Distance and dissimilarities

Contents


```r
knitr::opts_chunk$set(echo = TRUE)
#install.packages("dplyr")
#install.packages("stargazer")
#install.packages("ade4")
#install.packages("magrittr")
#install.packages("cluster")
```

Definition of a distance

- A distance function or a metric on $\mathbb{R}^n$, $n \geq 1$, is a function $d : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$.
- A distance function must satisfy some required properties or axioms.
- There are three main axioms.
- A1. $d(\mathbf{x}, \mathbf{y}) = 0 \iff \mathbf{x} = \mathbf{y}$ (identity of indiscernibles);
- A2. $d(\mathbf{x}, \mathbf{y}) = d(\mathbf{y}, \mathbf{x})$ (symmetry);
- A3. $d(\mathbf{x}, \mathbf{z}) \leq d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z})$ (triangle inequality), where $\mathbf{x} = (x_1, \cdots, x_n)$, $\mathbf{y} = (y_1, \cdots, y_n)$ and $\mathbf{z} = (z_1, \cdots, z_n)$ are all vectors of $\mathbb{R}^n$.
- We should use the term *dissimilarity* rather than *distance* when not all the three axioms A1-A3 are valid.
- Most of the time, we shall use, with some abuse of vocabulary, the term distance.

Exercice 1

- Prove that the three axioms A1-A3 imply the non-negativity condition:

$$d(\mathbf{x}, \mathbf{y}) \geq 0.$$

Euclidean distance

- It is defined by:

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

- A1-A2 are obvious.
- The proof of A3 is provided below.

Exercice 2

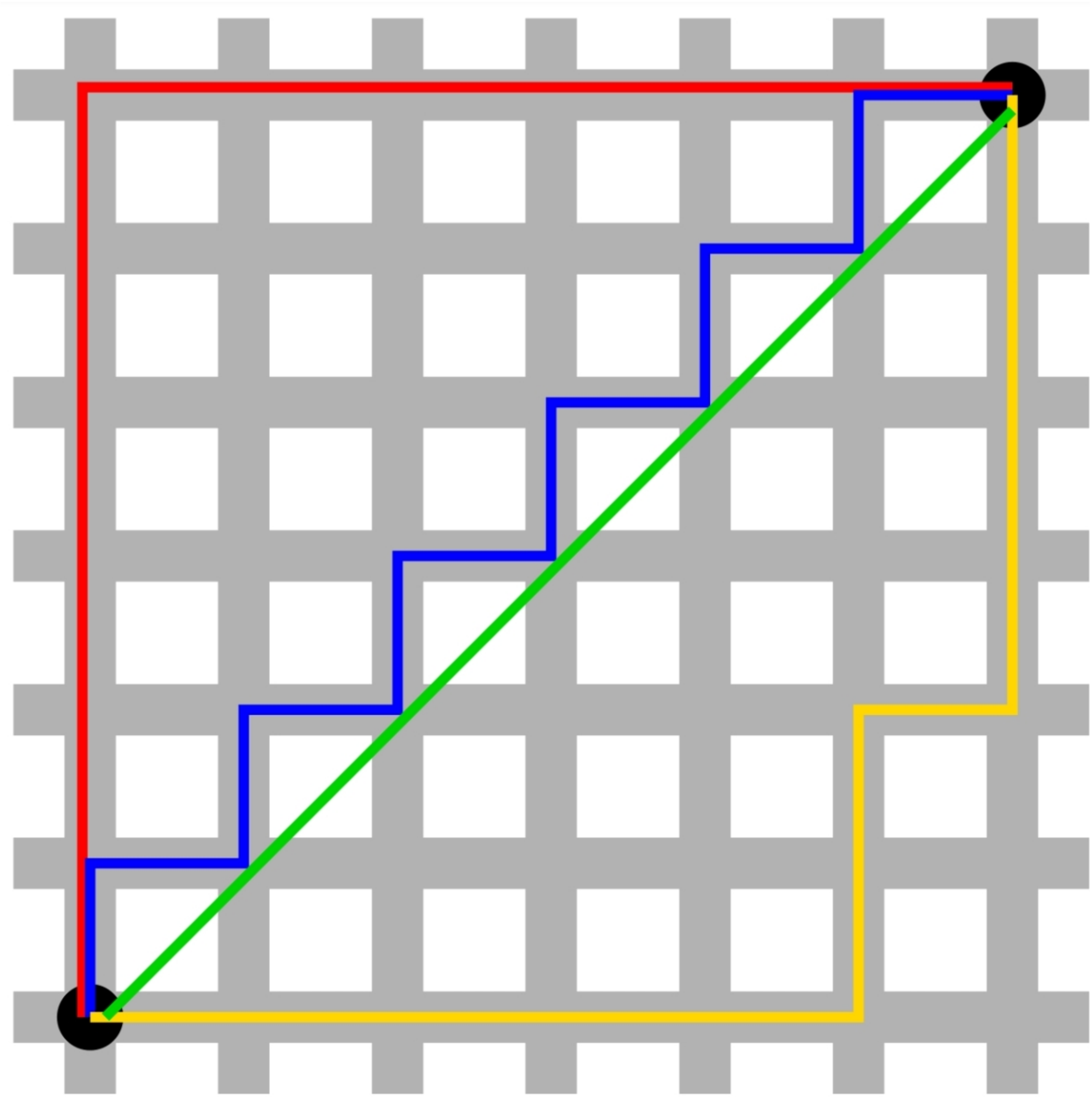
- Is the squared Euclidian distance a true distance?

