DATA ANALYTICS

Unit 2:Distance and Similarity Measures

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Similarity and Dissimilarity Measures

- Similarity and dissimilarity are important because they are used by a number of data mining, data analytics and machine learning techniques, such as clustering, nearest neighbor classification, and anomaly detection.

- In many cases, the initial data set is not needed once these similarities or dissimilarities have been computed.

- Such approaches can be viewed as transforming the data to a similarity (dissimilarity) space and then performing the analysis.

Similarity and Dissimilarity Measures

- Similarity measure
  - Numerical measure of how alike two data objects are.
  - Is higher when objects are more alike.
  - Often falls in the range [0,1]
- Dissimilarity measure
  - Numerical measure of how different two data objects are
  - Lower when objects are more alike
  - Minimum dissimilarity is often 0
  - Upper limit varies
- Proximity refers to a similarity or dissimilarity

Similarity/Dissimilarity for Simple Attributes

The following table shows the similarity and dissimilarity between two objects, *x* and *y,* with respect to a single, simple attribute.

Attribute Type	Dissimilarity	Similarity
Nominal	$d = \begin{cases} 0 & \text{if } x = y \\ 1 & \text{if } x \neq y \end{cases}$	$s = \begin{cases} 1 & \text{if } x = y \\ 0 & \text{if } x \neq y \end{cases}$
Ordinal	$d = \lvert x - y \rvert / (n-1)$ (values mapped to integers 0 to $n-1$, where n is the number of values)	$s = 1 - d$
Interval or Ratio	$d = \lvert x - y \rvert$	$s = -d$, $s = \frac{1}{1+d}$, $s = e^{-d}$, $s = 1 - \frac{d - min\_d}{max\_d - min\_d}$

Euclidean Distance

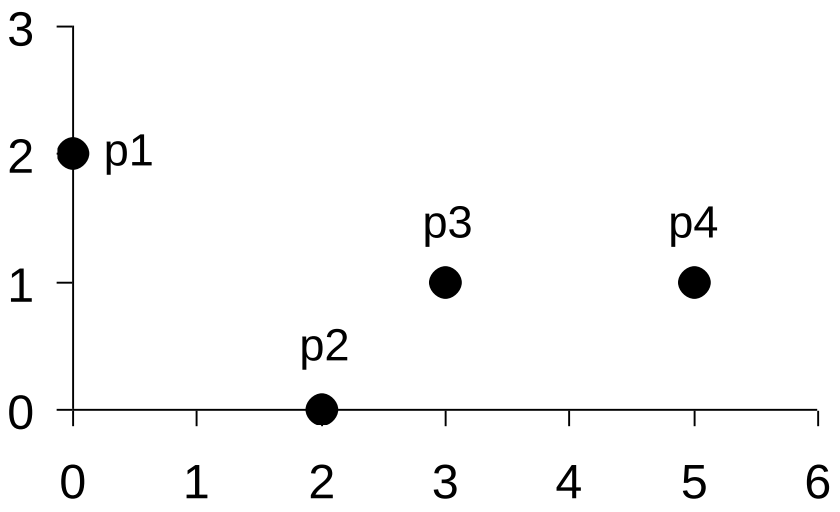
- Euclidean Distance

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_{k=1}^{n} (x_k - y_k)^2}$$

where n is the number of dimensions (attributes) and x_k and y_k are, respectively, the k^{th} attributes (components) or data objects **x** and **y**.

- Standardization is necessary, if scales differ.

Euclidean Distance



point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

Distance Matrix

Minkowski Distance

- Minkowski Distance is a generalization of Euclidean Distance

$$d(\mathbf{x}, \mathbf{y}) = \left(\sum_{k=1}^{n} |x_k - y_k|^r \right)^{1/r}$$

Where *r* is a parameter, *n* is the number of dimensions (attributes) and x_k and y_k are, respectively, the k^{th} attributes (components) or data objects ***x*** and ***y***.

