Clustering algorithms

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Unit 2

– Proximity measures

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Types of features

*Categorized with respect to their **domain***

Continuous (the domain is a continuous subset of $\Re$).
Discrete (the domain is a finite discrete set).
Binary or *dichotomous* (the domain consists of two possible values).

*Categorized with respect to the **relative significance of the values they take***

Nominal (the values code states, e.g., the gender of a person).
Ordinal (the values are meaningfully ordered, e.g., the rating of the services of a hotel (poor, good, very good, excellent)).
Interval-scaled (the difference of two values is meaningful but their ratio is meaningless, e.g., temperature in ^{o}C).
Ratio-scaled (the ratio of two values is meaningful, e.g., weight).

Proximity measures: Definitions

(A) Between vectors

(1) Dissimilarity measure (between vectors of X) is a function

$$d: X \times X \to \Re$$

with the following properties

1. $\exists d_0 \in \Re: 0 \le d_0 \le d(\boldsymbol{x}, \boldsymbol{y}) < +\infty, \forall \boldsymbol{x}, \boldsymbol{y} \in X$

2. $d(\boldsymbol{x}, \boldsymbol{x}) = d_0, \forall \boldsymbol{x} \in X$

3. $d(\boldsymbol{x}, \boldsymbol{y}) = d(\boldsymbol{y}, \boldsymbol{x}), \forall \boldsymbol{x}, \boldsymbol{y} \in X$

Examples: Euclidean distance, Manhattan distance etc.

If in addition:

4. $d(\boldsymbol{x}, \boldsymbol{y}) = d_0 \Leftrightarrow \boldsymbol{x} = \boldsymbol{y}$

5. $d(\boldsymbol{x}, \boldsymbol{z}) \le d(\boldsymbol{x}, \boldsymbol{y}) + d(\boldsymbol{y}, \boldsymbol{z}), \forall \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in X$ (triangular inequality)

d is called **metric** dissimilarity measure.

Proximity measures : Definitions

(A) Between vectors

(2) Similarity measure (between vectors of X) is a function

$$s: X \times X \rightarrow \Re$$

with the following properties

1. $\exists s_0 \in \Re: 0 \leq s(\boldsymbol{x}, \boldsymbol{y}) \leq s_0 < +\infty, \forall \boldsymbol{x}, \boldsymbol{y} \in X$
2. $s(\boldsymbol{x}, \boldsymbol{x}) = s_0, \forall \boldsymbol{x} \in X$
3. $s(\boldsymbol{x}, \boldsymbol{y}) = s(\boldsymbol{y}, \boldsymbol{x}), \forall \boldsymbol{x}, \boldsymbol{y} \in X$

If in addition:

4. $s(\boldsymbol{x}, \boldsymbol{y}) = s_0 \Leftrightarrow \boldsymbol{x} = \boldsymbol{y}$
5. $\frac{1}{s(\boldsymbol{x},\boldsymbol{z})} \leq \frac{1}{s(\boldsymbol{x},\boldsymbol{y})} + \frac{1}{s(\boldsymbol{y},\boldsymbol{z})}, \forall \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z} \in X$

s is called **metric** similarity measure.

Examples: inner product, Tanimoto distance etc.

NOTE:
Similarity measures and dissimilarity measures are also referred as **proximity measures**.

NOTATION:
- Similarity measure: *s*
  dissimilarity measure: *d*
- **proximity measures:** $\wp$

Proximity measures : Definitions

Exercise:

Consider the case where the elements of X are **scalars**.

Which of the following is

(a) a dissimilarity measure,

(b) a **metric** dissimilarity measure?

1. $d_1(x, y) = |x - y|$

2. $d_2(x, y) = |x^2 - y^2|$

3. $d_3(x, y) = \cos(x - y)$

4. $d_4(x, y) = \sin(|x - y|)$

Proximity measures: Definitions

(B) Between sets

Let $D_i \subset X, \quad i = 1, \ldots, k$, and $U = \{D_1, \ldots, D_k\}$.

A **proximity measure** (similarity or dissimilarity) $\wp$ on U is a function

$$\wp: U \times U \rightarrow \Re$$

For dissimilarity measure the following properties should hold

1. $\exists d_0 \in \Re: 0 \leq d_0 \leq d(D_i, D_j) < +\infty, \forall D_i, D_j \in X$
2. $d(D_i, D_i) = d_0, \forall D_i \in X$
3. $d(D_i, D_j) = d(D_j, D_i), \forall D_i, D_j \in X$

Question: What is the definition when $\wp$ stands for a similarity measure?

If in addition:

4. $d(D_i, D_j) = d_0 \Leftrightarrow D_i = D_j$
5. $d(D_i, D_k) \leq d(D_i, D_j) + d(D_j, D_k), \forall D_i, D_j, D_k \in X$

d is called **metric** dissimilarity measure.

Proximity measures: Definitions

(B) Between sets

NOTE: The **definition** of the *proximity functions between sets* **passes through** the definition of *proximity functions between a point and a set*.

Roadmap for the next few slides:

***Proximity** functions between a point and a set*

- **Nonparametric** case
- **Parametric** case
  - **Point** representatives
    - Mean vector
    - Mean center
    - Median center
  - **Hyperplane** representatives
  - **Hypersphere** representatives
  - …

Proximity measures: Definitions

(B) Between sets

NOTE: The **definition** of the *proximity functions between sets* **passes through** the definition of *proximity functions between a point and a set*.

