# Distance measures for clustering

- What is the distance between two objects (rows in the data matrix)?
- (Earlier we talked about distances between sets of objects, given the distance between objects; now we look at the distance between objects.)
- Examples: objects are documents; what is the distance between two documents
- Objects are gene sequences (strings in ACGT); what is the distance?
- Euclidean distances vs. non-Euclidean distances (points in space vs. some other properties)

## Desired properties of a distance measure

- Objects $X$, distance measure $d : X \times X \to R$
- Should be a metric
- $d(x, y) \geq 0$ for all $x$ and $y$
- $d(x, y) = 0$ if and only if $x = y$
- $d(x, y) = d(y, x)$
- $d(x, z) \leq d(x, y) + d(y, z)$ for all $x, y, z$ (triangle inequality)

## Examples of metrics

- Assume points are in $d$-dimensional space
- $x = (x_1, x_2, \ldots, x_d)$ and $y = (y_1, y_2, \ldots, y_d)$
- Normal Euclidean distance ($L_2$ distance)

$$d_2(x,y) = \sqrt{\sum_{i=1}^{d}(x_i - y_i)^2}.$$

- This is the $L_2$ norm of $x - y$, also written as $||x - y||_2$
- $L_p$ distance $p > 0$

$$d_p(x,y) = (\sum_{i=1}^{d}(x_i - y_i)^p)^(1/p)$$

- What is $L_1$ distance? What is $L_\infty$ distance?

## Distance and similarity

- Similarity $s(x, y) = M - d(x, y)$, where $M$ is the maximal value the distance can obtain
- About equivalent concepts
- Not always

## Other examples for vectors of 0s and 1s

- Jaccard distance: view $x = (x_1, x_2, \ldots, x_d) \in \{0,1\}^d$ and $y = (y_1, y_2, \ldots, y_d) \in \{0,1\}^d$ as sets
-
$$J(x,y) = 1 - \frac{|x \cap y|}{|x \cup y|}.$$

- Cosine distance: view $x$ and $y$ as vectors, similarity between the vectors is measured as the cosine of the angle between the vectors

$$s(x,y) = \frac{x \cdot y}{||x||_2||y||_2}$$

How does this behave?

## Distance notions for strings

- How close are two strings to each other?
- Edit distance
- Select a set of operations, say insert a character, delete a character, substitute one character for another
- $d(s, t)$: the smallest number of operations that is needed to transform string $s$ into string $t$
- This is a metric (why?)
- Can be computed efficiently

## Similarity for columns

- Similarity for columns of a 0-1 matrix $M$
- Jaccard coefficient for columns $A$ and $B$:

$$J(A,B) = \frac{|\{t \in M | t(A) = 1 \wedge t(B) = 1\}|}{|\{t \in M | t(A) = 1 \vee t(B) = 1\}|}$$

- How many rows $t$ of $M$ have both $A$ and $B$, divided by how many rows have at least one of $A$ and $B$
- $|\{t \in M | t(A) = 1 \vee t(B) = 1\}| = f(A) + f(B) - f(AB)$
- Thus $J(A,B) = f(AB)/(f(A) + f(B) - f(AB))$
- High if $A$ and $B$ are strongly associated
- Alternatives: correlation between variables $A$ and $B$

## Other measures of similarity

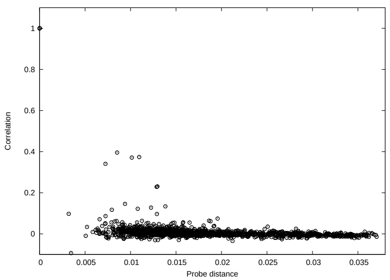
- Two columns $A$ and $B$ might actually be similar even if there are only a few rows with $A = B = 1$
- Example: retail data, two soft drinks $A$ and $B$
- $A$ and $B$ are similar in the sense that the behavior of the customers who buy $A$ is about the same as the behavior of the customers who buy $B$
- Can be very few customers who buy both $A$ and $B$
- How to formalize this?

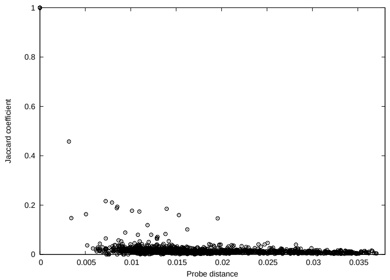
## Probe similarity

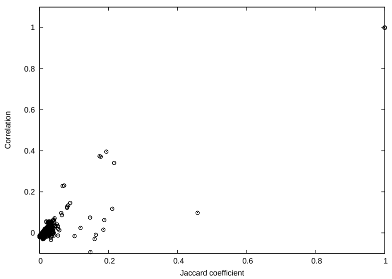
- Define the distance of $A$ and $B$ by the difference in the probabilities of the other variables
- $Pr(C|A=1)$: what fraction of the customers who buy $A$ also buy $C$ (conditional probability)
- $Pr(C|A=1) = f(AC)/f(A)$
- Let $U$ be the set of attributes, and $U_{AB} = U \setminus \{A, B\}$
- $d(A,B) = \sum_{C \in U_{AB}} |Pr(C|A=1) - Pr(C|B=1)|$

G. Das, H. Mannila, P. Ronkainen, KDD 1998

# Example: retail.over1000cols.01




Correlations between measures:

| Probe | Corr | Jaccard |
|---:|---:|---:|
| 1.00000 | -0.36364 | -0.34927 |
| -0.36364 | 1.00000 | 0.98819 |
| -0.34927 | 0.98819 | 1.00000 |

## Contextual similarity

- "Two words are similar, if they occur in similar sentences."
- "Two sentences are similar, if they contain similar words."
- How to implement this?