Manhattan distance

- The Manhattan distance also called taxi-cab metric or city-block metric is defined by:

$$d(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{n} |x_i - y_i|.$$

- A1-A2 hold.
- A3 also holds using the fact that $|a + b| \leq |a| + |b|$ for any reals a, b.
- There exists also a weighted version of the Manhattan distance called the Canberra distance.



```r
x = c(0, 0)
y = c(6,6)
dist(rbind(x, y), method = "euclidian")
```

```
##          x
## y 8.485281
```

```r
6*sqrt(2)
```

```
## [1] 8.485281
```

```r
dist(rbind(x, y), method = "manhattan")
```

```
##    x
## y 12
```

Canberra distance

- It is defined by:

$$d(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{n} \frac{|x_i - y_i|}{|x_i| + |y_i|}.$$

- Note that the term $|x_i - y_i|/(|x_i| + |y_i|)$ is not properly defined as:when $x_i = y_i = 0$.
- By convention we set the ratio to be zero in that case.
- The Canberra distance is specially sensitive to small changes near zero.

```r
x = c(0, 0)
y = c(6,6)
dist(rbind(x, y), method = "canberra")
```

```
##   x
## y 2
```

```r
6/6+6/6
```

```
## [1] 2
```

Exercice 3

- Prove that the Canberra distance is a true distance.

Minkowski distance

- Both the Euclidian and the Manattan distances are special cases of the Minkowski distance which is defined, for $p \geq 1$, by:

$$d(\mathbf{x}, \mathbf{y}) = \left[\sum_{i=1} |x_i - y_i|^p\right]^{1/p}.$$

- For $p = 1$, we get the Manhattan distance.
- For $p = 2$, we get the Euclidian distance.
- Let us also define:

$$\|\mathbf{x}\|_p \equiv \left[\sum_{i=1}^{n} |x_i|^p\right]^{1/p},$$

  where $\|\cdot\|_p$ is known as the p-norm or Minkowski norm.
- Note that the Minkowski distance and norm are related by:

$$d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_p.$$

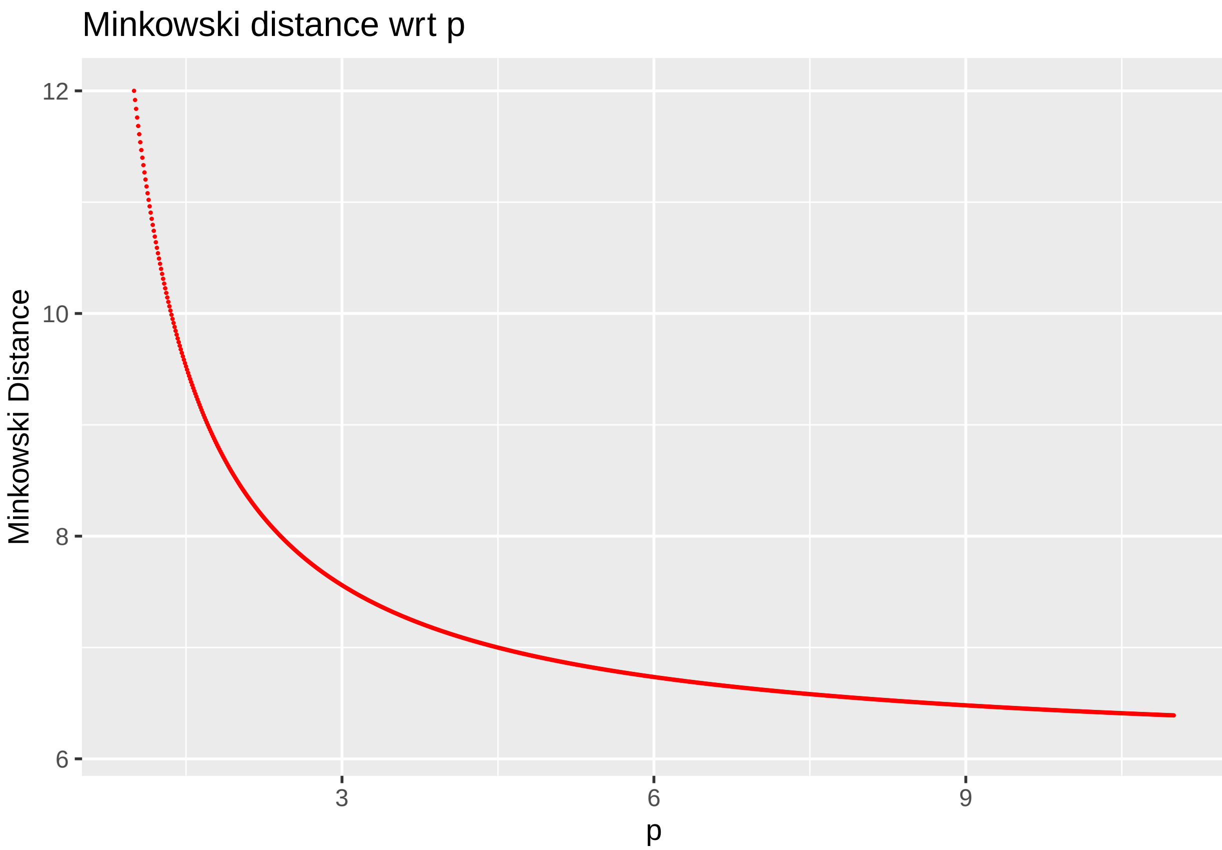
- Conversely, we have:

$$\|\mathbf{x}\|_p = d(\mathbf{x}, \mathbf{0}),$$

where $\mathbf{0}$ is the null-vetor of $\mathbb{R}^n$.

```
library("ggplot2")
x = c(0, 0)
y = c(6,6)
MinkowDist=c()
for (p in seq(1,30,.01))
{
MinkowDist=c(MinkowDist,dist(rbind(x, y), method = "minkowski", p = p))
}
ggplot(data =data.frame(x = seq(1,30,.01), y=MinkowDist ) , mapping = aes(x = x, y = y))+geom_point(siz
```

```
## Warning: Removed 1900 rows containing missing values (geom_point).
```



Chebyshev distance

- At the limit, we get the Chebyshev distance which is defined by:

$$d(\mathbf{x},\mathbf{y}) = \max_{i=1,\cdots,n}(|x_i - y_i|) = \lim_{p\to\infty}\left[\sum_{i=1}|x_i - y_i|^p\right]^{1/p}.$$

- The corresponding norm is:

$$\|\mathbf{x}|_\infty = \max_{i=1,\cdots,n}(|x_i|).$$

Minkowski inequality

- The proof of the triangular inequality A3 is based on the Minkowski inequality:
- For any nonnegative real numbers $a_1, \cdots, a_n$; $b_1, \cdots, b_n$, and for any $p \geq 1$, we have:

$$\left[\sum_{i=1}^{n}(a_i + b_i)^p\right]^{1/p} \leq \left[\sum_{i=1}^{n} a_i^p\right]^{1/p} + \left[\sum_{i=1}^{n} b_i^p\right]^{1/p}.$$

- To prove that the Minkowski distance satisfies A3, notice that

$$\sum_{i=1}^{n} |x_i - z_i|^p = \sum_{i=1}^{n} |(x_i - y_i) + (y_i - z_i)|^p.$$

- Since for any reals x, y, we have: $|x + y| \leq |x| + |y|$, and using the fact that x^p is increasing in $x \geq 0$, we obtain:

$$\sum_{i=1}^{n} |x_i - z_i|^p \leq \sum_{i=1}^{n}(|x_i - y_i| + |y_i - z_i|)^p.$$