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Proximity functions between a point and a set

Remark: Having in mind that a cluster is actually a set C, a proximity function between a point $\boldsymbol{x}$ and a set C actually **quantifies** the resemblance/relation of $\boldsymbol{x}$ with the cluster C.

Let $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ and $\boldsymbol{x} \in X, C \subset X$

Definitions of $\wp(\boldsymbol{x}, C)$:

(a) All points of C **contribute** to the definition of $\wp(\boldsymbol{x}, C)$ (**nonparametric** repr.).

Dissimilarity functions	Similarity functions
Max dissimilarity function $d_{max}^{ps}(\boldsymbol{x}, C) = max_{\boldsymbol{y} \in C} d(\boldsymbol{x}, \boldsymbol{y})$	*Min similarity function* $s_{min}^{ps}(\boldsymbol{x}, C) = min_{\boldsymbol{y} \in C} s(\boldsymbol{x}, \boldsymbol{y})$
Min dissimilarity function $d_{min}^{ps}(\boldsymbol{x}, C) = min_{\boldsymbol{y} \in C} d(\boldsymbol{x}, \boldsymbol{y})$	*Max similarity function* $s_{min}^{ps}(\boldsymbol{x}, C) = max_{\boldsymbol{y} \in C} s(\boldsymbol{x}, \boldsymbol{y})$
Average dissimilarity function $d_{avg}^{ps}(\boldsymbol{x}, C) = \frac{1}{n_C} \sum_{\boldsymbol{y} \in C} d(\boldsymbol{x}, \boldsymbol{y})$	*Average similarity function* $s_{avg}^{ps}(\boldsymbol{x}, C) = \frac{1}{n_C} \sum_{\boldsymbol{y} \in C} s(\boldsymbol{x}, \boldsymbol{y})$

n_C is the cardinality of C.

Proximity measures: Definitions

(B) Between sets

NOTE: The **definition** of the *proximity functions between sets* **passes through** the definition of *proximity functions between a point and a set*.

Roadmap for the next few slides:

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        - Median center
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    - **Hypersphere** representatives
    - …

Proximity functions between a point and a set

Definitions of $\wp(\boldsymbol{x}, C)$ (cont.):

(b) A representative of C, r_C, **contributes** to the definition of $\wp(\boldsymbol{x}, C)$ (**parametric** repr.).

In this case $\wp(\boldsymbol{x}, C) = \wp(\boldsymbol{x}, r_C)$

Typical **point** representatives are:

- The mean vector

$$\boldsymbol{m}_p = \frac{1}{n_C} \sum_{\boldsymbol{y} \in C} \boldsymbol{y}$$

n_C is the cardinality of C.

- The mean center

$$\boldsymbol{m}_C \in C: \sum_{\boldsymbol{y} \in C} d(\boldsymbol{m}_C, \boldsymbol{y}) \leq \sum_{\boldsymbol{y} \in C} d(\boldsymbol{z}, \boldsymbol{y}), \forall\, \boldsymbol{z} \in C$$

- The median center

$$\boldsymbol{m}_{med} \in C: med(d(\boldsymbol{m}_{med}, \boldsymbol{y}) | \boldsymbol{y} \in C) \leq med(d(\boldsymbol{z}, \boldsymbol{y}) | \boldsymbol{y} \in C), \forall\, \boldsymbol{z} \in C$$

d: dissimilarity measure.

NOTE: Other representatives (e.g., hyperplanes, hyperspheres) are useful in certain applications (e.g., object identification using clustering techniques).

Proximity functions between a point and a set

Definitions of $\wp(\boldsymbol{x}, C)$ (cont.):

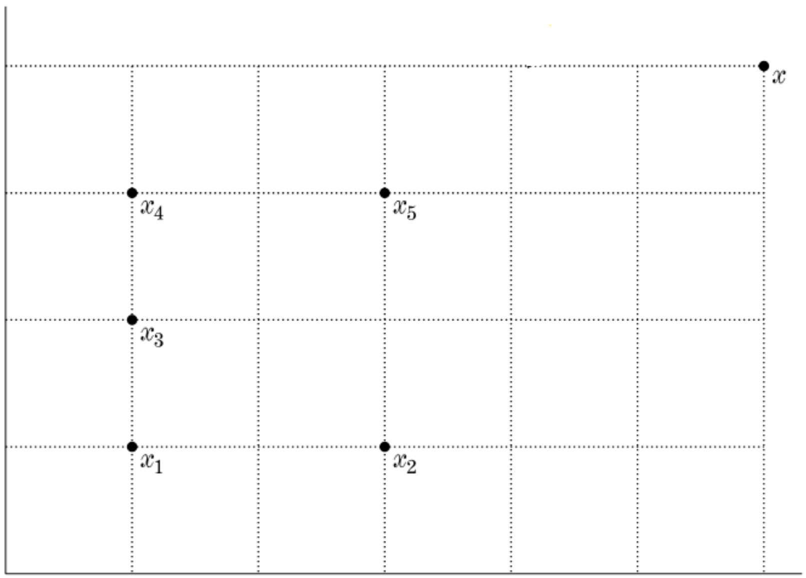
(b) A representative of C, r_C, **contributes** to the definition of $\wp(\boldsymbol{x}, C)$.

