Knowledge Discovery & Data Mining

Similarity and Distance Measures

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Outline

- Similarity and distance measures
 - Proximity Measures for
 - Nominal Attributes
 - Binary Attributes
 - Numeric Attributes
 - Ordinal attributes
 - Mixed types
 - Cosine Similarity

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Kullback-Leibler divergence

Knowledge Discovery & Data Mining

Similarity and distance measures

- Similarity
 - Numerical measure of how alike two data objects are
 - Value is higher when objects are more alike
 - Often falls in the range [0,1]
- Dissimilarity (e.g., distance)
 - 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

Dissimilarity matrix

Data matrix (or object-by-attribute structure):

- This structure stores the n data points with p dimensions (n objects ×p attributes)
- Two-mode

Dissimilarity matrix (or object-by-object structure):

- A triangular matrix
- d(i, j) is the measured dissimilarity or "difference" between objects i and j
- d(i, j)>=0, close to 0 when objects i and j are highly similar or "near" each other, and becomes larger the more they differ.
- $\bullet \quad d(i, j) = d(j, i).$
- One-mode

```
\begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix}
```

```
\begin{bmatrix} 0 \\ d(2,1) & 0 \\ d(3,1) & d(3,2) & 0 \\ \vdots & \vdots & \vdots \\ d(n,1) & d(n,2) & \cdots & 0 \end{bmatrix}
```

Simple matching

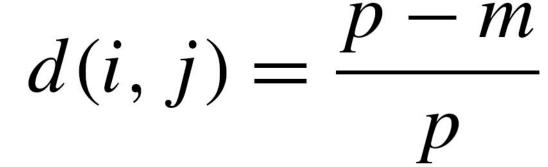
Dissimilarity: m: # of matches, p: total # of variables, then dissimilarity between two
objects i and j can be computed based on the ratio of mismatches

$$d(i,j) = \frac{p-m}{p}$$

• Similarity: $sim(i, j) = 1 - d(i, j) = \frac{m}{p}$

Encoding: creating a new binary attribute for each of the M states of a nominal attribute.

Example. Suppose that we have the sample data of following table, so the dissimilarity matrix is p-m





| Object Identifier | Test-1 (nominal) |
|-------------------|------------------|
| 1 | code A |
| 2 | code B |
| 3 | code C |
| 4 | code A |

Example. Suppose that we have the sample data of following table, so the dissimilarity matrix is p-m

 $d(i,j) = \frac{p-m}{p}$

$$\begin{bmatrix} 0 \\ d(2,1) & 0 \\ d(3,1) & d(3,2) & 0 \\ d(4,1) & d(4,2) & d(4,3) & 0 \end{bmatrix}$$

| Object Identifier | Test-1 (nominal) |
|-------------------|------------------|
| 1 | code A |
| 2 | code B |
| 3 | code C |
| 4 | code A |

Only one nominal attribute, so p = 1

Example. Suppose that we have the sample data of following table, so the dissimilarity

matrix is

| 1 | 0 | | |
|---|---|---|---|
| 1 | 1 | 0 | |
| 0 | 1 | 1 | 0 |

| d(i, | i | $\frac{p}{}$ | | <i>YYU</i> |
|------|------------|------------------|---|------------|
| a(i, | <i>J)</i> | | p | |

| Object Identifier | Test-1 (nominal) |
|-------------------|------------------|
| 1 | code A |
| 2 | code B |
| 3 | code C |
| 4 | code A |

If all binary attributes are thought of as having the same weight, we have the 2×2 contingency table, where q is the number of attributes that equal 1 for both objects i and j, r is the number of attributes that equal 1 for object i but equal 0 for object j, s is the number of attributes that equal 0 for object i but equal 1 for object j, and t is the number of attributes that equal 0 for both objects i and j. The total number of attributes is p, where p = q + r + s + t.

Object j

 1
 0
 Sum (row)

 1
 q
 r
 q+r

 0
 s
 t
 s+t

 Sum(col.)
 q+s
 r+t
 p

Object i

contingency table

Symmetric binary attributes: symmetric binary dissimilarity $d(i, j) = \frac{r + s}{a + r + s + t}$

Asymmetric binary attributes:

- the two states are not equally important,
- the agreement of two 1s (a positive match) is then considered more significant than that of two 0s (a negative match).

