Data Clustering

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Information Analysis Lab

Outline

- Clustering Definitions
- Distance/similarity measures
- Clustering categories
  - Exhaustive Clustering
  - Sequential Clustering
  - Clustering by optimization
  - Vector quantization
  - Graph-based clustering.

Introduction

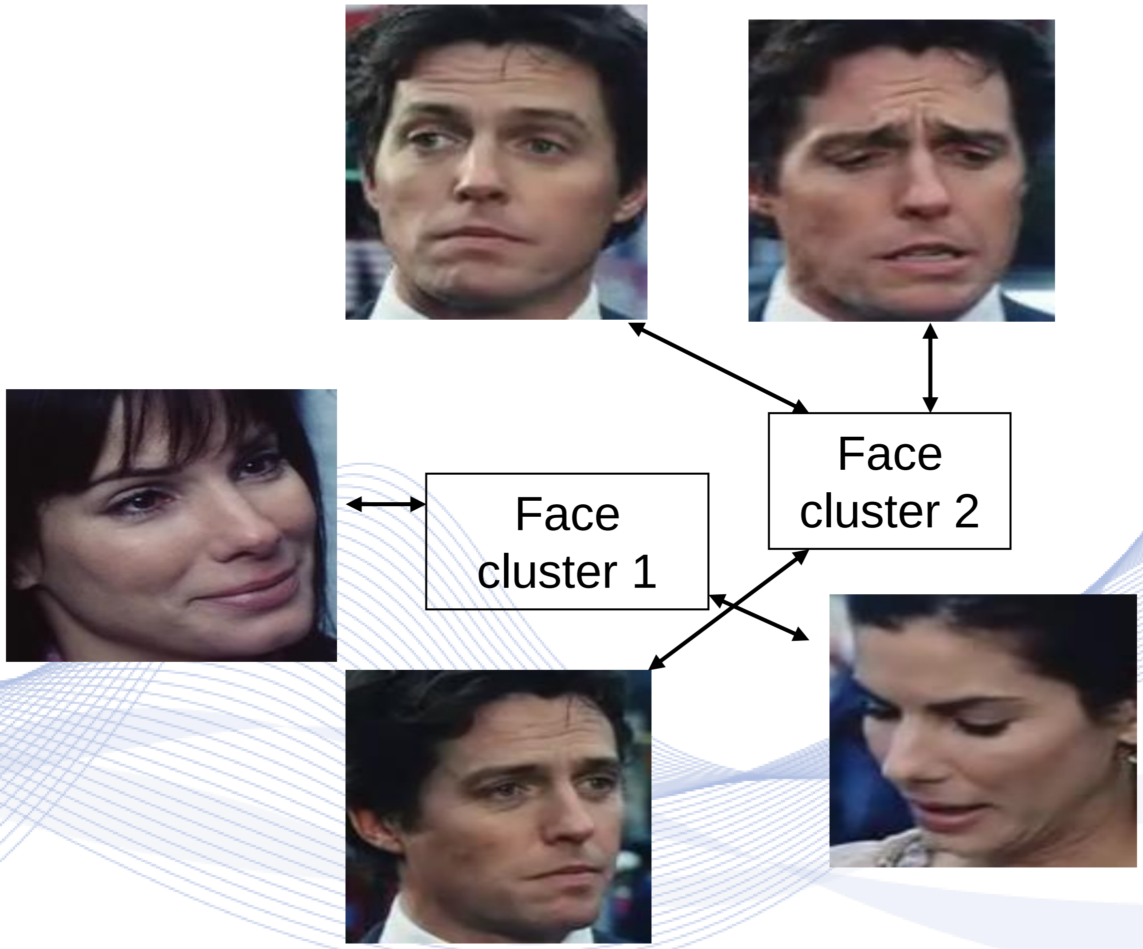
- ***Data clustering***: special case of ***unsupervised learning***.
  - class labelling of the training patterns is not available.
- Goal: to reveal the ***geometrical data organization*** into ***sensible clusters***, in order to:
  - discover data (dis)similarities.
  - discover geometrical cluster structure.
- Applications:
  - life sciences, earth sciences and engineering.

Face clustering

Problem statement:

- To cluster facial images
- ***Input***: many facial ROIs
- ***Output***: facial image clusters.

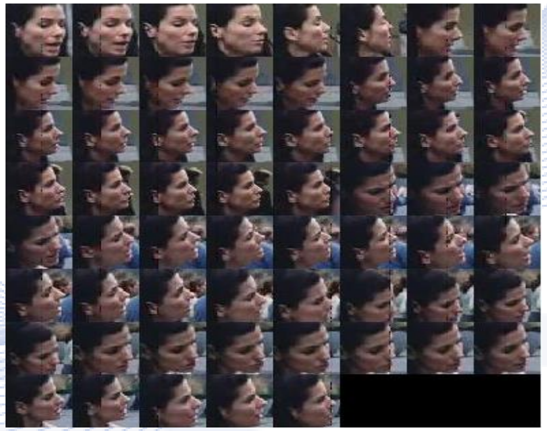
- Unsupervised learning
- Applications:
  Biometrics
  Surveillance applications
  Video analytics.



Face Clustering

Problem statement:

- To cluster a set of facial ROIs
- ***Input***: a set of face image ROIs
- ***Output***: several face clusters, each containing faces of only one person.
- Applications
  - Cluster actor images, even if they belong to different shots.
  - Cluster various views of the same actor.
  - Generate the cast of a movie.
  - Semi automatic face recognition.



Introduction

- Clustering criterion in image data:
  - ***Color similarity***: e.g., all facial image regions are pink.
  - ***Texture similarity***: tree foliage regions have fine unstructured visual texture.
  - ***Edge similarity***: building images have vertical/horizontal edges.
  - ***Intensity similarity***: black people have dark facial images.

Introduction

- ***Outliers***: black albinos have brighter facial images.

- Clusters may consist of ***sub-clusters***:
  - Caucasian and black facial images belong to ‘facial image’ cluster.

Introduction

- Clustering criterions greatly influence clustering results.
- Clustering is a key human cognitive ability:
  - Clusters are characterized by the common data attributes.
  - Cluster labeling leads to logical ***concepts***.

Introduction

Data clustering input: data samples described by feature vectors, without neither labels nor any information about the specific desired output:

$$\mathcal{D} = \{\mathbf{x}_i\}_{i=1}^{N}.$$

Typically: $\mathbf{x} \in \mathbb{R}^n$.

***Data clustering output*:**

- Sample data set $\mathcal{D} = \{\mathbf{x}_i\}_{i=1}^{N}$ partition to clusters $\mathcal{C}_i, i = 1, \ldots, m$.
  - Cluster samples are similar and dissimilar to the samples of other clusters based on similarity/distance metric ‖ . ‖.
  - Number of clusters m may be unknown.

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Feature types

- ***Real-valued feature vectors***: $\mathbf{x} \in \mathbb{R}^n$.
- ***Finite discrete set feature vectors***: $\mathbf{x} \in \mathcal{F}^n$.

- Discrete set cardinality k: $\mathcal{F} = \{0,1,\dots,k-1\}$.
- Special case:
  - binary set $k = 2$, $\mathcal{F} = \{0,1\}$.

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Feature types

- ***Labeled (nominal) features***: $\mathcal{F} = \{f_0, f_1, \dots, f_{k-1}\}$.
- Feature values $f_i, i = 0, \dots, k-1$ may have symbolic meaning (symbolic labels):
  - Facial image labels $\mathcal{F} = \{'\text{John}', '\text{Alice}', \dots, '\text{Vladimir}'\}$.
- Nominal feature vectors: $\mathbf{x} \in \mathcal{F}_1 \times \mathcal{F}_2 \times \cdots \times \mathcal{F}_n$.
  - Feature vector $\mathbf{x} \in \mathcal{F}_1 \times \mathcal{F}_2$ for describing apples:

    $\mathcal{F}_1 = \{'\text{small}', '\text{medium}', '\text{big}'\}$,

    $\mathcal{F}_2 = \{'\text{red}', '\text{yellow}', '\text{green}'\}$.

Feature types

- Feature categorization:
  - ***Nominal features***: $\mathcal{F}$ is a set.
    - No feature value ordering is possible.
  - ***Ordinal features***: e.g., $\mathcal{F} = \mathbb{R}$.
    - Feature values can be meaningfully ordered.
  - ***Angular features***: $\mathcal{F} = [0, 2\pi]$.
    - Feature values are angles (or on a unit circle).
  - Interval-scaled: feature value difference is meaningful.
  - Ratio-scaled: feature value ratio is meaningful.

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Introduction

Clustering subtasks:

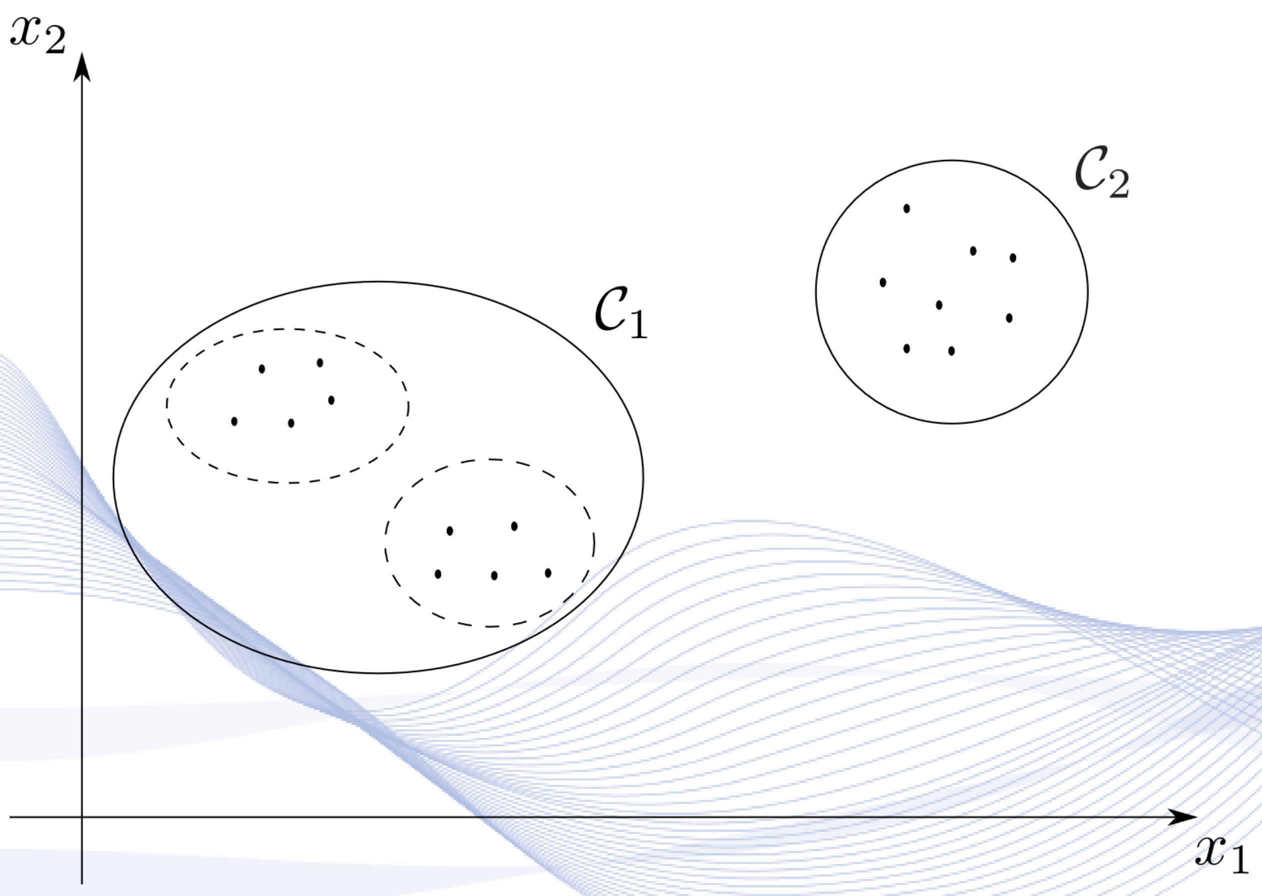
- ***Feature selection***: Create a feature vector $\mathbf{x}$ with minimum information redundancy.
- ***Data similarity measurement***: Quantify feature vector '(dis)similarity'.
- ***Clustering criterion***: It quantifies clustering 'sensibility'.
  - ***Cost function optimization***:
  - Maximize intra-class similarity and maximize inter-class dissimilarity.

Introduction

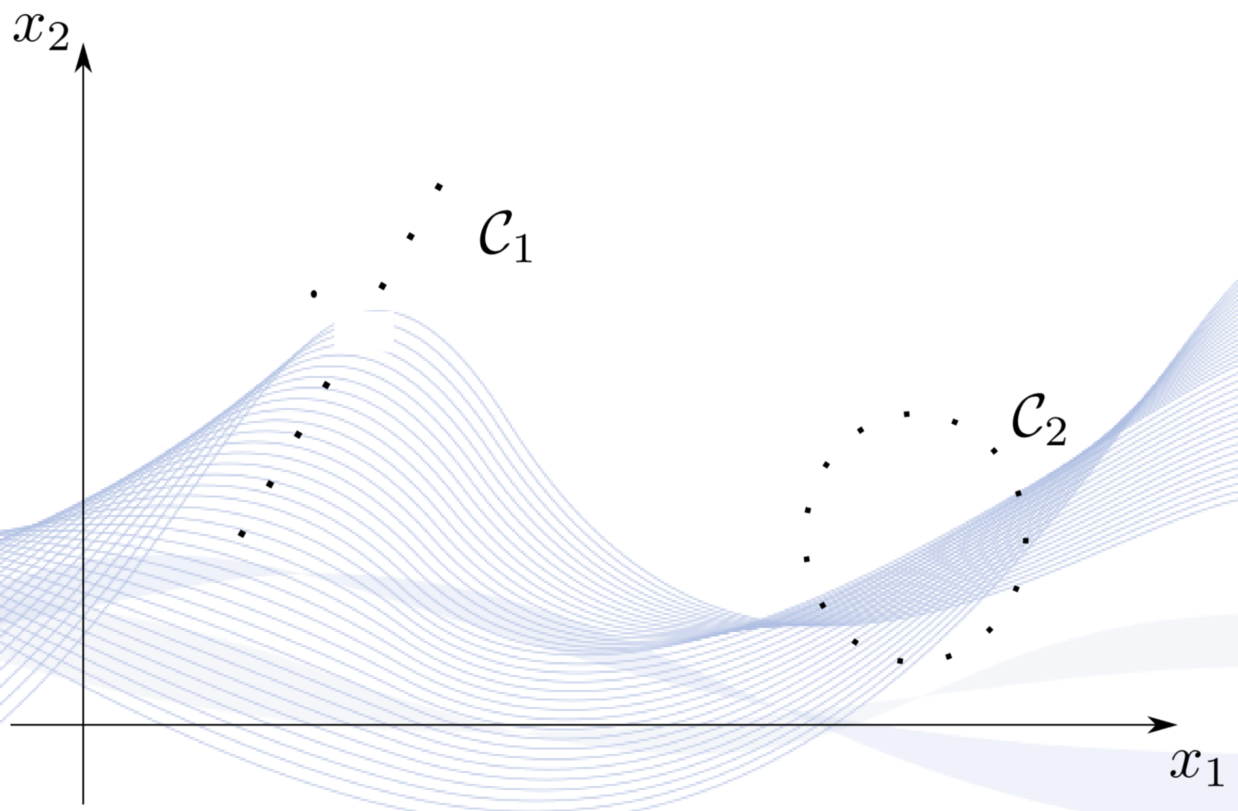
Clustering subtasks:

- ***Choosing a clustering algorithm***: to best unravel data structure.
- ***Clustering validation***: verify the correctness of clustering results using appropriate tests.
- ***Clustering explainability***: Interpretation clustering results.
- ***Concept creation***: Cluster labeling to create logical ‘concepts’.

Introduction



Clustering granularity.

