Similitud: ¿Cuánto se parecen dos elementos?

Disimilitud: ¿Cuánto se diferencian dos elementos?

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Distancia: \sim disimilitud, con una serie de condiciones:

► No negatividad:

$$d(a, b) \ge 0, \forall a, b \in \mathbb{R}$$

► Simetricidad:

$$d(a,b) = d(b,a), \forall a,b \in \mathbb{R}$$

► Identidad de los indiscernibles:

$$d(a,b) = 0 \Leftrightarrow a = b, \forall a, b \in \mathbb{R}$$

Desigualdad triangular:

$$d(a,b) \leq d(a,c) + d(c,b), \forall a,b,c \in \mathbb{R}$$

Variables aleatorias:

$$\boldsymbol{X} = (X_1, X_2, \dots, X_v)$$

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- ▶ Variable continua, X: valor numérico, $x \in \mathbb{R}$
- ▶ Variable categórica, X: valor discreto, $x \in \Omega_X$ con $\Omega_X = \{A, B, \dots, C\}$

Variables contínuas:

Una única variable

$$d(x_1, x_2) = |x_1 - x_2|$$

Variables contínuas:

Varias variables

$$d(\mathbf{x}_1, \mathbf{x}_2) = \sqrt{\sum_{j=1}^{v} (x_{1j} - x_{2j})^2} = \sqrt{(\mathbf{x}_1 - \mathbf{x}_2)^T (\mathbf{x}_1 - \mathbf{x}_2)}$$

Distancia euclidiana

Variables contínuas:

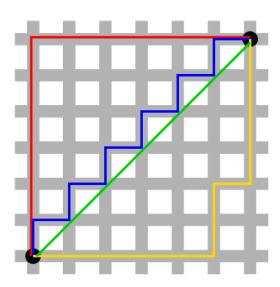
$$d_p(\mathbf{x}_1, \mathbf{x}_2) = ||\mathbf{x}_1 - \mathbf{x}_2||_p = \left(\sum_{j=1}^{v} |x_{1j} - x_{2j}|^p\right)^{(1/p)}$$

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▶ Manhattan (p = 1):

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• Euclidiana (p = 2):

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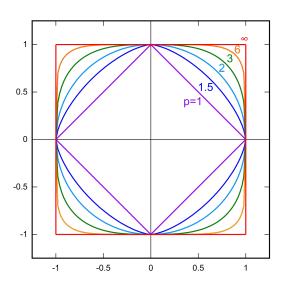
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▶ Máximo ($p = \infty$):

$$d(\mathbf{x}_1, \mathbf{x}_2) = \max_{j \in 1, \dots, v} |x_{1j} - x_{2j}| = ||\mathbf{x}_1 - \mathbf{x}_2||_{\infty}$$



Variables contínuas:

$$d(\mathbf{x}_1, \mathbf{x}_2) = \sqrt{(\mathbf{x}_1 - \mathbf{x}_2)^T \Sigma^{-1} (\mathbf{x}_1 - \mathbf{x}_2)}$$

Distancia Mahalanobis

$$\Sigma = \begin{bmatrix} \mathrm{E}[(X_1 - \mu_1)(X_1 - \mu_1)] & \mathrm{E}[(X_1 - \mu_1)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_1 - \mu_1)(X_n - \mu_n)] \\ \\ \mathrm{E}[(X_2 - \mu_2)(X_1 - \mu_1)] & \mathrm{E}[(X_2 - \mu_2)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_2 - \mu_2)(X_n - \mu_n)] \\ \\ \vdots & \vdots & \ddots & \vdots \\ \\ \mathrm{E}[(X_n - \mu_n)(X_1 - \mu_1)] & \mathrm{E}[(X_n - \mu_n)(X_2 - \mu_2)] & \cdots & \mathrm{E}[(X_n - \mu_n)(X_n - \mu_n)] \end{bmatrix}$$

$$\boldsymbol{\Sigma} = \mathsf{E}\left[(\boldsymbol{\textit{X}} - \mathsf{E}[\boldsymbol{\textit{X}}])(\boldsymbol{\textit{X}} - \mathsf{E}[\boldsymbol{\textit{X}}])^{\mathrm{T}} \right]$$

$$\sigma^2 = \text{var}(X) = \text{E}\left[(X - \text{E}[X])^2\right] = \text{E}\left[(X - \text{E}[X])(X - \text{E}[X])\right]$$

$$cov(X,Y) = E[(X - E[X])(Y - E[Y])]$$

Variables contínuas:

$$d(\mathbf{x}_1, \mathbf{x}_2) = \sqrt{(\mathbf{x}_1 - \mathbf{x}_2)^T \Sigma^{-1} (\mathbf{x}_1 - \mathbf{x}_2)}$$