 Object j
- asymmetric binary dissimilarity

$$d(i, j) = \frac{r + s}{q + r + s}$$

- asymmetric binary similarity:
 - is called the Jaccard coefficient

$$sim(i, j) = \frac{q}{q + r + s} = 1 - d(i, j)$$

| | 1 | 0 | Sum (row) |
|-----------|-----|-----|--------------|
| 1 | q | r | q+r |
| 0 | S | t | s+t |
| Sum(col.) | q+s | r+t | p |

contingency table

Object i

Example. Suppose that we have the sample data of following table, so the distance between each pair of the three patients—Jack, Mary, and Jim—is

| Name | Gender | Fever | Cough | Test-1 | Test-2 | Test-3 | Test-4 |
|------|--------|-------|-------|--------|--------|--------|--------|
| Jack | M | Y | N | P | N | N | N |
| Mary | F | Y | N | P | N | P | N |
| Jim | M | Y | P | N | N | N | N |

$$d(i,j) = \frac{r+s}{q+r+s}$$

Object j

- d(Jack, Jim) =
- d(Jack, Mary) =
- d(Jim, Mary) =



Object i

| | 1 | 0 | Sum (row) |
|-----------|-----|-----|--------------|
| 1 | q | r | q+r |
| 0 | S | t | s+t |
| Sum(col.) | q+s | r+t | p |

contingency table

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Example. Suppose that we have the sample data of following table, so the distance between each pair of the three patients—Jack, Mary, and Jim—is

| Name | Gender | Fever | Cough | Test-1 | Test-2 | Test-3 | Test-4 |
|------|--------|-------|-------|--------|--------|--------|--------|
| Jack | M | Y | N | P | N | N | N |
| Mary | F | Y | N | P | N | P | N |
| Jim | M | Y | P | N | N | N | N |

$$d(i, j) = \frac{r + s}{q + r + s}$$

Object j

$$d(Jack, Jim) = \frac{1+1}{1+1+1} = 0.67$$

$$d(Jack, Mary) = \frac{0+1}{2+0+1} = 0.33$$

$$d(Jim, Mary) = \frac{1+2}{1+1+2} = 0.75$$

 1
 0
 Sum (row)

 1
 q
 r
 q+r

 0
 s
 t
 s+t

 Sum(col.)
 q+s
 r+t
 p

contingency table

Object

Distance measures are commonly used for computing the dissimilarity of objects described by numeric attributes.

- Euclidean distance: The most popular distance measure
 - Let i = (xi1, xi2, . . . , xip) and j = (xj1, xj2, . . . , xjp) be two objects described by p numeric attributes.
 - The Euclidean distance between objects i and j is defined as

$$d(i,j) = \sqrt{(x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + \dots + (x_{ip} - x_{jp})^2}$$

Manhattan (or city block) distance:

$$d(i, j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \dots + |x_{ip} - x_{jp}|$$

Both the Euclidean and the Manhattan distance satisfy the following mathematical properties:

- Nonnegativity: $d(i, j) \ge 0$: Distance is a nonnegative number.
- Identity of indiscernibles: d(i, i) = 0: The distance of an object to itself is 0.
- Symmetry: d(i, j) = d(j, i): Distance is a symmetric function.
- Triangle inequality: d(i, j) ≤ d(i, k)+d(k, j): Going directly from object i to object j
 in space is no more than making a detour over any other object k.

A measure that satisfies these conditions is known as metric.

