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

Euclidean Distance

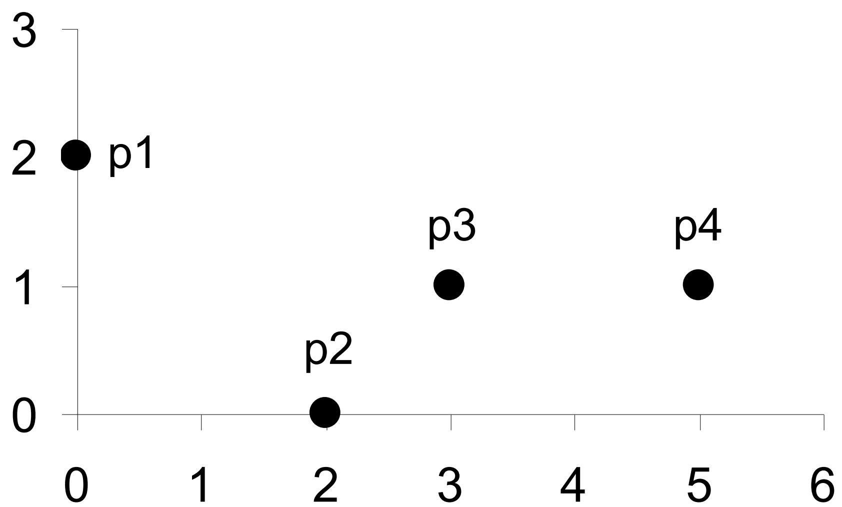
- Euclidean Distance

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

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

- 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 $\boldsymbol{x}$ and $\boldsymbol{y}$.

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

- $r \rightarrow \infty$. "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

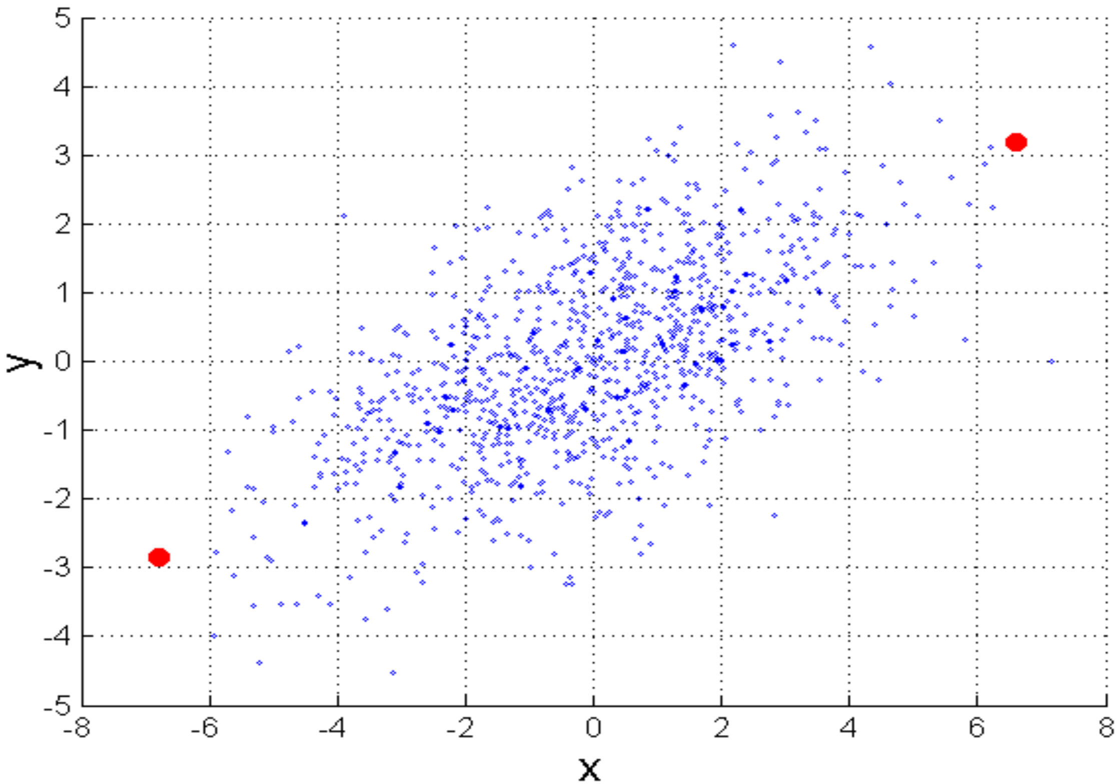
L2	p1	p2	p3	p4
p1	0	2.828	3.162	5.099
p2	2.828	0	1.414	3.162
p3	3.162	1.414	0	2
p4	5.099	3.162	2	0