Minkowski Distance: Examples

- $r = 1$. City block (Manhattan, taxicab, L_1 norm) distance.
  - A common example of this for binary vectors is the Hamming distance, which is just the number of bits that are different between two binary vectors

- $r = 2$. Euclidean distance

- $r \to \infty$. "supremum" (L_{max} norm, L_∞ norm) distance.
  - This is the maximum difference between any component of the vectors

- Do not confuse r with n, i.e., all these distances are defined for all numbers of dimensions.

Minkowski Distance

point	x	y
p1	0	2
p2	2	0
p3	3	1
p4	5	1

L1	p1	p2	p3	p4
p1	0	4	4	6
p2	4	0	2	4
p3	4	2	0	2
p4	6	4	2	0

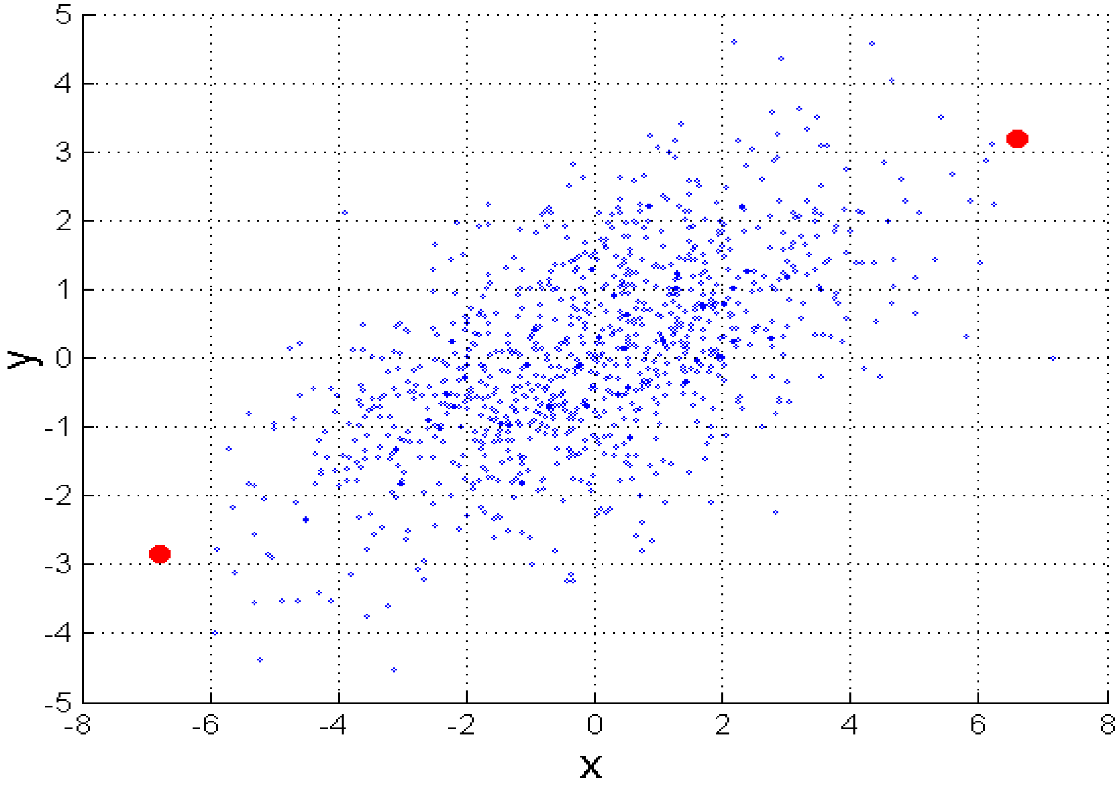
L2	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

