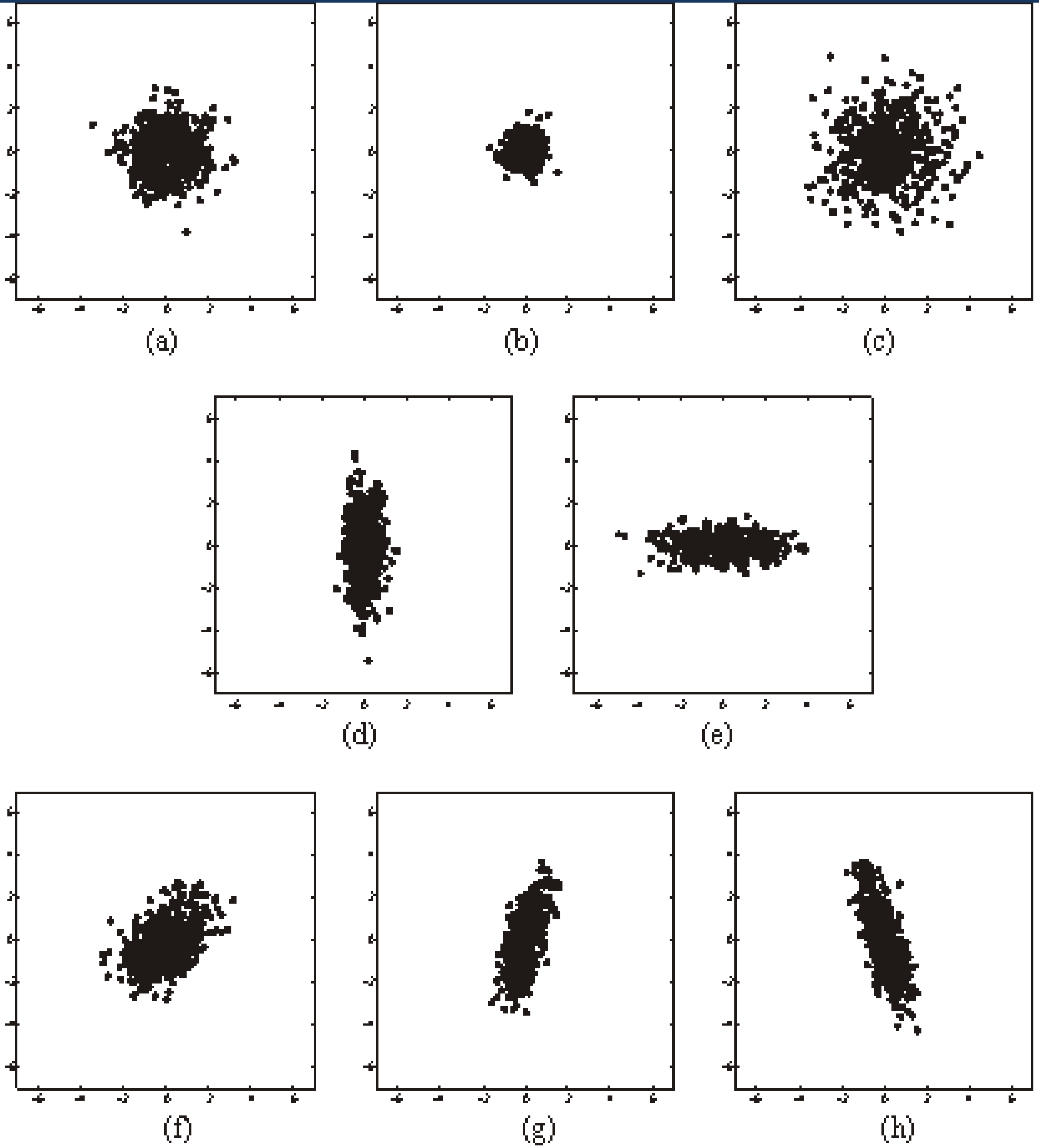


Σ: diagonal with $\sigma_1^2 << \sigma_2^2$



Σ: non diagonal

Probability and statistics: a brief review



$$\Sigma=\begin{bmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{bmatrix}$$

(α) $\sigma_1^2=\sigma_2^2=1, \sigma_{12}=0$

(β) $\sigma_1^2=\sigma_2^2=0.2, \sigma_{12}=0$

(γ) $\sigma_1^2=\sigma_2^2=2, \sigma_{12}=0$

(δ) $\sigma_1^2=0.2, \sigma_2^2=2, \sigma_{12}=0$

(ε) $\sigma_1^2=2, \sigma_2^2=0.2, \sigma_{12}=0$

(στ) $\sigma_1^2=\sigma_2^2=1, \sigma_{12}=0.5$

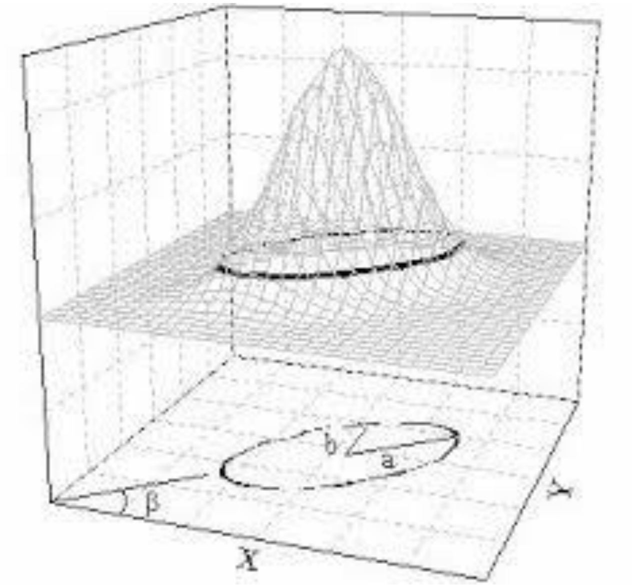
(ζ) $\sigma_1^2=0.3, \sigma_2^2=2, \sigma_{12}=0.5$

(η) $\sigma_1^2=0.3, \sigma_2^2=2, \sigma_{12}=-0.5$

Probability and statistics: a brief review

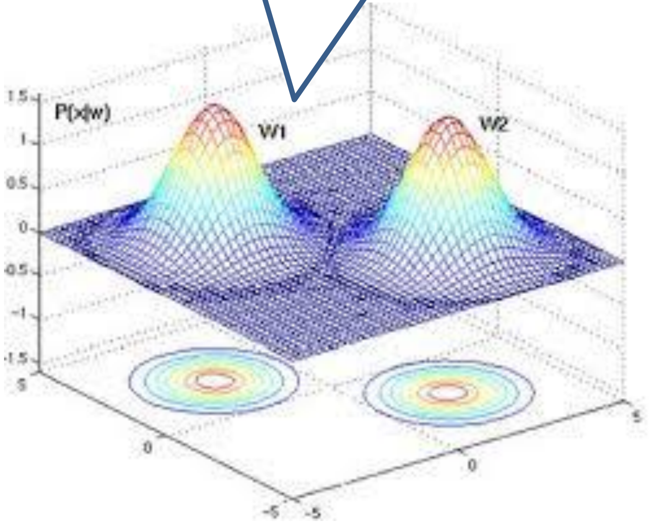
Continuous RV distributions (cont.)

- **Other examples of multi-dimensional pdfs**



Two-dim. pdfs

Bimodal distribution



Probability and statistics: a brief review

Likelihood function

- Let $X = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N\}$ a set of independent data vectors
- Let $p_{\boldsymbol{\theta}}(\cdot)$ be a pdf belonging to a known parametric set of pdf functions of parameter vector $\boldsymbol{\theta}$.
- $p(\boldsymbol{x}) = p_{\boldsymbol{\theta}}(\boldsymbol{x}) \equiv p(\boldsymbol{x}; \boldsymbol{\theta})$.

  Examples:

  ➢If $p_{\boldsymbol{\theta}}(\boldsymbol{x})$ is normal distribution parameterized on the mean vector $\boldsymbol{\mu}$, $\boldsymbol{\theta}$ will simply be $\boldsymbol{\mu}$.

  ➢If $p_{\boldsymbol{\theta}}(\boldsymbol{x})$ is normal distribution parameterized on both the mean vector $\boldsymbol{\mu}$ and the cov. matrix Σ, $\boldsymbol{\theta}$ will contain the coordinates of both $\boldsymbol{\mu}$ and Σ.

Likelihood function of $\boldsymbol{\theta}$ wrt X: $p(X; \boldsymbol{\theta}) = p(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N; \boldsymbol{\theta}) = \prod_{i=1}^{N} p(\boldsymbol{x}_i; \boldsymbol{\theta})$

Log-likelihood function of $\boldsymbol{\theta}$ wrt X:

$$L(\boldsymbol{\theta}) = \ln p(X; \boldsymbol{\theta}) = \ln p(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N; \boldsymbol{\theta}) = \sum_{i=1}^{N} \ln p(\boldsymbol{x}_i; \boldsymbol{\theta})$$

Probability and statistics: a brief review

Likelihood function

Example:

- $X = \{-2, -1, 0, 1, 2\}$

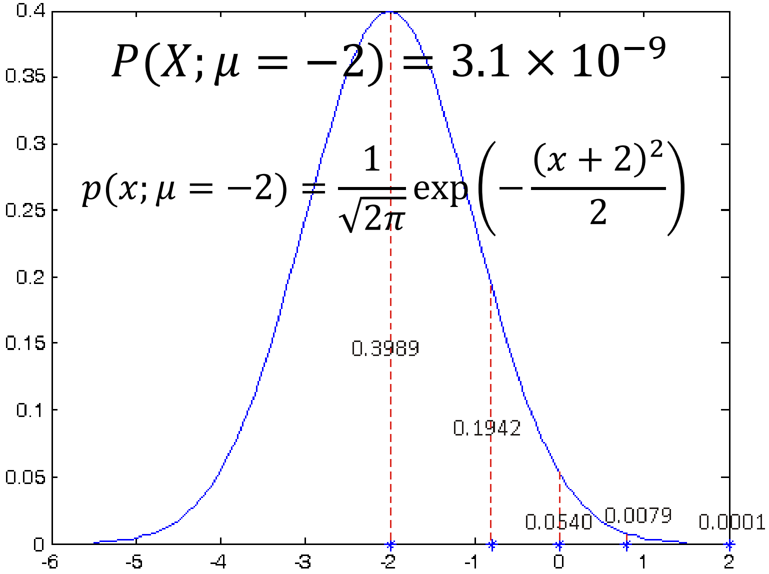
$$p(x) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{(x-\mu)^2}{2})$$