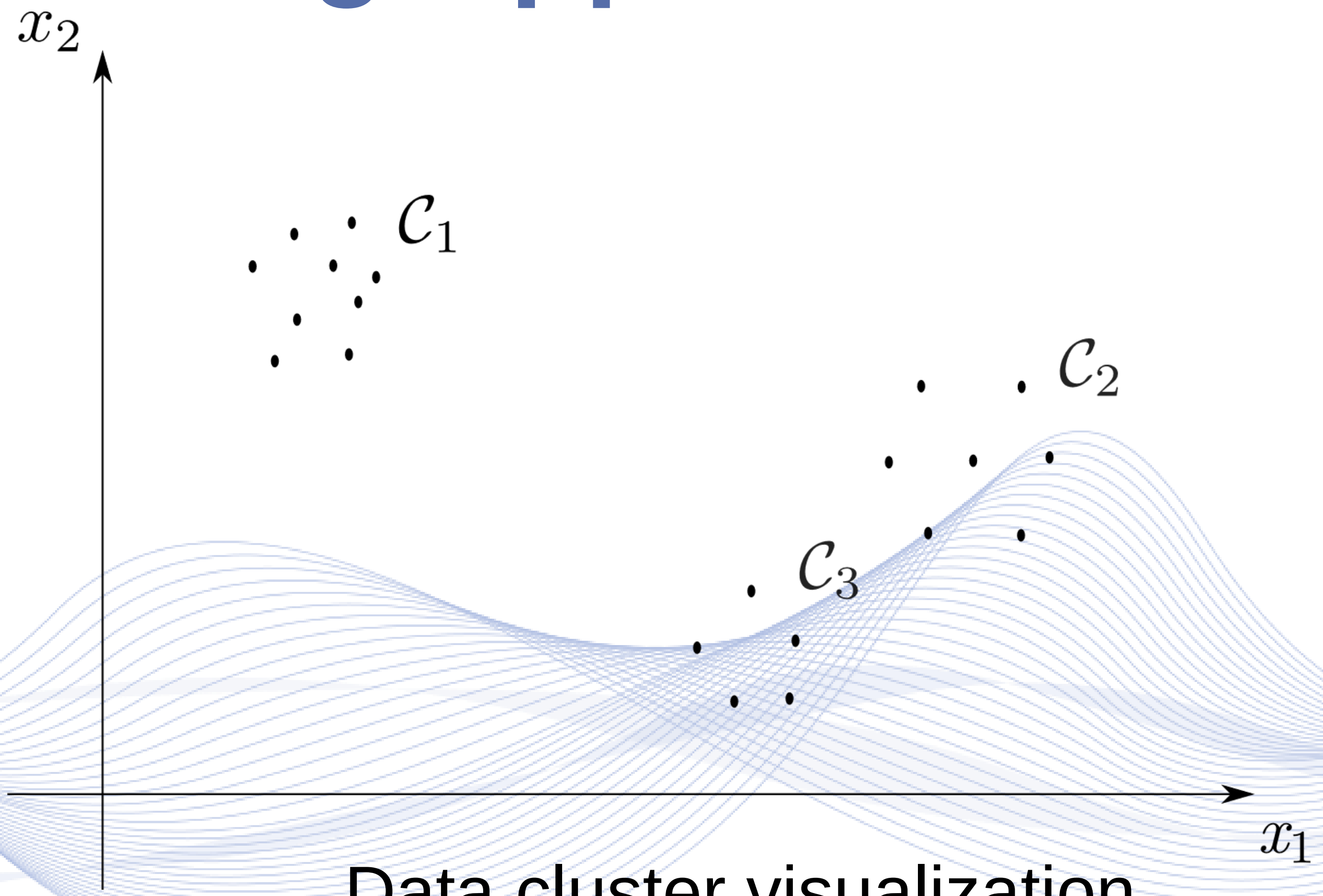


Cluster manifolds.

Clustering Applications

- ***Better data description***:
  - Data set $\mathcal{D} = \{\mathbf{x}_i\}_{i=1}^{N}$, $\mathbf{x} \in \mathbb{R}^n$ cardinality N or data dimensionality n may be too large;
  - Clustering groups the data into $m \ll N$ clusters, providing much better data description.
- ***Data cluster visualization***: clusters are well visualized if they are mapped on $\mathbb{R}^2$.
- ***Hypothesis generation***: Help forming and validating hypotheses on data structure.

Clustering Applications



Data cluster visualization.

Crisp/fuzzy Clustering

- Let $\mathcal{D}$ be a feature data set: $\mathcal{D} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$.
- ***Crisp clustering*** is the partition of $\mathcal{D}$ into m disjoint sets $\mathcal{C}_1, \dots, \mathcal{C}_m$, satisfying the following conditions:
  - $\mathcal{C}_i \neq \emptyset, \quad i = 1, \dots, m,$
  - $\cup_{i=1}^{m} \mathcal{C}_i = \mathcal{D},$
  - $\mathcal{C}_i \cap \mathcal{C}_j = \emptyset, \quad i \neq j, \quad i, j = 1, \dots, m.$

- Feature vectors in a cluster $\mathcal{C}_i$ are 'similar', while they are 'dissimilar' to the ones of other clusters $\mathcal{C}_j, i \neq j$.

Crisp/fuzzy Clustering

- ***Fuzzy clustering*** of $\mathcal{D}$ into m clusters:
  - For each sample $\mathbf{x}_i$, $i = 1, \dots, N$ find m ***membership functions*** u_j:

$$u_j\colon\ \mathcal{D} \rightarrow [0,1], \qquad j = 1, \dots, m.$$

$$\sum_{j=1}^{m} u_j(\mathbf{x}_i) = 1, \qquad i = 1, \dots, N,$$

$$0 < \sum_{j=1}^{m} u_j(\mathbf{x}_i) < N, \qquad j = 1, \dots, m.$$

Crisp/fuzzy Clustering

- Each vector $\mathbf{x}$ belongs to more than one clusters simultaneously, which depends on the value of u_j in [0,1].
- Fuzzy membership values $u_j \rightarrow 1$: high cluster membership possibility.
- Fuzzy membership values $u_j \rightarrow 0$: low cluster membership possibility.
- Feature vector similarity: the membership function vector difference $|\mathbf{u}_k - \mathbf{u}_n|$ for two feature vectors $\mathbf{x}_k, \mathbf{x}_n$ is small.

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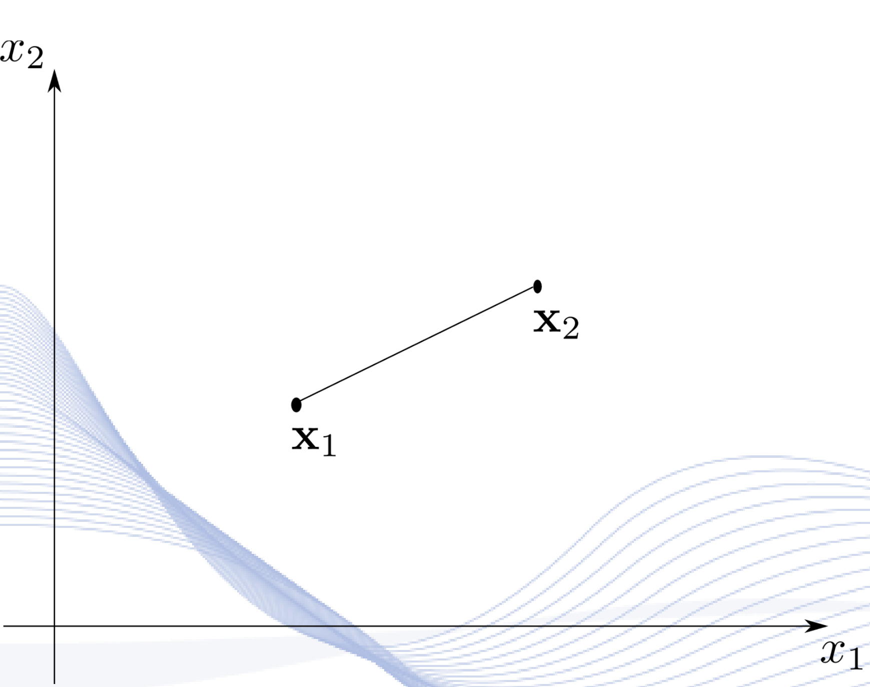
Distance/Similarity Measures

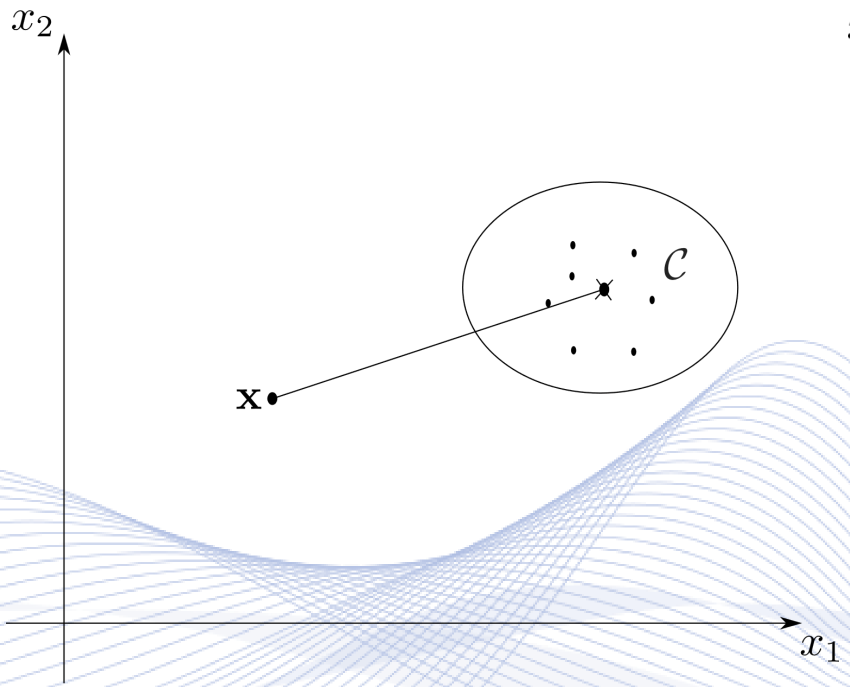
- Proximity or distance measures
- Similarity or dissimilarity measures.

- Distance between two feature points (feature vectors).
- Distance between a feature point and a feature point set.
- Distance between two feature point sets.

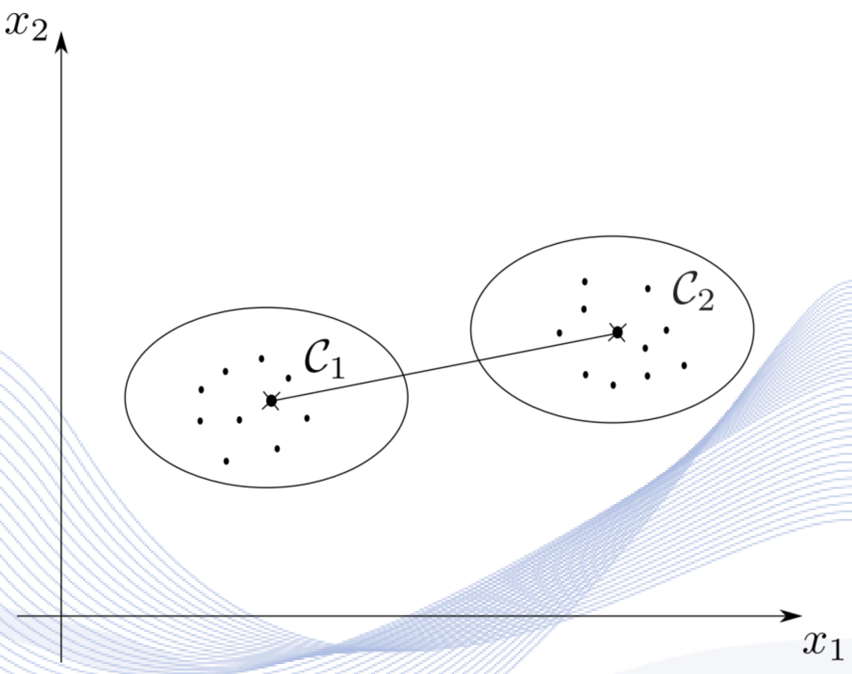
Distance Measures



Distance between two points.



Distance between point and set (set center).



Distance between sets (set center).

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Distance Measures

***Dissimilarity measure* (*DM*) $\boldsymbol{d}$:**

- a function $d: \mathcal{F} \times \mathcal{F} \rightarrow \mathbb{R}$, satisfying:

$$\exists\ d_0 \in \mathbb{R}: \quad -\infty < d_0 \leq d(\mathbf{x}, \mathbf{y}) < +\infty, \forall \mathbf{x}, \mathbf{y} \in \mathcal{F},$$

$$d(\mathbf{x}, \mathbf{x}) = d_0, \forall \mathbf{x} \in \mathcal{F},$$

$$d(\mathbf{x}, \mathbf{y}) = d(\mathbf{y}, \mathbf{x}), \forall \mathbf{x}, \mathbf{y} \in \mathcal{F}.$$

Typically: $d(\mathbf{x}, \mathbf{x}) = 0$.

- Also called ***distance measure*** for Euclidean spaces: $\mathcal{F} = \mathbb{R}^n$.

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Distance Measures

If:

- $d(\mathbf{x}, \mathbf{y}) = d_0$, if and only if $\mathbf{x} = \mathbf{y}$
- and **triangular inequality** holds:

$$d(\mathbf{x}, \mathbf{z}) \leq d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z}), \quad \forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathcal{F}.$$

d is a ***metric*** or ***norm***.

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Distance Measures

Weighted L_p metric between two real-valued feature points (vectors) $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$:

$$d(\mathbf{x}, \mathbf{y}) = \left(\sum_{i=1}^{n} w_i |x_i - y_i|^p\right)^{1/p}.$$

- $w_i \geq 0$: is weight coefficient.
- Unweighted L_p metric: $w_i = 1, \quad i = 1, \dots, n.$
- L_2 metric:

$$d(\mathbf{x}, \mathbf{y}) = \left(\sum_{i=1}^{n} (x_i - y_i)^2\right)^{1/2}.$$

Distance Measures

- ***Mahalanobis distance***:

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x} - \mathbf{y})^T \mathbf{A} (\mathbf{x} - \mathbf{y})}.$$

- $\mathbf{A}$ is a $n \times n$ symmetric, positive-definite matrix.
- ***Euclidean distance***:

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x} - \mathbf{y})^T (\mathbf{x} - \mathbf{y})}.$$

  - $\mathbf{A} = \mathbf{I}$.
  - It is equal to the length of the straight line segment connecting points $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$.

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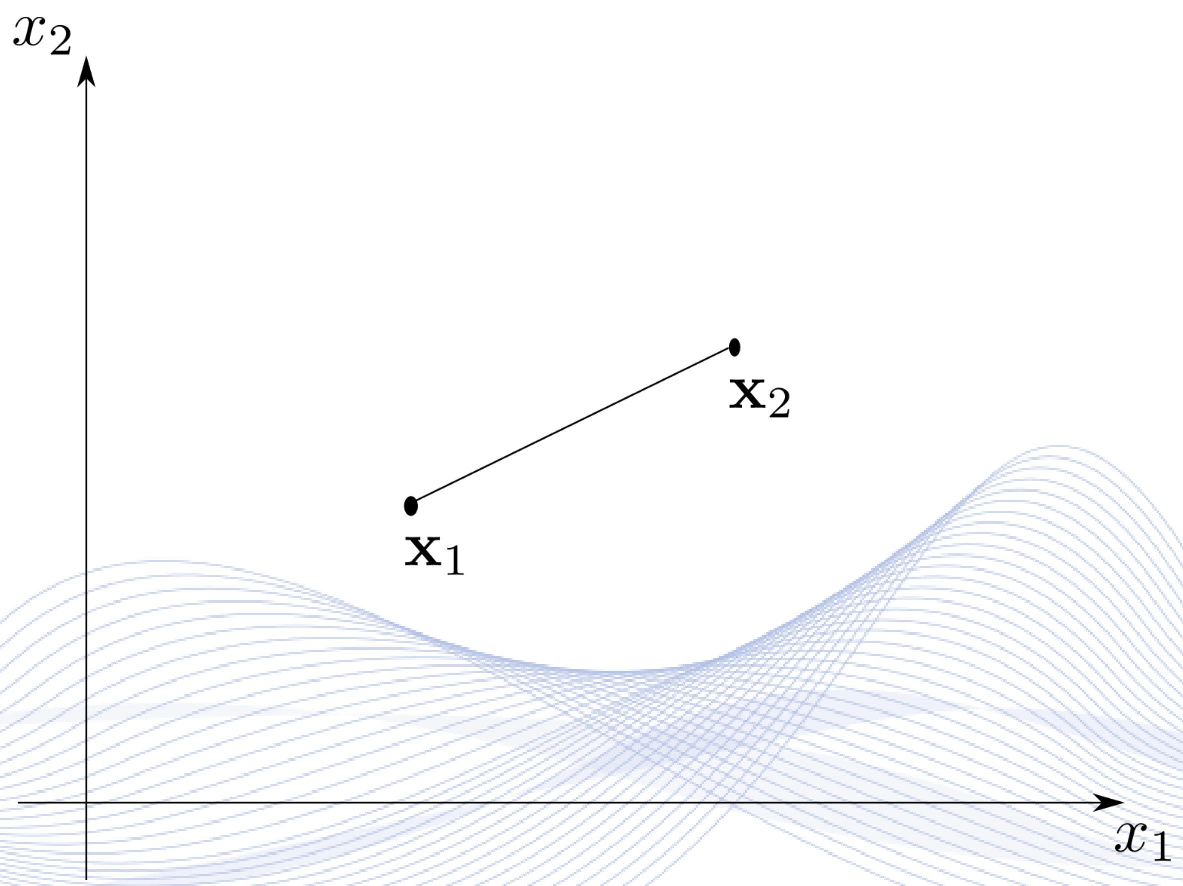
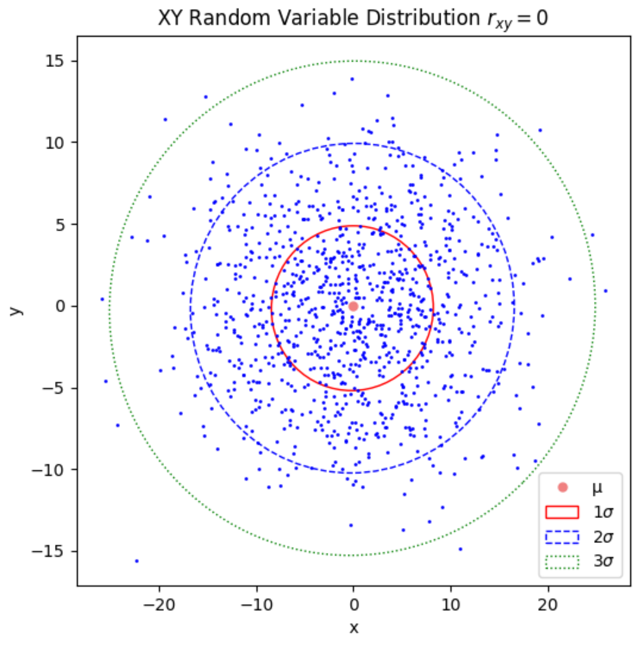
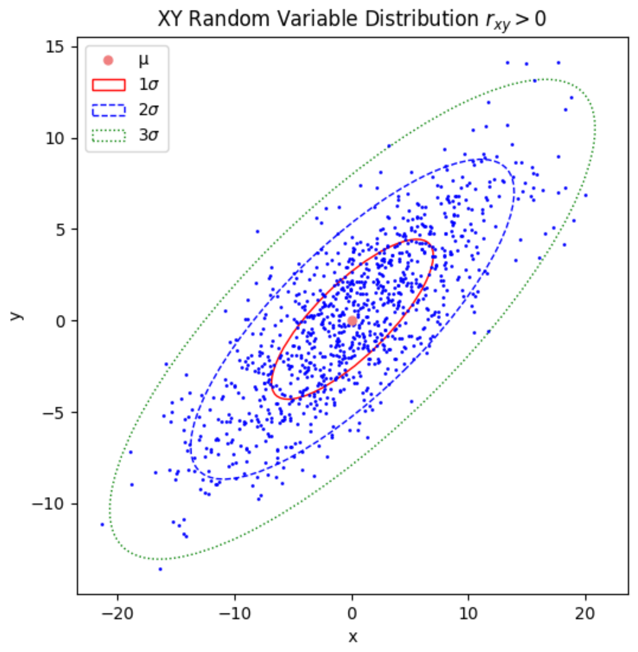
Distance Measures