In this case $\boxed{\wp(\boldsymbol{x}, C) = \wp(\boldsymbol{x}, r_C)}$

Exercise 5: Let $C = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4, \boldsymbol{x}_5\}$, where $\boldsymbol{x}_1 = [1,1]^T$, $\boldsymbol{x}_2 = [3,1]^T$, $\boldsymbol{x}_3 = [1,2]^T$, $\boldsymbol{x}_4 = [1,3]^T$, $\boldsymbol{x}_5 = [3,3]^T$. All points lie in the discrete space $\{0,1,2,\dots,6\}^2$. Use the Euclidean distance to measure the dissimilarity between two vectors in C.

(a) Determine the mean vector, the mean center and the median center of C.

(b) Compute the distance of point $\boldsymbol{x} = [6,4]^T$ from C using the above defined representatives (where it is valid).



Proximity functions between a point and a set

Definitions of $\wp(x, C)$ (cont.):

(b) A representative of C, r_C, **contributes** to the definition of $\wp(x, C)$.

In this case

$$\wp(x, C) = \wp(x, r_C)$$

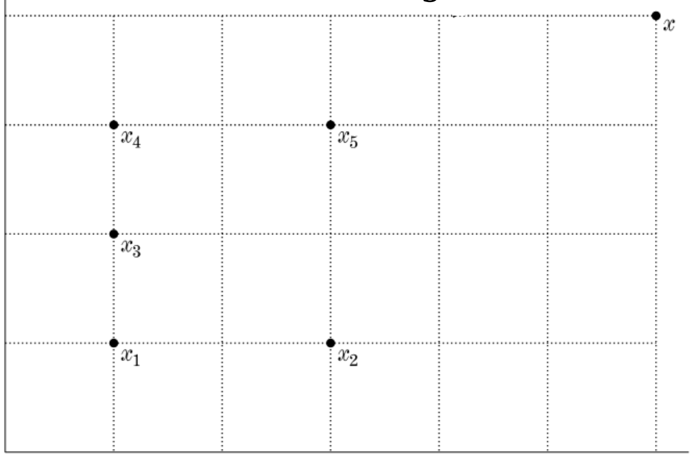
Exercise 5:

Mean vector: $\frac{1}{5}(x_1 + x_2 + x_3 + x_4 + x_5) = \frac{1}{5}\left(\begin{bmatrix}1\\1\end{bmatrix} + \begin{bmatrix}3\\1\end{bmatrix} + \begin{bmatrix}1\\2\end{bmatrix} + \begin{bmatrix}1\\3\end{bmatrix} + \begin{bmatrix}3\\3\end{bmatrix}\right) = \frac{1}{5}\begin{bmatrix}9\\10\end{bmatrix} = \begin{bmatrix}1.8\\2\end{bmatrix}$

Mean center:

	x_1	x_2	x_3	x_4	x_5	SUM
x_1	0	2	1	2	2.82	**7.82**
x_2	2	0	2.23	2.82	2	**9.05**
x_3	1	2.23	0	1	2.23	**6.46**
x_4	2	2.82	1	0	2	**7.82**
x_5	2.82	2	2.23	2	0	**9.05**

$\rightarrow$ ***Mean center*** $= x_3$



Median center:

	x_1	x_2	x_3	x_4	x_5	Med
x_1	0	2	1	2	2.82	**2**
x_2	2	0	2.23	2.82	2	**2**
x_3	1	2.23	0	1	2.23	**1**
x_4	2	2.82	1	0	2	**2**
x_5	2.82	2	2.23	2	0	**2**

$\rightarrow$ ***Median center*** $= x_3$

Proximity measures: Definitions

(B) Between sets

NOTE: The **definition** of the *proximity functions between sets* **passes through** the definition of *proximity functions between a point and a set*.

Roadmap for the next few slides:

***Proximity** functions between a point and a set*

- **Nonparametric** case

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  - **Hypersphere** representatives
  - …

Proximity functions between a point and a set

Definitions of $\wp(\boldsymbol{x}, C)$ (cont.):

(b) A representative of C, r_C, **contributes** to the definition of $\wp(\boldsymbol{x}, C)$.

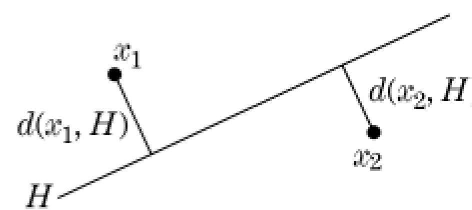
In this case $\wp(\boldsymbol{x}, C) = \wp(\boldsymbol{x}, r_C)$

Linear-shaped clusters:

- Such clusters occur e.g., in computer vision applications.
- In this case, a hyperplane is a better representative for such clusters
- Equation of a hyperplane H:

$$\sum_{j=1}^{l} a_j x_j + a_0 = \boldsymbol{a}^T \boldsymbol{x} + a_0 = 0$$

where $\boldsymbol{x} = [x_1, x_2, \dots, x_l]^T$, $\boldsymbol{a} = [a_1, a_2, \dots, a_l]^T$ is the direction vector of H and a_0 is its offset.