- Consider the parametric set of normal distributions of unit variance, parameterized on μ.
- The likelihood of μ wrt X is

$$p(X;\mu) = p(-2,-1,0,1,2;\mu) =$$
$$\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(-2-\mu)^2}{2}\right) \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(-1-\mu)^2}{2}\right) \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(0-\mu)^2}{2}\right)$$
$$\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(1-\mu)^2}{2}\right) \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(2-\mu)^2}{2}\right)$$

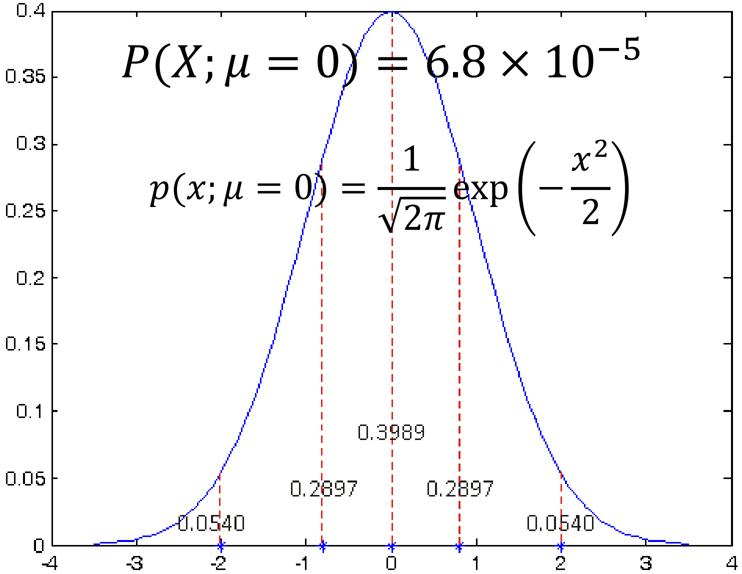
Probability and statistics: a brief review

Likelihood function



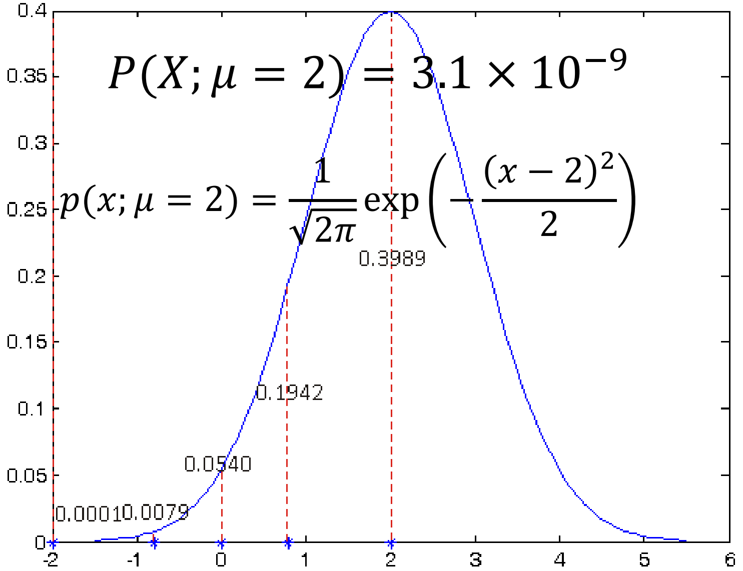
$$P(X;\mu = -2) = 3.1 \times 10^{-9}$$

$$p(x;\mu = -2) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x+2)^2}{2}\right)$$



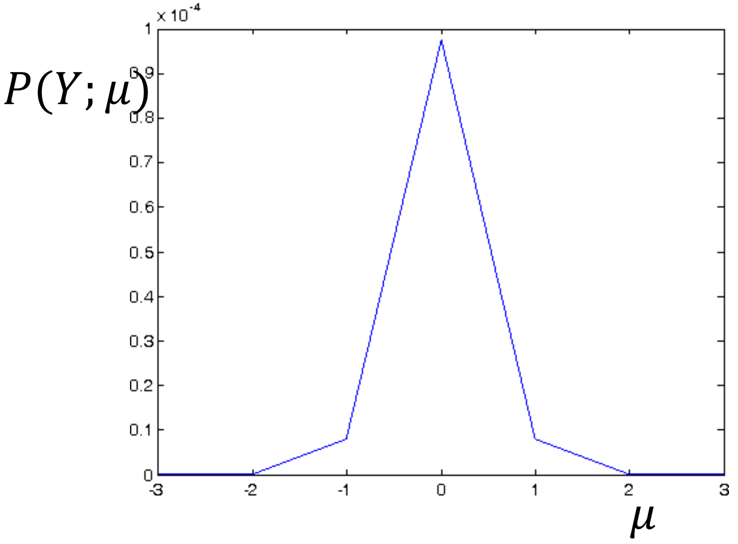
$$P(X;\mu = 0) = 6.8 \times 10^{-5}$$

$$p(x;\mu = 0) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$$



$$P(X;\mu = 2) = 3.1 \times 10^{-9}$$

$$p(x;\mu = 2) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x-2)^2}{2}\right)$$



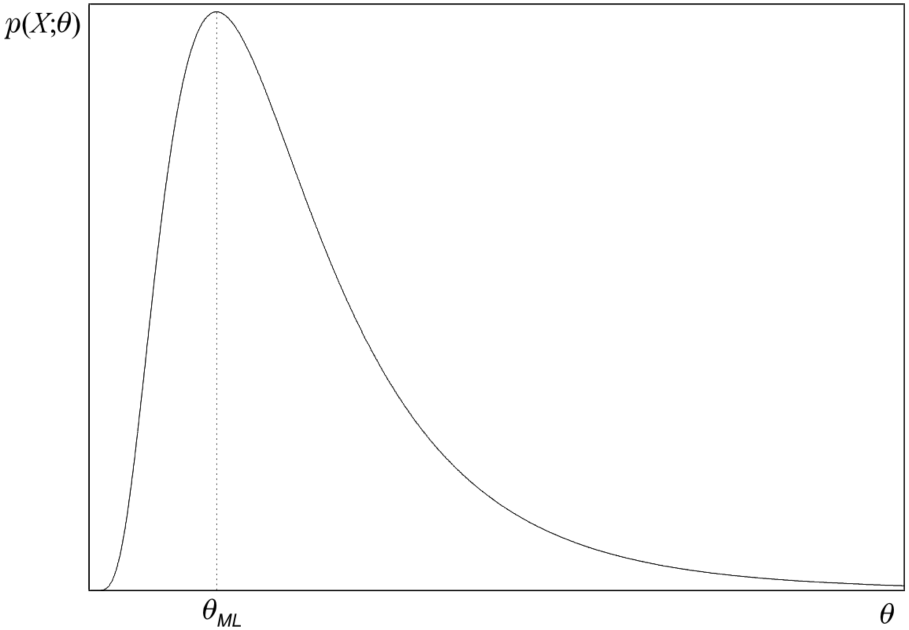
Probabilistic CFO clustering algorithms

Maximum likelihood (ML) method:

Given a set of independent data vectors $Y = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N\}$, estimate the parameter vector $\boldsymbol{\theta}$ as the maximum of the likelihood ($p(Y;\boldsymbol{\theta})$) or the log-likelihood ($L(\boldsymbol{\theta})$) function.

$$\boxed{\hat{\boldsymbol{\theta}}_{ML} = argmax_{\boldsymbol{\theta}}\, p(Y;\boldsymbol{\theta})} \rightarrow \boxed{\hat{\boldsymbol{\theta}}_{ML}: \frac{\partial L(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \sum_{\kappa=1}^{\mathrm{N}} \frac{1}{p(\boldsymbol{x}_k;\theta)} \frac{\partial p(\boldsymbol{x}_k;\theta)}{\partial \boldsymbol{\theta}} = \mathbf{0}}$$

Since $\ln(\cdot)$ is an increasing function, $p(Y;\boldsymbol{\theta})$ and $L(\boldsymbol{\theta})$ share the same maxima.



Probabilistic CFO clustering algorithms

Maximum likelihood (ML) method:

Assuming that

- the chosen model $p(\boldsymbol{x};\ \boldsymbol{\theta})$ is correct and
- there exists a true parameter $\boldsymbol{\theta}_{\boldsymbol{o}}$,

the ML estimator

(a) is asymptotically **unbiased** $lim_{N\to\infty}E\left[\widehat{\boldsymbol{\theta}}_{ML}\right]=\boldsymbol{\theta}_{o}$

(b) is asymptotically **consistent** $lim_{N\to\infty}Prob\left\{\left\|\widehat{\boldsymbol{\theta}}_{ML}-\boldsymbol{\theta}_{o}\right\|\right\}=0$

(c) is asymptotically **efficient** (it achieves the Cramer-Rao lower bound)

The **pdf** of the ML estimator approaches the normal distribution with mean $\boldsymbol{\theta}_{\boldsymbol{o}}$, as $N\to\infty$.

Maximum likelihood method

Example 1:

-Let Y be a set of N (independent from each other) data points, $\boldsymbol{x}_i$, $i = 1, \dots, N$, generated by a normal distribution $p(\boldsymbol{x};\ \boldsymbol{\theta})$ of known covariance matrix and unknown mean.