Euclidean distance between two points.

Distance Measures





a) Euclidean equidistant points (circles);

b) Mahalanobis equidistant points (ellipses).

Distance Measures

- Weighted $\boldsymbol{L_1}$ ***norm***:

$$d(\mathbf{x},\mathbf{y}) = \sum_{i=1}^{n} w_i |x_i - y_i|.$$

- ***Manhattan norm***:

$$d(\mathbf{x},\mathbf{y}) = \sum_{i=1}^{n} |x_i - y_i|.$$

- $\boldsymbol{L_\infty}$ **norm**:

$$d(\mathbf{x},\mathbf{y}) = \max_{1\le i\le n} |x_i - y_i|.$$

- L_∞ norm is a special case of L_p norm for $p \to \infty$.

Distance Measures

Discrete-Valued Vectors

- Vectors $\mathbf{x}$ with coordinates belonging to the finite set $\mathcal{F} = \{0,1,\ldots,k-1\}$, ($k$ is a positive integer).
- There are exactly k^n vectors $\mathbf{x}, \mathbf{y} \in \mathcal{F}^n$.

- $k \times k$ ***contingency table***:

$$\mathbf{A}(\mathbf{x}, \mathbf{y}) = [a_{ij}] \quad i,j = 0,1,\ldots,k-1.$$

- a_{ij} is the number of vectors $\mathbf{x}, \mathbf{y}$ entries having values $i, j \in \mathcal{F}$ symbols, respectively.

Distance Measures

Discrete-Valued Vectors

- ***Edit distance***.
- ***Hamming distance***:

$$d(\mathbf{x}, \mathbf{y}) = \sum_{i=0}^{k-1} \sum_{j=0, j \neq i}^{k-1} a_{ij} \,.$$

- Equal to the summation of all the off-diagonal elements of $\mathbf{A}$, indicating the entries, where $\mathbf{x}$ and $\mathbf{y}$ differ.

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Distance Measures

- For $k = 2$ the Hamming distance is:

$$d(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{n} (x_i - y_i)^2 .$$

- $\boldsymbol{L_1}$ ***distance***:

$$d_1(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{n} |x_i - y_i| .$$

Similarity Measures

- ***Similarity measure*** (***SM***):
- a function $s: \mathcal{F} \times \mathcal{F} \rightarrow \mathbb{R}$ such that:

$$\exists s_0 \in \mathbb{R}: -\infty < s(\mathbf{x}, \mathbf{y}) \leq s_0 < +\infty, \forall \mathbf{x}, \mathbf{y} \in \mathcal{F},$$

$$s(\mathbf{x}, \mathbf{x}) = s_0, \forall x \in \mathcal{F},$$
$$s(\mathbf{x}, \mathbf{y}) = s(\mathbf{y}, \mathbf{x}), \forall \mathbf{x}, \mathbf{y} \in \mathcal{F}.$$

- Typically, $s(\mathbf{x}, \mathbf{x}) = 1$.

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Similarity Measures

If:

- $s(\mathbf{x},\mathbf{y}) = s_0$, if and only if $\mathbf{x} = \mathbf{y}$
- and:

$$s(\mathbf{x},\mathbf{y})s(\mathbf{y},\mathbf{z}) \leq [s(\mathbf{x},\mathbf{y}) + s(\mathbf{y},\mathbf{z})]s(\mathbf{x},\mathbf{z}), \qquad \forall \mathbf{x},\mathbf{y},\mathbf{z} \in \mathcal{F}$$

then s is a ***metric SM***.

Similarity Measures

Similarity measures between two feature vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$:

- ***Inner vector product***:

$$s(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \mathbf{y} = \sum_{i=1}^{n} x_i y_i \,.$$

- If the vectors $\mathbf{x}, \mathbf{y}$ are normalized to length a: $s \in [-a^2, a^2]$.
- ***Cosine similarity*** measure:

$$s(\mathbf{x}, \mathbf{y}) = \frac{\mathbf{x}^T \mathbf{y}}{||\mathbf{x}|| \, ||\mathbf{y}||}, \quad ||\mathbf{x}|| = \sqrt{\sum_{i=1}^{n} x_i^2}\,, ||\mathbf{y}|| = \sqrt{\sum_{i=1}^{n} y_i^2}\,.$$

Similarity Measures

- ***Correlation coefficient***:

$$r(\mathbf{x}, \mathbf{y}) = \frac{\mathbf{x}_c^T \mathbf{y}_c}{||\mathbf{x}_c||\ ||\mathbf{y}_c||},$$

- $r(\mathbf{x}, \mathbf{y}) \in [-1,1]$.
- Central difference vectors:

$$\mathbf{x}_c = [x_1 - \bar{x}, \dots, x_n - \bar{x}]^T, \mathbf{y}_c = [y_1 - \bar{y}, \dots, y_l - \bar{y}]^T,$$

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i, \qquad \bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i.$$

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Similarity Measures

Fuzzy Similarity Measure between two vectors:

$$s(\mathbf{x}, \mathbf{y}) = \left(\sum_{i=1}^{n} s(x_i, y_i)\right)^{\frac{1}{q}}.$$

- Similarity between two real-valued variables x_i and y_i:

$$s(x_i, y_i) = \max(\min(1 - x_i, 1 - y_i), \min(x_i, y_i)).$$

Similarity Measures

- Motivation:
  - Equivalence between two logic variables a and b:

$$(a \equiv b) = \left(\bar{a}\ \mathrm{AND}\ \overline{b}\right)\ \mathrm{OR}\ (a\ AND\ b).$$

  - Fuzzy $\mathrm{AND}, \mathrm{OR}$, $\bar{a}$ (NOT) operators: $\max, \min, 1 - a$.

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Similarity Measures

Tanimoto similarity measure between two feature vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$:

$$s(\mathbf{x}, \mathbf{y}) = \frac{\mathbf{x}^T\mathbf{y}}{||\mathbf{x}-\mathbf{y}||^2} = \frac{\mathbf{x}^T\mathbf{y}}{||\mathbf{x}||^2 + ||\mathbf{y}||^2 - \mathbf{x}^T\mathbf{y}}.$$

- It is inversely proportional to the squared Euclidean distance divided by their inner product.
- Similarity measure:

$$s(\mathbf{x}, \mathbf{y}) = 1 - \frac{d_2(\mathbf{x}, \mathbf{y})}{||\mathbf{x}||+||\mathbf{y}||}.$$

- Maximum when $\mathbf{x} = \mathbf{y}$ and minimum when $\mathbf{x} = -\mathbf{y}$.

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Similarity Measures

Tanimoto measure for discrete-valued vectors:

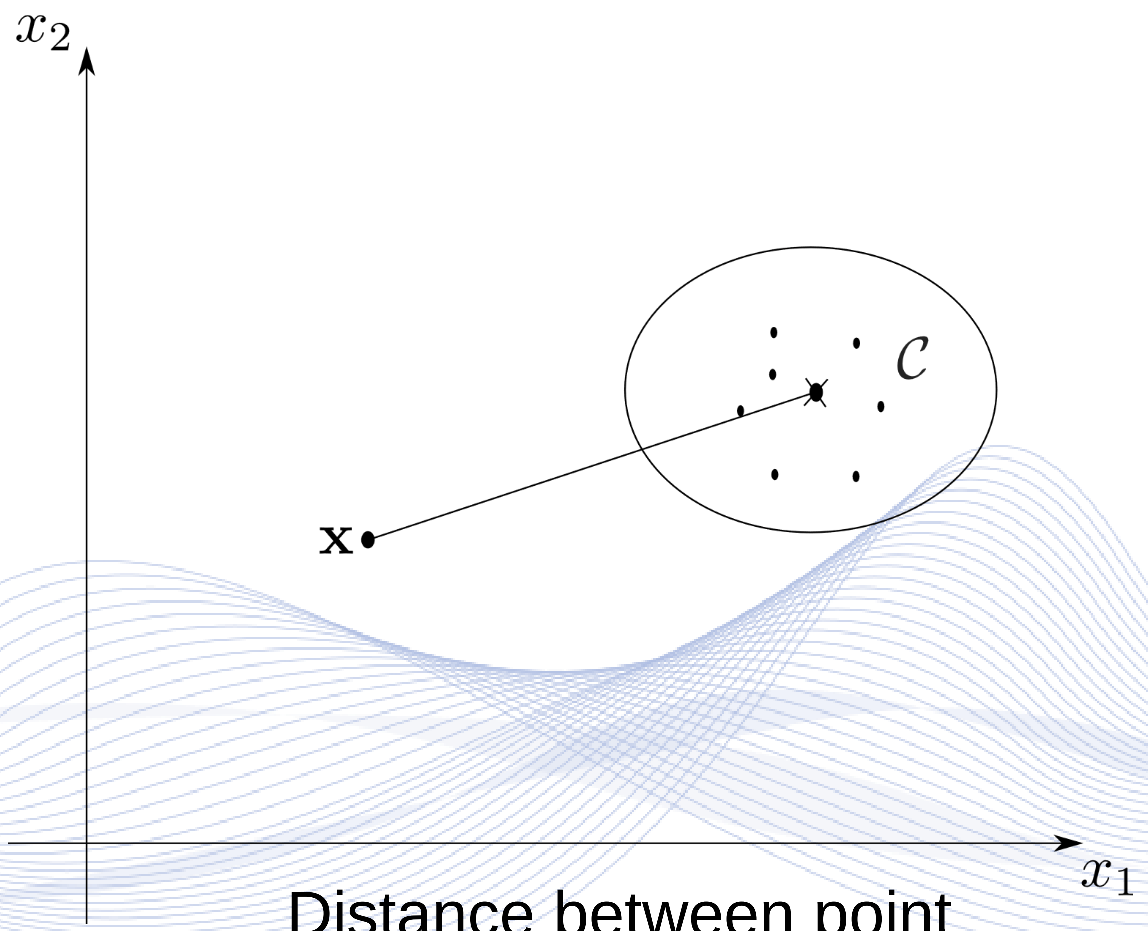
$$s(\mathbf{x},\mathbf{y}) = \frac{\sum_{i=1}^{k-1} a_{ii}}{n_x + n_y - \sum_{i=1}^{k-1}\sum_{j=1}^{k-1} a_{ij}},$$

$$n_x = \sum_{i=1}^{k-1}\sum_{j=0}^{k-1} a_{ij}\ ,\ n_y = \sum_{i=0}^{k-1}\sum_{j=1}^{k-1} a_{ij}.$$

- It takes into account all pairs of corresponding $\mathbf{x}$ and $\mathbf{y}$ coordinates, except when both $x_i = 0, y_i = 0$.
- Motivation: set ***Intersection over Union*** (***IoU***) for sets $\mathcal{X},\mathcal{Y}$:

$$s = \frac{|\mathcal{X} \cap \mathcal{Y}|}{|\mathcal{X} \cup \mathcal{Y}|}.$$

Distance Measures



Distance between point and set (set center).

Distance Measures

Distance functions between a point and a set (***cluster***).

- Distance $d'(\mathbf{x}, \mathcal{C})$ between vector $\mathbf{x}$ and cluster $\mathcal{C}$:
  - ***Distance to cluster center*** $\mathbf{m}$: $d'(\mathbf{x}, \mathcal{C}) = d(\mathbf{x}, \mathbf{m})$.
  - Max Distance function: $d'(\mathbf{x}, \mathcal{C}) = \max\limits_{\mathbf{y} \in \mathcal{C}} d(\mathbf{x}, \mathbf{y})$.
  - Min Distance function: $d'(\mathbf{x}, \mathcal{C}) = \min\limits_{\mathbf{y} \in \mathcal{C}} d(\mathbf{x}, \mathbf{y})$.
  - Average Distance function: $d'(\mathbf{x}, \mathcal{C}) = \frac{1}{|\mathcal{C}|} \sum_{\mathbf{y} \in \mathcal{C}} d(\mathbf{x}, \mathbf{y})$
    - $|\mathcal{C}|$: set $\mathcal{C}$ cardinality.

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Distance Measures

Cluster center is a representative vector of a data vector set:

- ***Mean vector***:

$$\mathbf{m} = \frac{1}{|\mathcal{C}|}\sum_{\mathbf{x}\in\mathcal{C}} \mathbf{x}.$$

- Sensitive to outliers.

Distance Measures

- ***Vector median***:

$$\sum_{\mathbf{y}\in\mathcal{C}} d(\mathbf{m}_v, \mathbf{y}) \leq \sum_{\mathbf{y}\in\mathcal{C}} d(\mathbf{z}, \mathbf{y}),\ \mathbf{m}_v \in \mathcal{C},\ \forall \mathbf{z} \in \mathcal{C}.$$

- ***Median center***:

  $\mathrm{med}(d(\mathbf{m}_m, \mathbf{y})|\mathbf{y} \in \mathcal{C}) \leq \mathrm{med}(d(\mathbf{z}, \mathbf{y})|\mathbf{y} \in \mathcal{C}),\ \mathbf{m}_m \in \mathcal{C},\ \forall \mathbf{z} \in \mathcal{C}.$

- med: ***median*** operator.

