

Distance and Similarity Measures

SIMILARITY AND DISSIMILARITY MEASURE FOR QUANTITATIVE FEATURES

		400	
Measures	Forms	Comments	Examples and Applications
Minkowski distance	$D_{ij} = \left(\sum_{l=1}^{d} \left \mathbf{x}_{il} - \mathbf{x}_{jl} \right ^{1/n} \right)^{n}$	Metric. Invariant to any translation and rotation only for $n=2$ (Euclidean distance). Features with large values and variances tend to dominate over other features.	Fuzzy c-means with measures based on Minkowski family [130].
Euclidean distance	$D_{ij} = \left(\sum_{l=1}^{d} \left x_{il} - x_{jl} \right ^{1/2} \right)^{2}$	The most commonly used metric. Special case of Minkowski metric at $n=2$. Tend to form hyperspherical clusters.	K-means algorithm [191]
City-block distance	$D_{ij} = \sum_{l=1}^{d} \left x_{il} - x_{jl} \right $	Special case of Minkowski metric at $n=1$. Tend to form hyperrecutangular clusters.	Fuzzy ART [57]
Sup distance	$D_{ij} = \max_{1 \le i \le d} \left x_{il} - x_{jl} \right $	Special case of Minkowski metric at $n \to \infty$.	Fuzzy c-means with sup norm [39].
Mahalanobis distance	$D_{ij} = (\mathbf{x}_i - \mathbf{x}_j)^T \mathbf{S}^{-1} (\mathbf{x}_i - \mathbf{x}_j)$, where S is the withingroup covariance matrix.	Invariant to any nonsingular linear transformation. S is calculated based on all objects. Tend to form hyperellipsoidal clusters. When features are not correlated, squared Mahalanobis distance is equivalent to squared Euclidean distance. May cause some computational burden.	Ellipsoidal ART [13], Hyperellipsoidal clustering algorithm [194].
Pearson correlation	$D_{ij} = (1 - r_{ij})/2, \text{ where } r_{ij} = \frac{\sum_{l=1}^{d} (x_{il} - \overline{x_i})(x_{jl} - \overline{x_j})}{\sqrt{\sum_{l=1}^{d} (x_{il} - \overline{x_i})^2 \sum_{l=1}^{d} (x_{jl} - \overline{x_j})^2}}$	Not a metric. Derived from correlation coefficient. Unable to detect the magnitude of differences of two variables.	Widely used as the measure for analyzing gene expression data [80].
Point symmetry distance	$D_{tr} = \min_{\substack{j=1,\dots,N\\ \text{and } j \neq i}} \frac{\left\ (\mathbf{x}_i - \mathbf{x}_r) + (\mathbf{x}_j - \mathbf{x}_r) \right\ }{\left\ (\mathbf{x}_i - \mathbf{x}_r) \right\ + \left\ (\mathbf{x}_j - \mathbf{x}_r) \right\ }$	Not a metric. Compute the distance between an object \mathbf{x}_i and a reference point \mathbf{x}_r . D_{ir} is minimized when a symmetric pattern exists.	SBKM (Symmetry-based K-means) [264].
Cosine similarity	$S_{ij} = \cos \alpha = \frac{\mathbf{x}_{t}^{T} \mathbf{x}_{j}}{\ \mathbf{x}_{i}\ \ \mathbf{x}_{j}\ }$	Independent of vector length. Invariant to rotation, but not to linear transformations.	The most commonly used measure in document clustering [261].