L_∞	p1	p2	p3	p4
p1	0	2	3	5
p2	2	0	1	3
p3	3	1	0	2
p4	5	3	2	0

Distance Matrix

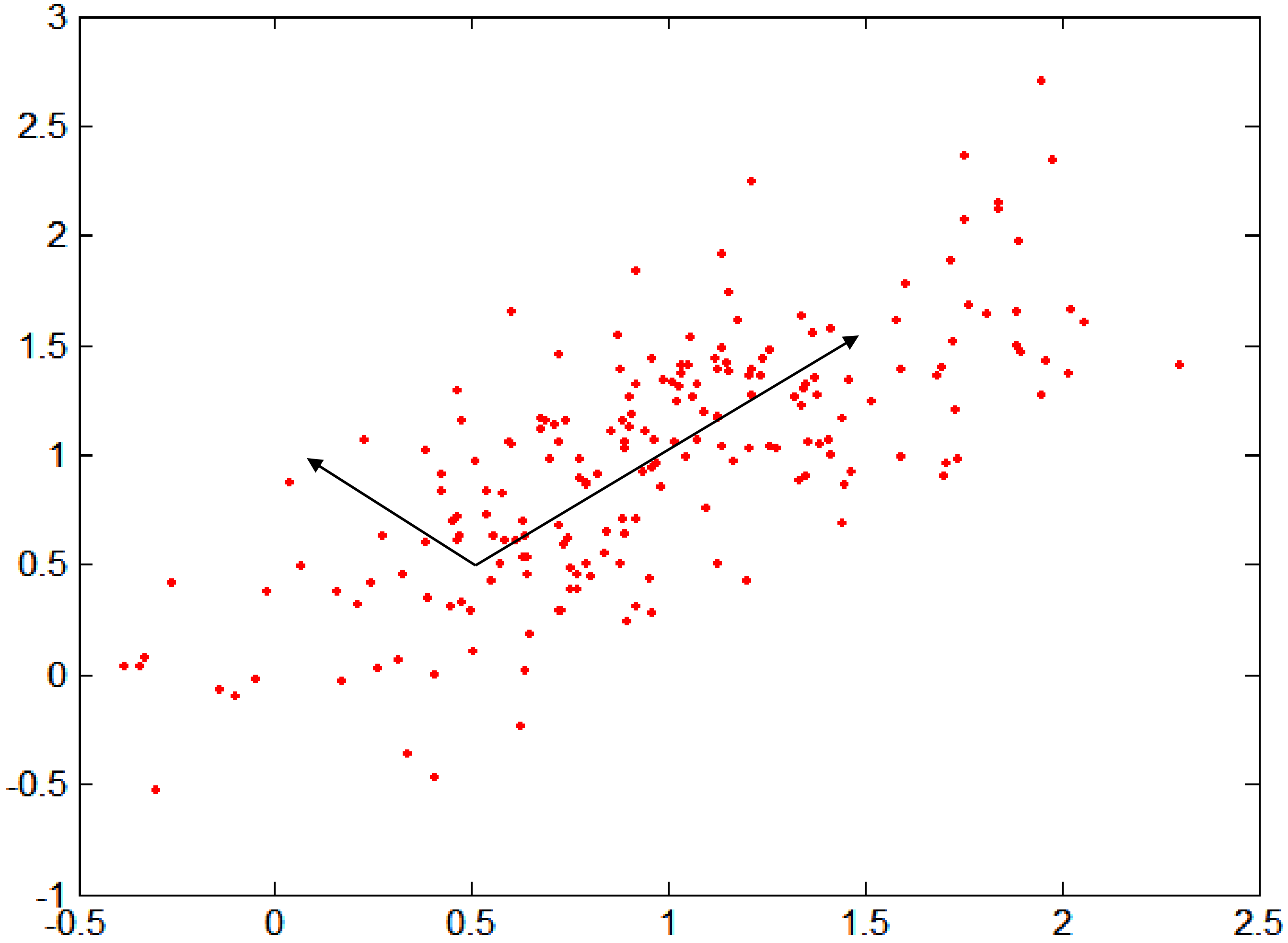
Mahalanobis Distance

$$\left(\mathbf{mahalanobis}(\mathbf{x},\mathbf{y})\right)^2 = (\mathbf{x}-\mathbf{y})^T\,\Sigma^{-1}(\mathbf{x}-\mathbf{y})$$



For red points, the Euclidean distance is 14.7, Mahalanobis distance is 6.