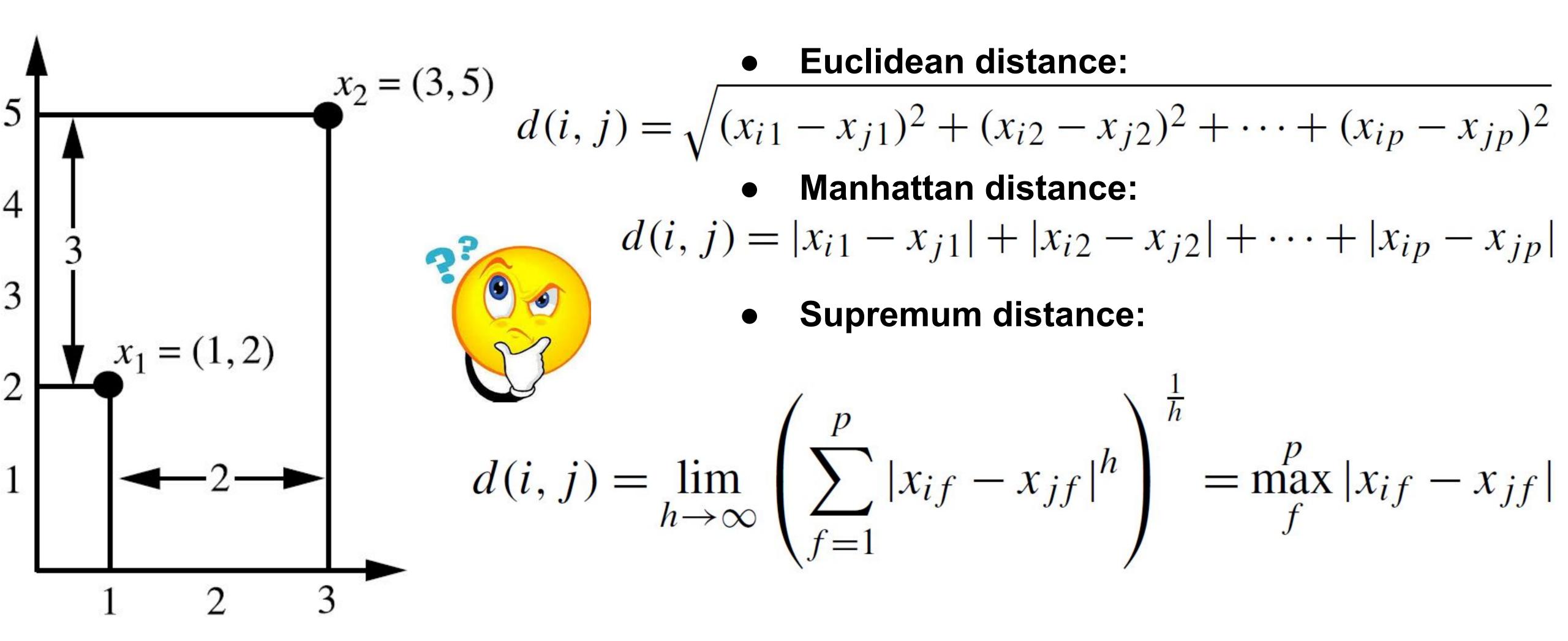
 Minkowski distance: is a generalization of the Euclidean and Manhattan distances. It is defined as

$$d(i,j) = \sqrt[h]{|x_{i1} - x_{j1}|^h + |x_{i2} - x_{j2}|^h + \dots + |x_{ip} - x_{jp}|^h}$$