- Applying the Minkowski inequality with $a_i = |x_i - y_i|$ and $b_i = |y_i - z_i|$, $i = 1, \cdots, n$, we get:

$$\sum_{i=1}^{n} |x_i - z_i|^p \leq \left(\sum_{i=1}^{n} |x_i - y_i|^p\right)^{1/p} + \left(\sum_{i=1}^{n} |y_i - z_i|^p\right)^{1/p}.$$

Hölder inequality

- The proof of the Minkowski inequality itself requires the Hölder inequality:
- For any nonnegative real numbers $a_1, \cdots, a_n$; $b_1, \cdots, b_n$, and any $p, q > 1$ with $1/p + 1/q = 1$, we have:

$$\sum_{i=1}^{n} a_i b_i \leq \left[\sum_{i=1}^{n} a_i^p\right]^{1/p} \left[\sum_{i=1}^{n} b_i^q\right]^{1/q}$$

- The proof of the Hölder inequality relies on the Young inequality:
- For any $a, b > 0$, we have

$$ab \leq \frac{a^p}{p} + \frac{b^q}{q},$$

  with equality occuring iff: $a^p = b^q$.
- To prove the Young inequality, one can use the (strict) convexity of the exponential function.
- For any reals x, y, we have:

$$e^{\frac{x}{p} + \frac{y}{q}} \leq \frac{e^x}{p} + \frac{e^y}{q}.$$

- We then set: $x = p \ln a$ and $y = q \ln b$ to get the Young inequality.
- A good reference on inequalities is: Z. Cvetkovski, Inequalities: theorems, techniques and selected problems, 2012, Springer Science & Business Media. # Cauchy-Schwartz inequality
- Note that the triangular inequality for the Minkowski distance implies:

$$\sum_{i=1}^{n} |x_i| \leq \left[\sum_{i=1}^{n} |x_i|^p\right]^{1/p}.$$

- Note that for $p = 2$, we have $q = 2$. The Hölder inequality implies for that special case

$$\sum_{i=1}^{n} |x_i y_i| \leq \sqrt{\sum_{i=1}^{n} x_i^2} \sqrt{\sum_{i=1}^{n} y_i^2}.$$

- Since the LHS od thes above inequality is greater then $|\sum_{i=1}^{n} x_i y_i|$, we get the Cauchy-Schwartz inequality

$$|\sum_{i=1}^{n} x_i y_i| \leq \sqrt{\sum_{i=1}^{n} x_i^2} \sqrt{\sum_{i=1}^{n} y_i^2}.$$

* Using the dot product notation called also scalar product noation: $\mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^{n} x_i y_i$, and the norm notation $\|\cdot\|_2\|$, the Cauchy-Schwart inequality is:

$$|\mathbf{x} \cdot \mathbf{y}| \leq \|\mathbf{x}\|_2 \|\mathbf{y}\|_2.$$

Pearson correlation distance

- The Pearson correlation coefficient is a similarity measure on $\mathbb{R}^n$ defined by:

$$\rho(\mathbf{x}, \mathbf{y}) = \frac{\sum_{i=1}^{n} (x_i - \bar{\mathbf{x}})(y_i - \bar{\mathbf{y}})}{\sqrt{\sum_{i=1}^{n} (x_i - \bar{\mathbf{x}})^2 \sum_{i=1}^{n} (y_i - \bar{\mathbf{y}})^2}},$$

where $\bar{\mathbf{x}}$ is the mean of the vector $\mathbf{x}$ defined by:

$$\bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^{n} x_i,$$

- Note that the Pearson correlation coefficient satisfies P2 and is invariant to any positive linear transformation, i.e.:

$$\rho(\alpha \mathbf{x}, \mathbf{y}) = \rho(\mathbf{x}, \mathbf{y}),$$

for any $\alpha > 0$.

- The Pearson distance (or correlation distance) is defined by:

$$d(\mathbf{x}, \mathbf{y}) = 1 - \rho(\mathbf{x}, \mathbf{y}).$$

- Note that the Pearson distance does not satisfy A1 since $d(\mathbf{x}, \mathbf{x}) = 0$ for any non-zero vector $\mathbf{x}$. It neither satisfies the triangle inequality. However, the symmetry property is fullfilled.