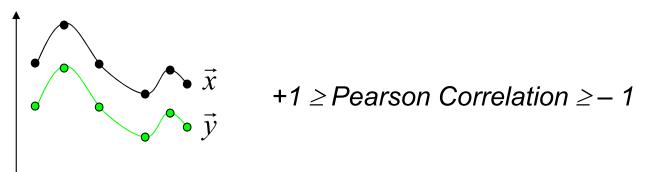
Pearson Correlation

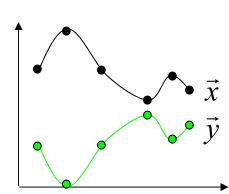
Two profiles (vectors)
$$\vec{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix}$$
 and $\vec{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$

$$C_{pearson}(\vec{x}, \vec{y}) = \frac{\sum_{i=1}^{N} (x_i - m_x)(y_i - m_y)}{\sqrt{\left[\sum_{i=1}^{N} (x_i - m_x)^2\right] \left[\sum_{i=1}^{N} (y_i - m_y)^2\right]}} \qquad m_x = \frac{1}{N} \sum_{n=1}^{N} x_n \\ m_y = \frac{1}{N} \sum_{n=1}^{N} y_n$$

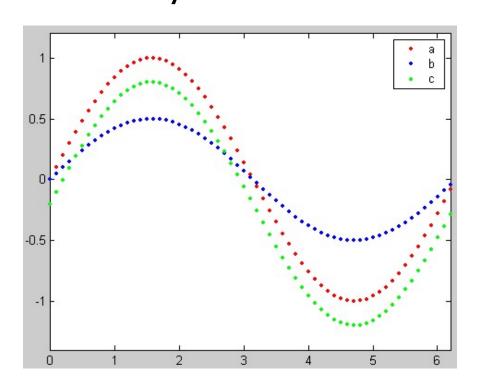
$$m_{x} = \frac{1}{N} \sum_{n=1}^{N} x_{n}$$

$$m_{y} = \frac{1}{N} \sum_{n=1}^{N} y_{n}$$





Pearson Correlation: Trend Similarity



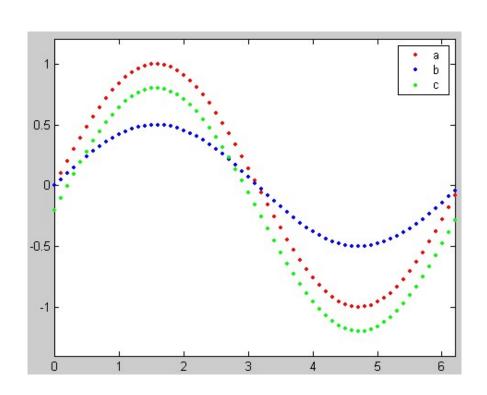
$$\vec{b} = 0.5\vec{a}$$
 $\vec{c} = \vec{a} - 0.2$
 $C_{pearson}(\vec{a}, \vec{b}) = 1$
 $C_{pearson}(\vec{a}, \vec{c}) = 1$
 $C_{pearson}(\vec{b}, \vec{c}) = 1$

Euclidean Distance

$$\vec{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} \vec{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$$

$$d(\vec{x}, \vec{y}) = \sqrt{\sum_{n=1}^{N} (x_n - y_n)^2}$$

Euclidean Distance: Absolute difference



$$\vec{b} = 0.5\vec{a}$$
 $\vec{c} = \vec{a} - 0.2$
 $d(\vec{a}, \vec{b}) = 2.8025$
 $d(\vec{a}, \vec{c}) = 1.5875$
 $d(\vec{b}, \vec{c}) = 3.2211$

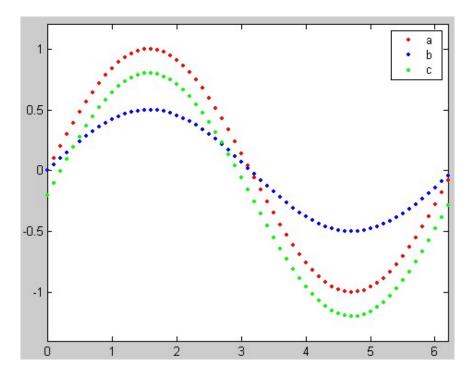
Cosine Correlation

$$\vec{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} \qquad \vec{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$$

$$C_{\text{cosine}}(\vec{x}, \vec{y}) = \frac{\frac{1}{N} \sum_{i=1}^{N} x_i \times y_i}{\|\vec{x}\| \times \|\vec{y}\|}$$