- **Distance** of a point $\boldsymbol{x}$ from H : $d(\boldsymbol{x}, H) = min_{\boldsymbol{z} \in H} d(\boldsymbol{x}, \boldsymbol{z})$
- If $d(\boldsymbol{x}, \boldsymbol{z})$ is the Euclidean distance, it is

$$d(\boldsymbol{x}, H) = \frac{|\boldsymbol{a}^T \boldsymbol{x} + a_0|}{||\boldsymbol{a}||} \qquad ||\boldsymbol{a}|| = \sqrt{\sum_{j=1}^{l} \alpha_j{}^2}$$

Proximity functions between a point and a set

Definitions of $\wp(\boldsymbol{x}, C)$ (cont.):

(b) A representative of C, r_C, **contributes** to the definition of $\wp(\boldsymbol{x}, C)$.

In this case $\wp(\boldsymbol{x}, C) = \wp(\boldsymbol{x}, r_C)$

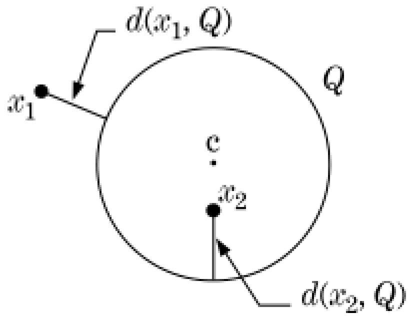
Hyperspherical clusters:

- Such clusters occur e.g., in computer vision applications.
- In this case, a hypersphere is a better representative of such clusters
- Equation of a hypersphere Q:

$$(\boldsymbol{x} - \boldsymbol{c})^T(\boldsymbol{x} - \boldsymbol{c}) = r^2$$

  where $\boldsymbol{x} = [x_1, x_2, \dots, x_l]^T$, $\boldsymbol{c} = [c_1, c_2, \dots, c_l]^T$ is the center of Q and r is its radius.

- **Distance** of a point $\boldsymbol{x}$ from Q: $d(\boldsymbol{x}, Q) = min_{\boldsymbol{z} \in Q} d(\boldsymbol{x}, \boldsymbol{z})$



- For Euclidean distance between two points, $d(\boldsymbol{x}, Q)$ has a geometric insight.

- However, other non-geometric alternatives have also been proposed.

Proximity functions between two sets

Remark: Having in mind that a cluster is actually a set C, a proximity function between two sets actually **quantifies** the resemblance/relation between two clusters.

Let $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ and $D_i, D_j \subset X$ with $n_i = |D_i|, n_j = |D_j|$.

Definitions of $\wp(D_i, D_j)$:

(a) All points of each set **contribute** to the definition of $\wp(D_i, D_j)$.

Dissimilarity functions	Similarity functions
Max dissimilarity function $$d_{max}^{ss}(D_i, D_j) = max_{x \in D_i, y \in D_j} d(\boldsymbol{x}, \boldsymbol{y})$$	*Min similarity function* $$s_{min}^{ss}(D_i, D_j) = min_{x \in D_i, y \in D_j} s(\boldsymbol{x}, \boldsymbol{y})$$
Min dissimilarity function $$d_{min}^{ss}(D_i, D_j) = min_{x \in D_i, y \in D_j} d(\boldsymbol{x}, \boldsymbol{y})$$	*Max similarity function* $$s_{max}^{ss}(D_i, D_j) = max_{x \in D_i, y \in D_j} s(\boldsymbol{x}, \boldsymbol{y})$$
Average dissimilarity function $$d_{avg}^{ss}(D_i, D_j) = \frac{1}{n_i n_j} \sum_{x \in D_i} \sum_{y \in D_j} d(\boldsymbol{x}, \boldsymbol{y})$$	*Average similarity function* $$s_{avg}^{ss}(D_i, D_j) = \frac{1}{n_i n_j} \sum_{x \in D_i} \sum_{y \in D_j} s(\boldsymbol{x}, \boldsymbol{y})$$

Proximity functions between two sets

Definitions of $\wp\left(D_i, D_j\right)$ (cont.):

(b) Each set D_i is **represented** by a point representative $\boldsymbol{m}_i$.

- Mean proximity function

$$\wp_{mean}^{ss}\left(D_i, D_j\right) = \wp(\boldsymbol{m}_i, \boldsymbol{m}_j)$$

$$d_{mean}^{ss}\left(D_i, D_j\right) = d(\boldsymbol{m}_i, \boldsymbol{m}_j)$$

$$s_{mean}^{ss}\left(D_i, D_j\right) = s(\boldsymbol{m}_i, \boldsymbol{m}_j)$$

- $\wp_e^{ss}\left(D_i, D_j\right) = \sqrt{\frac{n_i n_j}{n_i + n_j}}\,\wp(\boldsymbol{m}_i, \boldsymbol{m}_j)$

$$n_i = |D_i|$$

$$n_j = |D_j|$$

$$d_e^{ss}\left(D_i, D_j\right) = \sqrt{\frac{n_i n_j}{n_i + n_j}}\, d(\boldsymbol{m}_i, \boldsymbol{m}_j)$$

$$s_e^{ss}\left(D_i, D_j\right) = \sqrt{\frac{n_i n_j}{n_i + n_j}}\, s(\boldsymbol{m}_i, \boldsymbol{m}_j)$$

NOTE: Proximity functions between a vector $\boldsymbol{x}$ and a set C may be derived from the above functions if we set $D_i = \{\boldsymbol{x}\}$.