Cosine correlation distance

- The cosine of the angle θ between two vectors $\mathbf{x}$ and $\mathbf{y}$ is a measure of similarity given by:

$$\cos(\theta) = \frac{\mathbf{x} \cdot \mathbf{y}}{\|\mathbf{x}\|_2 \|\mathbf{y}\|_2} = \frac{\sum_{i=1}^{n} x_i y_i}{\sqrt{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i^2}}.$$

- Note that the cosine of the angle between the two centred vectors $\mathbf{x} - \bar{\mathbf{x}}\mathbf{1}$ and $\mathbf{y} - \bar{\mathbf{y}}\mathbf{1}$ coincides with the Pearson correlation coefficient of $\mathbf{x}$ and $\mathbf{y}$, where $\mathbf{1}$ is a vector of units of $\mathbb{R}^n$.
- The cosine correlation distance is defined by:

$$d(\mathbf{x}, \mathbf{y}) = 1 - \cos(\theta).$$

- It shares similar properties than the Pearson correlation distance. Likewise, Axioms A1 and A3 are not satisfied.

Spearman correlation distance

- To calculate the Spearman's rank-order correlation, we need to map seperately each of the vectors to ranked data values:
$$\mathbf{x} \to \text{rank}(\mathbf{x}) = (x_1^r, \cdots, x_n^r).$$
- Here, x_i^r is the rank of x_i among the set of values of $\mathbf{x}$.
- We illustrate this transformation with a simple example:
- If $\mathbf{x} = (3, 1, 4, 15, 92)$, then the rank-order vector is $\text{rank}(\mathbf{x}) = (2, 1, 3, 4, 5)$.

```
x=c(3, 1, 4, 15, 92)
rank(x)
```

```
## [1] 2 1 3 4 5
```

- The Spearman's rank correlation of two numerical variables $\mathbf{x}$ and $\mathbf{y}$ is simply the Pearson correlation of the two correspnding rank-order variables $\text{rank}(\mathbf{x})$ and $\text{rank}(\mathbf{y})$, i.e. $\rho(\text{rank}(\mathbf{x}), \text{rank}(\mathbf{y}))$. This measure is is useful because it is more robust against outliers than the Pearson correlation.
- If all the n ranks are distinct, it can be computed using the following formula:
$$\rho(\text{rank}(\mathbf{x}), \text{rank}(\mathbf{y})) = 1 - \frac{6 \sum_{i=1}^n d_i^2}{n(n^2 - 1)},$$
where $d_i = x_i^r - y_i^r$, $i = 1, \cdots, n$.
- The spearman distance is then defined by:
$$d(\mathbf{x}, \mathbf{y}) = 1 - \rho(\text{rank}(\mathbf{x}), \text{rank}(\mathbf{y})).$$
- It can be shown that easaly that it is not a proper distance.
- If all the n ranks are distinct, we get:
$$d(\mathbf{x}, \mathbf{y}) = \frac{6 \sum_{i=1}^n d_i^2}{n(n^2 - 1)}.$$

```
x=c(3, 1, 4, 15, 92)
rank(x)
```

```
## [1] 2 1 3 4 5
```

```
y=c(30,2 , 9, 20, 48)
rank(y)
```

```
## [1] 4 1 2 3 5
```

```
d=rank(x)-rank(y)
d
```

```
## [1] -2  0  1  1  0
```

```
cor(rank(x),rank(y))
```

```
## [1] 0.7
```

```
1-6*sum(d^2)/(5*(5^2-1))
```

```
## [1] 0.7
```

Kendall tau distance

- The Kendall rank correlation coefficient is calculated from the number of correspondances between the rankings of $\mathbf{x}$ and the rankings of $\mathbf{y}$.