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

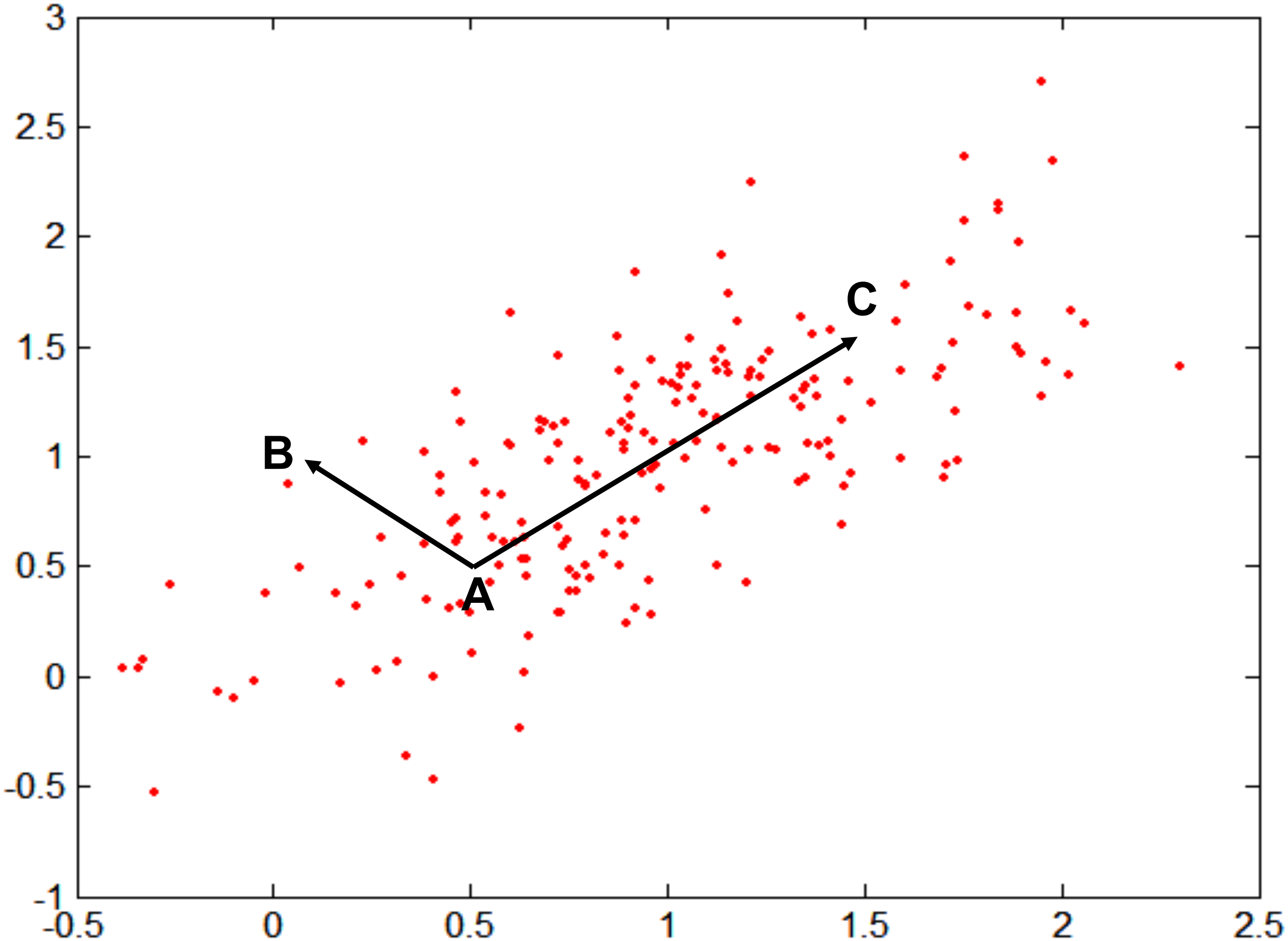
$$\mathbf{mahalanobis}(\mathbf{x},\mathbf{y}) = ((\mathbf{x}-\mathbf{y})^T\,\Sigma^{-1}(\mathbf{x}-\mathbf{y}))^{\mathbf{-0.5}}$$