Proximity measures between vectors

In the sequel we consider the cases:

$$\boldsymbol{x} = [x_1, \ldots, x_l]^T$$
$$\boldsymbol{y} = [y_1, \ldots, y_l]^T$$

(A) Real-valued vectors – **dissimilarity** measures (DMs)

(B) Real-valued vectors – **similarity** measures (SMs)

(C) Discrete-valued vectors – **similarity-dissimilarity** measures

(D) Mixed-valued vectors – **dissimilarity** and **similarity** measures

NOTE: Some of the measures below may seem “weird”. However, they have been **tailored** for certain types of applications.

Proximity measures between vectors

(A) Real-valued vectors – dissimilarity measures (DMs)

$\boldsymbol{x} = [x_1, \dots, x_l]^T$
$\boldsymbol{y} = [y_1, \dots, y_l]^T$

- Weighted l_p metric DMs

$$d_p(\boldsymbol{x}, \boldsymbol{y}) = \left(\sum_{i=1}^{l} w_i |x_i - y_i|^p \right)^{1/p}$$

Instances of special interest are obtained for:

$p = 1 \rightarrow d_1(\boldsymbol{x}, \boldsymbol{y}) = \sum_{i=1}^{l} w_i \, |x_i - y_i|$ (l_1 or Manhattan or city block dist.)

$p = 2 \rightarrow d_2(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{\sum_{i=1}^{l} w_i (x_i - y_i)^2}$ (l_2 or Euclidean distance)

$p = \infty \rightarrow d_\infty(\boldsymbol{x}, \boldsymbol{y}) = max_{i=1,\dots,l} w_i |x_i - y_i|$ (l_∞ or maximum distance)

NOTES:

✓ For $w_i = 1$, we obtain the unweighted versions of the l_p metrics.

✓ It holds: $d_\infty(\boldsymbol{x}, \boldsymbol{y}) \le d_2(\boldsymbol{x}, \boldsymbol{y}) \le d_1(\boldsymbol{x}, \boldsymbol{y})$

Proximity measures between vectors

(A) Real-valued vectors – dissimilarity measures (DMs)

$$\boldsymbol{x} = [x_1, \dots, x_l]^T$$
$$\boldsymbol{y} = [y_1, \dots, y_l]^T$$

- Mahalanobis distance

$$d(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{(\boldsymbol{x} - \boldsymbol{y})^T B (\boldsymbol{x} - \boldsymbol{y})}$$

B is symmetric, positive definite matrix

- *Other measures*

•Features may take positive and/or negative values

•Normalization per feature:

$$0 \leq \frac{|x_i - y_i|}{|b_i - a_i|} \leq 1$$

$$- \; d_G(\boldsymbol{x}, \boldsymbol{y}) = -log_{10}\left(1 - \frac{1}{l}\sum_{i=1}^{l} \frac{|x_i - y_i|}{|b_i - a_i|}\right)$$

where b_i and a_i are the maximum and the minimum values of the i-th feature, among the vectors of X (dependence on the current data set)

$$- \; d_Q(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{\frac{1}{l}\sum_{i=1}^{l} \left(\frac{x_i - y_i}{x_i + y_i}\right)^2}$$

•Features may take **only** non-negative values

•Normalization per feature:

$$0 \leq \frac{|x_i - y_i|}{x_i + y_i} \leq 1$$

Proximity measures between vectors

(B) Real-valued vectors –similarity measures (SMs)

$$\boldsymbol{x} = [x_1, \dots, x_l]^T$$
$$\boldsymbol{y} = [y_1, \dots, y_l]^T$$

- Inner product

$$s_{inner}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x}^T \boldsymbol{y} = \sum_{i=1}^{l} x_i y_i$$

- It is usually used either (i) for non-negative valued vectors or (ii) for normalized vectors, i.e., $||\boldsymbol{x}|| = \rho$.
- Concerning (ii), in order to comply with the non-negativity requirement in the definition of the similarity measure, we may consider the similarity measure $s_{inner}(\boldsymbol{x}, \boldsymbol{y}) + \rho^2$

- Cosine similarity measure

$$s_{cosine}(\boldsymbol{x}, \boldsymbol{y}) = \frac{\boldsymbol{x}^T \boldsymbol{y}}{||\boldsymbol{x}|| \cdot ||\boldsymbol{y}||}$$

where $||\boldsymbol{x}|| = \sqrt{\boldsymbol{x}^T \boldsymbol{x}} = \sqrt{\sum_{i=1}^{l} {x_i}^2}$ and $||\boldsymbol{y}|| = \sqrt{\boldsymbol{y}^T \boldsymbol{y}} = \sqrt{\sum_{i=1}^{l} {y_i}^2}$.

Proximity measures between vectors

(B) Real-valued vectors –similarity measures (SMs)

$\boldsymbol{x} = [x_1, \dots, x_l]^T$
$\boldsymbol{y} = [y_1, \dots, y_l]^T$

- Pearson's correlation coefficient

$$r_{Pearson}(\boldsymbol{x}, \boldsymbol{y}) = \frac{\boldsymbol{x_d}^T \boldsymbol{y_d}}{||\boldsymbol{x_d}|| \cdot ||\boldsymbol{y_d}||} \in [-1,1]$$

where $\boldsymbol{x}_d = [x_1 - \bar{x}, \dots, x_l - \bar{x}]^T$, $\boldsymbol{y}_d = [y_1 - \bar{y}, \dots, y_l - \bar{y}]^T$ with $\bar{x} = \frac{1}{l}\sum_{i=1}^{l} x_i$ and $\bar{y} = \frac{1}{l}\sum_{i=1}^{l} y_i$, respectively.