Distance Measures

Data manifold representations:

- Hyperplane $\mathbb{H}$:

$$\sum_{j=1}^{n} a_j x_j + a_0 = \mathbf{a}^T \mathbf{x} + a_0 = 0, \qquad \mathbf{x} = [x_1, \dots, x_n]^T.$$

  - Hyperplane parameters a_0 , $\mathbf{a} = [a_1, \dots, a_n]^T$.
- Distance of a point $\mathbf{x}$ from hyperplance $\mathbb{H}$:

$$d'(\mathbf{x}, \mathbb{H}) = \frac{|\mathbf{a}^T \mathbf{x} + a_0|}{||\mathbf{a}||}.$$

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Distance Measures

- ***Quadratic surface*** $\mathbb{S}$ representations:
  - ***Hypersphere*** equation: $(\mathbf{x}-\mathbf{c})^T(\mathbf{x}-\mathbf{c}) = r^2$.
  - $\mathbf{c}, r$: hypersphere center, radius.
  - ***Hyperellipsoid*** equation having parameters $\mathbf{A}, \mathbf{c}, r$:

$$(\mathbf{x}-\mathbf{c})^T\mathbf{A}(\mathbf{x}-\mathbf{c}) = r^2.$$

- Distance of a point $\mathbf{x}$ from $\mathbb{S}$:

$$d'(\mathbf{x}, \mathbb{S}) = \min_{\mathbf{z}\in\mathbb{S}} d(\mathbf{x}, \mathbf{z}).$$

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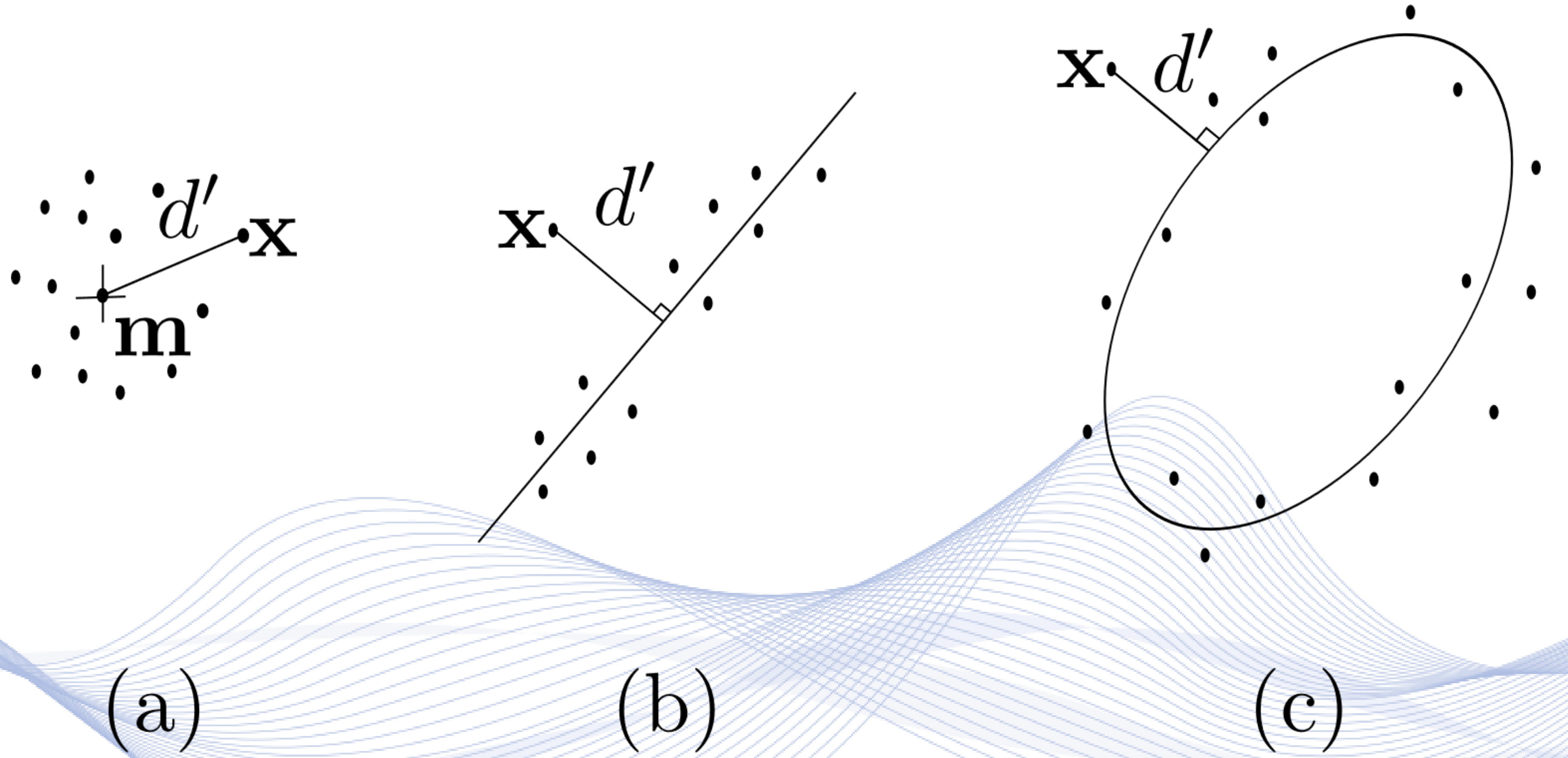
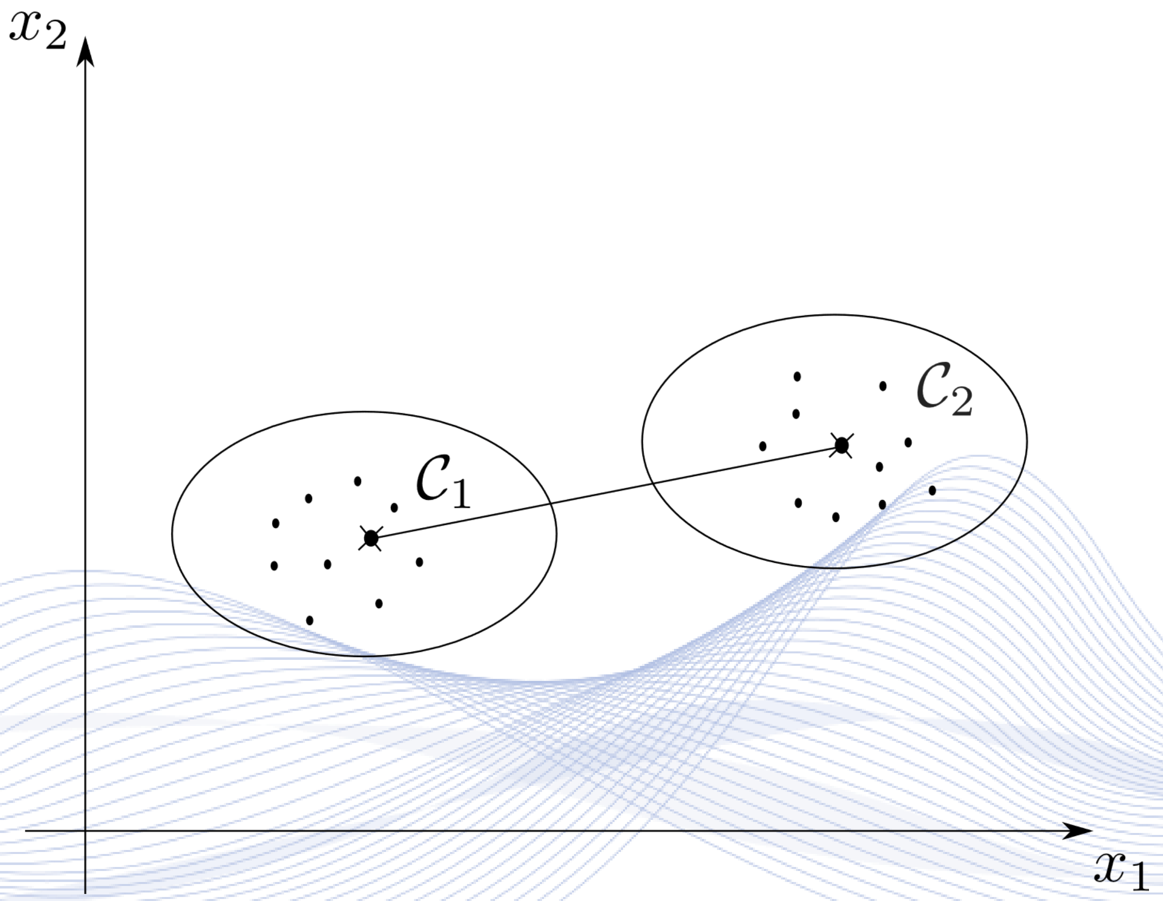
Distance Measures



a) Compact cluster; b) Linear cluster; c) Ellipsoid cluster representations.

Distance Measures



Distance between set centers.

Distance Measures

Distance Functions between Two Sets

- If $\mathcal{C}_i, \mathcal{C}_j$ are two sets of vectors the most common proximity functions are:
  - Max distance function: $d''(\mathcal{C}_i, \mathcal{C}_j) = \max_{\mathbf{x}\in\mathcal{C}_i,\, \mathbf{y}\in\mathcal{C}_j} d(\mathbf{x}, \mathbf{y})$.
  - Min distance function: $d''(\mathcal{C}_i, \mathcal{C}_j) = \min_{\mathbf{x}\in\mathcal{C}_i,\, \mathbf{y}\in\mathcal{C}_j} d(\mathbf{x}, \mathbf{y})$.
  - Min distance function is not a metric:

$$d''(\mathcal{C}_i, \mathcal{C}_j) = 0, \text{ even if } \mathcal{C}_i \neq \mathcal{C}_j, \text{ when } \mathcal{C}_i \cap \mathcal{C}_j \neq \emptyset.$$

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Distance Measures

Distance Functions between Two Sets

- Average proximity function:
- $d''(\mathcal{C}_i, \mathcal{C}_j) = \frac{1}{|\mathcal{C}_i||\mathcal{C}_j|} \sum_{\mathbf{x} \in \mathcal{C}} \sum_{\mathbf{y} \in \mathcal{C}} d(\mathbf{x}, \mathbf{y})$.
- ***Cluster center distance***:

$$d''(\mathcal{C}_i, \mathcal{C}_j) = d\left(\mathbf{m}_{\mathcal{C}_i}, \mathbf{m}_{\mathcal{C}_j}\right).$$

- $\mathbf{m}_{\mathcal{C}_i}, i = 1,2$: set representative vectors.

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Clustering Algorithms

- ***Exhaustive clustering.***
- ***Sequential Clustering***:
  - Produce single clustering with straightforward and fast methods.
  - Produce compact and hyperspherical/hyperellipsoidal clusters.
- ***Hierarchical Clustering***:
  - Cluster merge: produce a decreasing number of clusters at each step, by merging two clusters into one.
  - Cluster split: produce clusterings of increasing m.

Clustering Algorithms

- ***Clustering by cost function optimization***:
  - Optimization of cost function J representing a clustering criterion.
  - Optimization by differential calculus.
- ***Vector quantization***
- ***Graph-based clustering***

Exhaustive Clustering

Exhaustive clustering of a vector data set $\mathcal{D}$:

- identify all possible partition,
- select the one optimizing a clustering criterion.

- $S(N, m)$: number of all possible cluster outcomes, by clustering of N vectors into m groups.
- $S(N, m)$ properties:
  - $S(N, 1) = 1$ (one cluster of N vectors),
  - $S(N, N) = 1$ (N clusters of 1 vector each),
  - $S(N, m) = 0 \text{ for } m > N$.

Exhaustive Clustering

- ***Iterative equation***:

$$S(N,m) = mS(N-1,m) + S(N-1,m-1).$$

- Solution: ***Stirling numbers of the second kind***:

$$S(N,m) = \frac{1}{m!}\sum_{i=0}^{m} (-1)^{m-1} \binom{m}{i} i^N.$$

- Prohibitive computational complexity!

Sequential Clustering

Iterative sequential algorithm:

- Assigning data vectors $\mathbf{x}$ to its closest cluster $\mathcal{C}$.
- $d(\mathbf{x}, \mathcal{C})$: distance between a feature vector $\mathbf{x}$ and cluster $\mathcal{C}$.

- User-defined parameters:
  - the distance threshold ε.
  - the maximum allowable number of clusters M.

Sequential Clustering

- $d(\mathbf{x}, \mathcal{C}) = d(\mathbf{x}, \mathbf{m}_{\mathcal{C}})$, when $\mathcal{C}$ is represented by cluster center vector $\mathbf{m}_{\mathcal{C}}$.

- When $\mathbf{x}$ is assigned to its closest cluster $\mathcal{C}$ at iteration $(t+1)$, iterative cluster center vector update is given by:

$$\mathbf{m}_{\mathcal{C}}^{(t+1)} = \frac{n_{\mathcal{C}}^{(t)} \mathbf{m}_{\mathcal{C}_k}^{(t)} + \mathbf{x}}{n_{\mathcal{C}}^{(t+1)}}.$$

Sequential Clustering

Sequential clustering algorithm

```
$m = 1$
• $\mathcal{C}_m = \{\mathbf{x}_1\}$
• For $i = 2$ to $N$
    • Find $\mathcal{C}_k: d(\mathbf{x}_i, \mathcal{C}_k) = \min_{i \le j \le m} d(\mathbf{x}_i, \mathcal{C}_j)$
    • If $(d(\mathbf{x}_i, \mathcal{C}_k) > \varepsilon)$ AND $(m < M)$ then
        • $m = m + 1$
        • $\mathcal{C}_m = \{\mathbf{x}_i\}$
    • Else
        • $\mathcal{C}_k = \mathcal{C}_k \cup \{\mathbf{x}_i\}$
        • Update class $\mathcal{C}_k$ representation.
    • End{if}
• End{for}
```

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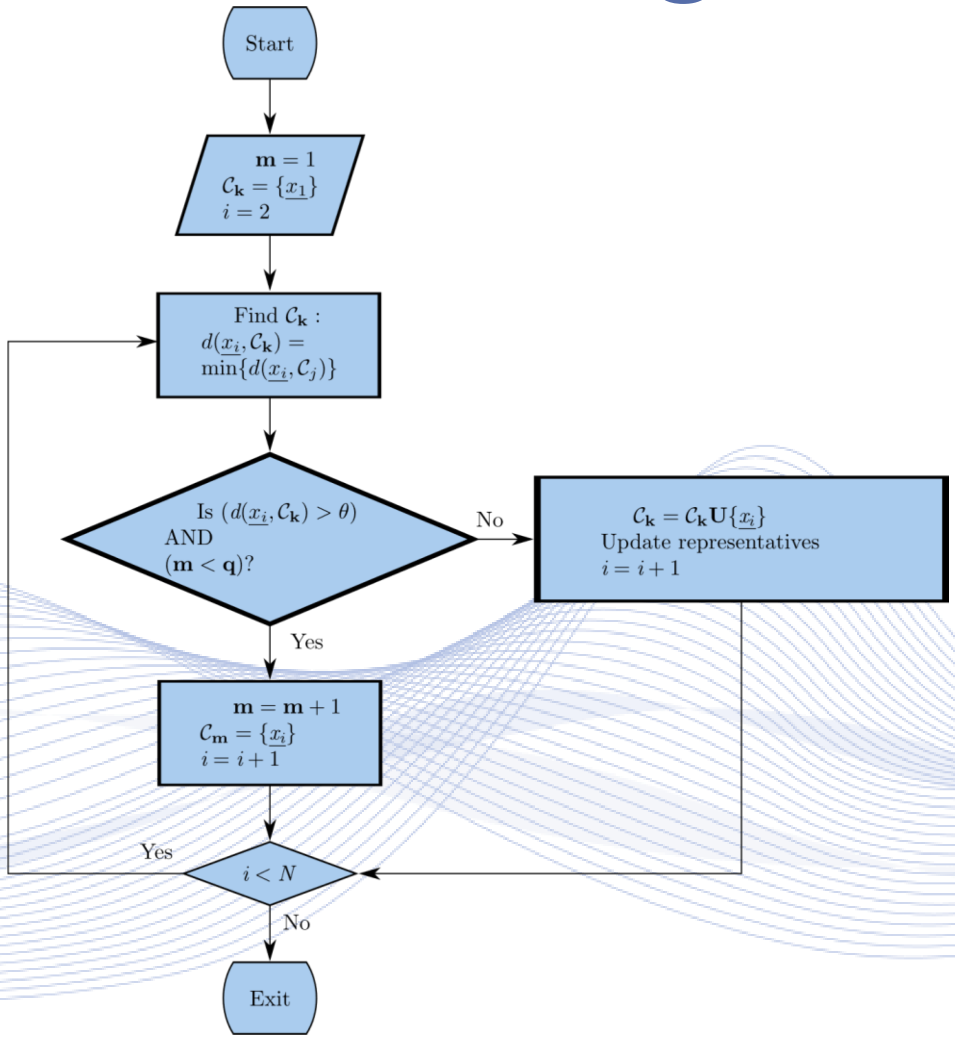
Sequential Clustering



Start
$\mathbf{m} = 1$
$\mathcal{C}_\mathbf{k} = \{\underline{x}_1\}$
$i = 2$
Find $\mathcal{C}_\mathbf{k}$:
$d(\underline{x}_i, \mathcal{C}_\mathbf{k}) = \min\{d(\underline{x}_i, \mathcal{C}_j)\}$
Is $(d(\underline{x}_i, \mathcal{C}_\mathbf{k}) > \theta)$ AND $(\mathbf{m} < \mathbf{q})$?
No
$\mathcal{C}_\mathbf{k} = \mathcal{C}_\mathbf{k} \mathbf{U} \{\underline{x}_i\}$
Update representatives
$i = i + 1$
Yes
$\mathbf{m} = \mathbf{m} + 1$
$\mathcal{C}_\mathbf{m} = \{\underline{x}_i\}$
$i = i + 1$
Yes
$i < N$
No
Exit

Block diagram of Sequential clustering algorithm.