$$\vec{x} = \vec{y}$$
 +1 \geq Cosine Correlation \geq -1 $\vec{x} = -\vec{y}$

Cosine Correlation: Trend + Mean Distance



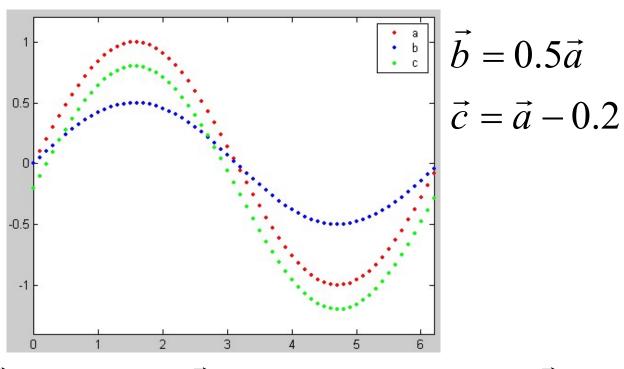
$$\vec{b} = 0.5\vec{a}$$

$$\vec{c} = \vec{a} - 0.2$$

$$C_{\text{cos ine}}(\vec{a}, \vec{b}) = 1$$

$$C_{\text{cos ine}}(\vec{a}, \vec{c}) = 0.9622$$

$$C_{\text{cos ine}}(\vec{b}, \vec{c}) = 0.9622$$



$$C_{pearson}(\vec{a}, \vec{b}) = 1$$

$$d(\vec{a}, \vec{b}) = 2.8025$$

$$C_{\text{cosine}}(\vec{a}, \vec{b}) = 1$$

$$C_{pearson}(\vec{a}, \vec{c}) = 1$$
 $d(\vec{a}, \vec{c}) = 1.5875$

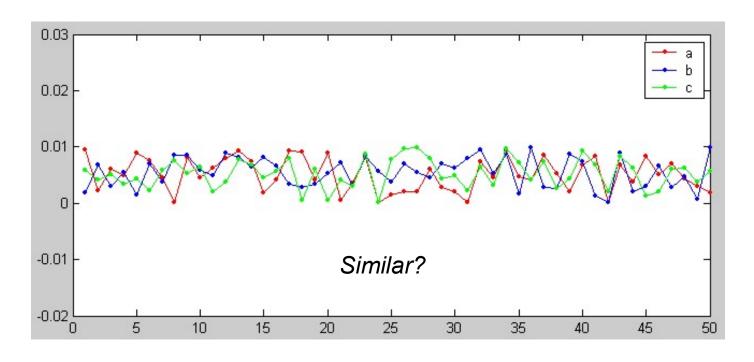
$$d(\vec{a}, \vec{c}) = 1.5875$$

$$C_{\text{cosine}}(\vec{a}, \vec{c}) = 0.9622$$

$$C_{pearson}(\vec{b}, \vec{c}) = 1$$
 $d(\vec{b}, \vec{c}) = 3.2211$

$$d(\vec{b}, \vec{c}) = 3.2211$$

$$C_{\text{cosine}}(\vec{b}, \vec{c}) = 0.9622$$



$$C_{pearson}(\vec{a}, \vec{b}) = -0.1175$$

$$d(\vec{a}, \vec{b}) = 0.0279$$

$$C_{\text{cosine}}(\vec{a}, \vec{b}) = 0.7544$$

$$C_{pearson}(\vec{a}, \vec{c}) = 0.1244$$

$$d(\vec{a}, \vec{c}) = 0.0255$$

$$C_{\text{cosine}}(\vec{a}, \vec{c}) = 0.8092$$

$$C_{pearson}(\vec{b}, \vec{c}) = 0.1779$$
 $d(\vec{b}, \vec{c}) = 0.0236$

$$d(\vec{b}, \vec{c}) = 0.0236$$

$$C_{\text{cosine}}(\vec{b}, \vec{c}) = 0.844$$