-Determine the ML estimate of the mean $\boldsymbol{\mu}$ of $p(\boldsymbol{x};\boldsymbol{\theta})$, based on Y.

Solution:

-The unknown parameter vector in this case is the mean vector $\boldsymbol{\mu}$, i.e. $\boldsymbol{\theta} \equiv \boldsymbol{\mu}$.

-It is

$$p(\boldsymbol{x};\boldsymbol{\theta}) \equiv p(\boldsymbol{x};\boldsymbol{\mu}) = \frac{1}{(2\pi)^{l/2}|\Sigma|^{1/2}} \cdot exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right) \Rightarrow$$

$$\ln p(\boldsymbol{x};\boldsymbol{\mu}) = \ln\frac{1}{(2\pi)^{l/2}|\Sigma|^{1/2}} - \frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\boldsymbol{x}-\boldsymbol{\mu}) = C - \frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^T\Sigma^{-1}(\boldsymbol{x}-\boldsymbol{\mu})$$

Then

$$L(\boldsymbol{\mu}) = \sum_{i=1}^{N} \ln p(\boldsymbol{x}_i;\boldsymbol{\mu}) = NC - \frac{1}{2}\sum_{i=1}^{N}(\boldsymbol{x}_i-\boldsymbol{\mu})^T\Sigma^{-1}(\boldsymbol{x}_i-\boldsymbol{\mu})$$

Maximum likelihood method

Example 1 (cont.):

Setting the gradient of $L(\boldsymbol{\mu})$ wrt $\boldsymbol{\mu}$ equal to $\mathbf{0}$ we have

$$\frac{\partial L(\boldsymbol{\mu})}{\partial \boldsymbol{\mu}} = \frac{\partial}{\partial \boldsymbol{\mu}}\left(NC - \frac{1}{2}\sum_{i=1}^{N}(\boldsymbol{x}_i - \boldsymbol{\mu})^T\Sigma^{-1}(\boldsymbol{x}_i - \boldsymbol{\mu})\right) = \mathbf{0} \Leftrightarrow$$

$$\sum_{i=1}^{N}\Sigma^{-1}(\boldsymbol{x}_i - \boldsymbol{\mu}) = \mathbf{0} \Leftrightarrow \sum_{i=1}^{N}(\boldsymbol{x}_i - \boldsymbol{\mu}) = \mathbf{0} \Leftrightarrow \sum_{i=1}^{N}\boldsymbol{x}_i - N\boldsymbol{\mu} = \mathbf{0}$$

$$\boldsymbol{\mu}_{ML} = \frac{1}{N}\sum_{i=1}^{N}\boldsymbol{x}_i$$

Remark: The ML estimate for the covariance matrix is

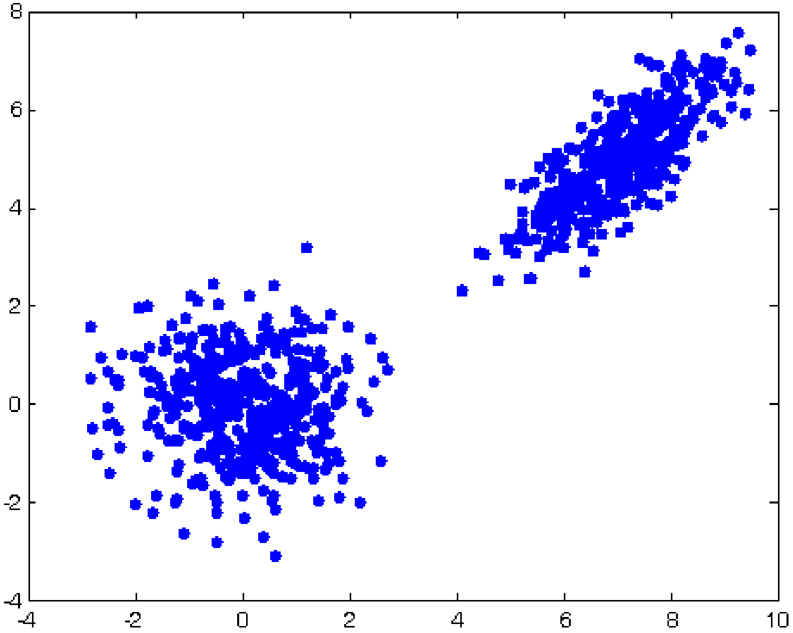
$$\Sigma_{ML} = \frac{1}{N}\sum_{i=1}^{N}(\boldsymbol{x}_i - \boldsymbol{\mu})(\boldsymbol{x}_i - \boldsymbol{\mu})^T$$

Probabilistic CFO clustering algorithms

Mixture models - The Expectation – Maximization (EM) algorithm

Mixture model: A weighted sum of known parametric form pdfs.

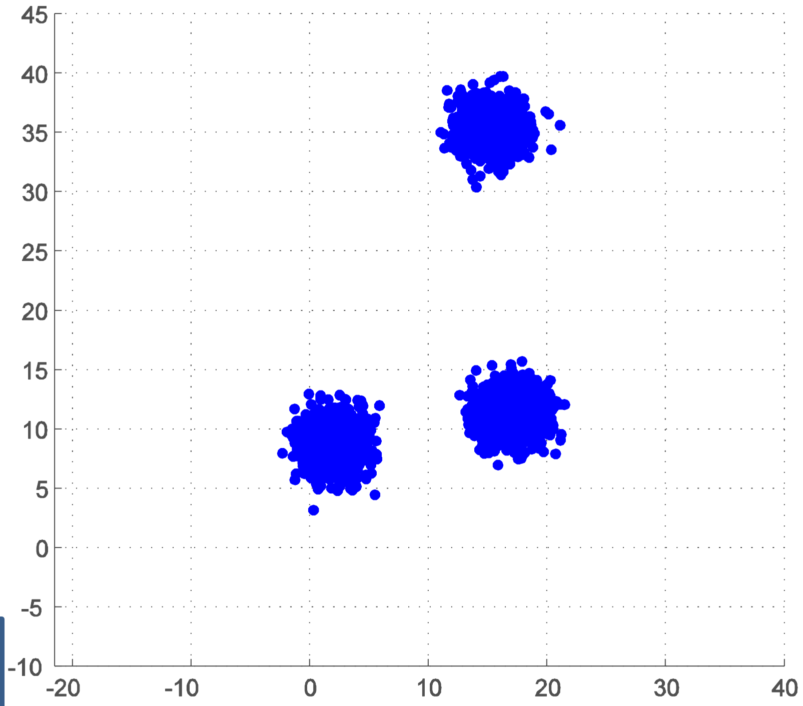
$$p(\boldsymbol{x}) = \sum_{j=1}^{m} P_j \, p(\boldsymbol{x} \mid j), \quad \sum_{j=1}^{m} P_j = 1, \quad \int_{-\infty}^{+\infty} p(\boldsymbol{x} \mid j) = 1$$



- Assume that $p(\boldsymbol{x})$ models the distribution of the data in X (each pdf models a cluster).

- The **aim** is to **move** each pdf so that to "cover" the area in the data space where the vectors of each cluster lie (**mixture decomposition**).

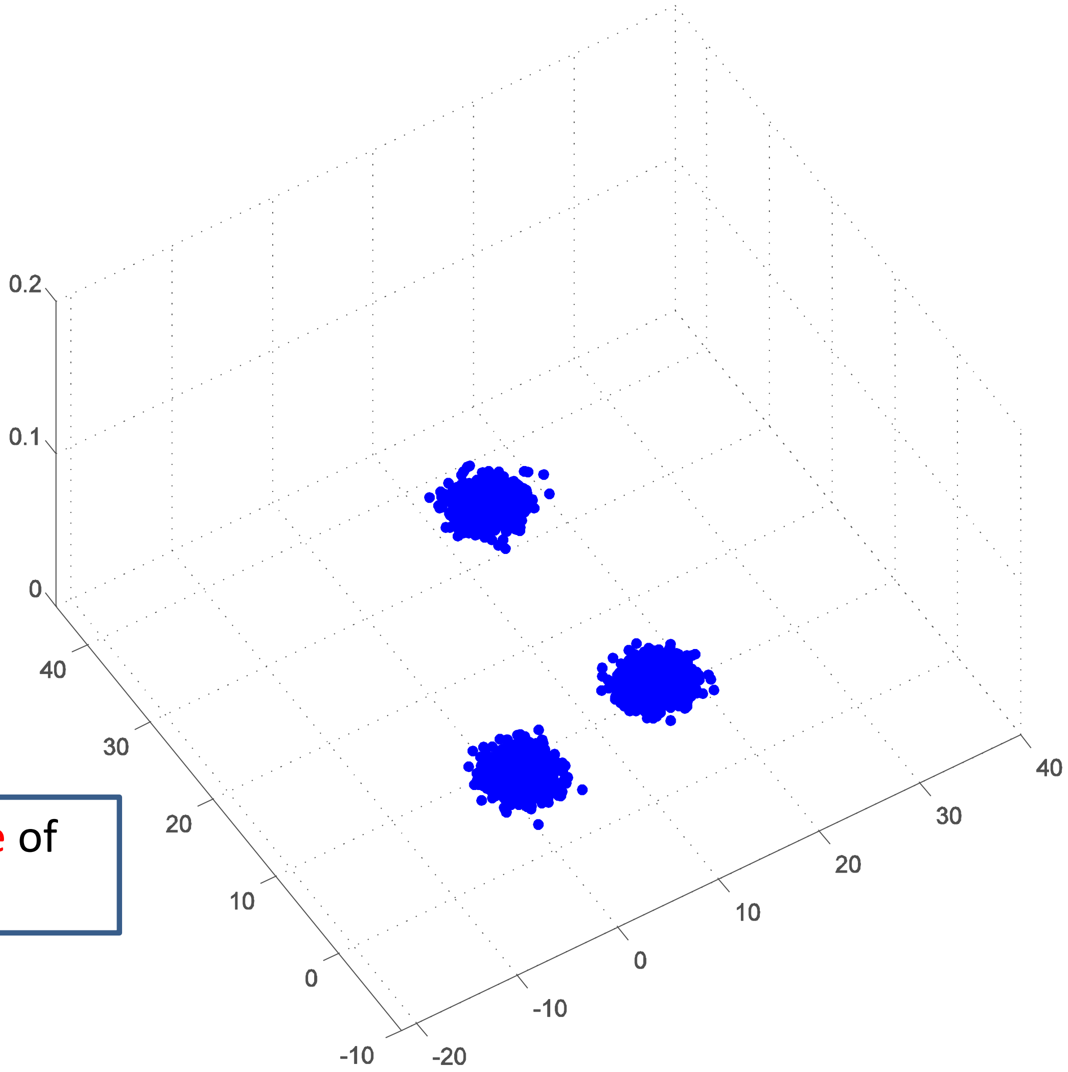
Probabilistic CFO clustering algorithms



Prerequisite: Knowledge of the number of clusters.