Sequential Clustering

Properties:

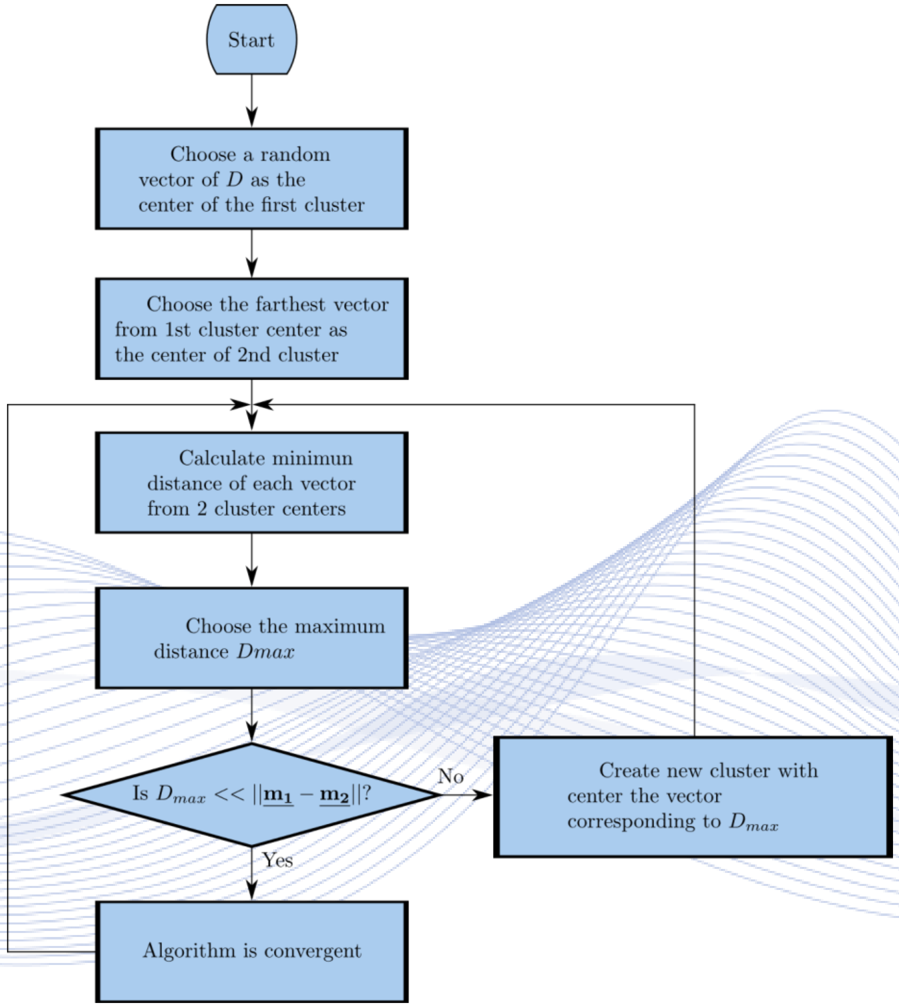
- Performance depends on data presentation to the algorithm.
- It may be used with similarity instead of distance measures by replacing $\min$ operator with $\max$.
- Class representation by its center favors compact clusters.
- A single pass on the entire data set has $O(Nm)$ complexity to compute $d(\mathbf{x}_i, \mathcal{C}_k)$ for N samples and $m < N$ clusters.

Sequential Clustering

Maximin Algorithm

```
• $m = 1$
• $C_m = \{\mathbf{x}_l\}$, $\mathbf{x}_l, l = 1, \dots, N$ is chosen randomly.
• For $i = 2$ to $N$
    • Find $d'(\mathbf{x}_l, C_k) = \max_{i \le j \le m} d'\left(\mathbf{x}_i, C_j\right)$
    • If $\left(d'(\mathbf{x}_l, C_k) \gg d''\left(C_i, C_j\right), \ i = 1, \dots, m, j = 1, \dots, m\right)$
        • $m = m + 1$
        • $C_m = \{\mathbf{x}_l\}$
    • Else
        • Find $C_k$:   $d(\mathbf{x}_i, C_k) = \min_{i \le j \le m} d\left(\mathbf{x}_i, C_j\right)$
        • $C_k = C_k \cup \{\mathbf{x}_i\}$
        • Where necessary, update representatives
    • End{if}
• End{for}
```

Sequential Clustering


Start
Choose a random vector of D as the center of the first cluster
Choose the farthest vector from 1st cluster center as the center of 2nd cluster
Calculate minimun distance of each vector from 2 cluster centers
Choose the maximum distance $Dmax$
Is $D_{max} << ||\underline{\mathbf{m_1}} - \underline{\mathbf{m_2}}||$?
No
Create new cluster with center the vector corresponding to D_{max}
Yes
Algorithm is convergent

Maximin Algorithm

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Clustering Based on Function Optimization

- Cost $J(\mathcal{D}, \boldsymbol{\Theta})$ is a function of:
  - data set $\mathcal{D}$ vectors and
  - an unknown cluster parameter vector/matrix/set $\boldsymbol{\Theta}$.
- Number of clusters m is fixed.
- Goal: estimate $\boldsymbol{\Theta}$ that optimizes cost function $J(\mathcal{D}, \boldsymbol{\Theta})$.
- $\boldsymbol{\Theta}$ is strongly depends on cluster topology.
- Compact clusters are best represented by their centers:

$$\boldsymbol{\Theta} = [\mathbf{m}_1^T, \ldots, \mathbf{m}_m^T]^T.$$

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K-means Algorithm

- Distances between a feature vector and a cluster:
  - Mahalanobis distance:

$$d(\mathbf{x}_i, \mathbf{m}_j) = (\mathbf{x}_i - \mathbf{m}_j)^T \mathbf{A} (\mathbf{x}_i - \mathbf{m}_j).$$

  - $\mathbf{A}$: symmetric, positive definite matrix.
  - Euclidean distance:

$$d(\mathbf{x}_i, \mathbf{m}_j) = (\mathbf{x}_i - \mathbf{m}_j)^T (\mathbf{x}_i - \mathbf{m}_j).$$

  - Minkowski distance: $d(\mathbf{x}_i, \mathbf{m}_j) = \left(\sum_{k=1}^{l} |\mathbf{x}_{ik} - \mathbf{m}_{jk}|^p\right)^{\frac{1}{p}}.$
  - $\mathbf{x}_{ik}, \mathbf{m}_{jk}$ are the j-th coordinates of $\mathbf{x}_i, \mathbf{m}_j$ respectively.

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K-means Algorithm

- Cost function minimization:

$$J(\mathbf{m}_1, \dots, \mathbf{m}_m) = \sum_{i=1}^{N} \sum_{j=1}^{m} d(\mathbf{x}_i, \mathbf{m}_j).$$

Using Euclidean distance:

$$J(\mathbf{m}_1, \dots, \mathbf{m}_m) = \sum_{i=1}^{N} \sum_{j=1}^{m} (\mathbf{x}_i - \mathbf{m}_j)^T (\mathbf{x}_i - \mathbf{m}_j).$$

K-means Algorithm

- Differentiation of $J(\mathbf{m}_1, \dots, \mathbf{m}_m)$:

$$\frac{\partial J(\mathbf{m}_1,\dots,\mathbf{m}_m)}{\partial \mathbf{m}_j} = 2\sum_{i=1}^{N}(\mathbf{m}_j - \mathbf{x}_i) = \mathbf{0}.$$

$$\mathbf{m}_j(t) = \frac{\sum_{i=1}^{N}\mathbf{x}_i}{N}.$$

K-means Algorithm

- Step 0: Initialize cluster centers $\mathbf{m}_1(0), \ldots, \mathbf{m}_m(0)$ randomly.
- Step 1: At each step (t) assign each data sample $\mathbf{x}_i, i = 1, \ldots N$ to the closest cluster center:

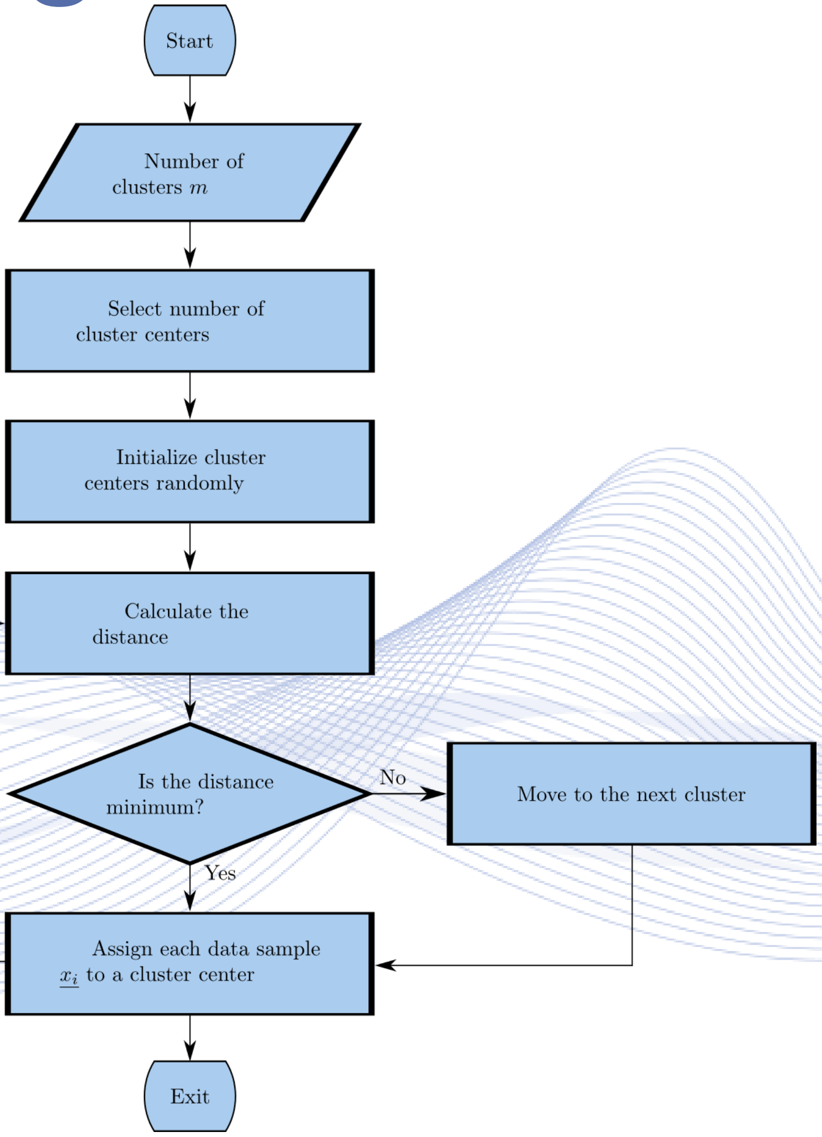
$$d(\mathbf{x}_i, \mathbf{m}_k(t)) < d\big(\mathbf{x}_i, \mathbf{m}_i(t)\big), \quad k \neq i$$

- Step 2: Update cluster $\mathcal{C}_j, j = 1, \ldots, m$ centers:

$$\mathbf{m}_j(t+1) = \frac{\sum_{i=1}^{|\mathcal{C}_j|} \mathbf{x}_i}{|\mathcal{C}_j|}.$$

- Step 3: If $\mathbf{m}_j(t+1) = \mathbf{m}_j(t)$, for every $j = 1, \ldots, m$, stop.

K-means Algorithm



Start
Number of clusters m
Select number of cluster centers
Initialize cluster centers randomly
Calculate the distance
Is the distance minimum?
No
Move to the next cluster
Yes
Assign each data sample $\underline{x}_i$ to a cluster center
Exit

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Isodata algorithm

- Step 1: Choose the initial cluster number m and initial cluster centers $\mathbf{m}_1(0), \dots, \mathbf{m}_m(0)$.
- Step 2: Classification of vectors of $\mathcal{D}$ in m clusters, based on their minimal distance from cluster centers.
- Step 3: Update the centers, as in the algorithm of K-means.
- Step 4: If cluster cardinality is smaller than a predetermined percentage of the cardinality of $\mathcal{D}$, this cluster is deleted.

Isodata algorithm

- Step 5 (***Cluster split***): Calculate the mean sample variance σ_{ij}^2 of each cluster $\mathcal{C}_j$ vectors along each data axis i :

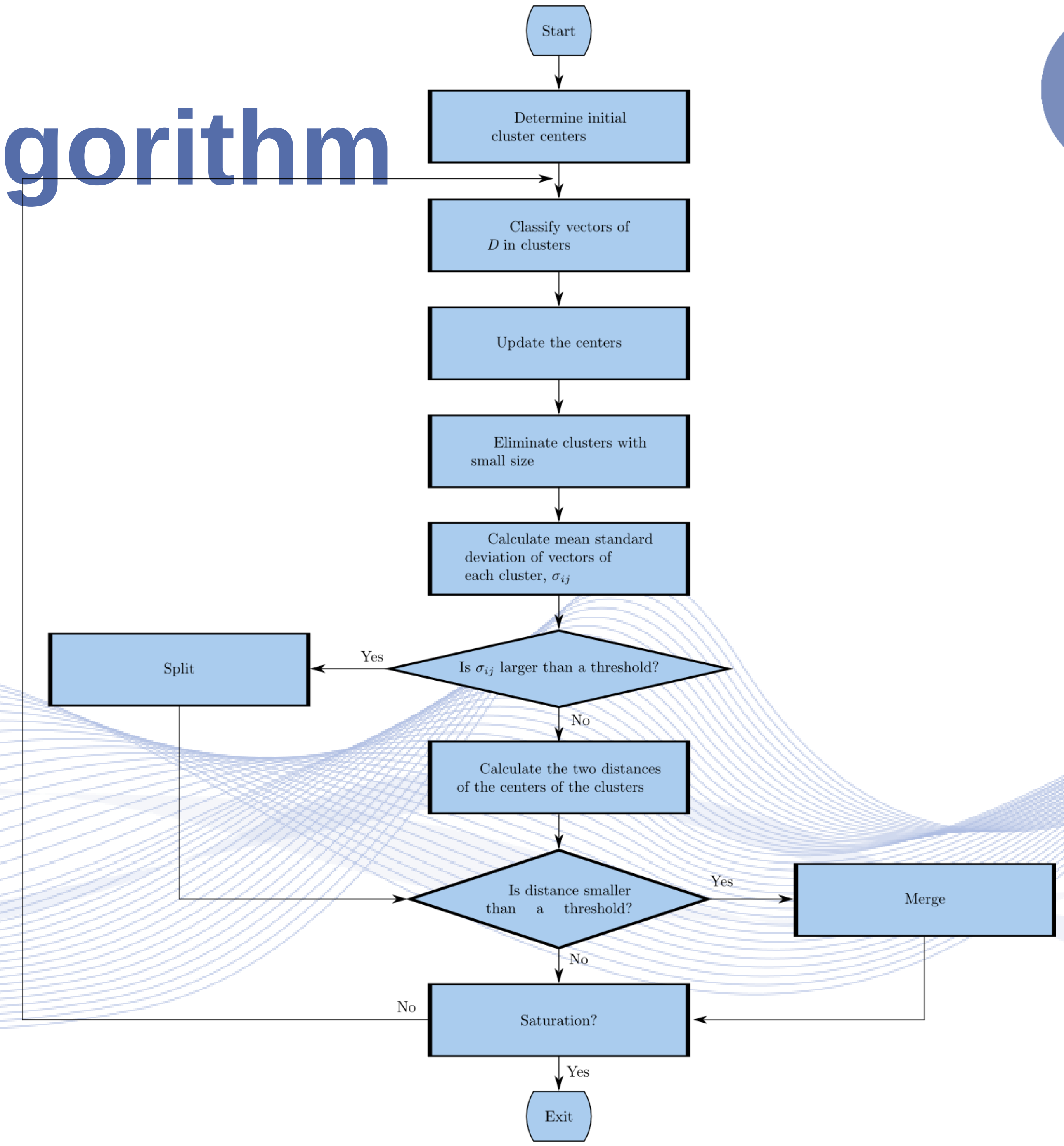
$$\sigma_{ij}^2 = \frac{1}{|\mathcal{C}_j|}\sum_{\mathbf{x}\in\mathcal{C}_j}(x_{ij} - m_{ij})^2, \qquad i = 1, \dots, n, j = 1, \dots, m.$$

  - If some σ_{ij} is larger than a predetermined threshold, split $\mathcal{C}_j$ in two and create their centers $\mathbf{m}_j - \mathbf{c}, \mathbf{m}_j + \mathbf{c}$.
  - Update number of clusters m.

Isodata algorithm

- Step 6 (***Cluster merge***):
  - Calculate the distances $d''(\mathcal{C}_i, \mathcal{C}_j)$, $i = 1, \dots, m, j = 1, \dots, m$ of any two clusters $\mathcal{C}_i$, $\mathcal{C}_j$.
  - If $d''(\mathcal{C}_i, \mathcal{C}_j)$ is smaller than a threshold, merge two clusters $\mathcal{C}_i$, $\mathcal{C}_j$.
  - Update number of clusters m.