Mahalanobis Distance



Covariance Matrix:

$$\Sigma = \begin{bmatrix} 0.3 & 0.2 \\ 0.2 & 0.3 \end{bmatrix}$$

A: (0.5, 0.5)

B: (0, 1)

C: (1.5, 1.5)

Mahal(A,B) = 5

Mahal(A,C) = 4

Common Properties of a Distance

- Distances, such as the Euclidean distance, have some well known properties.

1. $d(\mathbf{x}, \mathbf{y}) \geq 0$ for all x and y and $d(\mathbf{x}, \mathbf{y}) = 0$ only if $\mathbf{x} = \mathbf{y}$. (Positive definiteness)
2. $d(\mathbf{x}, \mathbf{y}) = d(\mathbf{y}, \mathbf{x})$ for all $\mathbf{x}$ and $\mathbf{y}$. (Symmetry)
3. $d(\mathbf{x}, \mathbf{z}) \leq d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z})$ for all points $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$. (Triangle Inequality)

where $d(\mathbf{x}, \mathbf{y})$ is the distance (dissimilarity) between points (data objects), $\mathbf{x}$ and $\mathbf{y}$.

- A distance that satisfies these properties is a metric

Common Properties of a Similarity

- Similarities, also have some well known properties.

1. $s(\mathbf{x}, \mathbf{y}) = 1$ (or maximum similarity) only if $\mathbf{x} = \mathbf{y}$. (does not always hold, e.g., cosine)
2. $s(\mathbf{x}, \mathbf{y}) = s(\mathbf{y}, \mathbf{x})$ for all $\mathbf{x}$ and $\mathbf{y}$. (Symmetry)

where $s(\mathbf{x}, \mathbf{y})$ is the similarity between points (data objects), $\mathbf{x}$ and $\mathbf{y}$.

Similarity Between Binary Vectors

- Common situation is that objects, **x** and **y**, have only binary attributes

- Compute similarities using the following quantities

  f_{01} = the number of attributes where **x** was 0 and **y** was 1
  f_{10} = the number of attributes where **x** was 1 and **y** was 0
  f_{00} = the number of attributes where **x** was 0 and **y** was 0
  f_{11} = the number of attributes where **x** was 1 and **y** was 1

- Simple Matching and Jaccard Coefficients

  SMC = number of matches / number of attributes
  $= (f_{11} + f_{00}) / (f_{01} + f_{10} + f_{11} + f_{00})$

  J = number of 11 matches / number of non-zero attributes
  $= (f_{11}) / (f_{01} + f_{10} + f_{11})$

SMC versus Jaccard: Example

x = 1 0 0 0 0 0 0 0 0 0

y = 0 0 0 0 0 0 1 0 0 1

$f_{01} = 2$ (the number of attributes where **x** was 0 and **y** was 1)

$f_{10} = 1$ (the number of attributes where **x** was 1 and **y** was 0)

$f_{00} = 7$ (the number of attributes where **x** was 0 and **y** was 0)

$f_{11} = 0$ (the number of attributes where **x** was 1 and **y** was 1)

SMC $= (f_{11} + f_{00}) / (f_{01} + f_{10} + f_{11} + f_{00})$

$= (0+7) / (2+1+0+7) = 0.7$

$J = (f_{11}) / (f_{01} + f_{10} + f_{11}) = 0 / (2 + 1 + 0) = 0$

Cosine Similarity

- If $\mathbf{d}_1$ and $\mathbf{d}_2$ are two document vectors, then

$$\cos(\mathbf{d_1}, \mathbf{d_2}) = \langle \mathbf{d_1},\mathbf{d_2} \rangle / ||\mathbf{d}_1|| \; ||\mathbf{d}_2||,$$

where $\langle \mathbf{d_1},\mathbf{d_2} \rangle$ indicates inner product or vector dot product of vectors, $\mathbf{d_1}$ and $\mathbf{d_2}$, and $\mathbf{|| \, d \, ||}$ is the length of vector **d**.