- **Adopt** a parametric mixture of distributions, each one corresponding to a cluster (e.g., mixture of Gaussians), initialized randomly.
- **Move** iteratively the distributions each one above a cluster, **optimizing** a criterion.

Probabilistic CFO clustering algorithms



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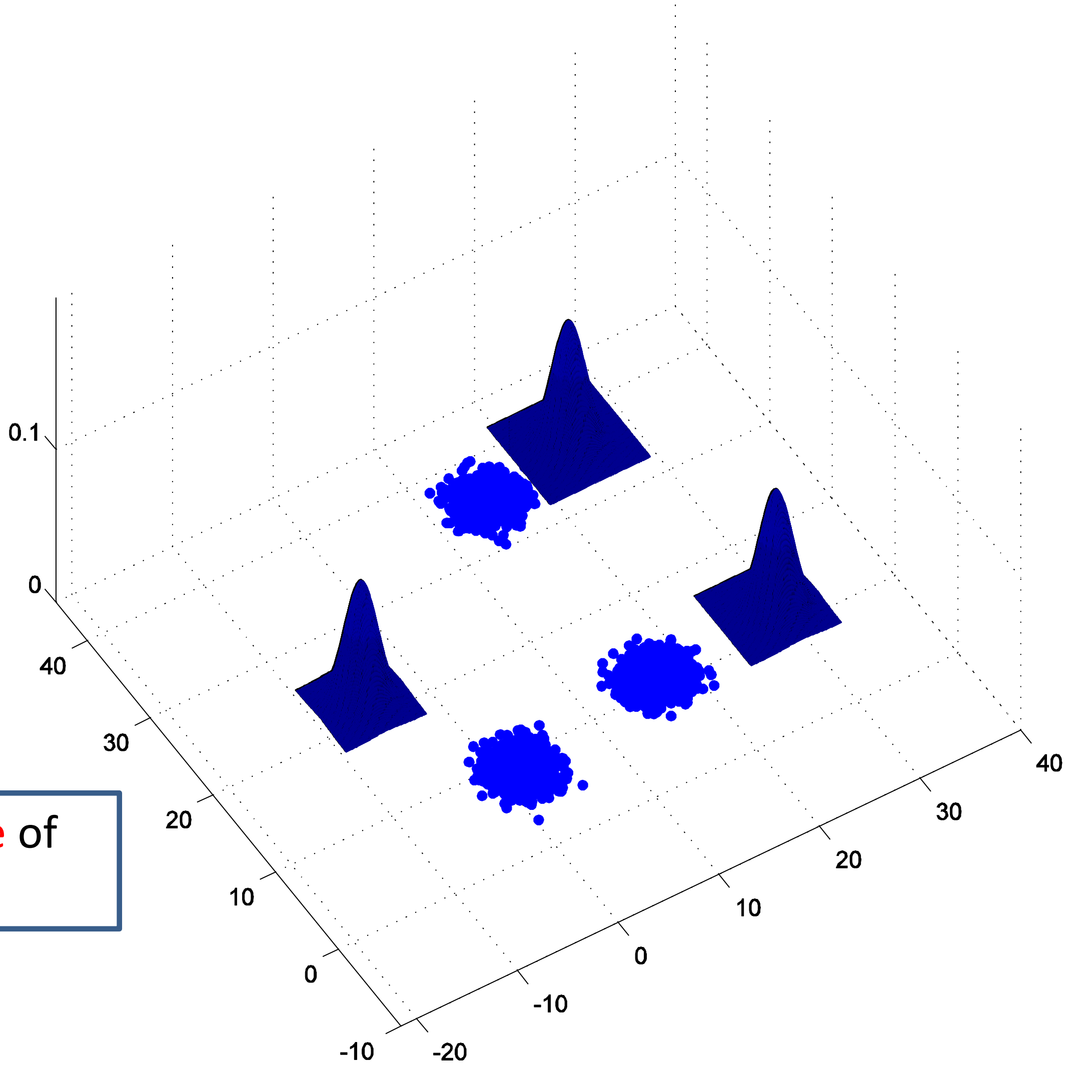
Probabilistic CFO clustering algorithms



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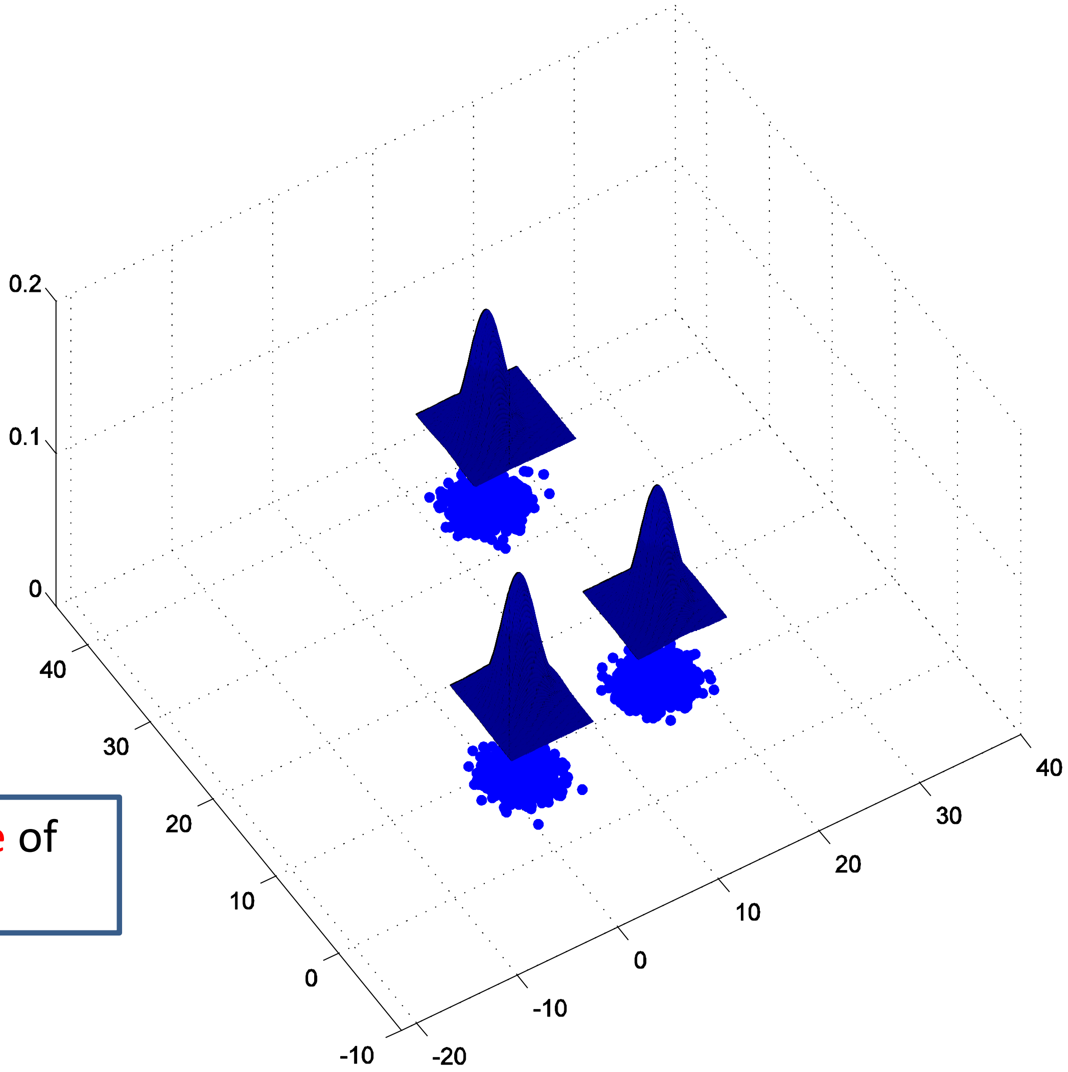
Probabilistic CFO clustering algorithms