Isodata algorithm



Start
Determine initial cluster centers
Classify vectors of D in clusters
Update the centers
Eliminate clusters with small size
Calculate mean standard deviation of vectors of each cluster, σ_{ij}
Is σ_{ij} larger than a threshold?
Yes
Split
No
Calculate the two distances of the centers of the clusters
Is distance smaller than a threshold?
Yes
Merge
No
Saturation?
No
Yes
Exit

Fuzzy Clustering

- In fuzzy set partitions, a vector belongs simultaneously to more than one cluster:
  - Fuzzy membership functions $u_j, j = 1, \dots, m$: $\mathcal{D} \rightarrow [0,1]$.
- $\mathbf{m}_j$: representative vector of j -th cluster (cluster center).
- $\boldsymbol{\Theta} = [\mathbf{m}_1^T, \dots, \mathbf{m}_m^T]^T$
- $\mathbf{U}$: $N \times m$ matrix whose element (i, j) equals to $u_j(\mathbf{x}_i)$.

- $d(\mathbf{x}_i, \mathbf{m}_j)$: distance between $\mathbf{x}_i$ and $\mathbf{m}_j$.

Fuzzy Clustering

- Distances between a feature vector and a cluster:
  - Mahalanobis distance:

$$d(\mathbf{x}_i, \mathbf{m}_j) = (\mathbf{x}_i - \mathbf{m}_j)^T \mathbf{A} (\mathbf{x}_i - \mathbf{m}_j).$$

  - $\mathbf{A}$: symmetric, positive definite matrix.
  - Euclidean distance:

$$d(\mathbf{x}_i, \mathbf{m}_j) = (\mathbf{x}_i - \mathbf{m}_j)^T (\mathbf{x}_i - \mathbf{m}_j).$$

  - Minkowski distance: $d(\mathbf{x}_i, \mathbf{m}_j) = \left(\sum_{k=1}^{l} |\mathbf{x}_{ik} - \mathbf{m}_{jk}|^p\right)^{\frac{1}{p}}.$
  - $\mathbf{x}_{ik}, \mathbf{m}_{jk}$ are the jth coordinates of $\mathbf{x}_i, \mathbf{m}_j$ respectively.

Fuzzy Clustering Algorithms

- Cost function minimization:

$$J_q(\boldsymbol{\Theta}, \mathbf{U}) = \sum_{i=1}^{N} \sum_{j=1}^{m} u_{ij}^q d(\mathbf{x}_i, \mathbf{m}_j),$$

with respect to $\boldsymbol{\Theta}$ and $\mathbf{U}$, subject to the constraints:

$$\sum_{j=1}^{m} u_{ij} = 1, \qquad i = 1, \dots, N.$$

- $u_{ij} \in [0,1], i = 1, \dots, N, \;\; j = 1, \dots, m,$
- $0 < \sum_{i=1}^{N} u_{ij} < N \,, \; j = 1, \dots, m.$
- $q > 1$: ***fuzzifier parameter***.

Fuzzy Clustering Algorithms

Minimization of $J_q(\boldsymbol{\Theta}, \mathbf{U})$ with respect to $\mathbf{U}$ under constraints:

- Lagrangian function minimization:

$$\mathcal{J}(\boldsymbol{\Theta}, \mathbf{U}) = \sum_{i=1}^{N} \sum_{j=1}^{m} u_{ij}^{q} d(\mathbf{x}_i, \mathbf{m}_j) - \sum_{i=1}^{N} \lambda_i \left(\sum_{j=1}^{m} u_{ij} - 1 \right).$$

- Partial differentiation of $\mathcal{J}(\boldsymbol{\Theta}, \mathbf{U})$ with respect to u_{rs}:

$$\frac{\partial \mathcal{J}(\boldsymbol{\Theta}, \mathbf{U})}{\partial u_{rs}} = q u_{rs}^{q-1} d(\mathbf{x}_r, \mathbf{m}_s) - \lambda_r = 0.$$

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Fuzzy Clustering Algorithms

Solution:

$$u_{rs} = \left(\frac{\lambda_r}{q d(\mathbf{x}_r, \mathbf{m}_s)}\right)^{\frac{1}{q-1}}, \; s = 1, \dots, m.$$

Substitution of u_{rs} in the constraint $\sum_{j=1}^{m} u_{rj} = 1$ leads to:

$$\lambda_r = \frac{q}{\left(\sum_{j=1}^{m}\left(\frac{1}{d\left(\mathbf{x}_r, \mathbf{m}_j\right)}\right)^{\frac{1}{q-1}}\right)^{q-1}}.$$

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Fuzzy Clustering Algorithms

- Combining the two previous equations:

$$u_{rs} = \frac{1}{\sum_{j=1}^{m}\left(\frac{d(\mathbf{x}_r,\mathbf{m}_s)}{d(\mathbf{x}_r,\mathbf{m}_j)}\right)^{\frac{1}{q-1}}}, \qquad r = 1,\dots,N, \qquad s = 1,\dots,m.$$

- Gradient of $J(\mathbf{\Theta},\mathbf{U})$ with respect to $\mathbf{m}_j$:

$$\frac{\partial J(\mathbf{\Theta},\mathbf{U})}{\partial \mathbf{m}_j} = \sum_{i=1}^{N} u_{ij}^{q}\frac{\partial d(\mathbf{x}_i,\mathbf{m}_j)}{\partial \mathbf{m}_j} = \mathbf{0}, \qquad j = 1,\dots,m.$$

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Fuzzy Clustering Algorithms

Fuzzy k-means algorithm:

- Using Mahalanobis distance:

$$\frac{\partial d(\mathbf{x}_i,\mathbf{m}_j)}{\partial \mathbf{m}_j} = 2\mathbf{A}(\mathbf{m}_j - \mathbf{x}_i).$$

- Substituting the above equation in $\frac{\partial J(\mathbf{\Theta},\mathbf{U})}{\partial \mathbf{m}_j}$, we obtain:

$$\sum_{i=1}^{N} u_{ij}^{q}(t-1)\,\mathbf{A}(\mathbf{m}_j - \mathbf{x}_i) = \mathbf{0}\ .$$

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Fuzzy Clustering Algorithms

- Since $\mathbf{A}$ is positive definite, it can be discarded:

$$\mathbf{m}_j(t) = \frac{\sum_{i=1}^{N} u_{ij}^{q}(t-1)\mathbf{x}_i}{\sum_{i=1}^{N} u_{ij}^{q}(t-1)}.$$

- Termination criterion:

$$||\mathbf{m}_j(t) - \mathbf{m}_j(t-1)\,|| < \epsilon,\ j = 1, \ldots, m.$$

Vector Quantization

Vector Quantization:

- Compact representation of the data set $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$, $\mathbf{x}_i \in \mathbb{R}^n$ by much fewer vectors $\mathbf{m}_i \in \mathbb{R}^n$, $i = 1, \ldots, m$, $m \ll N$ of the same dimensionality.

- Each $\mathbf{m}_i \in \mathbb{R}^n$ corresponds to one cluster $\mathcal{C}_i$, $i = 1, \ldots, m$.

Vector Quantization

- A data set $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$, $\mathbf{x}_i \in \mathbb{R}^{\boldsymbol{n}}$ is to be clustered (partitioned).
- Desired cluster number $m \ll N$.
- Distance measure $d(\mathbf{x}, \mathbf{y})$ between two vectors $\mathbf{x}, \mathbf{y}$.
- Calculation of cluster centers.
- Sorting algorithm to decide vector proximity.

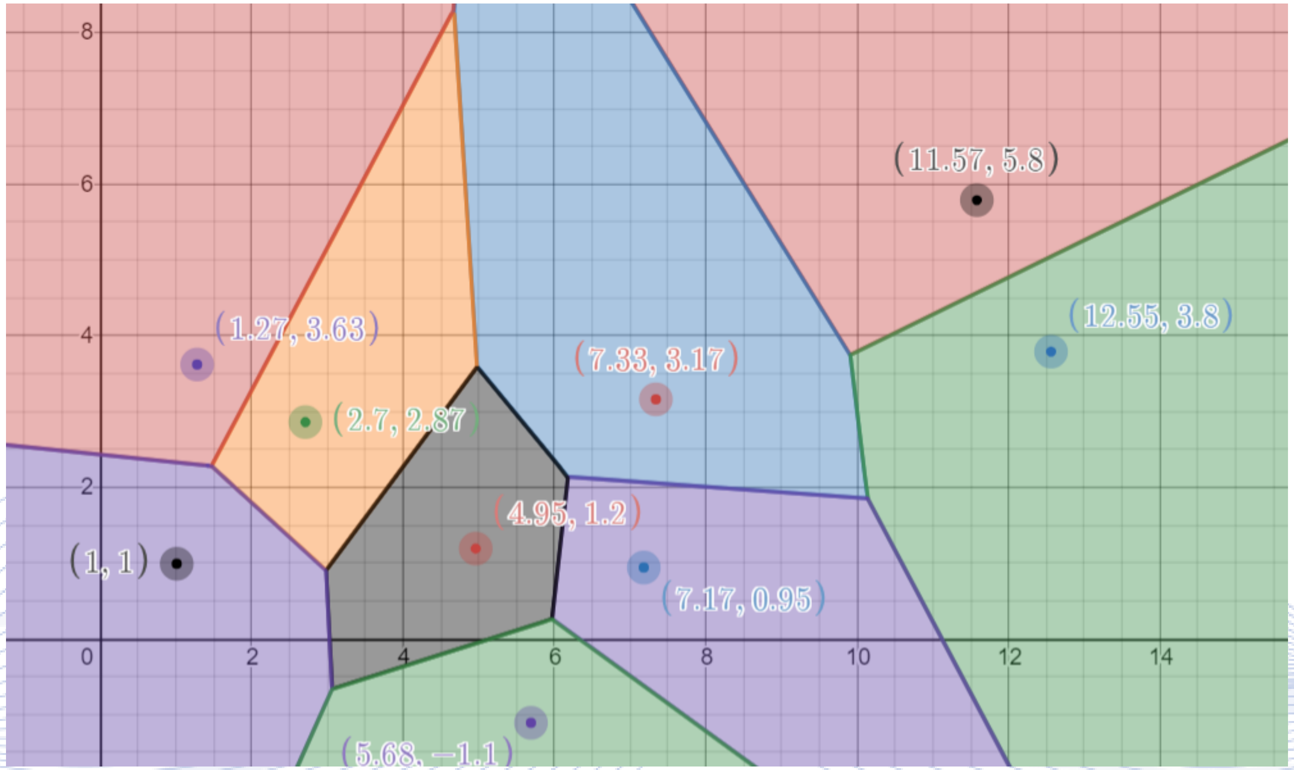
Vector Quantization

- Data vectors are partitioned in m clusters $\{\mathcal{C}_i, i = 1, \dots, m\}$.
- Mapping: $\mathbf{m} = \boldsymbol{Q}(\mathbf{x})$.
- $\mathbb{R}^n$ is partitioned in m ***Voronoi regions*** (one per cluster).
- Each Voronoi region (cell) $\mathcal{R}_i$ is represented by $\mathbf{m}_i \in \mathbb{R}^n$, $i = 1, \dots, m$:

$$|\mathbf{x} - \mathbf{m}_i| < |\mathbf{x} - \mathbf{m}_j|, \quad i \neq j.$$

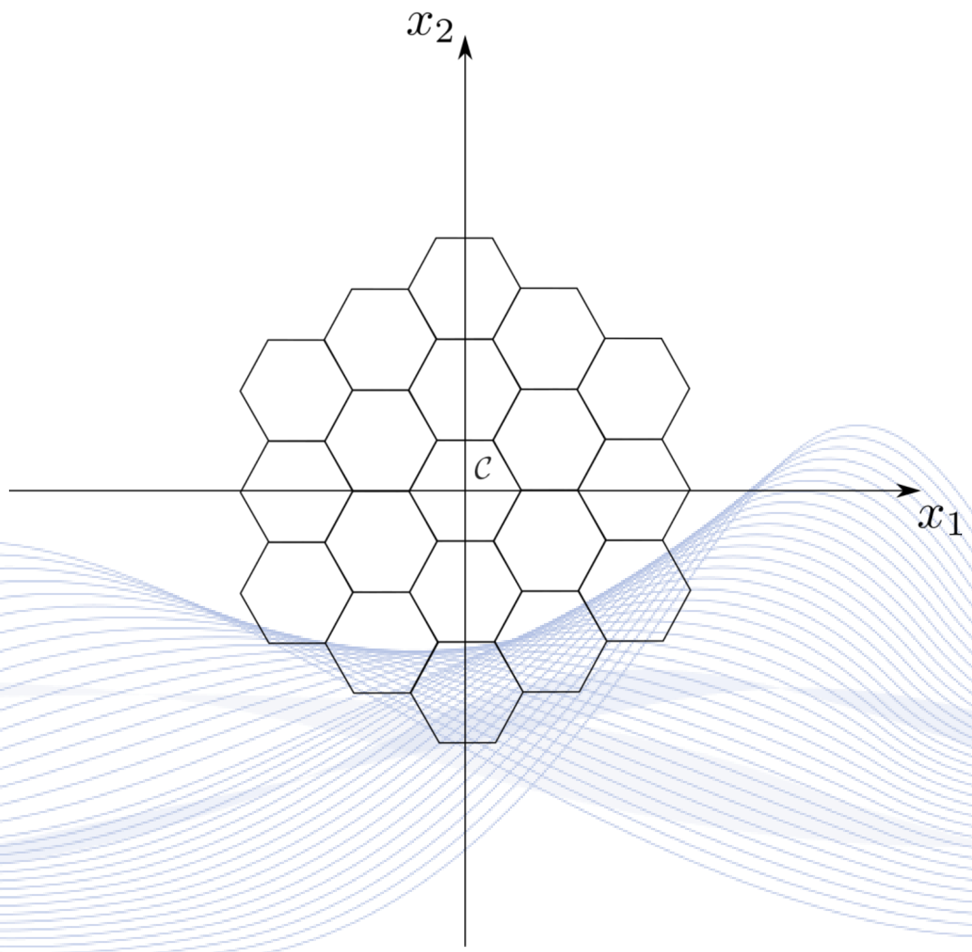
- Cluster $\mathcal{C}_i, i = 1, \dots, m$ vectors reside in $\mathcal{R}_i$.
- Voronoi cells may have regular structure.

Vector Quantization



Voronoi regions and clusters in $\mathbb{R}^2$.

Vector Quantization



Hexagonal Voronoi cells in $\mathbb{R}^2$.

Vector Quantization

- ***Codevectors*** $\mathbf{m}_i \in \mathbb{R}^n,\ i = 1, \dots, m$: cluster centers.
- Any vector in Voronoi region $\mathcal{C}_i$ are represented by $\mathbf{m}_i$.
- ***Quantization error*** (***distortion***) $|\mathbf{x} - \mathbf{m}_i|$.

- If $x_i \in \mathbb{R}$, classical (scalar) quantization:

$$|x - m_i| < |x - m_j|, \qquad i \neq j.$$

$$\mathcal{R}_i = [(m_{i-1} + m_i)/2,\ (m_i + m_{i+1})/2].$$

- It can be applied for 1D ***histogram thresholding***.

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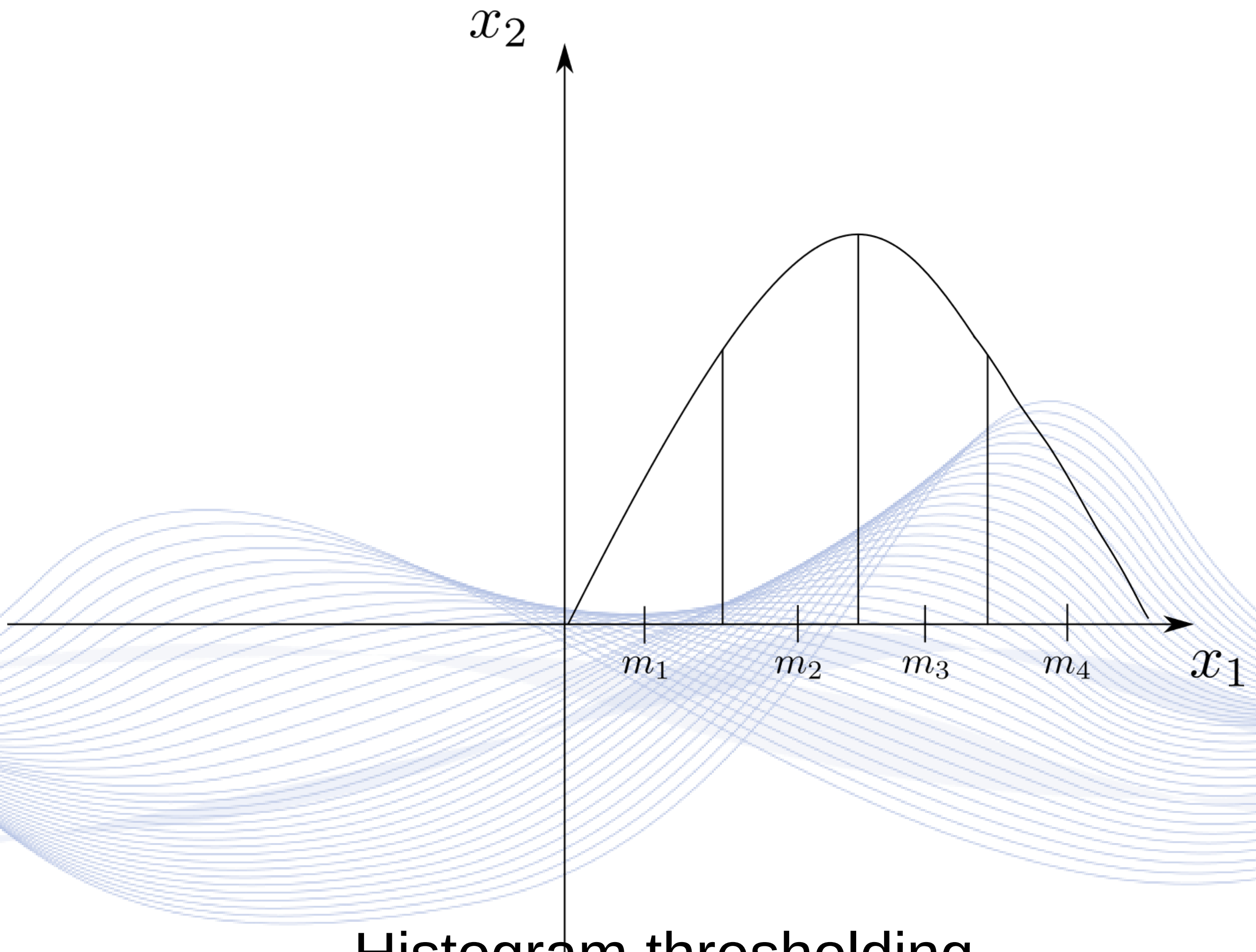
Vector Quantization



Histogram thresholding.