Σ is the covariance matrix

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 $d(\mathbf{x}, \mathbf{y}) = 0$ if and only if $\mathbf{x} = \mathbf{y}$.
  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, $\mathbf{x}$ and $\mathbf{y}$, have only binary attributes

- Compute similarities using the following quantities

  f_{01} = the number of attributes where $\mathbf{x}$ was 0 and $\mathbf{y}$ was 1

  f_{10} = the number of attributes where $\mathbf{x}$ was 1 and $\mathbf{y}$ was 0

  f_{00} = the number of attributes where $\mathbf{x}$ was 0 and $\mathbf{y}$ was 0

  f_{11} = the number of attributes where $\mathbf{x}$ was 1 and $\mathbf{y}$ 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

$\mathbf{x} = 1\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0$

$\mathbf{y} = 0\ 0\ 0\ 0\ 0\ 0\ 1\ 0\ 0\ 1$

$f_{01} = 2$ (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)

$$\begin{aligned} \text{SMC} &= (f_{11} + f_{00}) / (f_{01} + f_{10} + f_{11} + f_{00}) \\ &= (0+7) / (2+1+0+7) = 0.7 \end{aligned}$$

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

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 $\mathbf{d}$.

- Example:

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

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

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

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

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

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

Correlation measures the linear relationship between objects

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

where we are using the following standard statistical notation and definitions

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

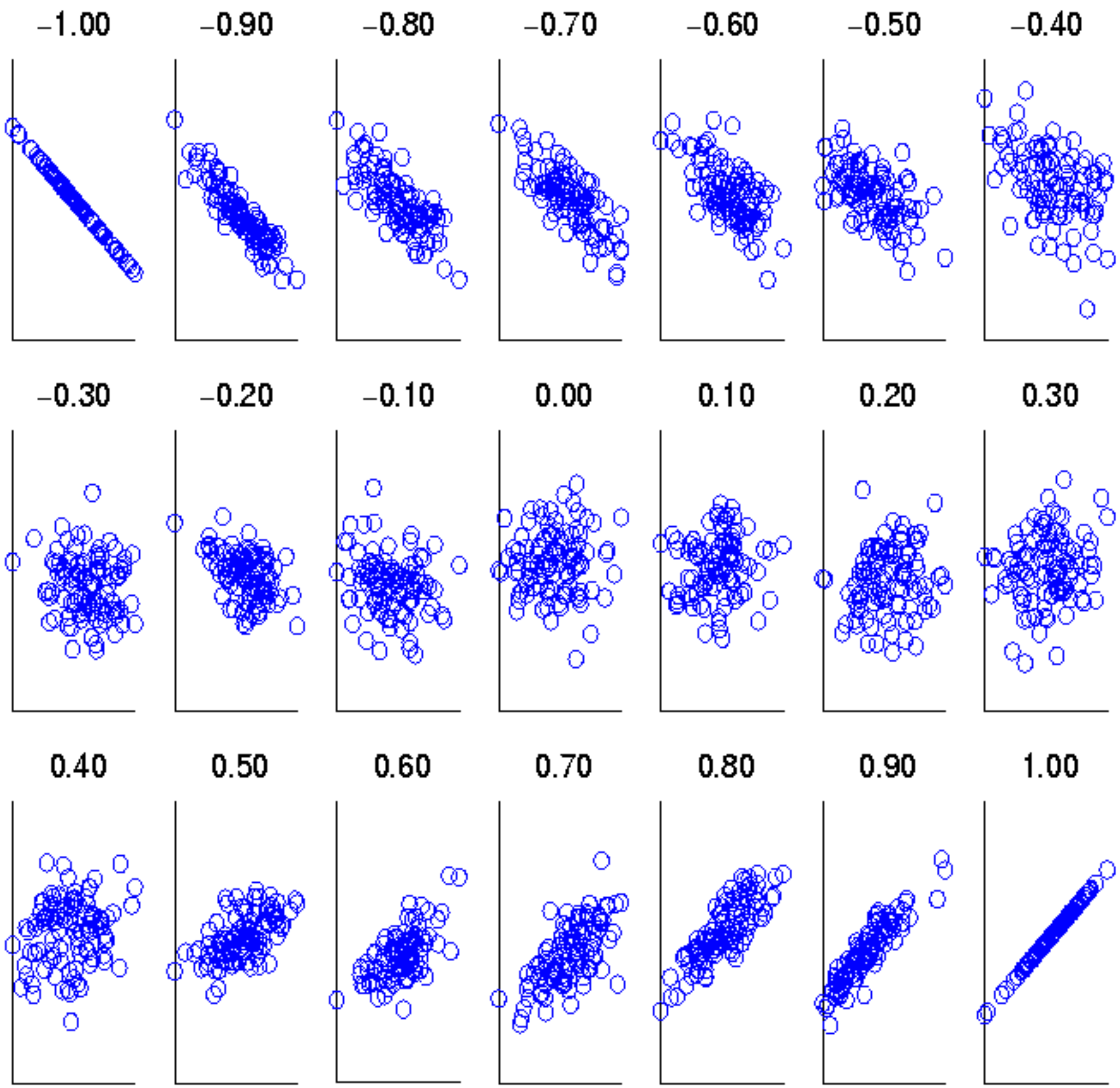
$$\text{standard\_deviation}(\mathbf{x}) = s_x = \sqrt{\frac{1}{n-1} \sum_{k=1}^{n} (x_k - \overline{x})^2}$$

