Lecture 05b

Distance Measures

Similarity and Dissimilarity

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

Euclidean Distance

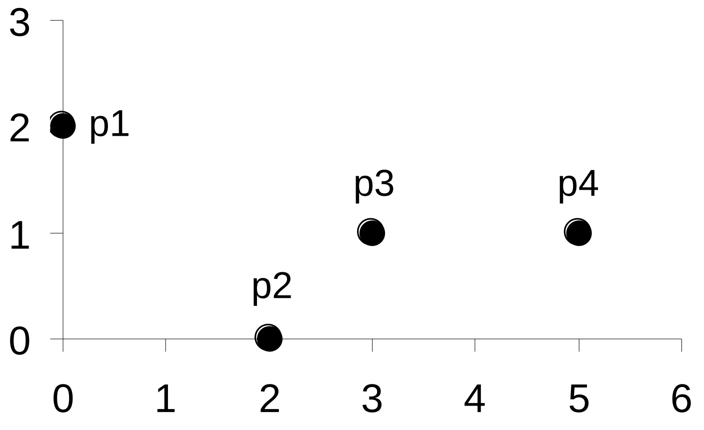
- Euclidean Distance

$$dist = \sqrt{\sum_{k=1}^{n} (p_k - q_k)^2}$$

Where *n* is the number of dimensions (attributes) and p_k and q_k are, respectively, the k^th attributes (components) or data objects *p* and *q*.

- 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

$$dist = \left(\sum_{k=1}^{n} |p_k - q_k|^r \right)^{\frac{1}{r}}$$

Where *r* is a parameter, *n* is the number of dimensions (attributes) and p_k and q_k are, respectively, the kth attributes (components) or data objects *p* and *q*.

Minkowski Distance: Examples

- *r* = 1. Cityblock (Manhattan, taxicab, L_1 norm) distance.
  - A common example of this is the Hamming distance, which is just the number of bits that are different between two binary vectors
- *r* = 2. Euclidean (L_2 norm) distance.
- $r \rightarrow \infty$. Chebyshev (L_{max} norm, L_∞ norm, maximum, supremum) distance.
  - This is the maximum difference between any component of the vectors
  - Example: L_infinity of (1, 0, 2) and (6, 0, 3) = ??
  - 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

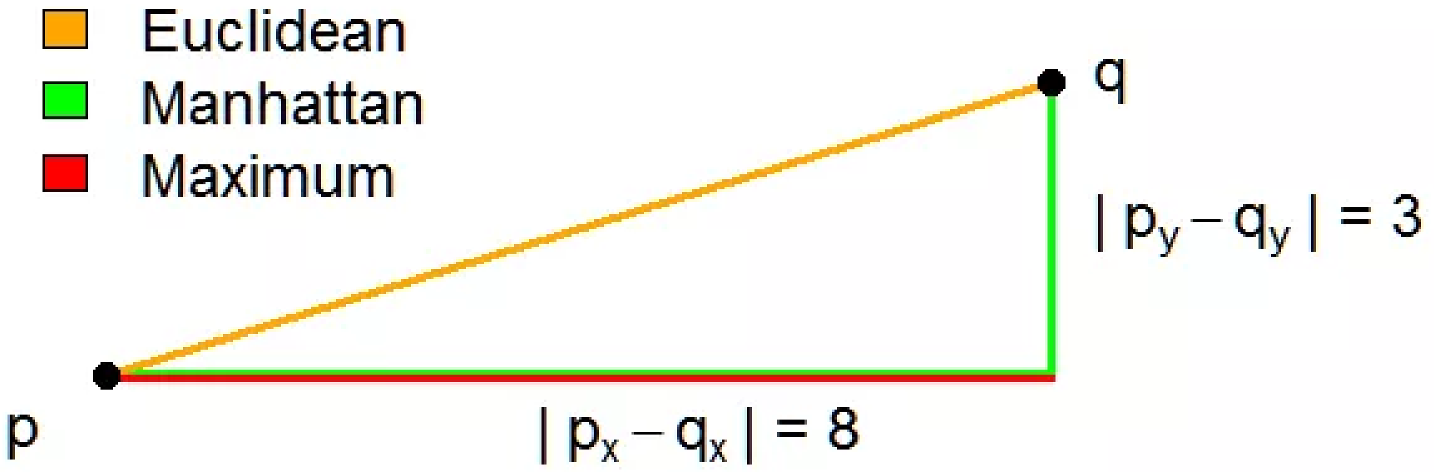
L1	p1	p2	p3	p4
p1	0	4	4	6
p2	4	0	2	4
p3	4	2	0	2
p4	6	4	2	0