- The number of pairs of observations among n observations or values is:

$$\binom{n}{2} = \frac{n(n-1)}{2}.$$

- The pairs of observations (x_i, x_j) and (y_i, y_j) are said to be *concordant* if:

$$\text{sign}(x_j - x_i) = \text{sign}(y_j - y_i),$$

and to be *discordant* if:

$$\text{sign}(x_j - x_i) = -\text{sign}(y_j - y_i),$$

where sign$(\cdot)$ returns 1 for positive numbers and -1 negative numbers and 0 otherwise.
- If $x_i = x_j$ or $y_i = y_j$ (or both), there is a tie.
- The Kendall τ coefficient is defined by (neglecting ties):

$$\tau = \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j=1}^{n} \text{sign}(x_j - x_i)\text{sign}(y_j - y_i).$$

- Let n_c (resp. n_d) be the number of concordant (resp. discordant) pairs, we have

$$\tau = \frac{2(n_c - n_d)}{n(n-1)}.$$

- The Kendall tau distance is then:

$$d(\mathbf{x}, \mathbf{y}) = 1 - \tau.$$

- Remark: the triangular inequality may fail in cases where there are ties.

```
x=c(3, 1, 4, 15, 92)
y=c(30,2 , 9, 20, 48)
tau=0
for (i in 1:5)
{
tau=tau+sign(x -x[i])%*%sign(y -y[i])
}
tau=tau/(5*4)
tau
```

```
##      [,1]
## [1,]  0.6
```

```
cor(x,y, method="kendall")
```

```
## [1] 0.6
```

Variables standardization

- Variables are often standardized before measuring dissimilarities.
- Standardization converts the original variables into uniteless variables.
- A well known method is the z-score transformation:

$$\mathbf{x} \to (\frac{x_1 - \bar{\mathbf{x}}}{s_{\mathbf{x}}}, \cdots, \frac{x_n - \bar{\mathbf{x}}}{s_{\mathbf{x}}}),$$

where $s_{\mathbf{x}}$ is the sample standard deviation given by:

$$s_{\mathbf{x}} = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{\mathbf{x}})^2.$$

- The transformed variable will have a mean of 0 and a variance of 1.
- The result obtained with Pearson correlation measures and standardized Euclidean distances are comparable.
- For other methods, see: Milligan, G. W., & Cooper, M. C. (1988). A study of standardization of variables in cluster analysis. *Journal of classification*, *5*(2), 181-204.

```
x=c(3, 1, 4, 15, 92)
y=c(30,2 , 9, 20, 48)
(x-mean(x))/sd(x)
```

```
## [1] -0.5134116 -0.5647527 -0.4877410 -0.2053646  1.7712699
```

```
scale(x)
```

```
##            [,1]
## [1,] -0.5134116
## [2,] -0.5647527
## [3,] -0.4877410
## [4,] -0.2053646
## [5,]  1.7712699
## attr(,"scaled:center")
## [1] 23
## attr(,"scaled:scale")
## [1] 38.9551
```

```
(y-mean(y))/sd(y)
```

```
## [1]  0.45263128 -1.09293895 -0.70654639 -0.09935809  1.44621214
```

```
scale(y)
```

```
##             [,1]
## [1,]  0.45263128
## [2,] -1.09293895
## [3,] -0.70654639
## [4,] -0.09935809
## [5,]  1.44621214
## attr(,"scaled:center")
## [1] 21.8
## attr(,"scaled:scale")
## [1] 18.11629
```

Similarity measures for binary data

- A common simple situation occurs when all information is of the presence/absence of 2-level qualitative characters.
- We assume there are n characters.
- *The presence of the character is coded by 1 and the absence by 0.
- We have have at our disposal two vectors.
- $\mathbf{x}$ is observed for a first individual (or object).
- $\mathbf{y}$ is observed for a second individual.
- We can then calculate the following four statistics:

$a = \mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^{n} x_i y_i$.

$b = \mathbf{x} \cdot (\mathbf{1} - \mathbf{y}) = \sum_{i=1}^{n} x_i (1 - y_i)$.

$c = (\mathbf{1} - \mathbf{x}) \cdot \mathbf{y} = \sum_{i=1}^{n} (1 - x_i) y_i$.

$d = (\mathbf{1} - \mathbf{x}) \cdot (\mathbf{1} - \mathbf{y}) = \sum_{i=1}^{n} (1 - x_i)(1 - y_i)$.

- The counts of matches are a for $(1, 1)$ and d for $(0, 0)$;
- The counts of mismatches are b for $(1, 0)$ and c for $(0, 1)$.
- Note that obviously: $a + b + c + d = n$.
- This gives a very useful 2×2 association table.