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

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

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

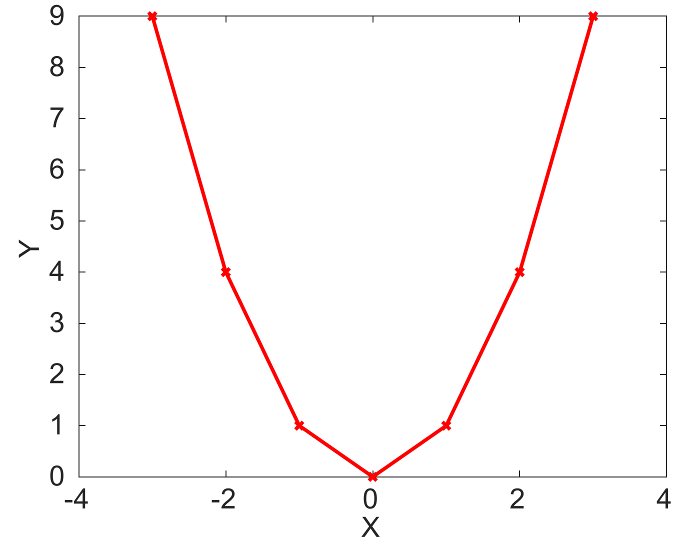
Visually Evaluating Correlation



Scatter plots showing the similarity from –1 to 1.

Drawback of Correlation

- $\mathbf{x} = (-3, -2, -1, 0, 1, 2, 3)$
- $\mathbf{y} = (9, 4, 1, 0, 1, 4, 9)$



$y_i = x_i^2$

- $\text{mean}(\mathbf{x}) = 0$, $\text{mean}(\mathbf{y}) = 4$
- $\text{std}(\mathbf{x}) = 2.16$, $\text{std}(\mathbf{y}) = 3.74$

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

  = 0

Correlation vs Cosine vs Euclidean Distance

- Compare the three proximity measures according to their behavior under variable transformation
  - scaling: multiplication by a value
  - translation: adding a constant

Property	Cosine	Correlation	Euclidean Distance
Invariant to scaling (multiplication)	Yes	Yes	No
Invariant to translation (addition)	No	Yes	No