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

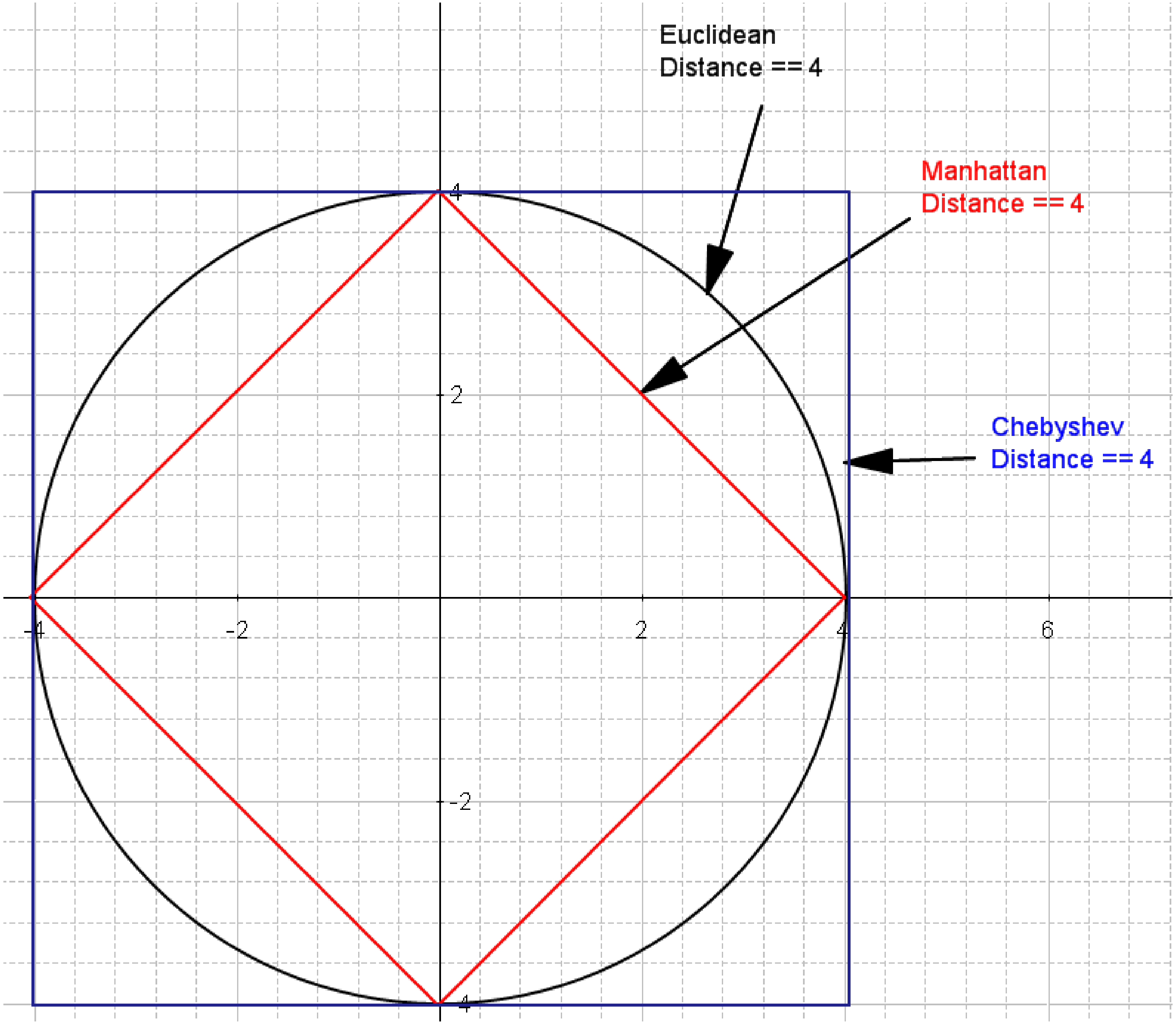
L∞	p1	p2	p3	p4
p1	0	2	3	5
p2	2	0	1	3
p3	3	1	0	2
p4	5	3	2	0