- Example:

$$\mathbf{d_1 = 3\ 2\ 0\ 5\ 0\ 0\ 0\ 2\ 0\ 0}$$

$$\mathbf{d_2 = 1\ 0\ 0\ 0\ 0\ 0\ 0\ 1\ 0\ 2}$$

$\mathbf{\langle d_1, d2 \rangle}$ = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5

$||\ \mathbf{d_1}\ || = (3*3+2*2+0*0+5*5+0*0+0*0+0*0+2*2+0*0+0*0)^{\mathbf{0.5}} = (42)^{\mathbf{0.5}} = 6.481$

$||\ \mathbf{d_2}\ || = (1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{\mathbf{0.5}} = (6)^{\mathbf{0.5}} = 2.449$

$\cos(\mathbf{d_1}, \mathbf{d_2}) = 0.3150$

Extended Jaccard Coefficient (Tanimoto)

- Variation of Jaccard for continuous or count attributes
  - Reduces to Jaccard for binary attributes

$$EJ(\mathbf{x},\mathbf{y}) = \frac{\mathbf{x}\cdot\mathbf{y}}{\|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 - \mathbf{x}\cdot\mathbf{y}}$$

Correlation measures the linear relationship between objects

$$\operatorname{corr}(\mathbf{x},\mathbf{y}) = \frac{\operatorname{covariance}(\mathbf{x},\mathbf{y})}{\text{standard\_deviation}(\mathbf{x}) * \text{standard\_deviation}(\mathbf{y})} = \frac{s_{xy}}{s_x\, s_y}, \quad (2.11)$$

where we are using the following standard statistical notation and definitions

$$\operatorname{covariance}(\mathbf{x},\mathbf{y}) = s_{xy} = \frac{1}{n-1}\sum_{k=1}^{n}(x_k-\overline{x})(y_k-\overline{y}) \quad (2.12)$$

$$\text{standard\_deviation}(\mathbf{x}) = s_x = \sqrt{\frac{1}{n-1}\sum_{k=1}^{n}(x_k-\overline{x})^2}$$

$$\text{standard\_deviation}(\mathbf{y}) = s_y = \sqrt{\frac{1}{n-1}\sum_{k=1}^{n}(y_k-\overline{y})^2}$$

$$\overline{x} = \frac{1}{n}\sum_{k=1}^{n}x_k \text{ is the mean of } \mathbf{x}$$

$$\overline{y} = \frac{1}{n}\sum_{k=1}^{n}y_k \text{ is the mean of } \mathbf{y}$$