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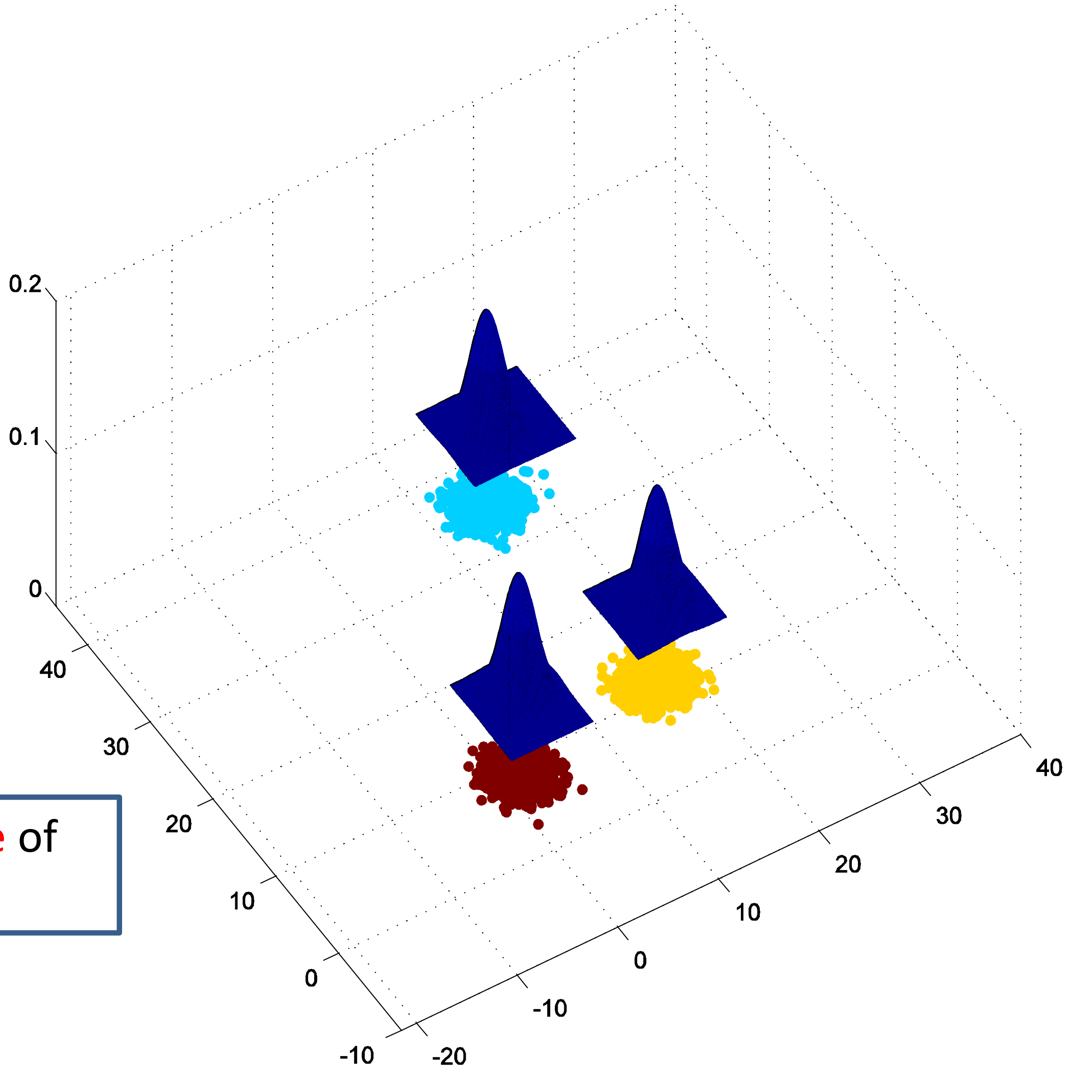
Probabilistic CFO clustering algorithms



Prerequisite: Knowledge of the number of clusters.

- **Adopt** a parametric mixture of distributions, each one corresponding to a cluster (e.g., mixture of Gaussians), initialized randomly.
- **Move** iteratively the distributions each one above a cluster, **optimizing** a criterion.

Probabilistic CFO clustering algorithms

Let $X = \{x_1, x_2, \dots, x_N\}$ be a set of data points.

Each vector belongs exclusively to a single cluster, with a certain probability.

Each cluster is **modeled** by a pdf $p(\boldsymbol{x}|j)$, parameterized by the vector $\boldsymbol{\theta}_j$.

Let:

$\Theta = \{\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \dots, \boldsymbol{\theta}_m\}$

$P = \{P_1, P_2, \dots, P_m\}$, the set of a priori probabilities of the clusters.

$P(j|\boldsymbol{x}) \equiv P\left(j\middle|\boldsymbol{x}; \boldsymbol{\theta}_j\right)$ the (a posteriori) probability of cluster j, given $\boldsymbol{x}$.

$p(\boldsymbol{x}|j) \equiv p\left(\boldsymbol{x}\middle|j; \boldsymbol{\theta}_j\right)$ the pdf that models cluster j.

It is $p(\boldsymbol{x}) = \sum_{j=1}^{m} p(\boldsymbol{x}, j) = \sum_{j=1}^{m} p(\boldsymbol{x}|j)\, P_j$

Bayes rule $P(j|\boldsymbol{x}) = \frac{p(\boldsymbol{x},j)}{p(\boldsymbol{x})} = \frac{p(\boldsymbol{x}|j)\boldsymbol{P_j}}{p(\boldsymbol{x})}$

Probabilistic CFO clustering algorithms

It is

- $\sum_{j=1}^{m} P(j|\boldsymbol{x}_i) = 1\,, i = 1, \ldots, N$
- $\sum_{j=1}^{m} P_j = 1\,.$

ML: $L(\boldsymbol{\theta}) = \sum_{i=1}^{N} \ln(p(\boldsymbol{x}_i; \boldsymbol{\theta}))$

Define the cost function

$$\ln p(X; \Theta, P) = \sum_{i=1}^{N} \sum_{j=1}^{m} P(j|\boldsymbol{x}_i) \ln p(\boldsymbol{x}_i, j; \boldsymbol{\theta}_j)$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{m} P(j|\boldsymbol{x}_i) \ln\left(p\left(\boldsymbol{x}_i \middle| j; \boldsymbol{\theta}_j\right) P_j\right)$$

When $\ln p(X; \Theta, P)$ is **maximized**?

When large $P(j|\boldsymbol{x}_i)$’s are **multiplied** by large $\ln p(\boldsymbol{x}_i, j; \boldsymbol{\theta}_j)$ ‘s.

Probabilistic CFO clustering algorithms

For **fixed $\boldsymbol{\theta}_j$'s:** Use the Bayes rule $P(j|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|j;\boldsymbol{\theta}_j)\boldsymbol{P_j}}{p(\boldsymbol{x};\boldsymbol{\Theta})}$

For **fixed $P(j|\boldsymbol{x})$'s:** Solve the following maximization problem

$$max_{\Theta,P} \sum_{i=1}^{N} \sum_{j=1}^{m} P(j|\boldsymbol{x}_i) \ln\left(p\left(\boldsymbol{x}_i\middle|j;\boldsymbol{\theta}_j\right)P_j\right)$$

$$= max_{\Theta,P} \left[\sum_{i=1}^{N} \sum_{j=1}^{m} P(j|\boldsymbol{x}_i) \ln\left(p\left(\boldsymbol{x}_i\middle|j;\boldsymbol{\theta}_j\right)\right) + \sum_{i=1}^{N} \sum_{j=1}^{m} P(j|\boldsymbol{x}_i) \ln P_j\right]$$

Subject to the constraint $\sum_{j=1}^{m} P_j = 1$.

Mixture models – Expectation-Maximization (EM) algorithm

For **fixed $\boldsymbol{\theta}_j$‘s:** Use the Bayes rule $P(j|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|j;\boldsymbol{\theta}_j)\boldsymbol{P_j}}{p(\boldsymbol{x};\boldsymbol{\Theta})}$

For **fixed $P(j|\boldsymbol{x})$‘s:** Solve the following maximization problem

$$max_{\Theta,P} \sum_{i=1}^{N} \sum_{j=1}^{m} P(j|\boldsymbol{x}_i) \ln\left(p(\boldsymbol{x}_i|j;\boldsymbol{\theta}_j)P_j\right) =$$

$$max_{\Theta} \sum_{i=1}^{N} \sum_{j=1}^{m} P(j|\boldsymbol{x}_i) \ln\left(p(\boldsymbol{x}_i|j;\boldsymbol{\theta}_j)\right) + max_P \sum_{i=1}^{N} \sum_{j=1}^{m} P(j|\boldsymbol{x}_i) \ln P_j$$

$$= max_{\Theta} \sum_{j=1}^{m} \sum_{i=1}^{N} P(j|\boldsymbol{x}_i) \ln\left(p(\boldsymbol{x}_i|j;\boldsymbol{\theta}_j)\right) + max_P \sum_{i=1}^{N} \sum_{j=1}^{m} P(j|\boldsymbol{x}_i) \ln P_j$$

Subject to the **constraint** $\sum_{j=1}^{m} P_j = 1$.

The above maximization problem is equivalent to the following maximization sub-problems

– $\boldsymbol{\theta}_j = argmax_{\boldsymbol{\theta}_j} \sum_{i=1}^{N} P(j|\boldsymbol{x_i}) \ln\left(p(\boldsymbol{x}_i|j;\boldsymbol{\theta}_j)\right), j = 1, \dots, m$

– $P \equiv \{P_1, P_2, \dots, P_m\} = argmax_P \sum_{i=1}^{N} \sum_{j=1}^{m} P(j|\boldsymbol{x_i}) \ln P_j, s.t. \sum_{j=1}^{m} P_j = 1 \Leftrightarrow$

$$P_j = \frac{1}{N} \sum_{i=1}^{N} P(j|\boldsymbol{x_i}), j = 1, \dots, m$$

Probabilistic CFO clustering algorithms

Generalized probabilistic Algorithmic Scheme (GPrAS)

```
• Choose $\boldsymbol{\theta}_j(0)$, $P_j(0)$ as initial estimates for $\boldsymbol{\theta}_j, P_j,$ respectively, $j = 1, \dots, m$
• t=0
• Repeat
    – For i=1 to N  % Expectation step
        o For j=1 to m
            $P(j|\boldsymbol{x}_i;\Theta^{(t)},P^{(t)}) = \frac{p(x_i|j;\theta_j{}^{(t)})P_j{}^{(t)}}{\sum_{q=1}^{m} p(x_i|q;\theta_q{}^{(t)})P_q{}^{(t)}} \equiv \gamma_{ji}{}^{(t)}$
        o End {For-j}
    – End {For-i}
    – t=t+1
    – For j=1 to m % Parameter updating – Maximization step
        o Set
            $\boldsymbol{\theta}_j{}^{(t)} = argmax_{\boldsymbol{\theta}_j} \sum_{i=1}^{N} \gamma_{ji}{}^{(t-1)} \ln\left(p\left(\boldsymbol{x}_i\middle|j;\boldsymbol{\theta}_j\right)\right), j = 1, \dots, m$
            $P_j{}^{(t)} = \frac{1}{N}\sum_{i=1}^{N} \gamma_{ji}{}^{(t-1)}, j = 1, \dots, m$
    - End {For-j}
• Until a termination criterion is met.
```

Probabilistic CFO clustering algorithms

Remark: The above algorithm is an instance of the more general Expectation-Maximization (EM) framework.