Distance Matrix

Minkowski Distance

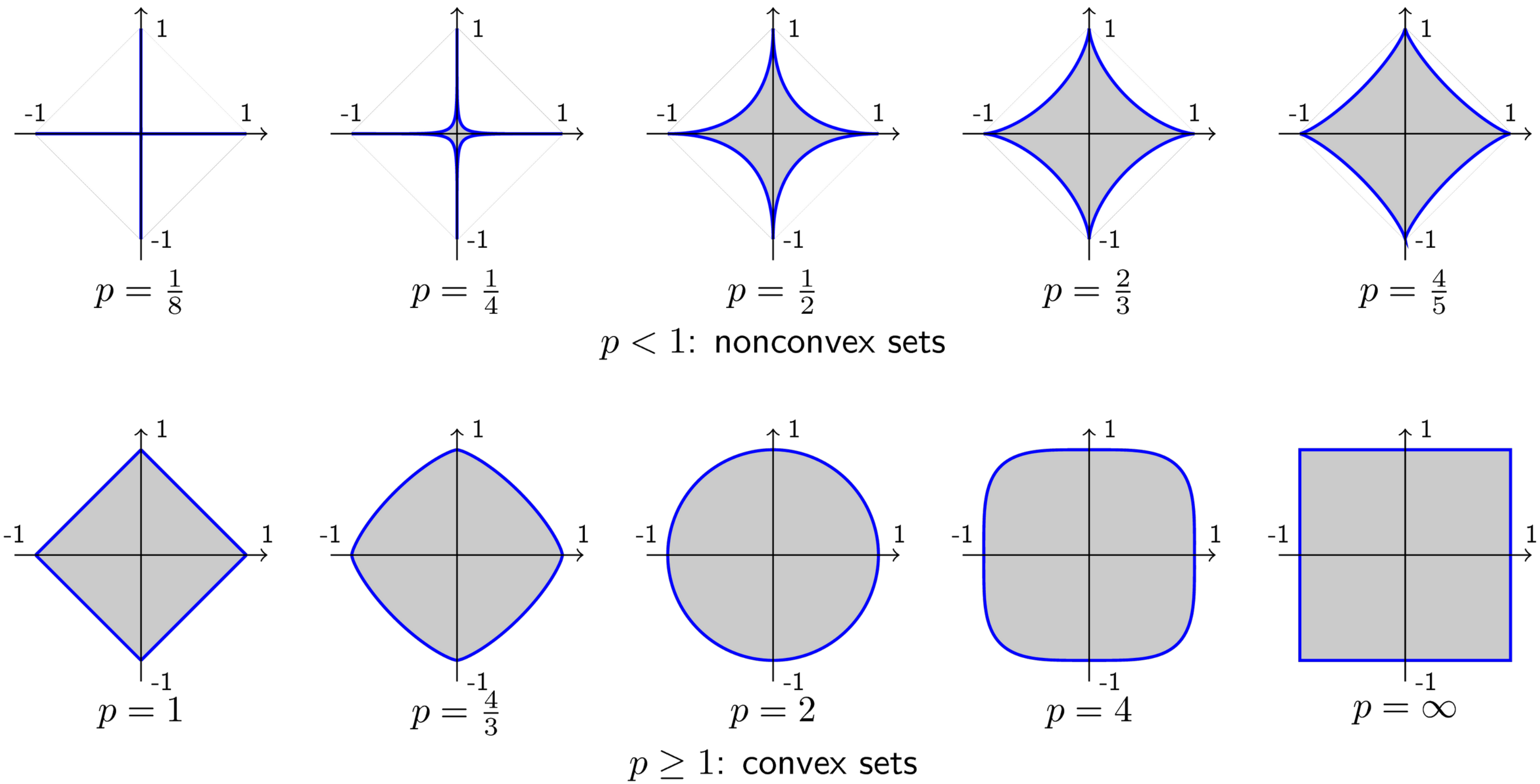


Minkowski Distance

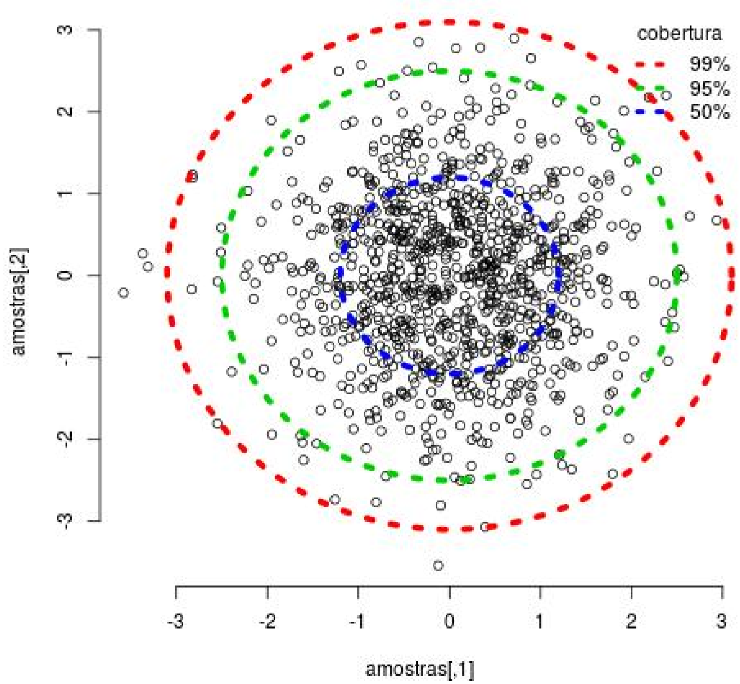


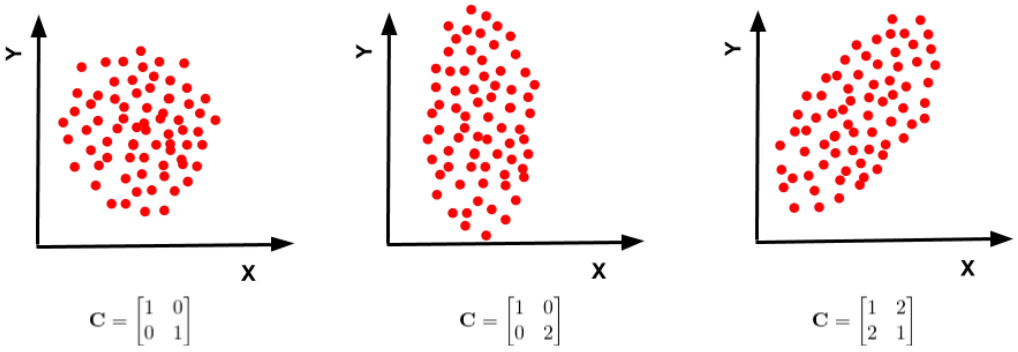
Minkowski Distance

$$\mathcal{C}_p = \{(x,y) \mid (|x|^p + |y|^p)^{1/p} \leq 1\}$$



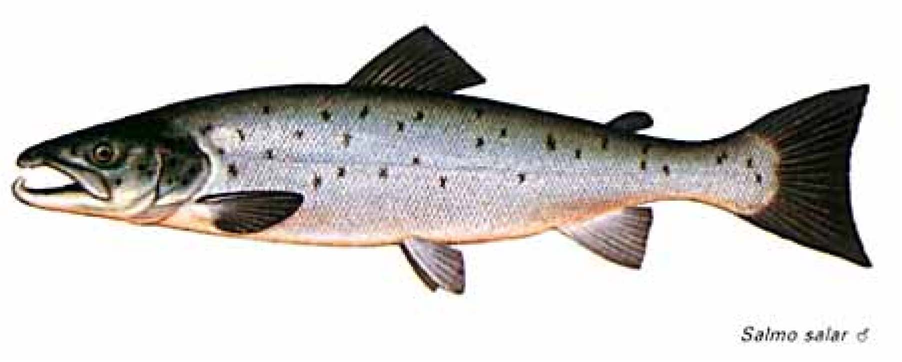
Normalized Euclidean



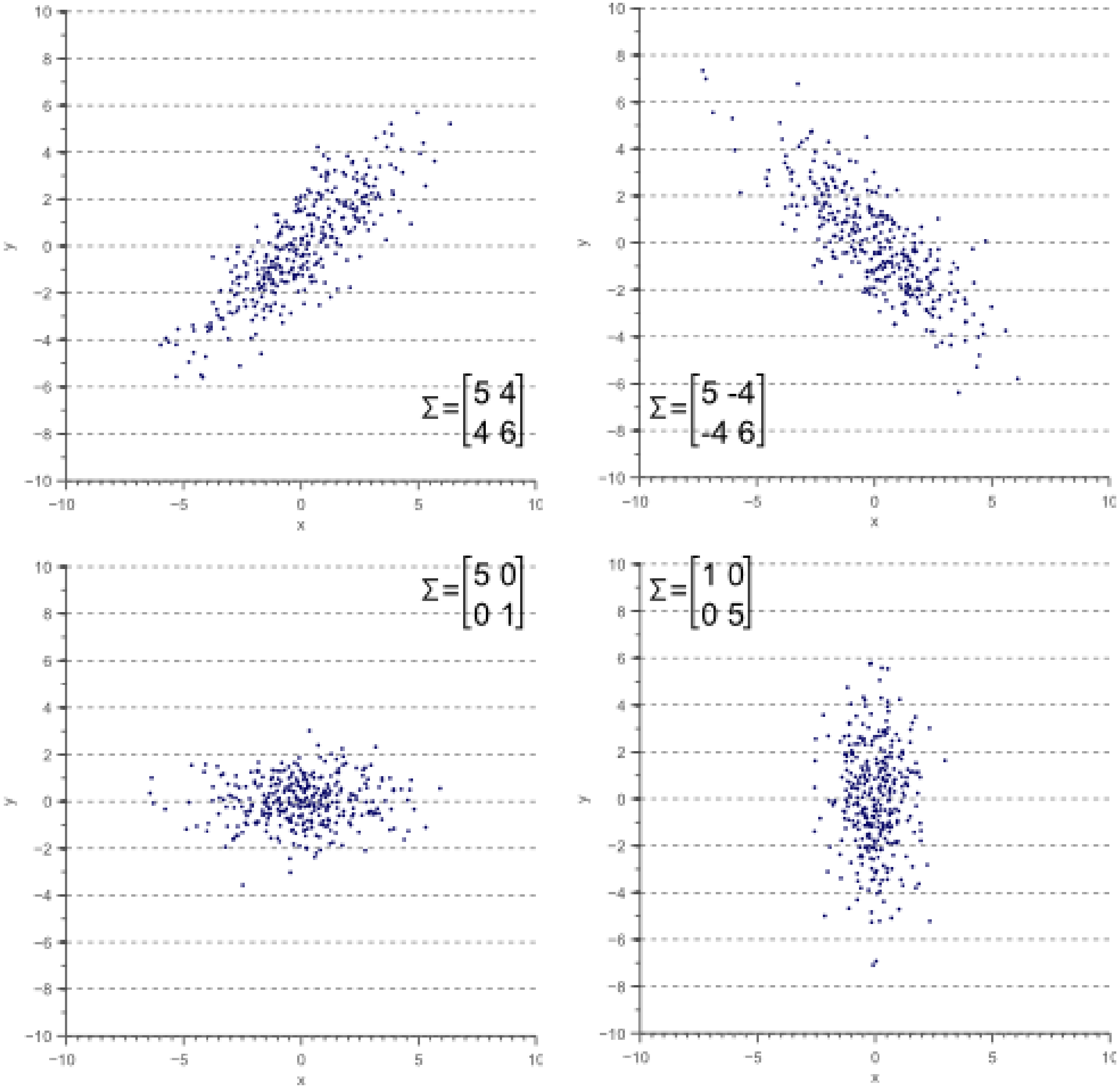


Normalized Euclidean

- Um pescador quer medir a dissimilaridade entre os salmões, para assim classificá-los em tipos e vender por um melhor preço os mais grandes
- Para cada salmão ele mede a comprimento e a largura
- O comprimento dos salmões é uma variável aleatória entre 50 e 100cm
- A largura dos salmões é uma variável aleatória entre 10 e 20cm
- Observa-se que a largura tem valores menores, portanto menos importância terá na distância euclidiana



Normalized Euclidean



Normalized Euclidean

- Por essa razão o pescador resolve incorporar a estatística dos dados, segundo sua variância
  - As variáveis com menos variância terão mais importância que as de maior variância
- Dessa forma pretende-se igualar a importância do comprimento e da largura na métrica de distância

$$d_e(\overrightarrow{x_1}, \overrightarrow{x_2}) = \sqrt{(x_{11} - x_{12})^2 + (x_{21} - x_{22})^2}$$

$$d_2(\overrightarrow{x_1}, \overrightarrow{x_2}) = \sqrt{\left(\frac{(x_{11} - x_{12})}{\sigma_1}\right)^2 + \left(\frac{(x_{21} - x_{22})}{\sigma_2}\right)^2}$$

$$d_e(\overrightarrow{x_1}, \overrightarrow{x_2}) = \sqrt{(\vec{x}_1 - \vec{x}_2)^T S^{-1} (\vec{x}_1 - \vec{x}_2)}$$

Mahalanobis Distance

- Euclidean distance

$$d_e(\overrightarrow{x_1}, \overrightarrow{x_2}) = \sqrt{(\vec{x}_1 - \vec{x}_2)^T(\vec{x}_1 - \vec{x}_2)}$$