Distancia Mahalanobis

$$d(\mathbf{x}_1,\mathbf{x}_2) = \sqrt{\sum_{j=1}^{\nu} \left(\frac{x_{1j} - x_{2j}}{\sigma_j}\right)^2} = \sqrt{(\mathbf{x}_1 - \mathbf{x}_2)^T S^{-1}(\mathbf{x}_1 - \mathbf{x}_2)}$$

Distancia euclidiana estandarizada

Variables contínuas:

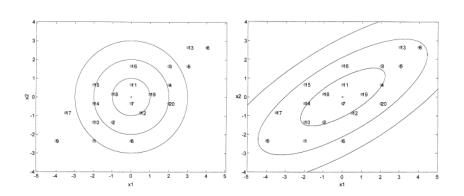
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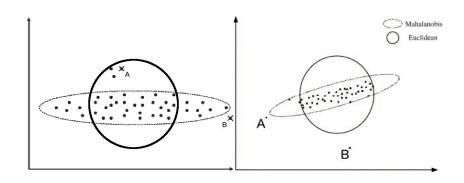
Distancia Mahalanobis

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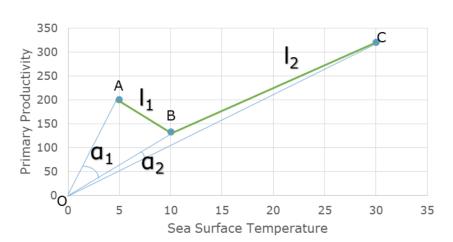
Variable continuas:

$$s(\mathbf{x}_1, \mathbf{x}_2) = \frac{\mathbf{x}_1, \mathbf{x}_2}{||\mathbf{x}_1|| \cdot ||\mathbf{x}_2||} = \frac{\sum_{j=1}^{\nu} x_{1j} \cdot x_{2j}}{\sqrt{\sum_{j=1}^{\nu} x_{1j}^2} \sqrt{\sum_{j=1}^{\nu} x_{2j}^2}}$$

Similitud coseno

Variable continuas:

Similitud coseno



Variable binarias:

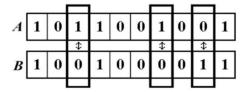
$$d(\mathbf{x}_1, \mathbf{x}_2) = |x_{1j} = x_{2j}|_{j \in \{1, \dots, v\}}$$

Distancia de Hamming

$$s(\mathbf{x}_1, \mathbf{x}_2) = \frac{|x_{1j} = 1 \land x_{2j} = 1|_{j \in \{1, \dots, \nu\}}}{|x_{1j} = 1 \lor x_{2j} = 1|_{j \in \{1, \dots, \nu\}}}$$

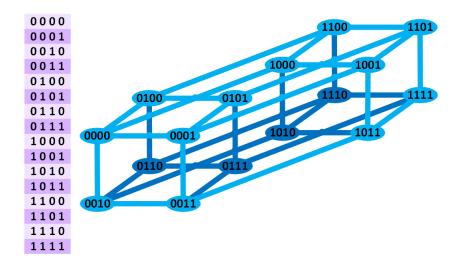
Similitud de Jaccard

Variable binarias:

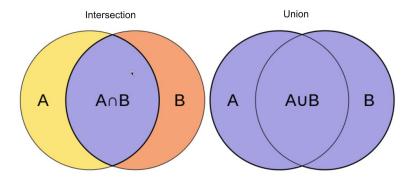


Distancia de Hamming

Variable binarias:



Variable binarias:



Similitud de Jaccard

Variable categórica:

$$d_j(x_{1j}, x_{2j}) = \begin{cases} 1, & \text{si } x_{1j} \neq x_{2j} \\ 0, & \text{si } x_{1j} = x_{2j} \end{cases}$$

Combinar medidas por variable:

$$d(\mathbf{x}_1, \mathbf{x}_2) = \sum_{j=1}^{v} d_j(x_{1j}, x_{2j})$$

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Propuesta de Hastie et al. (2008):

$$w_j = 1/\hat{d}_j$$
, con $\hat{d}_j = \frac{1}{n^2} \sum_{i=1}^n \sum_{i'=1}^n d_j(x_{ij}, x_{i'j})$

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Si $d_j(x_{ij},x_{i'j})=(x_{ij}-x_{i'j})^2$ para todo j, entonces: $w_j=1/(2\mathsf{var}_j)$

Transformar matriz de ejemplos $D(n \times v)$ en...

matriz de distancias, $M(n \times n)$, tal que:

$$M_{ij}=d(\mathbf{x}_i,\mathbf{x}_j)$$

y ésta, a su vez, en una matriz de similitudes, $S(n \times n)$:

$$S_{ij} = \exp(-M_{ij}^2/c)$$