- Consider the example
  - **x** = (1, 2, 4, 3, 0, 0, 0), **y** = (1, 2, 3, 4, 0, 0, 0)
  - $\mathbf{y_s = y * 2}$ (scaled version of y), $\mathbf{y_t = y + 5}$ (translated version)

Measure	(x , y)	(x , y_s)	(x , y_t)
Cosine	0.9667	0.9667	0.7940
Correlation	0.9429	0.9429	0.9429
Euclidean Distance	1.4142	5.8310	14.2127

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

Information Based Measures

- Information theory is a well-developed and fundamental disciple with broad applications

- Some similarity measures are based on information theory
  - Mutual information in various versions
  - Maximal Information Coefficient (MIC) and related measures
  - General and can handle non-linear relationships
  - Can be complicated and time intensive to compute

Information and Probability

- Information relates to possible outcomes of an event
  - transmission of a message, flip of a coin, or measurement of a piece of data

- The more certain an outcome, the less information that it contains and vice-versa
  - For example, if a coin has two heads, then an outcome of heads provides no information
  - More quantitatively, the information is related the probability of an outcome
    - The smaller the probability of an outcome, the more information it provides and vice-versa
  - Entropy is the commonly used measure

Entropy

- For
  - a variable (event), X,
  - with n possible values (outcomes), $x_1, x_2 \ldots, x_n$
  - each outcome having probability, $p_1, p_2 \ldots, p_n$
  - the entropy of X , $H(X)$, is given by

$$H(X) = -\sum_{i=1}^{n} p_i \log_2 p_i$$

- Entropy is between 0 and $\log_2 n$ and is measured in bits
  - Thus, entropy is a measure of how many bits it takes to represent an observation of X on average

Entropy Examples

- For a coin with probability p of heads and probability $q = 1 - p$ of tails

$$H = -p \log_2 p - q \log_2 q$$

  - For $p= 0.5$, $q = 0.5$ (fair coin) $H = 1$
  - For $p = 1$ or $q = 1$, $H = 0$

- What is the entropy of a fair four-sided die?

Entropy for Sample Data: Example

Hair Color	Count	p	$-p\log_2 p$
Black	75	0.75	0.3113
Brown	15	0.15	0.4105
Blond	5	0.05	0.2161
Red	0	0.00	0
Other	5	0.05	0.2161
Total	100	1.0	1.1540

Maximum entropy is $\log_2 5 = 2.3219$

Entropy for Sample Data

- Suppose we have
  - a number of observations (m) of some attribute, X, e.g., the hair color of students in the class,
  - where there are n different possible values
  - And the number of observation in the i^{th} category is m_i
  - Then, for this sample

$$H(X) = -\sum_{i=1}^{n} \frac{m_i}{m} \log_2 \frac{m_i}{m}$$

- For continuous data, the calculation is harder

Mutual Information

- Information one variable provides about another

Formally, $I(X,Y) = H(X) + H(Y) - H(X,Y)$, where

$H(X,Y)$ is the joint entropy of X and Y,

$$H(X,Y) = -\sum_i \sum_j p_{ij} \log_2 p_{ij}$$

Where p_{ij} is the probability that the i^{th} value of X and the j^{th} value of Y occur together

- For discrete variables, this is easy to compute

- Maximum mutual information for discrete variables is $\log_2(\min(n_X, n_Y))$, where n_X (n_Y) is the number of values of X (Y)

Mutual Information Example

Student Status	Count	p	$-p\log_2 p$
Undergrad	45	0.45	0.5184
Grad	55	0.55	0.4744
Total	100	1.00	0.9928

Grade	Count	p	$-p\log_2 p$
A	35	0.35	0.5301
B	50	0.50	0.5000
C	15	0.15	0.4105
Total	100	1.00	1.4406

Student Status	Grade	Count	p	$-p\log_2 p$
Undergrad	A	5	0.05	0.2161
Undergrad	B	30	0.30	0.5211
Undergrad	C	10	0.10	0.3322
Grad	A	30	0.30	0.5211
Grad	B	20	0.20	0.4644
Grad	C	5	0.05	0.2161
Total		100	1.00	2.2710

Mutual information of Student Status and Grade = 0.9928 + 1.4406 - 2.2710 = 0.1624