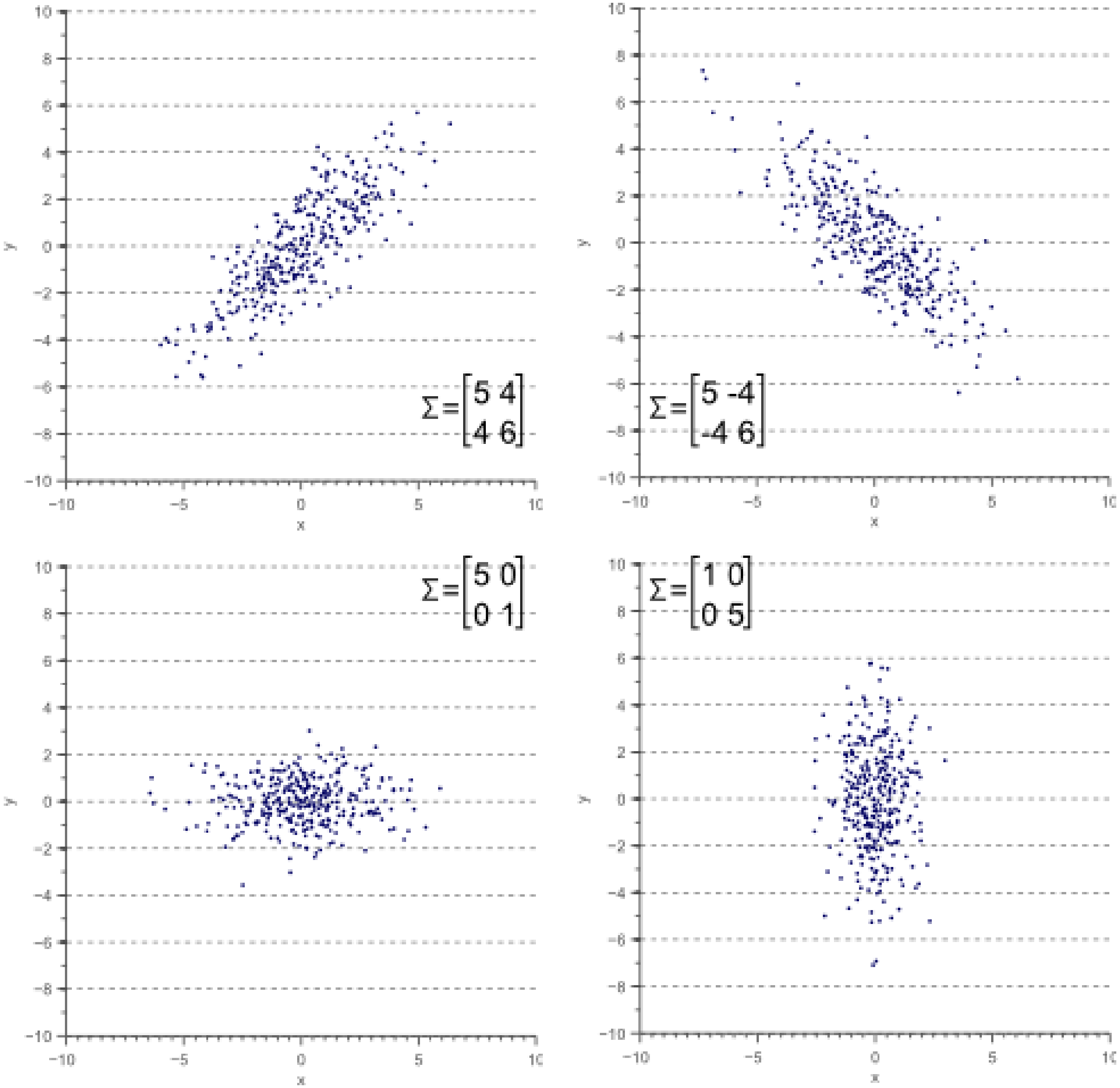
- Normalized Euclidean distance

$$d_e(\overrightarrow{x_1}, \overrightarrow{x_2}) = \sqrt{(\vec{x}_1 - \vec{x}_2)^T S^{-1}(\vec{x}_1 - \vec{x}_2)}$$

- Ambas as medidas têm um problema, que é o fato do comprimento e da largura dos salmões não são independentes.
- Ou seja, a largura depende, de certa forma, do comprimento, pois é mais provável que um salmão mais comprido seja também mais largo.
- Para incorporar essa dependência o pescador pode substituir a matriz diagonal (usada na distância euclidiana normalizada) pela matriz de covariância