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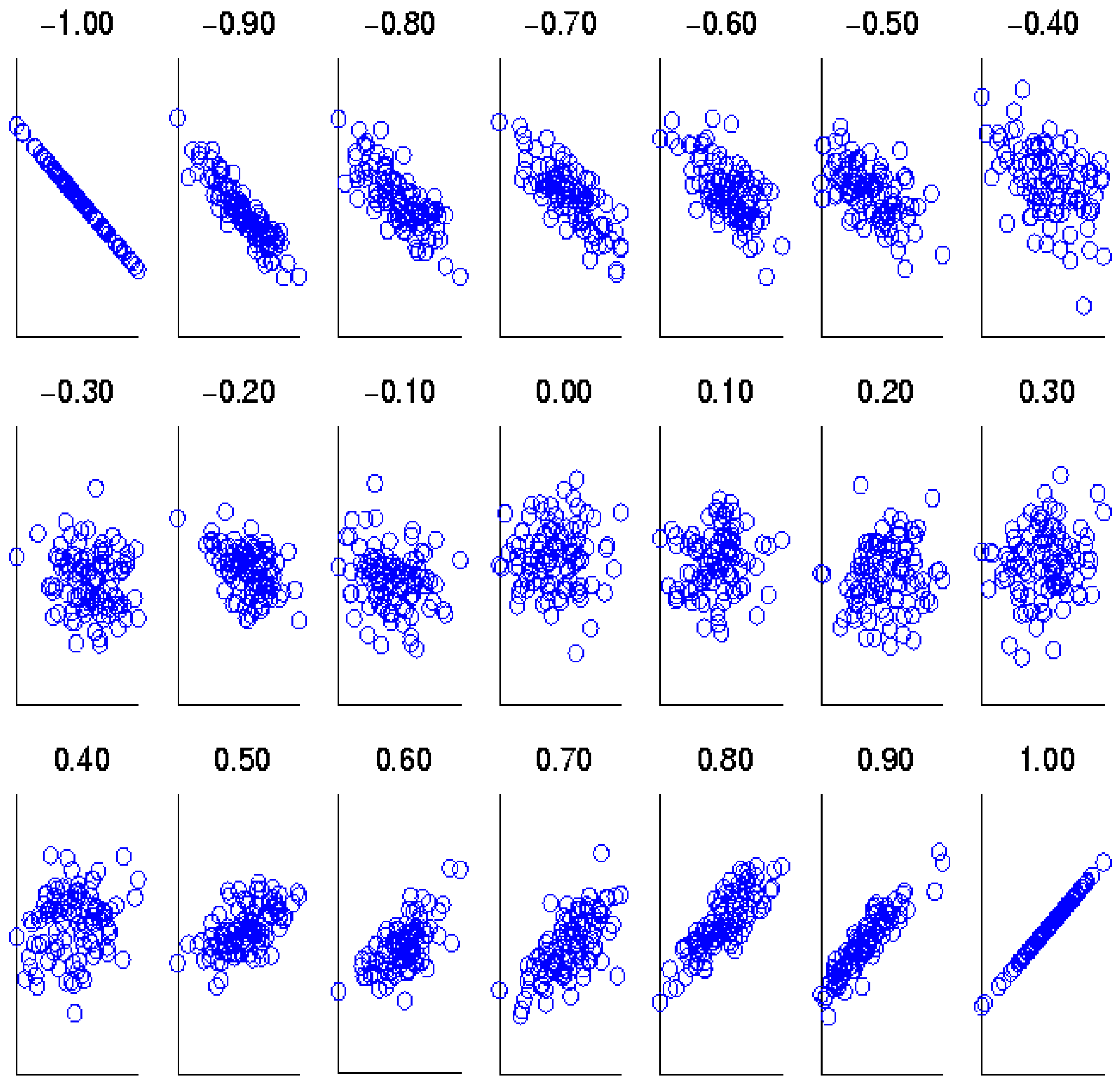
Visually Evaluating Correlation



Scatter plots showing the similarity from –1 to 1.

Drawback of Correlation

- **x** = (-3, -2, -1, 0, 1, 2, 3)
- **y** = (9, 4, 1, 0, 1, 4, 9)

$y_i = x_i^2$

- mean(**x**) = 0, mean(**y**) = 4
- std(**x**) = 2.16, std(**y)** = 3.74

- corr = (-3)(5)+(-2)(0)+(-1)(-3)+(0)(-4)+(1)(-3)+(2)(0)+3(5) / (6 * 2.16 * 3.74)

  = 0

Comparison of Proximity Measures

- Domain of application
  - Similarity measures tend to be specific to the type of attribute and data
  - Record data, images, graphs, sequences, 3D-protein structure, etc. tend to have different measures
- However, one can talk about various properties that you would like a proximity measure to have
  - Symmetry is a common one
  - Tolerance to noise and outliers is another
  - Ability to find more types of patterns?
  - Many others possible
- The measure must be applicable to the data and produce results that agree with domain knowledge

General Approach for Combining Similarities

- Sometimes attributes are of many different types, but an overall similarity is needed.

1: For the k^{th} attribute, compute a similarity, $s_k(\mathbf{x}, \mathbf{y})$, in the range [0, 1].

2: Define an indicator variable, δ_k, for the k^{th} attribute as follows:

$\delta_k = 0$ if the k^{th} attribute is an asymmetric attribute and both objects have a value of 0, or if one of the objects has a missing value for the kth attribute

$\delta_k = 1$ otherwise

3. Compute

$$\text{similarity}(\mathbf{x}, \mathbf{y}) = \frac{\sum_{k=1}^{n} \delta_k s_k(\mathbf{x}, \mathbf{y})}{\sum_{k=1}^{n} \delta_k}$$

Using Weights to Combine Similarities

- May not want to treat all attributes the same.
  - Use non-negative weights ω_k
  - $similarity(\mathbf{x}, \mathbf{y}) = \frac{\sum_{k=1}^{n} \omega_k \delta_k s_k(\mathbf{x},\mathbf{y})}{\sum_{k=1}^{n} \omega_k \delta_k}$
- Can also define a weighted form of distance