		Second individual		
		1	0	*Totals*
First individual	1	a	b	$a+b$
	0	c	d	$c+d$
Totals		$a+c$	$b+d$	n

Table 9 Binary Variables for Eight People

Person	Sex (Male = 1, Female = 0)	Married (Yes = 1, No = 0)	Fair Hair = 1, Dark Hair = 0	Blue Eyes = 1, Brown Eyes = 0	Wears Glasses (Yes = 1, No = 0)	Round Face = 1, Oval Face = 0	Pessimist = 1, Optimist = 0	Evening Type = 1, Morning Type = 0	Is an Only Child (Yes = 1, No = 0)	Left-Handed = 1, Right-Handed = 0
Ilan	1	0	1	1	0	0	1	0	0	0
Jacqueline	0	1	0	0	1	0	0	0	0	0
Kim	0	0	1	0	0	0	1	0	0	1
Lieve	0	1	0	0	0	0	0	1	1	0
Leon	1	1	0	0	1	1	0	1	1	0
Peter	1	1	0	0	1	0	1	1	0	0
Talia	0	0	0	1	0	1	0	0	0	0
Tina	0	0	0	1	0	1	0	0	0	0

Table from Kaufman, L., & Rousseeuw, P. J. (2009). Finding groups in data: an introduction to cluster analysis *(Vol. 344). John Wiley & Sons* * The data shows 8 people (individuals) and 10 binary variables: *

Sex, Married, Fair Hair, Blue Eyes, Wears Glasses, Round Face, Pessimist, Evening Type, Is an Only Child, Left-Handed.

```
data=c(
1,0,1,1,0,0,1,0,0,0,
0,1,0,0,1,0,0,0,0,0,
0,0,1,0,0,0,1,0,0,1,
0,1,0,0,0,0,0,1,1,0,
1,1,0,0,1,1,0,1,1,0,
1,1,0,0,1,0,1,1,0,0,
0,0,0,1,0,1,0,0,0,0,
0,0,0,1,0,1,0,0,0,0
)
data=data.frame(matrix(data, nrow=8,byrow=T))
row.names(data)=c("Ilan","Jacqueline","Kim","Lieve","Leon","Peter","Talia","Tina")
names(data)=c("Sex", "Married", "Fair Hair", "Blue Eyes", "Wears Glasses", "Round Face", "Pessimist", "
```

- We are comparing the records for Ilan with Talia.

```
x=data["Ilan",]
y=data["Talia",]
knitr::kable(table(x, y)[2:1,2:1],"pipe")
```

	1	0
1	1	3
0	1	5

- Therefore: $a = 1$, $b = 3$, $c = 1$, $d = 5$.
- Note that interchanging Ilan and Talia would permute b and c while leaving a and d unchanged.
- A good similarity or dissimilarity coefficient must treat b and c symmetrically.
- A similarity measure is denoted by: $s(\mathbf{x}, \mathbf{y})$.
- The corresponding distance is then defined as:

$$d(\mathbf{x}, \mathbf{y}) = 1 - s(\mathbf{x}, \mathbf{y}).$$

- Alternatively, we have:

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{1 - s(\mathbf{x}, \mathbf{y})}.$$

- A list of some of the similarity measures $s(\mathbf{x}, \mathbf{y})$ that have been suggested for binary data is shown below.
- A more extensive list can be found in: Gower, J. C., & Legendre, P. (1986). Metric and Euclidean properties of dissimilarity coefficients. *Journal of classification*, *3*(1), 5-48.

Coefficient	$s(\mathbf{x}, \mathbf{y})$	$d(\mathbf{x}, \mathbf{y}) = 1 - s(\mathbf{x}, \mathbf{y})$
Simple matching	$\frac{a+d}{a+b+c+d}$	$\frac{b+c}{a+b+c+d}$
Jaccard	$\frac{a}{a+b+c}$	$\frac{b+c}{a+b+c}$
Rogers and Tanimoto (1960)	$\frac{a+d}{a+2(b+c)+d}$	$\frac{2(b+c)}{a+2(b+c)+d}$
Gower and Legendre (1986)	$\frac{2(a+d)}{2(a+d)+b+c}$	$\frac{b+c}{2(a+d)+b+c}]$
Gower and Legendre (1986)	$\frac{2a}{2a+b+c}$	$\frac{b+c}{2a+b+c}$