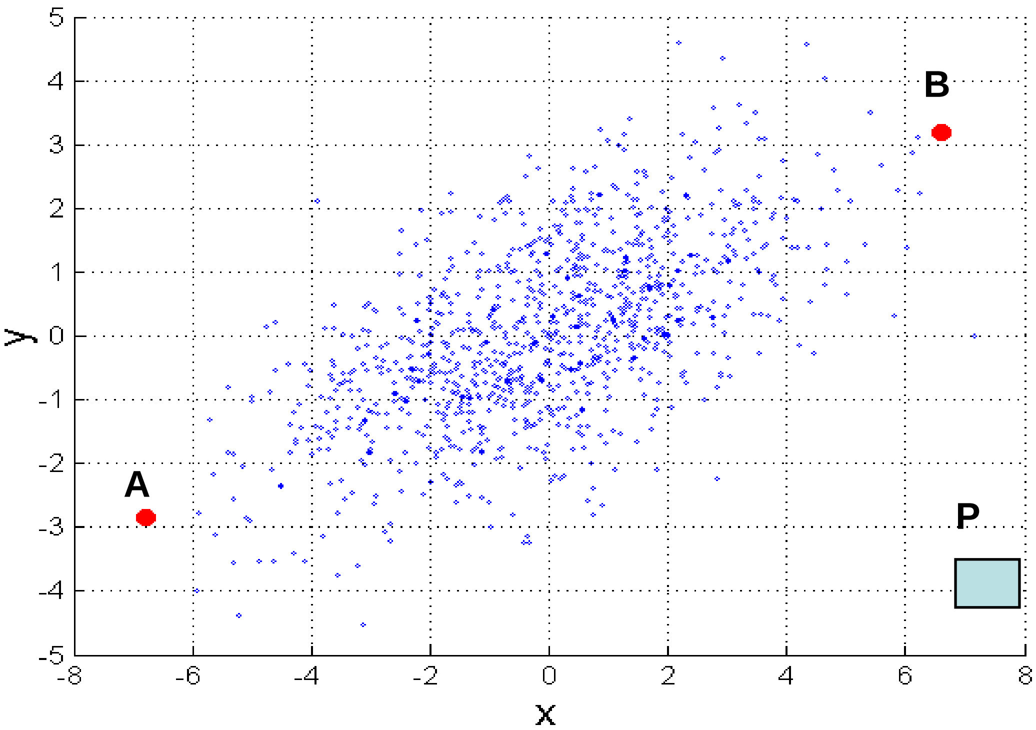
$$d_m(\overrightarrow{x_1}, \overrightarrow{x_2}) = \sqrt{(\vec{x}_1 - \vec{x}_2)^T \Sigma^{-1}(\vec{x}_1 - \vec{x}_2)}$$

Normalized Euclidean



Mahalanobis Distance

$$mahalanobis(p,q) = (p-q)\Sigma^{-1}(p-q)^T$$



Σ is the covariance matrix of the input data *X*

$$\Sigma_{j,k} = \frac{1}{n-1}\sum_{i=1}^{n}(X_{ij}-\overline{X}_j)(X_{ik}-\overline{X}_k)$$

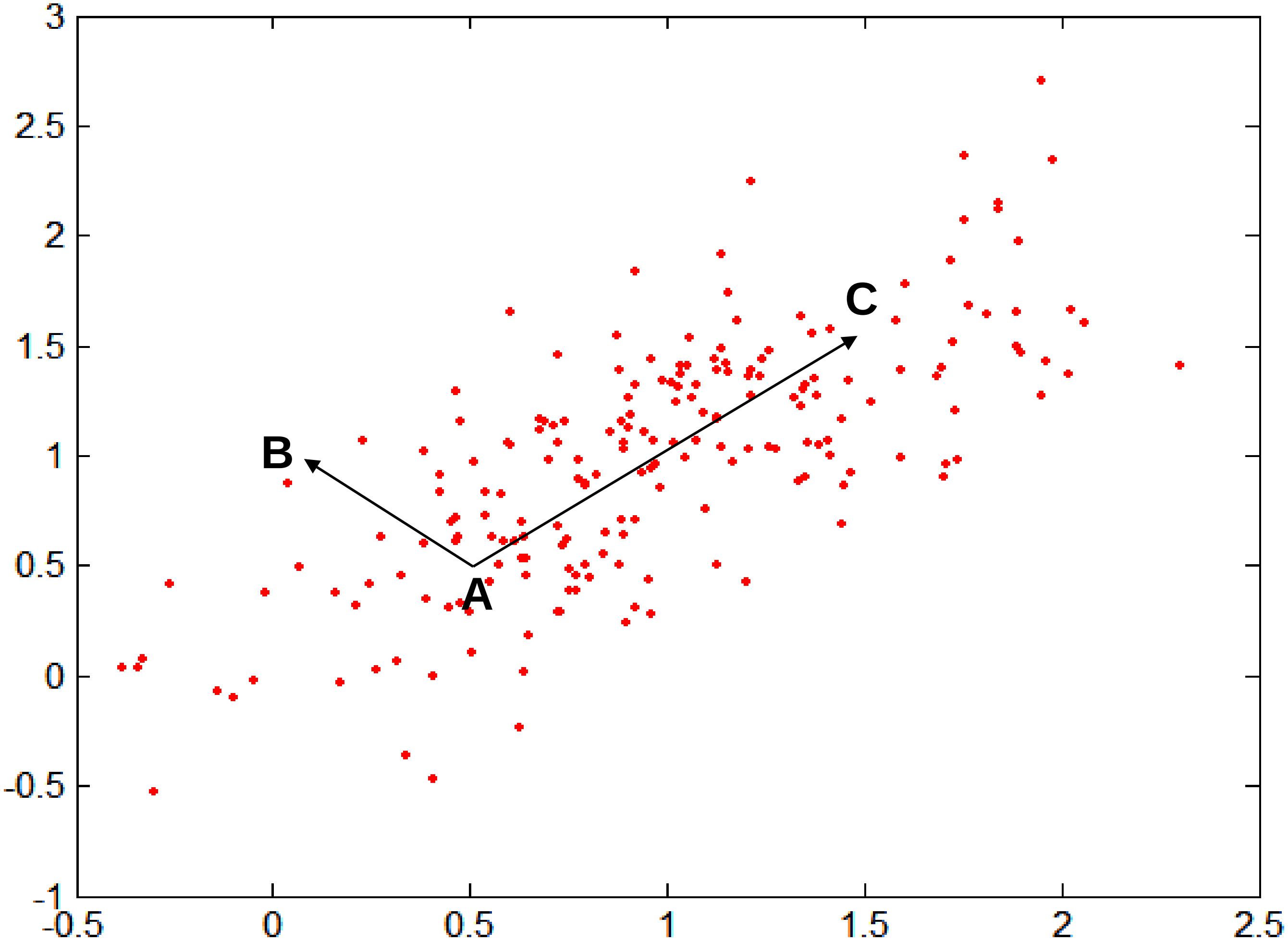
When the covariance matrix is identity Matrix, the mahalanobis distance is the same as the Euclidean distance.