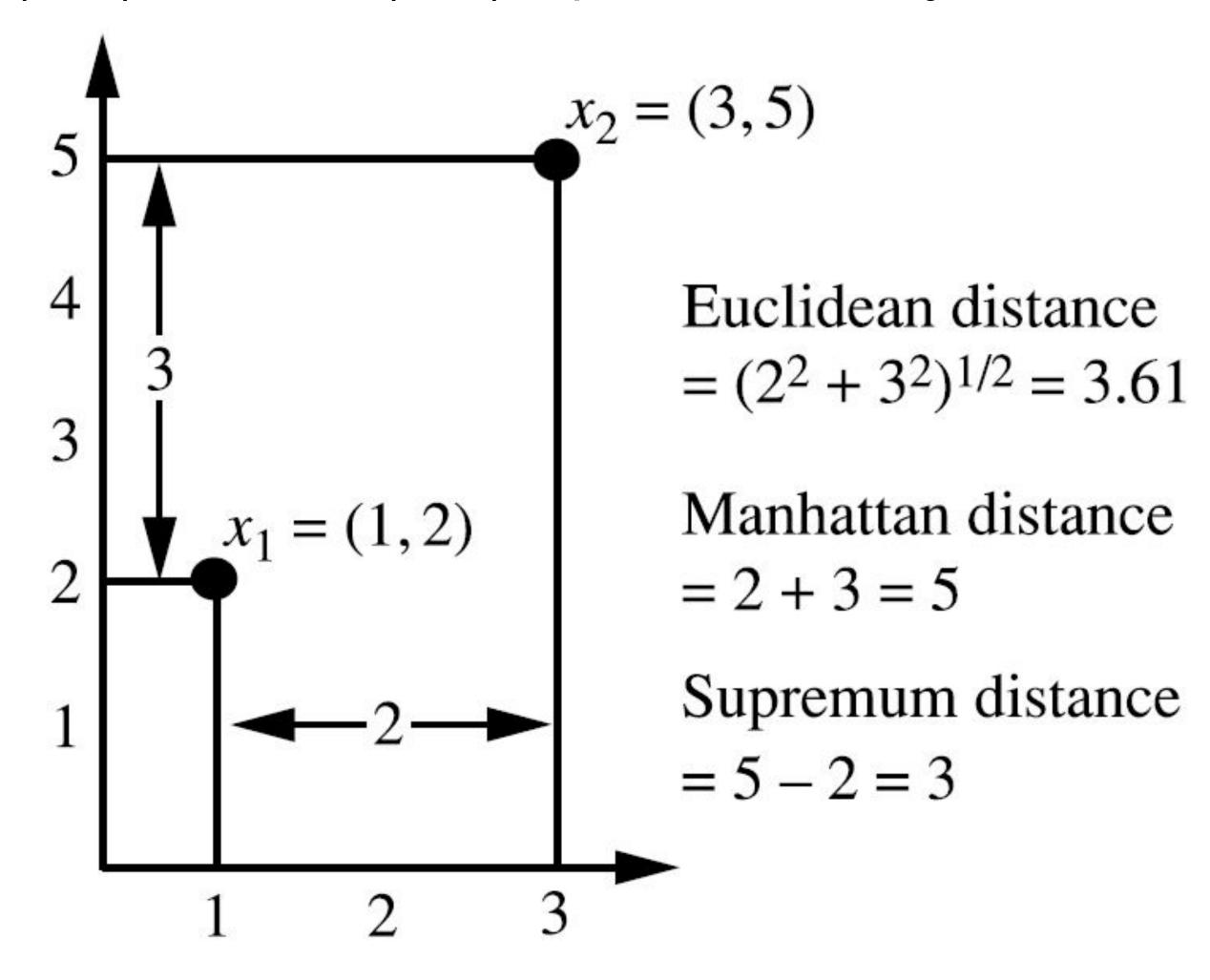
- o where h is a real number such that h ≥ 1
 - Manhattan distance when h = 1 (L1 norm)
 - Euclidean distance when h = 2 (L2 norm)
- Supremum distance (Lmax, L∞ norm, and the Chebyshev distance): a generalization of the Minkowski distance for h→∞

$$d(i, j) = \lim_{h \to \infty} \left(\sum_{f=1}^{p} |x_{if} - x_{jf}|^h \right)^{\frac{1}{h}} = \max_{f} |x_{if} - x_{jf}|$$

Example. Let x1 = (1, 2) and x2 = (3, 5) represent two objects as shown



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The values of an ordinal attribute have a meaningful order or ranking about them. e.g. drink_size = {small, medium, large} Suppose that f is an ordinal attribute and has Mf ordered states. Let 1, . . . , Mf

represent ranking of these ordered states. The dissimilarity of f can be calculated by:

- 1. Normalize the rank rif of the object i and attribute f by
- 2.Compute the dissimilarity using distance methods

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

Example. Suppose that we have the sample data shown as follows. use the Euclidean distance, the dissimilarity matrix is?



$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

| Object Identifier | Test-2 (ordinal) |
|-------------------|------------------|
| 1 | excellent |
| 2 | fair |
| 3 | good |
| 4 | excellent |

Example. Suppose that we have the sample data shown as follows. use the Euclidean distance, the dissimilarity matrix is?

Z1f =

Z2f =

Z3f =

Z4f =



$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

| Object Identifier | Test-2 (ordinal) |
|-------------------|------------------|
| 1 | excellent |
| 2 | fair |
| 3 | good |
| 4 | excellent |

Example. Suppose that we have the sample data shown as follows. use the Euclidean distance, the dissimilarity matrix is?

$$M_f = 3$$
, [fair, good, excellent] = [1,2,3]

$$Z1f = 1$$

$$Z_{2f} = 0$$

$$Z3f = 0.5$$

$$Z4f = 1$$

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

| Object Identifier | Test-2 (ordinal) |
|-------------------|------------------|
| 1 | excellent |
| 2 | fair |
| 3 | good |
| 4 | excellent |