It **measures** the correlation (covariance) between $\boldsymbol{x}, \boldsymbol{y}$

A related dissimilarity measure:

$$D(\boldsymbol{x}, \boldsymbol{y}) = \frac{1 - r_{Pearson}(\boldsymbol{x}, \boldsymbol{y})}{2} \in [0,1]$$

Proximity measures between vectors

(B) Real-valued vectors –similarity measures (SMs)

$\boldsymbol{x} = [x_1, \dots, x_l]^T$
$\boldsymbol{y} = [y_1, \dots, y_l]^T$

- Tanimoto distance

$$s_T(\boldsymbol{x}, \boldsymbol{y}) = \frac{\boldsymbol{x}^T \boldsymbol{y}}{||\boldsymbol{x}||^2 + ||\boldsymbol{y}||^2 - \boldsymbol{x}^T \boldsymbol{y}}$$

Algebraic manipulations give

$$s_T(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{1 + \frac{(\boldsymbol{x}-\boldsymbol{y})^T(\boldsymbol{x}-\boldsymbol{y})}{\boldsymbol{x}^T \boldsymbol{y}}}$$

The larger the agreement between $\boldsymbol{x}, \boldsymbol{y}$, the larger the $s_T(\boldsymbol{x}, \boldsymbol{y})$.

NOTE: $s_T(\boldsymbol{x}, \boldsymbol{y})$ is inversely proportional to the Euclidean distance and proportional to the inner product.

- *Other measure:*

$$s_C(\boldsymbol{x}, \boldsymbol{y}) = 1 - \frac{\sqrt{(\boldsymbol{x}-\boldsymbol{y})^T(\boldsymbol{x}-\boldsymbol{y})}}{||\boldsymbol{x}|| + ||\boldsymbol{y}||} \in [0,1]$$

Proximity measures between vectors

(C) Discrete-valued vectors – similarity & dissimilarity measures (SMs-DMs)

Let F_i be the **discrete** set of values the i-th feature (nominal/categorical attribute) can take and n_i be its cardinality, $i = 1, \dots, l$.

$$\boldsymbol{x} = [x_1, \dots, x_l]^T$$
$$\boldsymbol{y} = [y_1, \dots, y_l]^T$$

Consider two l-dimensional vectors

$$\boldsymbol{x} = [x_1, x_2, \dots, x_k, \dots, x_l]^T \in F_1 \mathrm{x} F_2 \mathrm{x} \dots \mathrm{x} F_k \mathrm{x} \dots \mathrm{x} F_l$$
$$\boldsymbol{y} = [y_1, y_2, \dots, y_k, \dots, y_l]^T \in F_1 \mathrm{x} F_2 \mathrm{x} \dots \mathrm{x} F_k \mathrm{x} \dots \mathrm{x} F_l$$

The similarity measure $s(\boldsymbol{x}, \boldsymbol{y})$ is defined as

$$s(\boldsymbol{x}, \boldsymbol{y}) = \sum_{k=1}^{l} w_k s_k(x_k, y_k)$$

where $s_k(x_k, y_k)$ is the **feature** similarity measure between the values x_k, y_k of the k-th feature.

Thus, in order to define $s(\boldsymbol{x}, \boldsymbol{y})$, we need to **define** $s_k(x_k, y_k)$.

Proximity measures between vectors

(C) Discrete-valued vectors – similarity & dissimilarity measures (SMs-DMs)

Example: Let l=3 and

$$\boldsymbol{x} = [x_1, \dots, x_l]^T$$
$$\boldsymbol{y} = [y_1, \dots, y_l]^T$$

$$F_1 = \{a, b, c\}$$
$$F_2 = \{1,2,3,4\}$$
$$F_3 = \{A, B, C\}$$

Consider the vectors:

$$\boldsymbol{x} = [x_1, x_2, x_3]^T = [a, 2, A]^T$$
$$\boldsymbol{y} = [y_1, y_2, y_3]^T = [a, 3, B]^T$$

That is, $x_1 = a$, $y_1 = a$,
$x_2 = 2$, $y_2 = 3$,
$x_3 = A$, $y_3 = B$.

Thus

$$s_1(x_1, y_1) = s_1(a, a)$$
$$s_2(x_2, y_2) = s_2(2, 3)$$
$$s_3(x_3, y_3) = s_3(A, B)$$

and

$$s(\boldsymbol{x}, \boldsymbol{y}) = w_1 \cdot s_1(a, a) + w_2 \cdot s_2(2, 3) + w_3 \cdot s_3(A, B)$$

Proximity measures between vectors

(C) Discrete-valued vectors – similarity & dissimilarity measures (SMs-DMs)

Let F_i be the **discrete** set of values the i-th (nominal/categorical) feature can take
and n_i be its cardinality, $i=1,\ldots,l$.

$$\boldsymbol{x} = [x_1, \ldots, x_l]^T$$
$$\boldsymbol{y} = [y_1, \ldots, y_l]^T$$

$$s(\boldsymbol{x}, \boldsymbol{y}) = \sum_{k=1}^{l} w_k s_k(x_k, y_k)$$

Recall that, in order to define $s(\boldsymbol{x}, \boldsymbol{y})$, we need to **define** $s_k(x_k, y_k)$.