Useful for detecting outliers.

Q: what is the shape of data when covariance matrix is identity?
Q: A is closer to P or B?

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)

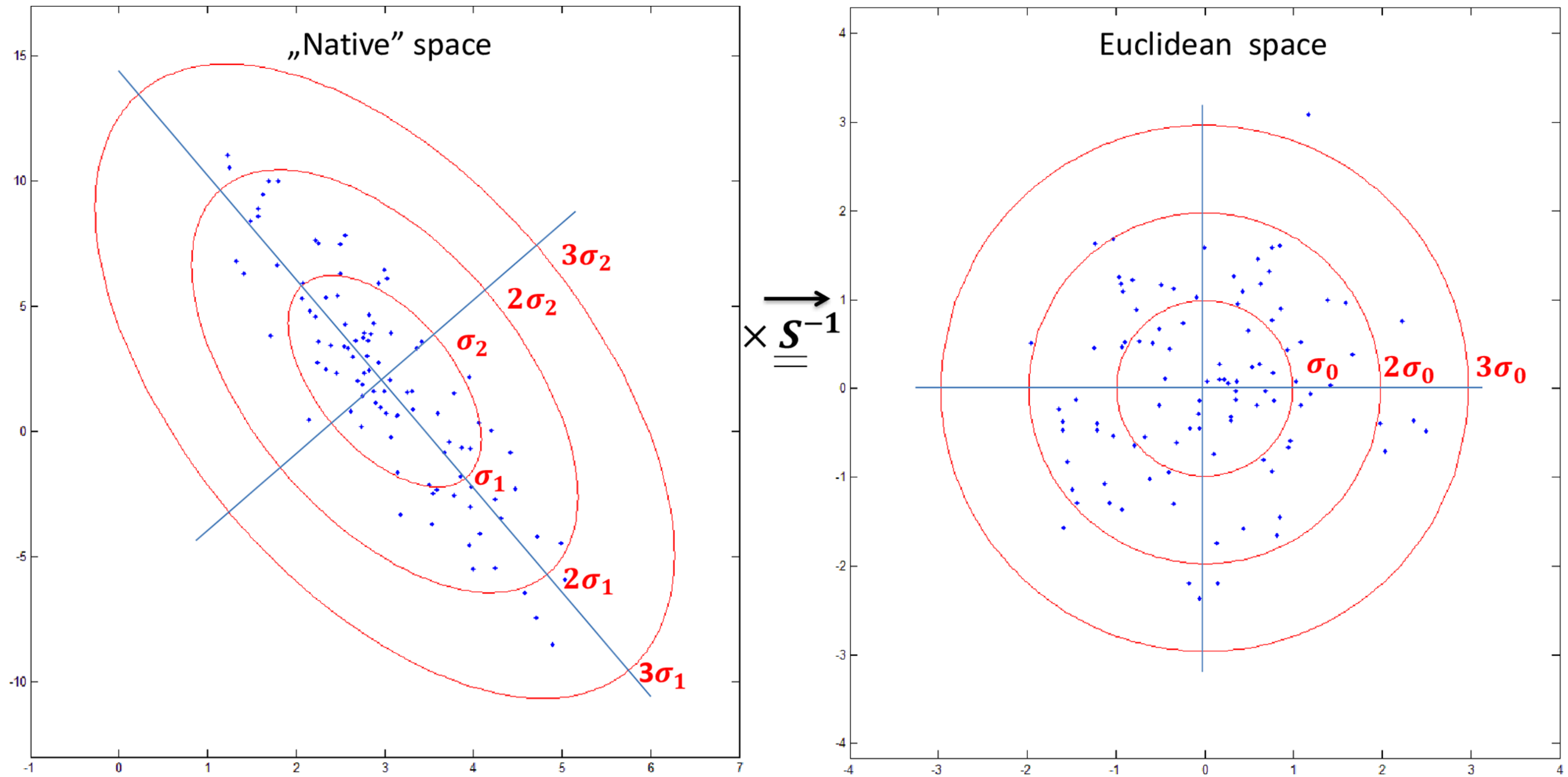
B: (0, 1)

C: (1.5, 1.5)