Example. Suppose that we have the sample data shown as follows. use the Euclidean distance, the dissimilarity matrix is?

$$M_f = 3$$
, [fair, good, excellent] = [1,2,3]

$$Z1f = 1$$

$$Z_{2f} = 0$$

$$Z3f = 0.5$$

$$Z4f = 1$$

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

| Object Identifier | Test-2 (ordinal) |
|-------------------|------------------|
| 1 | excellent |
| 2 | fair |
| 3 | good |
| 4 | excellent |

A database may contain all attribute types

Nominal, symmetric binary, asymmetric binary, numeric, ordinal

Suppose that the data set contains p attributes of mixed types. The dissimilarity d(i, j)

between objects i and j is defined as

ween objects i and j is defined as
$$d(i,j) = \frac{\sum_{f=1}^p \delta_{ij}^{(f)} d_{ij}^{(f)}}{\sum_{f=1}^p \delta_{ij}^{(f)}}$$
 where the indicator $\delta_{ij}^{(f)}$ = 0 if

- 1. x_{if} or x_{if} is missing (i.e., there is no measurement of attribute f for object i or object j),
- 2. $x_{if} = x_{if} = 0$ and attribute f is asymmetric binary;
- 3. otherwise, $\delta_{ii}^{(f)} = 1$.

The contribution of attribute f to the dissimilarity between i and j (i.e., $d_{ij}^{(f)}$) is computed dependent on its type:

- If f is numeric: $d_{ij}^{(f)} = \frac{|x_{if} x_{jf}|}{max_f min_f}$, where max_f and min_f are the maximum and minimum values of attribute f, respectively;
- If f is nominal or binary: $d_{ij}^{(f)} = 0$ if $x_{if} = x_{jf}$; otherwise, $d_{ij}^{(f)} = 1$; and
- If f is ordinal: compute the ranks r_{if} and $z_{if} = \frac{r_{if}-1}{M_f-1}$, and treat z_{if} as numeric.



| Object Identifier | Test-1 (nominal) | Test-2 (ordinal) | Test-3 (numeric) |
|-------------------|------------------|------------------|------------------|
| 1 | code A | excellent | 45 |
| 2 | code B | fair | 22 |
| 3 | code C | good | 64 |
| 4 | code A | excellent | 28 |

- If f is numeric: $d_{ij}^{(f)} = \frac{|x_{if} x_{jf}|}{max_f min_f}$, where max_f and min_f are the maximum and minimum values of attribute f, respectively;
- If f is nominal or binary: $d_{ij}^{(f)} = 0$ if $x_{if} = x_{jf}$; otherwise, $d_{ij}^{(f)} = 1$; and
- If f is ordinal: compute the ranks r_{if} and $z_{if} = \frac{r_{if}-1}{M_f-1}$, and treat z_{if} as numeric.

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$$d_{ij}^{(1)} = \begin{bmatrix} 0 \\ 1 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

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$$d_{ij}^{(1)} = \begin{bmatrix} 0 \\ 1 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

$$d_{ij}^{(1)} = \begin{bmatrix} 0 \\ 1 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix} \qquad d_{ij}^{(2)} = \begin{bmatrix} 0 \\ 1.0 & 0 \\ 0.5 & 0.5 & 0 \\ 0 & 1.0 & 0.5 & 0 \end{bmatrix}$$

| Object Identifier | Test-1 (nominal) | Test-2 (ordinal) | Test-3(numeric) |
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$$d_{ij}^{(1)} = \begin{bmatrix} 0 \\ 1 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

$$d_{ij}^{(2)} = \begin{bmatrix} 0 \\ 1.0 & 0 \\ 0.5 & 0.5 & 0 \\ 0 & 1.0 & 0.5 & 0 \end{bmatrix}$$

$$d_{ij}^{(1)} = \begin{bmatrix} 0 & & & \\ 1 & 0 & & \\ 1 & 1 & 0 & \\ 0 & 1 & 1 & 0 \end{bmatrix} \quad d_{ij}^{(2)} = \begin{bmatrix} 0 & & & \\ 1.0 & 0 & & \\ 0.5 & 0.5 & 0 & \\ 0 & 1.0 & 0.5 & 0 \end{bmatrix} \quad d_{ij}^{(3)} = \begin{bmatrix} 0 & & & \\ 0.55 & 0 & & \\ 0.45 & 1.00 & 0 & \\ 0.40 & 0.14 & 0.86 & 0 \end{bmatrix}$$