<u>GPrAS – The case of normal pdfs</u>

Each cluster is **modeled** by a normal distribution

$$p(\boldsymbol{x}|j;\mu_j,\Sigma_j)=\frac{1}{(2\pi)^l|\Sigma_j|^{1/2}}\exp\left(-\frac{(\boldsymbol{x}-\boldsymbol{\mu}_j)^T{\Sigma_j}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_j)}{2}\right), j=1,\dots m$$

In this case $\boldsymbol{\theta}_j=\{\boldsymbol{\mu}_j,\Sigma_j\}$.

$$\{\boldsymbol{\mu}_j,\Sigma_j\}=argmax_{\{\boldsymbol{\mu}_j,\Sigma_j\}}\sum_{i=1}^{N}P(j|\boldsymbol{x}_i)\ln\left(p(\boldsymbol{x}_i|j;\boldsymbol{\mu}_j,\Sigma_j)\right)$$

Equating the gradient of the above function wrt $\boldsymbol{\mu}_j,\Sigma_j$ to **0** and *O*, respectively, we have

$$\boldsymbol{\mu}_j=\frac{\sum_{i=1}^{N}P(j|\boldsymbol{x}_i)\boldsymbol{x}_i}{\sum_{i=1}^{N}P(j|\boldsymbol{x}_i)}$$

$$\Sigma_j=\frac{\sum_{i=1}^{N}P(j|\boldsymbol{x}_i)(\boldsymbol{x}_i-\boldsymbol{\mu}_j)\,(\boldsymbol{x}_i-\boldsymbol{\mu}_j)^{\boldsymbol{T}}}{\sum_{i=1}^{N}P(j|\boldsymbol{x}_i)}$$

Probabilistic CFO clustering algorithms

GPrAS – The normal pdfs case

```
•  Choose $\boldsymbol{\mu}_j(0)$, $\Sigma_j(0)$, $P_j(0)$ as initial estimates for $\boldsymbol{\mu}_j, \Sigma_j, P_j$, resp., $j = 1, \dots, m$
•  $t$=0
•  Repeat
     – For $i$=1 to $N$  % Expectation step
          o For $j$=1 to $m$
               $P(j|\boldsymbol{x}_i; \Theta^{(t)}, P^{(t)}) = \frac{p(x_i|j;\theta_j^{(t)})P_j^{(t)}}{\sum_{q=1}^{m} p(x_i|q;\theta_q^{(t)})P_q^{(t)}} \equiv \gamma_{ji}^{(t)}$
          o End {For-$j$}
     – End {For-$i$}
     –$t$=$t$+1
     – For $j$=1 to $m$ % Parameter updating – Maximization step
          o Set
               $\boldsymbol{\mu}_j^{(t)} = \frac{\sum_{i=1}^{N} \gamma_{ji}^{(t-1)} \boldsymbol{x}_i}{\sum_{i=1}^{N} \gamma_{ji}^{(t-1)}}, \quad \Sigma_j^{(t)} = \frac{\sum_{i=1}^{N} \gamma_{ji}^{(t-1)} (\boldsymbol{x}_i - \boldsymbol{\mu}_j)(\boldsymbol{x}_i - \boldsymbol{\mu}_j)^{\boldsymbol{T}}}{\sum_{i=1}^{N} \gamma_{ji}^{(t-1)}} \quad j = 1, \dots, m$
               $P_j^{(t)} = \frac{1}{N} \sum_{i=1}^{N} \gamma_{ji}^{(t-1)}, j = 1, \dots, m$
     - End {For-$j$}
•  Until a termination criterion is met.
```

Probabilistic CFO clustering algorithms

GPrAS – The normal pdfs case

```
• Choose $\boldsymbol{\mu}_j(0), \Sigma_j(0), P_j(0)$ as initial estimates for $\boldsymbol{\mu}_j, \Sigma_j, P_j$, resp., $j = 1, \ldots, m$
• t=0
• Repeat
    – For i=1 to N  % Expectation step
        $P(C_j|\boldsymbol{x};\Theta(t)) = \dfrac{|\Sigma_j(t)|^{-1/2}\exp\left(-\frac{1}{2}(\boldsymbol{x}-\mu_j(t))^T\Sigma_j^{-1}(t)(\boldsymbol{x}-\mu_j(t))\right)P_j(t)}{\sum_{k=1}^{m}|\Sigma_k(t)|^{-1/2}\exp\left(-\frac{1}{2}(\boldsymbol{x}-\mu_k(t))^T\Sigma_k^{-1}(t)(\boldsymbol{x}-\mu_k(t))\right)P_k(t)}$
        o End {For-j}
    – End {For-i}
    –t=t+1
    – For j=1 to m % Parameter updating – Maximization step
        o Set
            $\boldsymbol{\mu}_j{}^{(t)} = \dfrac{\sum_{i=1}^{N}\gamma_{ji}{}^{(t-1)}\boldsymbol{x}_i}{\sum_{i=1}^{N}\gamma_{ji}{}^{(t-1)}}, \qquad \Sigma_j{}^{(t)} = \dfrac{\sum_{i=1}^{N}\gamma_{ji}{}^{(t-1)}(\boldsymbol{x}_i-\boldsymbol{\mu}_j)(\boldsymbol{x}_i-\boldsymbol{\mu}_j)^T}{\sum_{i=1}^{N}\gamma_{ji}{}^{(t-1)}} \quad j = 1, \ldots, m$
            $P_j{}^{(t)} = \dfrac{1}{N}\sum_{i=1}^{N}\gamma_{ji}{}^{(t-1)}, j = 1, \ldots, m$
    - End {For-j}
• Until a termination criterion is met.
```

Probabilistic CFO clustering algorithms

Remark:

- The above scheme is more computationally demanding since it requires the inversion of the m covariance matrices at each iteration step. Two ways to deal with this problem are:
    - The use of a single covariance matrix for all clusters.
    - The use of different diagonal covariance matrices.

Example: (a) Consider three two-dimensional normal distributions with mean values:

$$\boldsymbol{\mu}_1=[1,\ 1]^T,\ \boldsymbol{\mu}_2=[3.5,\ 3.5]^T,\ \boldsymbol{\mu}_3=[6,\ 1]^T$$

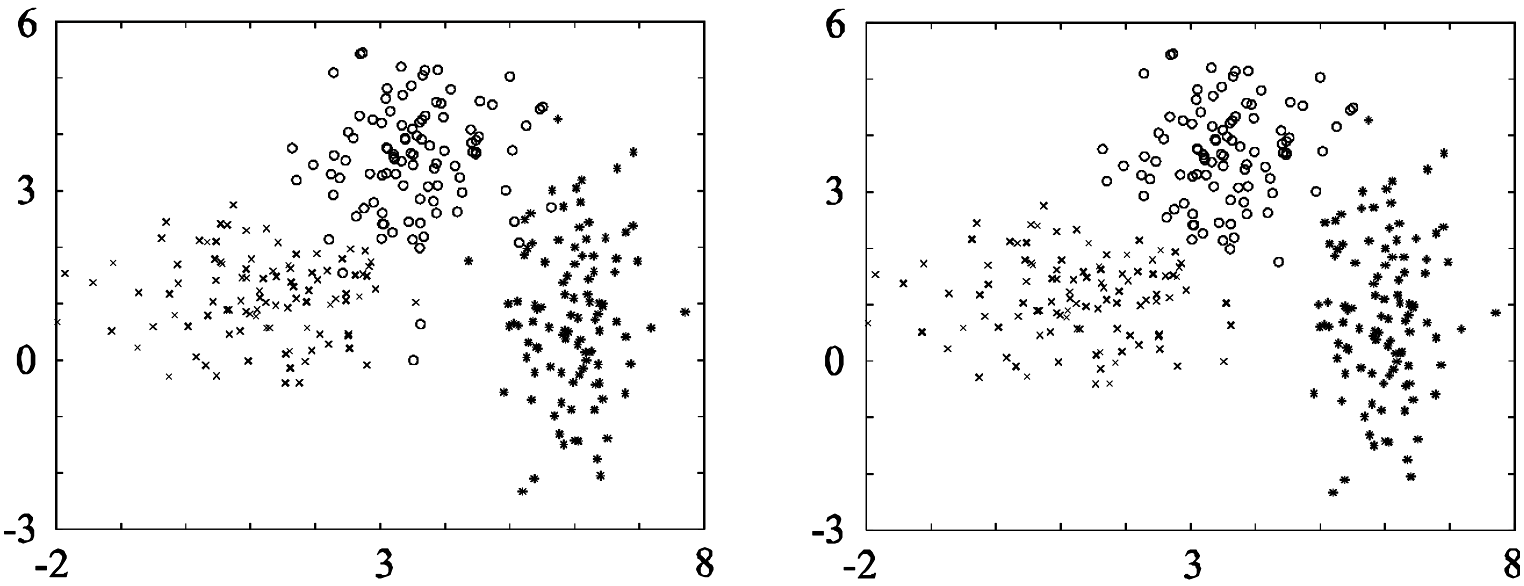
and covariance matrices

$$\Sigma_1=\begin{bmatrix} 1 & -0.3 \\ -0.3 & 1 \end{bmatrix},\quad \Sigma_2=\begin{bmatrix} 1 & 0.3 \\ 0.3 & 1 \end{bmatrix},\quad \Sigma_3=\begin{bmatrix} 1 & 0.7 \\ 0.7 & 1 \end{bmatrix},$$

respectively.