Each $s_k(\cdot,\cdot)$ is completely **defined** by the associated similarity matrix.

If $F_k = \{1,2, \ldots, q\}$, the similarity matrix associated with the k-th feature is

	1	**2**	**. . .**	**q**
1	$s_k(1,1)$	$s_k(1,2)$	. . .	$s_k(1,q)$
2	$s_k(2,1)$	$s_k(2,2)$	. . .	$s_k(2,q)$
. . .	. . .	. . .	$\ddots$	. . .
q	$s_k(q,1)$	$s_k(q,2)$	. . .	$s_k(q,q)$

NOTE: (a) The similarity matrix is **completely defined** if all of its entries are defined.
(b) Such a similarity matrix is **associated** with a similarity measure for a **single** discrete-valued feature.

Proximity measures between vectors

(C) Discrete-valued vectors – similarity & dissimilarity measures (SMs-DMs)

There are plenty of similarity measures for single discrete-valued features.

Defining such a similarity measure ⇔ **filling** the entries of the similarity matrix.

The entries filling may be carried out by utilizing:

- Simply 0 and 1 entries
- The size of the data set N
- The number of attributes/features n involved in the current problem
- The cardinality of F_q, n_q.
- The number of times, $f_k(j)$, the j-th symbol is encountered as k-th feature in the data set
- The frequency of occurrence of the j-th symbol as k-th feature in the data set, defined as $\hat{p}_k(j) = f_k(j)/N$, or, in some cases, $p_k{}^2(j) = \frac{f_k(j)(f_k(j)-1)}{N(N-1)}$

	1	2	$\cdots$	q
1	$s_k(1,1)$	$s_k(1,2)$	$\cdots$	$s_k(1,q)$
2	$s_k(2,1)$	$s_k(2,2)$	$\cdots$	$s_k(2,q)$
$\cdots$	$\cdots$	$\cdots$	$\ddots$	$\cdots$
q	$s_k(q,1)$	$s_k(q,2)$	$\cdots$	$s_k(q,q)$

Proximity measures between vectors

(C) Discrete-valued vectors – similarity & dissimilarity measures (SMs-DMs)

These similarity measures can be categorized in terms of:

- ✓ The *way they fill the entries of the similarity matrix*
  - **I.** **Fill** the diagonal entries only
  - **II.** **Fill** the non-diagonal entries only
  - **III.** **Fill** both diagonal and non-diagonal entries

- ✓ The *arguments they use to define the measure* (information theoretic, probabilistic etc).

Proximity measures between vectors

(C) Discrete-valued vectors – similarity & dissimilarity measures (SMs-DMs)

Indicative measures from category **I**: **Fill** the diagonal entries only.

- Overlap measure

$$s_k(x_k, y_k) = \begin{cases} 1, & if\ x_k = y_k \\ 0, & otherwise \end{cases}, \quad w_k = \frac{1}{l}$$

$$s(\boldsymbol{x}, \boldsymbol{y}) = \sum_{k=1}^{l} w_k s_k(x_k, y_k)$$

$$s_k(x_k, y_k) \in \{0,1\}$$

- Goodall3 measure

$$s_k(x_k, y_k) = \begin{cases} 1 - {p_k}^2(x_k), & if\ x_k = y_k \\ 0, & otherwise \end{cases}, \quad w_k = \frac{1}{l}$$

$$s_k(x_k, y_k) \in [0, 1 - \frac{2}{N(N-1)}]$$

Comment: It **assigns** a high similarity **if** the matching values are **infrequent** regardless of the frequencies of the other values.

Proximity measures between vectors

(C) Discrete-valued vectors – similarity & dissimilarity measures (SMs-DMs)

Indicative measures from category **II: Fill** the non-diagonal entries only.

- Eskin measure

$s_k(x_k, y_k) \in [\frac{2}{3}, 1]$

$$s_k(x_k, y_k) = \begin{cases} 1, & if\ x_k = y_k \\ \frac{{n_k}^2}{{n_k}^2+2}, & otherwise \end{cases}, \quad w_k = \frac{1}{l}$$

Comments:

- It **gives** more weight to mismatches for attributes that take **many** values.
- It has been **used** for record-based network intrusion detection data.

- Inverse Occurrence Frequency (**IOF**) measure

$s_k(x_k, y_k) \in [\frac{1}{1 + (log\,\frac{N}{2})^2}, 1]$

$$s_k(x_k, y_k) = \begin{cases} 1, & if\ x_k = y_k \\ \frac{1}{1+log f_k(x_k) \cdot log f_k(y_k)}, & otherwise \end{cases}, \quad w_k = \frac{1}{l}$$

Comments:

- It **assigns** lower similarity to mismatches on **more frequent** values..
- It is related to the concept of inverse document frequency which comes from information retrieval, where it is used to signify the relative number of documents that contain a specific word.