| Object Identifier | Test-1 (nominal) | Test-2 (ordinal) | Test-3(numeric) |
|-------------------|------------------|------------------|-----------------|
| 1 | code A | excellent | 45 |
| 2 | code B | fair | 22 |
| 3 | code C | good | 64 |
| 4 | code A | excellent | 28 |

$$d_{ij}^{(1)} = \begin{bmatrix} 0 & & & \\ 1 & 0 & & \\ 1 & 1 & 0 & \\ 0 & 1 & 1 & 0 \end{bmatrix} \qquad d_{ij}^{(2)} = \begin{bmatrix} 0 & & & \\ 1.0 & 0 & & \\ 0.5 & 0.5 & 0 & \\ 0 & 1.0 & 0.5 & 0 \end{bmatrix} \qquad d_{ij}^{(3)} = \begin{bmatrix} 0 & & & \\ 0.55 & 0 & & \\ 0.45 & 1.00 & 0 & \\ 0.40 & 0.14 & 0.86 & 0 \end{bmatrix}$$

$$\delta_{ij}^{(f)} = 1, \quad d(3, 1) = \frac{1(1) + 1(0.50) + 1(0.45)}{3} = 0.65$$

| Object Identifier | Test-1 (nominal) | Test-2 (ordinal) | Test-3(numeric) |
|-------------------|------------------|------------------|-----------------|
| 1 | code A | excellent | 45 |
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| 4 | code A | excellent | 28 |

$$d(i, j) = \begin{bmatrix} 0 \\ 0.85 & 0 \\ 0.65 & 0.83 & 0 \\ 0.13 & 0.71 & 0.79 & 0 \end{bmatrix}$$

Cosine similarity: measures the similarity between two vectors of an inner product space. It is measured by the cosine of the angle between two vectors and determines whether two vectors are pointing in roughly the same direction.

- Often used to measure document similarity in text analysis.
- A document can be represented by thousands of attributes, each recording the frequency of a particular word (such as keywords) or phrase in the document. Thus each document is an object represented by what is called a **term-frequency vector**.

Let x and y be two term-frequency vectors for comparison. Using the cosine measure as a similarity function, we have $x \cdot v$

$$sim(x, y) = \frac{x \cdot y}{||x||||y||}$$

where ||x|| is the Euclidean norm of vector $\mathbf{x} = (x_1, x_2, \dots, x_p)$, defined as $\sqrt{x_1^2 + x_2^2 + \dots + x_p^2}$. ||y|| is the Euclidean norm of vector \mathbf{y}

Example. Suppose that x and y are the first two term-frequency vectors in the following table, That is, x = (5, 0, 3, 0, 2, 0, 0, 2, 0, 0) and y = (3, 0, 2, 0, 1, 1, 0, 1, 0, 1).

How similar are x and y?

$$sim(x, y) = \frac{x \cdot y}{||x||||y||}$$

Document vector or term-frequency vector.

| Document | Team | Coach | Hockey | Baseball | Soccer | Penalty | Score | Win | Loss | Season |
|----------|------|-------|--------|----------|--------|---------|-------|-----|------|--------|
| 1 | 5 | 0 | 3 | 0 | 2 | 0 | 0 | 2 | 0 | 0 |
| 2 | 3 | 0 | 2 | 0 | 1 | 1 | 0 | 1 | 0 | 1 |
| 3 | 0 | 7 | 0 | 2 | 1 | 0 | 0 | 3 | 0 | 0 |
| 4 | 0 | 1 | 0 | 0 | 1 | 2 | 2 | 0 | 3 | 0 |

Example. Suppose that x and y are the first two term-frequency vectors in the following table, That is, x = (5, 0, 3, 0, 2, 0, 0, 2, 0, 0) and y = (3, 0, 2, 0, 1, 1, 0, 1, 0, 1).