A group of 100 vectors stem from each distribution. These form the data set X.

Probabilistic CFO clustering algorithms



(a) The data set

(b) Results of GMDAS

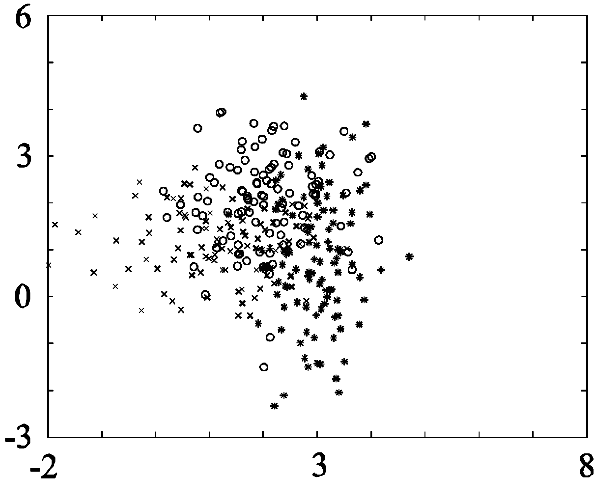
Confusion matrix:

	Cluster 1	*Cluster 2*	*Cluster 3*
1st distribution	99	0	1
2nd distribution	0	100	0
3rd distribution	3	4	93

The algorithm reveals accurately the underlying structure.

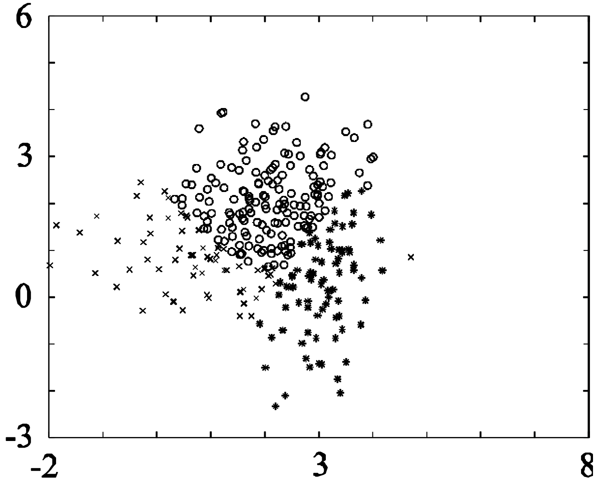
Probabilistic CFO clustering algorithms

(b) The same as (a) but now $\underline{\mu}_1=[1, 1]^T$, $\underline{\mu}_2=[2, 2]^T$, $\underline{\mu}_3=[3, 1]^T$ (The clusters are closer).



(a)

The data set



(b)

Results of GMDAS

Confusion matrix:

	Cluster 1	*Cluster 2*	*Cluster 3*
1st distribution	85	4	11
2nd distribution	35	56	9
3rd distribution	26	0	74

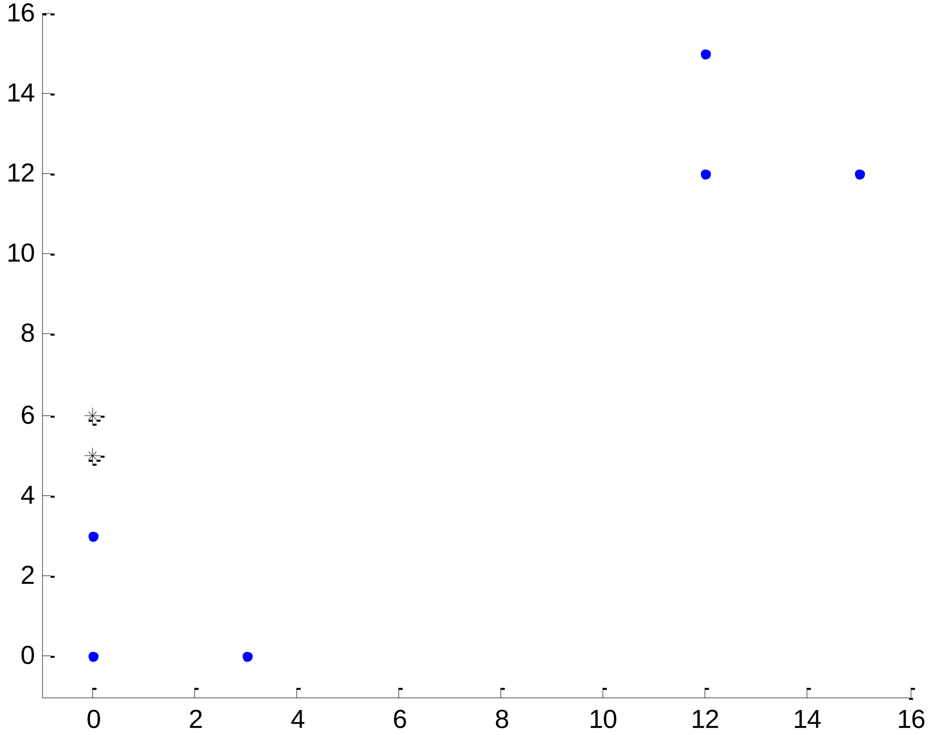
The algorithm reveals the underlying structure less accurately.

Probabilistic CFO clustering algorithms

<u>*Example*</u> $\boldsymbol{x}_1 = [0\ 0]^T, \boldsymbol{x}_2 = [3\ 0]^T, \boldsymbol{x}_3 = [0\ 3]^T, \boldsymbol{x}_4 = [12\ 12]^T, \boldsymbol{x}_5 = [15\ 12]^T, \boldsymbol{x}_6 = [12\ 15]^T$

Initially:

$$\theta_1(0) = [0, 5]^{\mathrm{T}}$$
$$\theta_2(0) = [0, 6]^{\mathrm{T}}$$
$$\mathrm{P}_1(0) = 0.1$$
$$P_2(0) = 0.9$$



$$p(\boldsymbol{x}|1) = \frac{1}{2\pi} exp(-0.5 \cdot \|\boldsymbol{x} - \boldsymbol{\theta}_1\|^2), \qquad P(1|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|1)P_1}{p(\boldsymbol{x})}$$

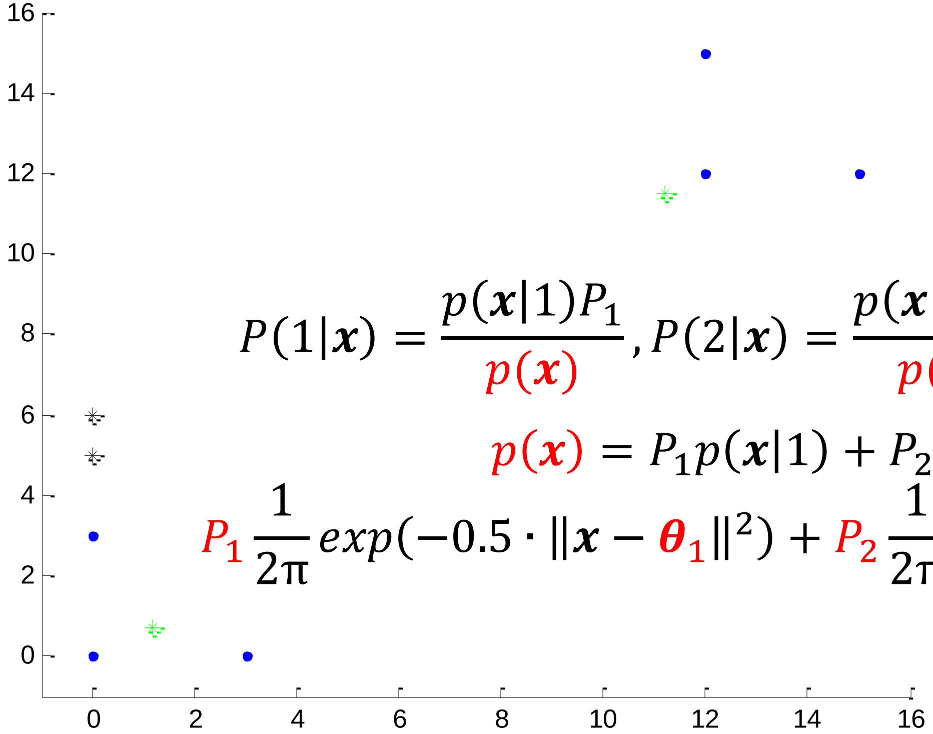
$$p(\boldsymbol{x}|2) = \frac{1}{2\pi} exp(-0.5 \cdot \|\boldsymbol{x} - \boldsymbol{\theta}_2\|^2), \qquad P(2|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|2)P_2}{p(\boldsymbol{x})}$$

$$p(\boldsymbol{x}) = P_1 p(\boldsymbol{x}|1) + P_2 p(\boldsymbol{x}|2) = P_1 \frac{1}{2\pi} exp(-0.5 \cdot \|\boldsymbol{x} - \boldsymbol{\theta}_1\|^2) + P_2 \frac{1}{2\pi} exp(-0.5 \cdot \|\boldsymbol{x} - \boldsymbol{\theta}_2\|^2)$$

$$\ln p(X; \Theta, P) = \sum_{i=1}^{N} [P(1|\boldsymbol{x}_i) \ln(p(\boldsymbol{x}_i|1; \boldsymbol{\theta}_1)P_1) + P(2|\boldsymbol{x}_i) \ln(p(\boldsymbol{x}_i|2; \boldsymbol{\theta}_2)P_2)]$$