Mahal(A,B) = 5

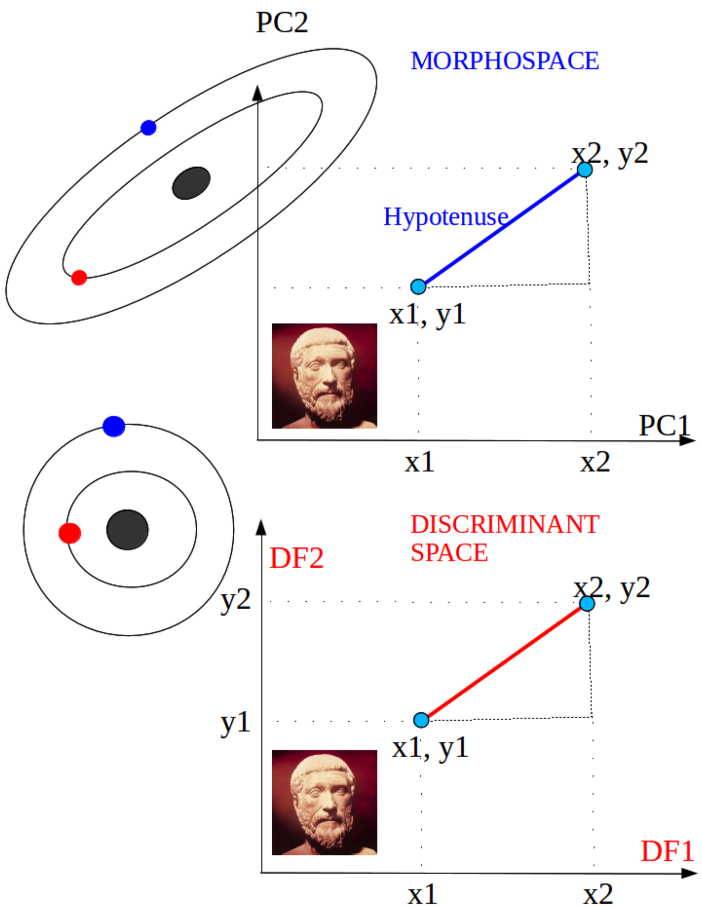
Mahal(A,C) = 4

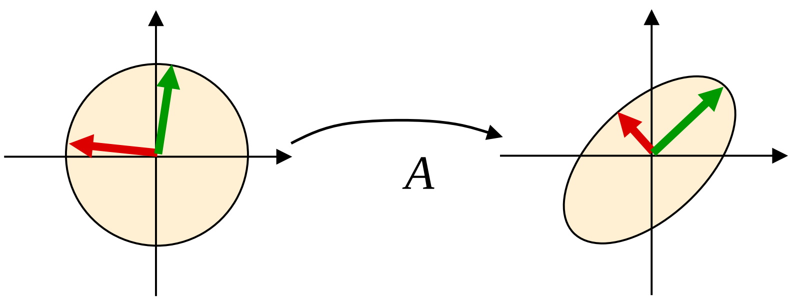
Mahalanobis Distance

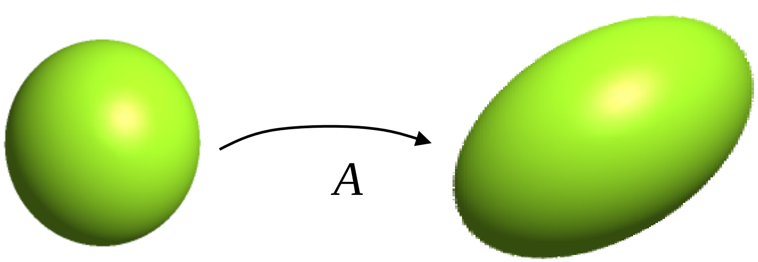


https://doi.org/10.1371/journal.pone.0222720.g001

Mahalanobis Distance







Common Properties of a Distance

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

1. *$d(p, q) \geq 0$* for all *p* and *q* and *$d(p, q) = 0$* only if *$p = q$*. (**Positive definiteness**)
2. *$d(p, q) = d(q, p)$* for all *p* and *q*. (**Symmetry**)
3. $d(p, r) \leq d(p, q) + d(q, r)$ for all points *p*, *q*, and *r*. (**Triangle Inequality**)

where *$d(p, q)$* is the distance (**dissimilarity**) between points (data objects), *p* and *q*.

- A distance that satisfies these properties is a metric, and a space is called a metric space

Common Properties of a Similarity

- Similarities, also have some well known properties.

  1. $s(p, q) = 1$ (or maximum similarity) only if $p = q$.

  2. $s(p, q) = s(q, p)$ for all p and q. (Symmetry)

  where $s(p, q)$ is the similarity between points (data objects), p and q.

Similarity Between Binary Vectors

- Common situation is that objects, *p* and *q*, have only binary attributes
- Compute similarities using the following quantities
  M_{01} = the number of attributes where p was 0 and q was 1
  M_{10} = the number of attributes where p was 1 and q was 0
  M_{00} = the number of attributes where p was 0 and q was 0
  M_{11} = the number of attributes where p was 1 and q was 1
- Simple Matching and Jaccard Distance/Coefficients
  SMC = number of matches / number of attributes
  $= (M_{11} + M_{00}) / (M_{01} + M_{10} + M_{11} + M_{00})$

  J = number of value-1-to-value-1 matches / number of not-both-zero attributes values
  $= (M_{11}) / (M_{01} + M_{10} + M_{11})$

SMC versus Jaccard: Example

p = 1 0 0 0 0 0 0 0 0 0

q = 0 0 0 0 0 0 1 0 0 1

$M_{01} = 2$ (the number of attributes where p was 0 and q was 1)
$M_{10} = 1$ (the number of attributes where p was 1 and q was 0)
$M_{00} = 7$ (the number of attributes where p was 0 and q was 0)
$M_{11} = 0$ (the number of attributes where p was 1 and q was 1)

SMC = $(M_{11} + M_{00})/(M_{01} + M_{10} + M_{11} + M_{00}) = (0+7) / (2+1+0+7) = 0.7$

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

Cosine Similarity

- If d_1 and d_2 are two document vectors, then

$$\cos(d_1, d_2) = (d_1 \bullet d_2) / ||d_1||\ ||d_2|| ,$$

where $\bullet$ indicates vector dot product and $|| d ||$ is the length of vector d.

- Example:

d_1 **= 3 2 0 5 0 0 0 2 0 0**

d_2 **= 1 0 0 0 0 0 0 1 0 2**

$d_1 \bullet d_2 = 3*1 + 2*0 + 0*0 + 5*0 + 0*0 + 0*0 + 0*0 + 2*1 + 0*0 + 0*2 = 5$

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

$||d_2|| = (1*1+0*0+0*0+0*0+0*0+0*0+0*0+1*1+0*0+2*2)^{0.5} = (6)^{0.5} = 2.245$

$\cos(d_1, d_2) = .3150$, distance=1-cos(d1,d2)