How similar are x and y?

$$sim(x, y) = \frac{x \cdot y}{||x||||y||}$$

$$\mathbf{x} \cdot \mathbf{y} = 5 \times 3 + 0 \times 0 + 3 \times 2 + 0 \times 0 + 2 \times 1 + 0 \times 1 + 0 \times 0 + 2 \times 1 + 0 \times 0 + 0 \times 1 = 25$$

$$||x|| = \sqrt{5^2 + 0^2 + 3^2 + 0^2 + 2^2 + 0^2 + 0^2 + 2^2 + 0^2 + 0^2 + 0^2} = 6.48$$

$$||\mathbf{y}|| = \sqrt{3^2 + 0^2 + 2^2 + 0^2 + 1^2 + 1^2 + 0^2 + 1^2 + 0^2 + 1^2} = 4.12$$

Example. Suppose that x and y are the first two term-frequency vectors in the following table, That is, x = (5, 0, 3, 0, 2, 0, 0, 2, 0, 0) and y = (3, 0, 2, 0, 1, 1, 0, 1, 0, 1).

How similar are x and y?

$$sim(x, y) = \frac{x \cdot y}{||x||||y||}$$

$$\mathbf{x} \cdot \mathbf{y} = 5 \times 3 + 0 \times 0 + 3 \times 2 + 0 \times 0 + 2 \times 1 + 0 \times 1 + 0 \times 0 + 2 \times 1 + 0 \times 0 + 0 \times 1 = 25$$

$$||x|| = \sqrt{5^2 + 0^2 + 3^2 + 0^2 + 2^2 + 0^2 + 0^2 + 2^2 + 0^2 + 0^2 + 0^2} = 6.48$$

$$||\mathbf{y}|| = \sqrt{3^2 + 0^2 + 2^2 + 0^2 + 1^2 + 1^2 + 1^2 + 0^2 + 1^2 + 0^2 + 1^2} = 4.12$$

$$sim(x, y) = 0.94$$

Kullback-Leibler divergence(the KL divergence): a measure that has been popularly used in the data mining literature to measure the difference between two probability distributions over the same variable x.

- closely related to relative entropy, information divergence, and information for discrimination
- is a nonsymmetric measure of the difference between two probability distributions p(x) and q(x)
- the KL divergence of q(x) from p(x), denoted $D_{KL}(p(x)||q(x))$, is a measure of the information loss when q(x) is used to approximate p(x).

Let p(x) and q(x) be two probability distributions of a discrete random variable x. That is, both p(x) and q(x) sum up to 1, and p(x) > 0 and q(x) > 0 for any x in X. $D \ltimes L(p(x) || q(x))$ is defined as

$$D_{KL}(p(x)||q(x)) = \sum_{x \in X} p(x) \ln \frac{p(x)}{q(x)}$$

Typically p(x) represents the "true" distribution of data. The measure q(x) typically represents a theory, model, description, or approximation of p(x).

- it is not a distance measure, because it is not a metric measure.
- It is not symmetric: the KL from p(x) to q(x) is generally not the same as the KL from q(x) to p(x).
- DKL(p(x)||q(x)) is a nonnegative measure. DKL(p(x)||q(x)) ≥ 0 and DKL(p(x)||q(x)) = 0 if and only if p(x) = q(x)

Example. Suppose there are two sample distributions P and Q as follows: P: (a: 3/5, b: 1/5, c: 1/5) and Q: (a: 5/9, b: 3/9, d: 1/9). Compute the KL divergence Dkl(P ||Q)



Example. Suppose there are two sample distributions P and Q as follows: P: (a: 3/5, b: 1/5, c: 1/5) and Q: (a: 5/9, b: 3/9, d: 1/9). Compute the KL divergence Dkl(P ||Q)



No sample d in P, and no sample c in Q?

Avoiding the Zero-Probability Problem

Kullback-Leibler divergence: smoothing

Example. Suppose there are two sample distributions P and Q as follows: P: (a: 3/5, b: 1/5, c: 1/5) and Q: (a: 5/9, b: 3/9, d: 1/9). Compute the KL divergence Dkl(P ||Q)

- Introduce a small constant e = 0.001,
- **smoothing:** the missing symbols can be added to each distribution accordingly, with the small probability e.

```
P': (a: 3/5 - e/3, b: 1/5 - e/3, c: 1/5 - e/3, d: e)
Q': (a: 5/9 - e/3, b: 3/9 - e/3, c: e, d: 1/9 - e/3)
```

DKL(P',Q') can be calculated.

Summary

- Similarity and distance measures
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 - Mixed types
 - Cosine Similarity
 - Kullback-Leibler divergence