Probabilistic CFO clustering algorithms

<u>*Example*</u> $\boldsymbol{x}_1 = [0\ 0]^T, \boldsymbol{x}_2 = [3\ 0]^T \boldsymbol{x}_3 = [0\ 3]^T, \boldsymbol{x}_4 = [12\ 12]^T, \boldsymbol{x}_5 = [15\ 12]^T, \boldsymbol{x}_6 = [12\ 15]^T$



$$P(1|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|1)P_1}{p(\boldsymbol{x})}, P(2|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|2)P_2}{p(\boldsymbol{x})}$$

$$p(\boldsymbol{x}) = P_1 p(\boldsymbol{x}|1) + P_2 p(\boldsymbol{x}|2) =$$

$$P_1 \frac{1}{2\pi} exp(-0.5 \cdot \|\boldsymbol{x} - \boldsymbol{\theta}_1\|^2) + P_2 \frac{1}{2\pi} exp(-0.5 \cdot \|\boldsymbol{x} - \boldsymbol{\theta}_2\|^2)$$

1st iteration:

A posteriori probs

	$\boldsymbol{x}_1$	$\boldsymbol{x}_2$	$\boldsymbol{x}_3$	$\boldsymbol{x}_4$	$\boldsymbol{x}_5$	$\boldsymbol{x}_6$
$P(1\|x)$	0.9645	0.9645	0.5751	0.0002	0.0002	0.0000
$P(2\|x)$	0.0355	0.0355	0.4249	0.9998	0.9998	1.0000

$\boldsymbol{\theta}_1(1) = [1.1572 \quad 0.6906]^{\mathrm{T}}$

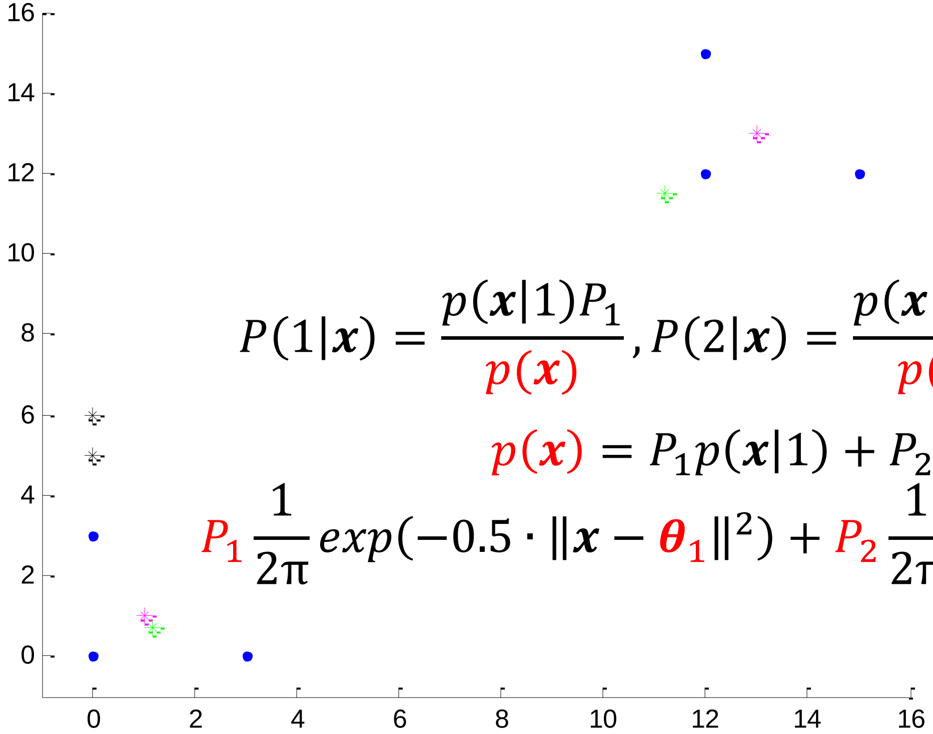
$\boldsymbol{\theta}_2(1) = [11.1864 \quad 11.5207]^{\mathrm{T}}$

$\mathrm{P}_1(1) = 0.4174$

$P_2(1) = 0.5826$

Probabilistic CFO clustering algorithms

<u>*Example*</u> $\boldsymbol{x}_1 = [0\ 0]^T, \boldsymbol{x}_2 = [3\ 0]^T \boldsymbol{x}_3 = [0\ 3]^T, \boldsymbol{x}_4 = [12\ 12]^T, \boldsymbol{x}_5 = [15\ 12]^T, \boldsymbol{x}_6 = [12\ 15]^T$



$$P(1|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|1)P_1}{p(\boldsymbol{x})}, P(2|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|2)P_2}{p(\boldsymbol{x})}$$

$$p(\boldsymbol{x}) = P_1 p(\boldsymbol{x}|1) + P_2 p(\boldsymbol{x}|2) =$$

$$P_1 \frac{1}{2\pi} exp(-0.5 \cdot \|\boldsymbol{x} - \boldsymbol{\theta}_1\|^2) + P_2 \frac{1}{2\pi} exp(-0.5 \cdot \|\boldsymbol{x} - \boldsymbol{\theta}_2\|^2)$$

2nd iteration:

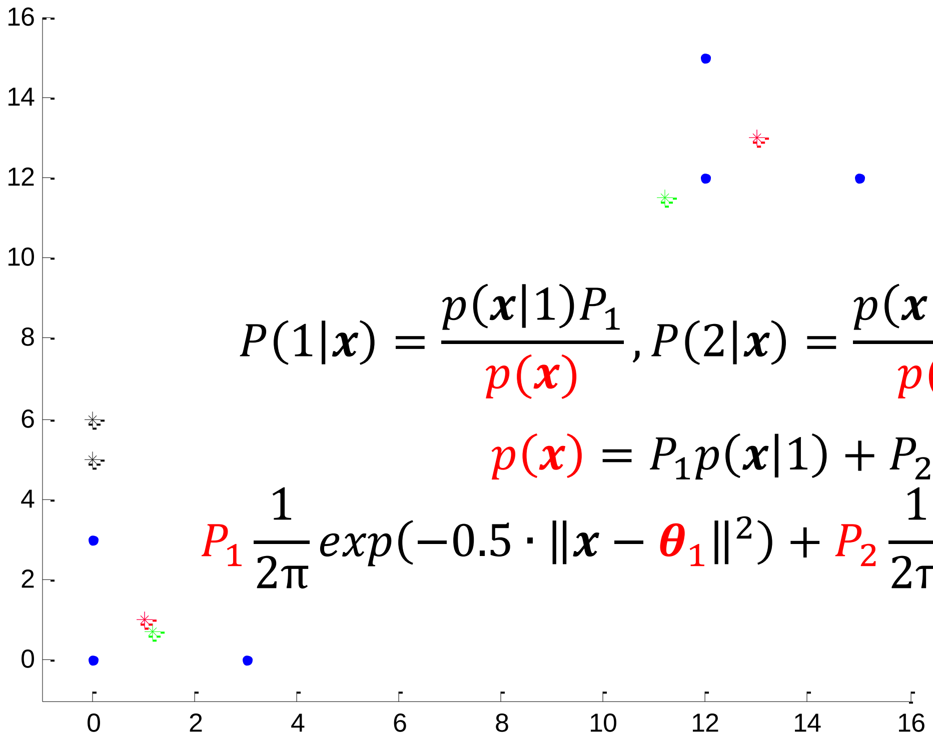
A posteriori probs

	$\boldsymbol{x}_1$	$\boldsymbol{x}_2$	$\boldsymbol{x}_3$	$\boldsymbol{x}_4$	$\boldsymbol{x}_5$	$\boldsymbol{x}_6$
$P(1\|x)$	1.0000	1.0000	1.0000	0.0000	0.0000	0.0000
$P(2\|x)$	0.0000	0.0000	0.0000	1.0000	1.0000	1.0000

$$\boldsymbol{\theta}_1(2) = [1\ 1]^{\mathrm{T}}$$
$$\boldsymbol{\theta}_2(2) = [13\ 13]^{\mathrm{T}}$$
$$\mathrm{P}_1(2) = 0.5$$
$$P_2(2) = 0.5$$

Probabilistic CFO clustering algorithms

<u>*Example*</u> $\boldsymbol{x}_1 = [0\ 0]^T, \boldsymbol{x}_2 = [3\ 0]^T \boldsymbol{x}_3 = [0\ 3]^T, \boldsymbol{x}_4 = [12\ 12]^T, \boldsymbol{x}_5 = [15\ 12]^T, \boldsymbol{x}_6 = [12\ 15]^T$



$$P(1|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|1)P_1}{p(\boldsymbol{x})}, P(2|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|2)P_2}{p(\boldsymbol{x})}$$

$$p(\boldsymbol{x}) = P_1 p(\boldsymbol{x}|1) + P_2 p(\boldsymbol{x}|2) =$$

$$P_1 \frac{1}{2\pi} exp(-0.5 \cdot \|\boldsymbol{x} - \boldsymbol{\theta}_1\|^2) + P_2 \frac{1}{2\pi} exp(-0.5 \cdot \|\boldsymbol{x} - \boldsymbol{\theta}_2\|^2)$$

3rd iteration:

A posteriori probs

	$\boldsymbol{x}_1$	$\boldsymbol{x}_2$	$\boldsymbol{x}_3$	$\boldsymbol{x}_4$	$\boldsymbol{x}_5$	$\boldsymbol{x}_6$
$P(1\|x)$	1.0000	1.0000	1.0000	0.0000	0.0000	0.0000
$P(2\|x)$	0.0000	0.0000	0.0000	1.0000	1.0000	1.0000

$$\boldsymbol{\theta}_1(3) = [1\ 1]^{\mathrm{T}}$$
$$\boldsymbol{\theta}_2(3) = [13\ 13]^{\mathrm{T}}$$
$$\mathrm{P}_1(3) = 0.5$$
$$P_2(3) = 0.5$$