Vector Quantization

- Advantages:
  - Reduced storage requirements and faster processing.
  - Comparing two vectors has little computational complexity, thus VQ algorithms are not time-consuming.

- Disadvantages:
  - Quantization error.

Vector Quantization

Linde-Buzo-Gray Algorithm

- Initialization: Choose m random vectors $\mathbf{m}_i, i = 1, \dots, m$.
- Recursion:
  - Each vector $\mathbf{x}$ from set $\mathcal{D}$ is assigned to vector $\mathbf{m}_k$:

$$k = \arg_i \min d(\mathbf{x}, \mathbf{m}_i).$$

  - Calculate total quantization error: $J = \sum_i \sum d(\mathbf{x}, \mathbf{m}_i)$.
  - If $J < \varepsilon$ is smaller than a threshold, stop.
  - Else calculate new centers $\mathbf{m}_i, i = 1, \dots, m$ and repeat previous steps until convergence.
- Very similar to k-means algorithm.

Vector Quantization

Binary Split Algorithm

Initialization: Define a random cluster center. All vectors of data set $\mathcal{D}$ belong to the same cluster.

- Iteration t: (Total L iterations producing 2^L codevectors)
  - Each codevector $\mathbf{m}_i$ is broken into two vectors $\mathbf{m}_i(1+\epsilon)$, $\mathbf{m}_i(1-\epsilon)$ **,** $\epsilon \in [0.01, 0.005]$
  - Each vector $\mathbf{x}$ from training set is assigned to the closest vector $\mathbf{m}_k$:
    $$k = \arg_i \min d(\mathbf{x}, \mathbf{m}_i).$$
  - Calculate total quantization error: $J = \sum_i \sum d(\mathbf{x}, \mathbf{m}_i)$.
  - If J is smaller than a threshold, stop.
  - Calculate new center for each i. If $\mathrm{t} < L$ repeat previous steps, else stop.

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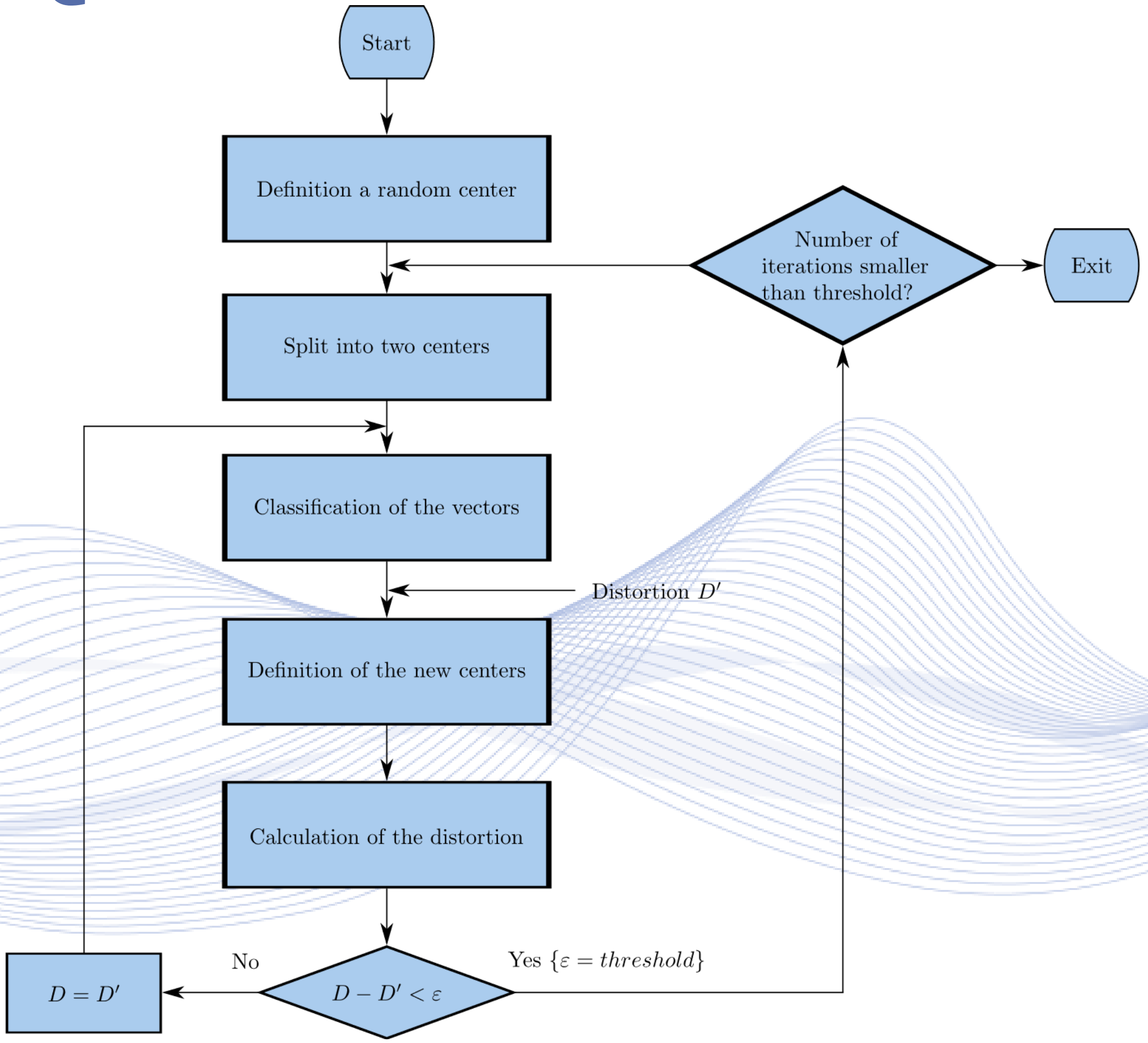
Vector Quantization


Start
Definition a random center
Split into two centers
Classification of the vectors
Distortion D'
Definition of the new centers
Calculation of the distortion
$D - D' < \varepsilon$
No
$D = D'$
Yes $\{\varepsilon = threshold\}$
Number of iterations smaller than threshold?
Exit

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Learning Vector Quantization

- ***Learning Vector Quantization*** (***LVQ***) was proposed by Kohonen.
- Also called ***Self-Organizing Maps*** (***SOM***).
- Initial values are set based on classic cluster algorithms.
- Code vectors $\mathbf{m}_i$ are iteratively optimized.
- Goal: clustering based on the nearest-neighbor rule.
- Clusters are described by their codevectors.
- Cluster boundaries matter.

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Learning Vector Quantization

Mathematical model of vector quantization

- $\mathbf{x}$: vector to be assigned to a cluster.
- Employ Euclidean distance.
- Find the winner cluster:
  - Closest cluster center $\mathbf{m}_k$:

$$d(\mathbf{x}, \mathbf{m}_k) = \min_i \{d(\mathbf{x}, \mathbf{m}_i)\}, \qquad \forall i \neq k .$$

Learning Vector Quantization

- Cluster center updating:

$$\mathbf{m}_k(t+1) = \mathbf{m}_k(t) + a(t)[\mathbf{x} - \mathbf{m}_k(t)]$$

$$\mathbf{m}_i(t+1) = \mathbf{m}_i(t), \qquad \text{for } i \neq k,$$

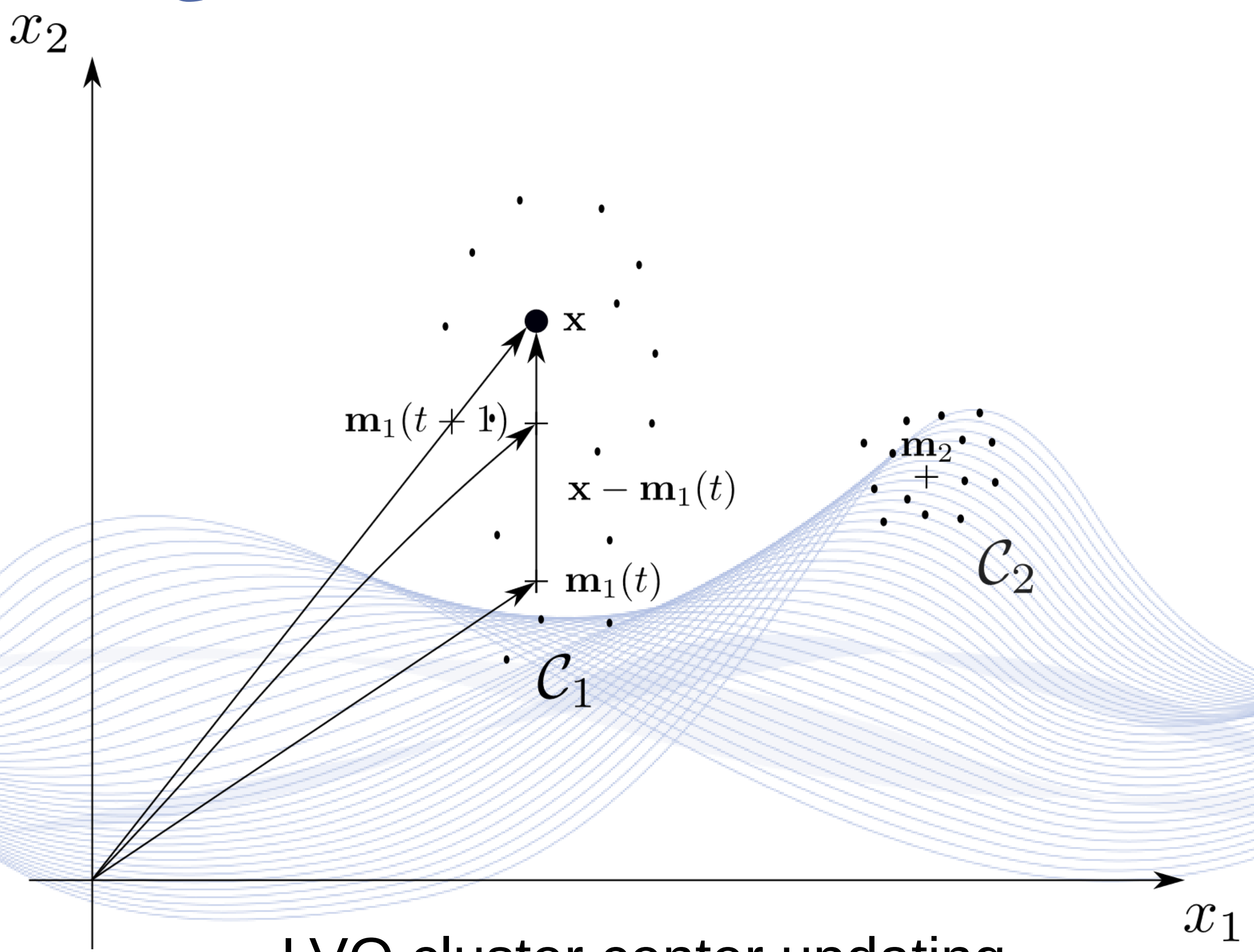
- $0 \leq a(t) \leq 1$.
- Distance $d(\mathbf{x}, \mathbf{m}_k)$ is monotonically decreasing:
  - If $\boldsymbol{\delta}\mathbf{x}_i = \mathbf{m}_i(t+1) - \mathbf{m}_i(t)$, then $[\nabla_{\mathbf{m}_k} d(\mathbf{x}, \mathbf{m}_k)]^T \boldsymbol{\delta}\mathbf{m}_i < 0$.

Learning Vector Quantization

- Incremental algorithm: data may come on the fly.
- For the first steps, $a(t)$ value shall be close to 1.
- Depending on total number of steps, $a(t)$ decreases:
  - Linear, exponential decrease.

- When $a(t)$ falls below the threshold, the algorithm freezes.
- Updating of winning cluster neighborhood $\mathcal{N}(\mathcal{C})$ can be performed.

Vector Quantization



LVQ cluster center updating.

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Learning Vector Quantization Algorithms

Competitive cluster center updating

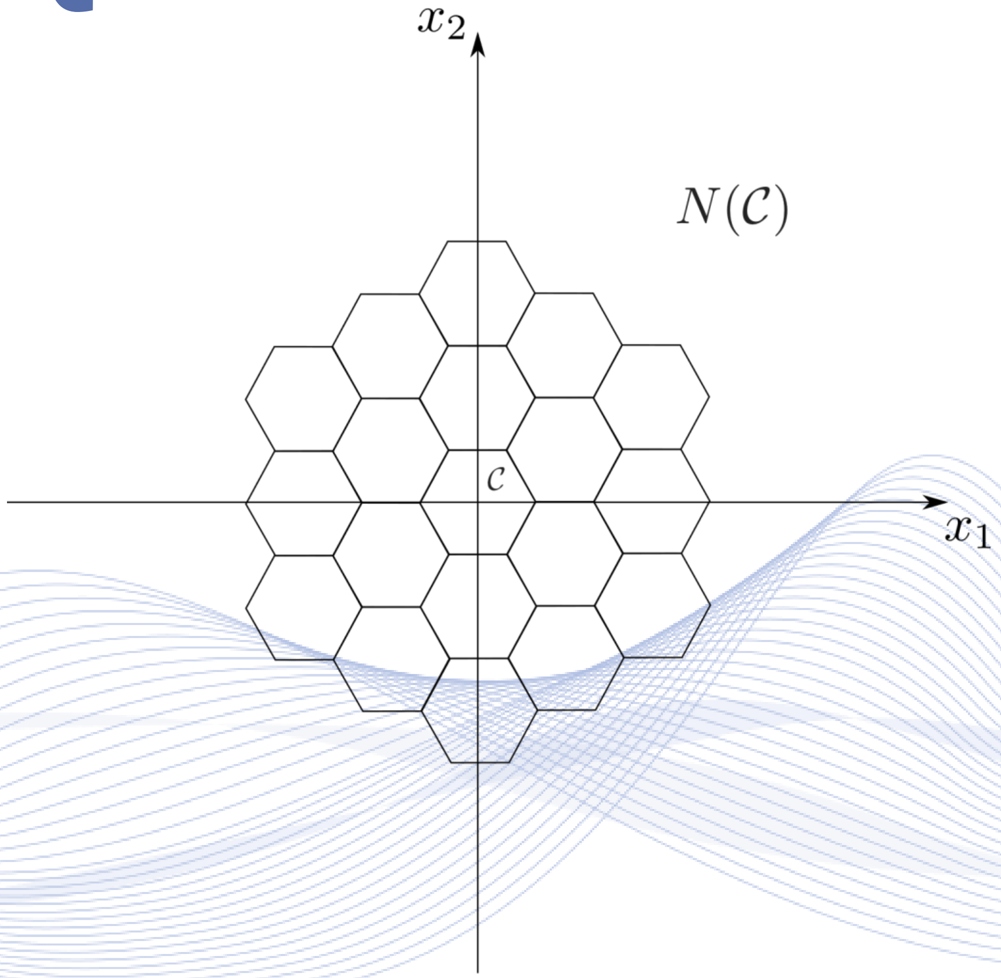
- For the winner cluster:

$$\mathbf{m}_k(t+1) = \mathbf{m}_k(t) + a(t)[\mathbf{x}(t) - \mathbf{m}_k(t)].$$

- For the rest of the clusters:

$$\mathbf{m}_k(t+1) = \mathbf{m}_k(t) - a(t)[\mathbf{x}(t) - \mathbf{m}_k(t)].$$

Vector Quantization



Hexagonal Voronoi cell neighborhood $\mathcal{N}(\mathcal{C})$ in $\mathbb{R}^2$.