Proximity measures between vectors

(C) Discrete-valued vectors – similarity & dissimilarity measures (SMs-DMs)

Indicative measures from category **III**: **Fill** both diagonal & non-diagonal entries

- Lin measure

$$s_k(x_k, y_k) = \begin{cases} 2 \cdot log\hat{p}_k(x_k), & if\ x_k = y_k \\ 2 \cdot \log(\hat{p}_k(x_k) + \hat{p}_k(y_k)), & otherwise \end{cases},$$

$$w_k = \frac{1}{\sum_{i=1}^{l}(\log \hat{p}_i(x_i) + log\hat{p}_i(y_i))}$$

$s_k(x_k, y_k) \in [-2logN, 0]$ for **match**

$s_k(x_k, y_k) \in [-2log\frac{N}{2}, 0]$ for **mismatch**

Comments:

It **gives**

- higher weight to matches on frequent values, and
- lower weight to mismatches on infrequent values.

It has been **used** in word similarity procedure.

(*) S. Boriah, V. Chandola, and V. Kumar, "Similarity measures for categorical data: A Comparative Evaluation," in *Proc. SDM*, pp. 243-254, 2008.

Proximity measures between vectors

(C) Discrete-valued vectors – similarity & dissimilarity measures (SMs-DMs)

	Feat. 1	Feat. 2	Feat. 3
$\boldsymbol{x}_1$	a	1	A
$\boldsymbol{x}_2$	b	4	B
$\boldsymbol{x}_3$	a	3	B
$\boldsymbol{x}_4$	c	2	A
$\boldsymbol{x}_5$	a	2	A
$\boldsymbol{x}_6$	a	2	B
$\boldsymbol{x}_7$	b	1	B
$\boldsymbol{x}_8$	c	1	A
$\boldsymbol{x}_9$	b	1	A
$\boldsymbol{x}_{10}$	a	3	B
$\boldsymbol{x}_{11}$	a	4	A
$\boldsymbol{x}_{12}$	b	4	C
$\boldsymbol{x}_{13}$	b	3	A
$\boldsymbol{x}_{14}$	c	2	A
$\boldsymbol{x}_{15}$	a	2	C

Exercise 1: Consider the data set *X* given in the adjacent table.
Determine the similarity between the vectors
$\boldsymbol{x} = [a, 2, A]^T$ and
$\boldsymbol{y} = [a, 3, B]^T$ utilizing

(a) The overlap measure
(b) The Goodall3 measure
(c) The Eskin measure
(d) The IOF measure
(e) The Lin measure.

Exercise 2: Define corresponding dissimilarity measures for the above defined similarity measures.

Proximity measures between vectors

(D) Mixed-valued vectors –similarity measures (SMs)

Here some coordinates of the feature vectors are real-valued, while others are discrete-valued.

$\boldsymbol{x} = [x_1, \dots, x_l]^T$
$\boldsymbol{y} = [y_1, \dots, y_l]^T$

How to **measure** the proximity between $\boldsymbol{x}$ and $\boldsymbol{y}$?

- **Adopt** a proximity measure **suitable** for real-valued vectors (**only** for ordinal discrete-valued features).

- **Convert** the real-valued features **to** discrete-valued ones (e.g., via quantization) and **employ** a discrete proximity measure (again, **only** for ordinal discrete-valued features).

- For the more general case where nominal, ordinal, interval-scaled and ratio-scaled features **co-exist**, we treat each one of them separately, as follows:

Proximity measures between vectors

(D) Mixed-valued vectors –similarity measures (SMs)

$\boldsymbol{x} = [x_1, \dots, x_l]^T$
$\boldsymbol{y} = [y_1, \dots, y_l]^T$

The similarity between $\boldsymbol{x}$ and $\boldsymbol{y}$ is defined as:

$$s(\boldsymbol{x}, \boldsymbol{y}) = \frac{\sum_{k=1}^{l} s_k(x_k, y_k)}{\sum_{k=1}^{l} w_k}$$

where:

- $w_k = 0$, if **at least one** of x_k and y_k is **undefined** or (optionally) both x_k and y_k are equal to 0. Otherwise $w_k = 1$.

- If x_k and y_k are **binary**, $s_k(x_k, y_k) = \begin{cases} 1, & if\, x_k = y_k = 1 \ (or\ x_k = y_k) \\ 0, & otherwise \end{cases}$

- If x_k and y_k are **nominal** or **ordinal**, $s_k(x_k, y_k) = \begin{cases} 1, & x_k = y_k \\ 0, & otherwise \end{cases}$.

This is the overlap measure. Other options can also be used.

- If x_k and y_k are **interval** or **ratio scaled**-valued

$$s_k(x_k, y_k) = 1 - \frac{|x_k - y_k|}{r_k}$$

where r_k is the width of the interval where the k-th coordinates of the vectors of X lie.

Proximity measures between vectors

(D) Mixed-valued vectors –similarity measures (SMs)

Exercise 2: Consider the data set given in the following table. Each row corresponds to a vector and each column to a feature. The first three features are ratio scaled, the 4th one is nominal and the 5th one is ordinal. Utilizing the previous similarity measure, compute the similarities between any pair of feature vectors.

Company	1st year budget	2nd year budget	3rd year budget	Activity abroad	Rate of services 0: not good 1: good 2: very good
1 (x_1)	1.2	1.5	1.9	0	1
2 (x_2)	0.3	0.4	0.6	0	0
3 (x_3)	10	13	15	1	2
4 (x_4)	6	6	7	1	1