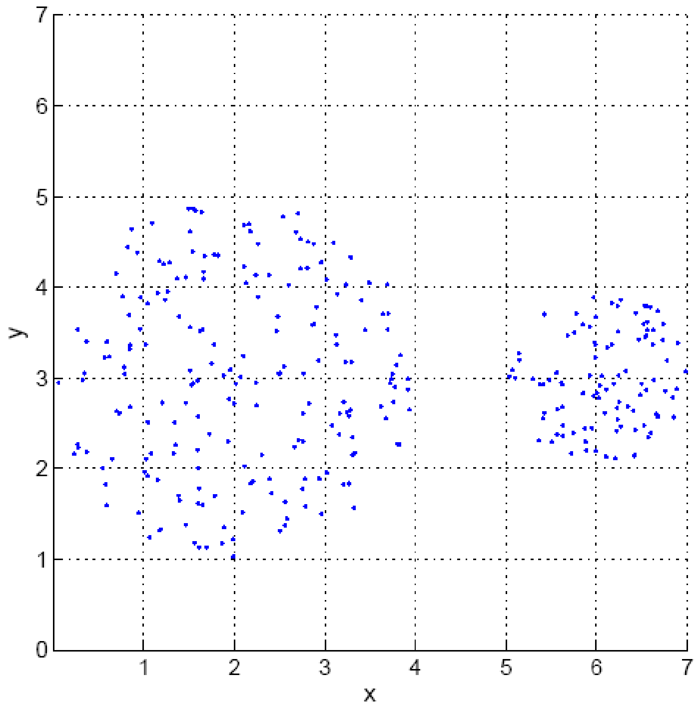
$$d(\mathbf{x}, \mathbf{y}) = \left(\sum_{k=1}^{n} w_k |x_k - y_k|^r \right)^{1/r}$$

Density

- Measures the degree to which data objects are close to each other in a specified area
- The notion of density is closely related to that of proximity
- Concept of density is typically used for clustering and anomaly detection
- Examples:
  - Euclidean density
    - Euclidean density = number of points per unit volume
  - Probability density
    - Estimate what the distribution of the data looks like
  - Graph-based density
    - Connectivity

Euclidean Density: Grid-based Approach

- Simplest approach is to divide region into a number of rectangular cells of equal volume and define density as # of points the cell contains



0	0	0	0	0	0	0
0	0	0	0	0	0	0
4	17	18	6	0	0	0
14	14	13	13	0	18	27
11	18	10	21	0	24	31
3	20	14	4	0	0	0
0	0	0	0	0	0	0

Euclidean Density: Center-Based

- Euclidean density is the number of points within a specified radius of the point

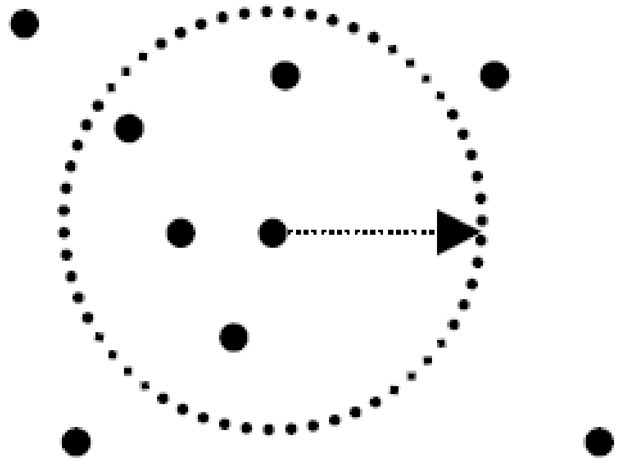


Illustration of center-based density.

Exercise

- Mention and explain the different distance measures.
- For each of the distance measure, find out an application and explore how it is used in that application.

References

Text Book:

- Introduction to Data Mining , Tan, Steinbach, Kumar, 2nd Edition

THANK YOU

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