Learning Vector Quantization Algorithms

Cooperative cluster center updating

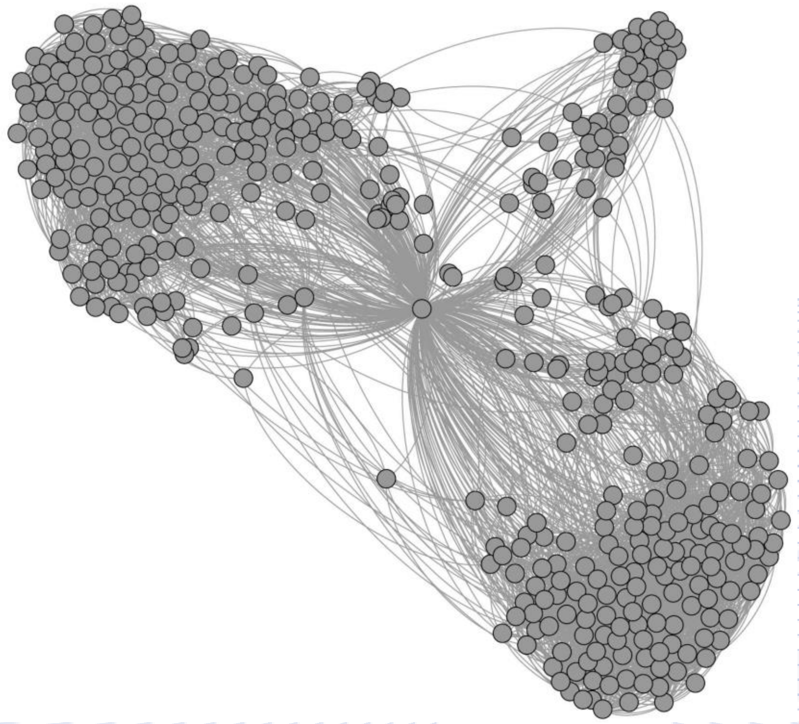
- For clusters within neighborhood $\mathcal{N}(\mathcal{C}_k)$:

$$\mathbf{m}_k(t+1) = \mathbf{m}_k(t) - a(t)[\mathbf{x}(t) - \mathbf{m}_k(t)].$$

- For the rest of the clusters:

$$\mathbf{m}_k(t+1) = \mathbf{m}_k(t), \quad i \neq k.$$

Graph-based Clustering


Data graph visualization.

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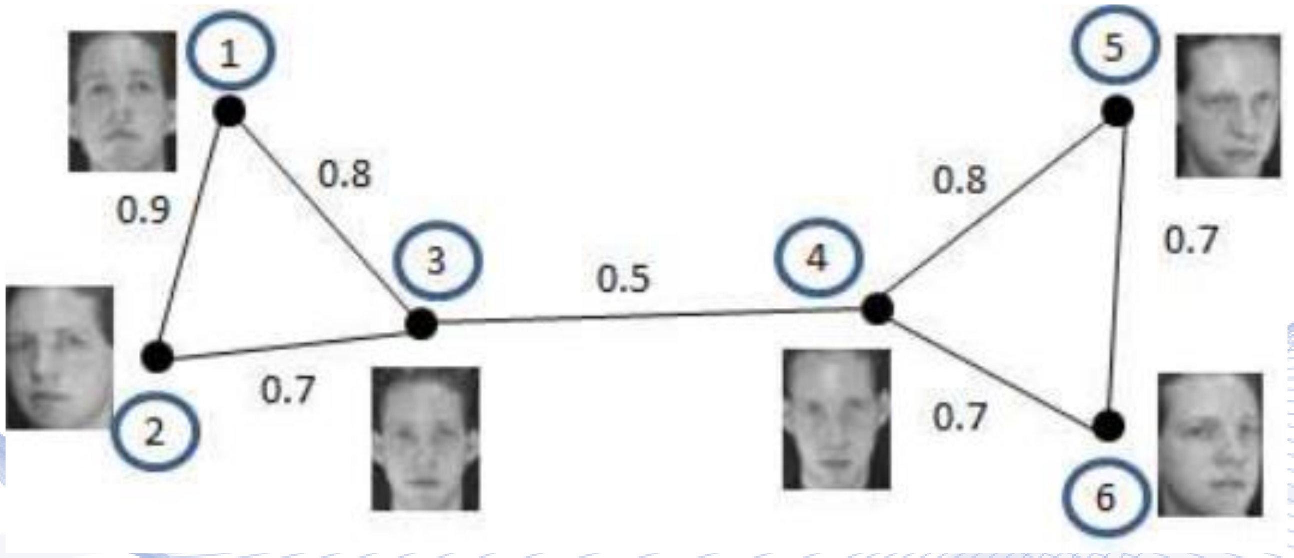
Graph-based Clustering

Similarity graph, Adjacency/Similarity matrix

- Let $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ be the data set where $\mathbf{x}_i \in \mathbb{R}^n$.
- Construct a graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$, where each graph vertex corresponds to a point $\mathbf{x}_i$, $i = 1, \dots, N$.
- Similarity graphs can be weighted connected and undirected.
- Graph $N \times N$ ***adjacency matrix***: $\mathbf{A} \in \{0,1\}^{N \times N}$.
- ***Similarity*** (***weight***) ***matrix***: $\mathbf{W} = [W_{ij}] \in \mathbb{R}^{N \times N}$.

Graph-based Clustering



1	0.9	0.8	0	0	0
0.9	1	0.7	0	0	0
0.8	0.7	1	0.5	0	0
0	0	0.5	1	0.8	0.7
0	0	0	0.8	1	0.7
0	0	0	0.7	0.7	1

a) Similarity graph; b) Similarity matrix.

Graph-based Clustering

- ***Vertex degree***: number of vertex connection in $\mathbf{A}$.
- ***Gaussian kernel*** for edge weight calculation:

$$W(i,j) = \begin{cases} e^{-\frac{||\mathbf{x}_i - \mathbf{x}_j||^2}{2\sigma^2}}, & \text{if } ||\mathbf{x}_i - \mathbf{x}_j|| < e, \\ 0, & \text{otherwise.} \end{cases}$$

- e: is a user-defined constant.
- || . || is Euclidean norm.

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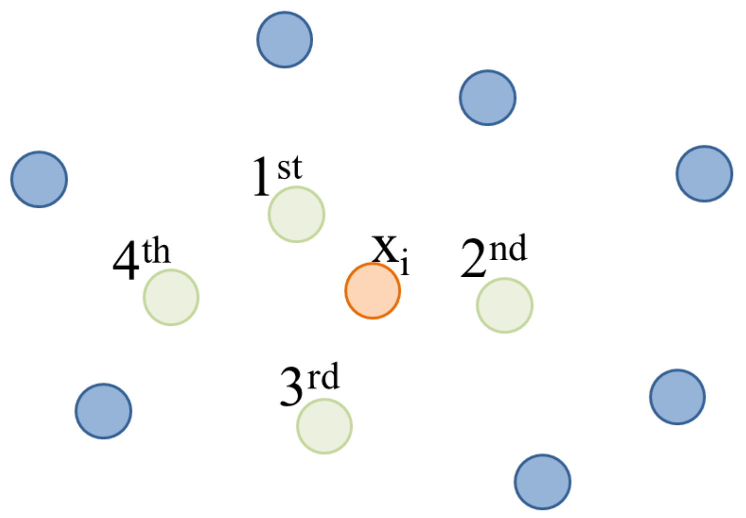
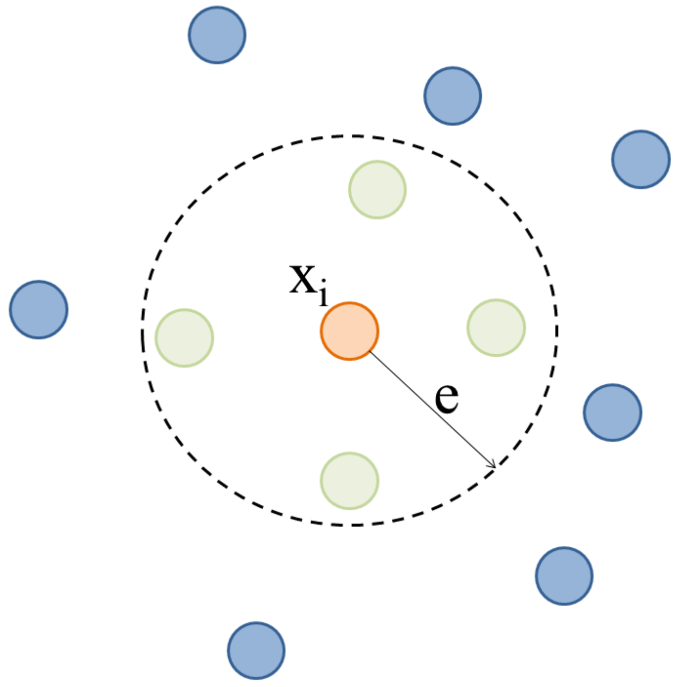
Graph-based Clustering

Nearest neighbor graphs





a) k-nearest neighbors graph; b) e-neighborhood graph.

Graph-based Clustering

Graph Clustering

- Cluster graph vertices (data vectors) into tightly linked clusters.
- Vertices of the same cluster are:
  - Strongly connected to each other and
  - sparsely connected to the rest of the graph.
- ***Intra-cluster connectivity***: measured by the cluster density.
- ***Inter-cluster connectivity***: measured by ***graph cut*** cardinality.

Graph-based Clustering

Global clustering algorithms

- ***Iterative methods***:
  - Go through all vertices and assign them to clusters.
  - Decisions based on optimization of a node connectivity metric.
  - ***Online method***:
    - Process one vertex at a time and update clusters based on what has been encountered thus far.

Graph-based Clustering

- ***Hierarchical structure***:
  - Clusters not rigidly defined.
  - Subclusters can be contained in the same cluster.

Graph-based Clustering

Adjacency matrix eigenanalysis:

- Adjacency matrix eigenvalues and eigenvectors:

$$\mathbf{A}\mathbf{u}_i = \lambda_i \mathbf{u}_i, \quad i = 0, \dots, N - 1.$$

- $\lambda_i, i = 0, \dots, N - 1$: roots of ***characteristic polynomial***:

$$\det(\mathbf{A} - \lambda \mathbf{I}) = 0.$$

- Adjacency matrix eigen-decomposition: $\mathbf{A} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T$.

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Graph-based Clustering

Laplacian matrix eigenanalysis:

$$\mathbf{L} = \mathbf{D} - \mathbf{A}.$$

- $\mathbf{D}$: $N \times N$ diagonal ***vertex degree*** matrix.

- Symmetric Laplacian matrix :

$$\mathbf{L}_S \triangleq \mathbf{D}^{-\frac{1}{2}}\mathbf{L}\mathbf{D}^{-\frac{1}{2}} = \mathbf{I} - \mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}}.$$

- Random walk Laplacian matrix :

$$\mathbf{L}_R \triangleq \mathbf{D}^{-1} = \mathbf{I} - \mathbf{D}^{-1}\mathbf{A}.$$

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Graph-based Clustering

Laplacian matrix eigenanalysis:

- Non-decreasing eigenvalue order:

$$\lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{N-1}.$$

- ***Graph spectrum*** is the eigenvalue set: $\{\lambda_i, \quad i = 0, \ldots, N - 1\}$
- It is invariant to ***graph isomorphism***
  - Graph vertex permutations.
- Non-isomorphic graphs can be co-spectral.

Graph-based Clustering

- λ_0 is always zero, $0 = \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{N-1} \leq \ 2$.

$$\sum_{i=0}^{N-1} \lambda_i = N.$$

- $\lambda_{N-1} = 2$, if graph $\mathcal{G}$ is ***bipartite***.

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Graph-based Clustering

- ***Algebraic connectivity*** (eigenvalue λ_1):

- If $\lambda_1 > 0$:
  - graph $\mathcal{G}$ is connected.
- else:
  - multiplicity of eigen value 0 is equal number of connected graph components.

Graph-based Clustering

- Graph comprised of k disjoint ***cliques***:
  - k smallest eigenvalues of normalized Laplacian matrix are 0.
  - i-th corresponding eigenvector $(0 \leq i \leq k-1)$ has non-zero values for vertices of the i –th clique.

- Adding edges cause the eigenvalues to increase and change slightly corresponding eigenvectors.

Graph-based Clustering

Graph clustering based on ***spectral bisection***:

- 2-way graph partitioning.

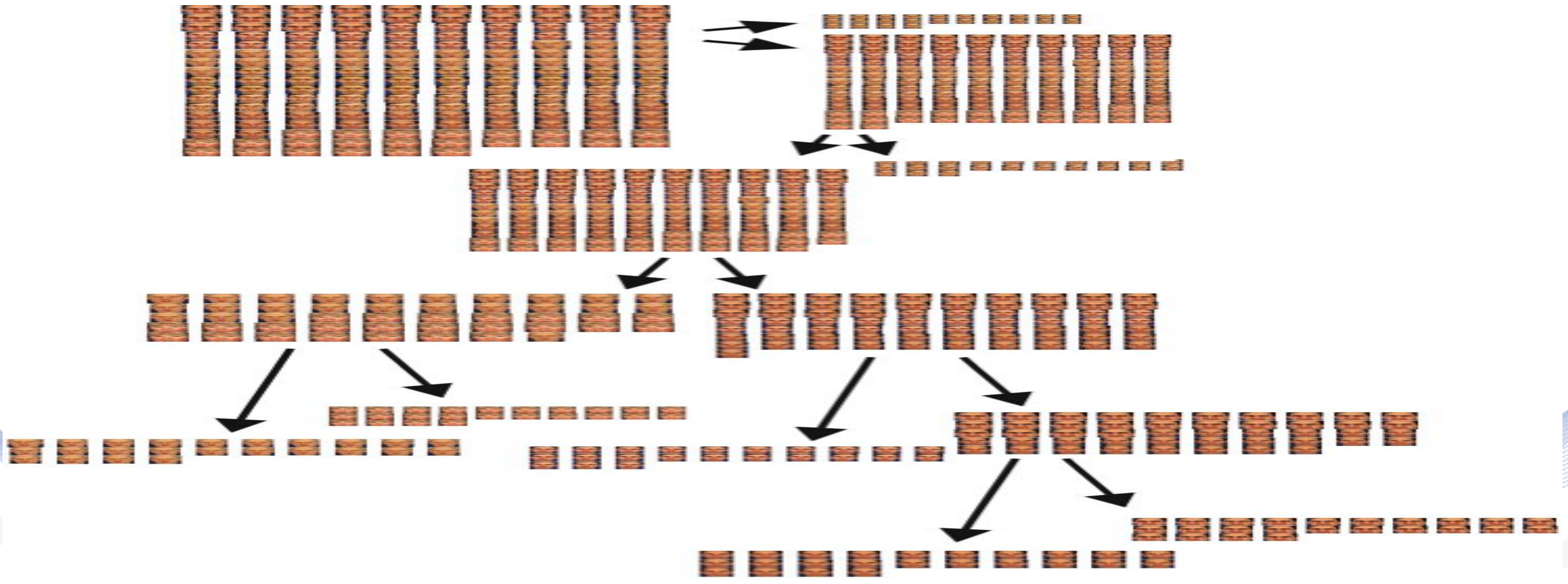
- It uses the so-called ***Fiedler vector***:
  - eigenvector $\mathbf{u}_1$ corresponding to eigenvalue λ_1 of Laplacian matrix.

Graph-based Clustering

N-Cut Graph Clustering

- When there are 2 clusters with strong internal connectivity and sparsely connected:
  - Positive Fiedler vector entries correspond to one cluster and negative to the other.
  - This provide a bisection of the graph in two subgraphs.
- Iterative bisection of the resulting subgraphs.

Graph-based Clustering



N-Cut Graph Clustering (2-way partitioning).

Graph-based Clustering

***Edge-based bisection*:**

- Compute Fiedler vector.
- Split vertices into 2 groups:
  - their relevant Fiedler vector entries are below/above the Fiedler vector entries median.
- Edges between these two groups are cut.

Graph-based Clustering

Vertex-based bisection:

- Compute Fiedler vector.
- Find the largest gap in Fiedler vector entries
- Split Fiedler vector entries accordingly.
- Split the graph at the cut provides the best cut quotient.

Graph-based Clustering

Spectral graph clustering:

- Perform eigenanalysis on one of the normalized Laplacians.
- extract r eigenvectors corresponding to the smallest eigenvalues excluding λ_0.
- Store eigenvectors in a $N \times r$ matrix $\mathbf{U}$.
- Its rows are the new data representation.
- Use any standard clustering algorithm to cluster them.

Graph-based Clustering

Graph-based clustering properties:

- Little user input is needed.
- Trivial clusters easily avoided.
- Unlikely to get bad clustering results.
- They cannot be employed in extremely large graphs:
  - memory limitations.
- Eigenanalysis has $O(N^3)$ computational complexity.

Q & A

Thank you very much for your attention!

More material in
http://icarus.csd.auth.gr/cvml-web-lecture-series/

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