- To calculate these coefficients, we use the function: dist.binary().
- All the distances in this package are of type $d(\mathbf{x}.\mathbf{y}) = \sqrt{1 - s(\mathbf{x}.\mathbf{y})}$.

```r
library(ade4)
a=1
b=3
c=1
d=5
dist.binary(data[c("Ilan","Talia"),],method=2)^2
```

```
  Ilan
```

Talia 0.4

```r
1-(a+d )/(a+b+c+d)
```

[1] 0.4

```r
dist.binary(data[c("Ilan","Talia"),],method=1)^2
```

```
  Ilan
```

Talia 0.8

```r
1-a/(a+b+c)
```

[1] 0.8

```r
dist.binary(data[c("Ilan","Talia"),],method=4)^2
```

```
        Ilan
```

Talia 0.5714286

```r
1-(a+d )/(a+2*(b+c)+d)
```

[1] 0.5714286

```r
# One Gower coefficient is missing
dist.binary(data[c("Ilan","Talia"),],method=5)^2
```

```
        Ilan
```

Talia 0.6666667

```r
1-2*a/(2*a+b+c)
```

[1] 0.6666667 * The reason for such a large number of possible measures has to do with the apparent uncertainty as to how to deal with the count of zero-zero matches d. * The measues embedding d are sometimes called symmetrical. * The other measues are called assymmetrical. * In some cases, of course, zero_zero matches are completely equivalent to one–one matches, and therefore should be included in the calculated similarity measure. * An example is gender, where there is no preference as to which of the two categories should be coded zero or one. * But in other cases the inclusion or otherwise of d is more problematic; for example, when the zero category corresponds to the genuine absence of some property, such as wings in a study of insects. # Exercice 4 * Prove that the distances based on the SimplemMatching coefficient and the Jaccard coefficient satisfy A3. * Prove that the distances proposed by Gower and Legendre (1986) do not satisfy A3. * Hint: Proofs and counterexamples have to be adapted from in the paper: * Gower, J. C., & Legendre, P. (1986). Metric and Euclidean properties of dissimilarity coefficients. *Journal of classification*, *3*(1), 5-48.

Nominal variables

- We previuosly studied above binary variables which can only take on two states coded as $0, 1$.

- We generalize this approach to nominal variables which may take on more than two states.
- Eye's color may have for example four states: blue, brown, green, grey .
- Le M be the number of states and code the outcomes as $1, \cdots, M$.
- We could choose 1 = blue, 2 = brown, 3 = green, and 4 = grey.
- These states are not ordered in any way
- One strategy would be creating a new binary variable for each of the M nominal states.
- Then to put it equal to 1 if the corresponding state occurs and to 0 otherwise.
- After that, one could resort to one of the dissimilarity coeffi- cients of the previous subsection.
- The most common way of measuring the similarity or dissimilarity between two objects through categorial variables is the simple matching approach.
- If $\mathbf{x}, \mathbf{y}$, are both n nominal records for two individuals,
- Let define the function:

$$\delta(x_i, y_i) \equiv \begin{cases} 0, & \text{if } x_i = y_i; \\ 1, & \text{if } x_i \neq y_i. \end{cases}$$

- Let N_{a+d} be the number of attributes of the two individuals on which the two records match:

$$N_{a+d} = \sum_{i=1}^{n} \delta(x_i, y_i).$$

- Let N_{b+c} be the number of attributes on which the two records do not match:

$$N_{b+c} = n - N_{a+d}.$$

- Let N_d be the number of attributes on which the two records match in a "not applicable" category:

$$N_d = \sum_{i=1}^{n} \delta(x_i, y_i).$$

- The distance corresponding to the simple matching approach is:

$$d(\mathbf{x}, \mathbf{y}) = \frac{\sum_{i=1}^{n} \delta(x_i, y_i)}{n}.$$

- Therefore:

$$d(\mathbf{x}, \mathbf{y}) = \frac{N_{a+d}}{N_{a+d} + N_{b+c}}.$$

- Note that simple matching has exactly the same meaning as in the preceding section.

Gower's dissimilarity

- Gower's coefficient is a dissimilarity measure specifically designed for handling mixed attribute types or variables.
- See: GOWER, John C. A general coefficient of similarity and some of its properties. *Biometrics*, 1971, p. 857-871.
- The coefficient is calculated as the weighted average of attribute contributions.

- Weights usually used only to indicate which attribute values could actually be compared meaningfully.
- The formula is:

$$d(\mathbf{x}, \mathbf{y}) = \frac{\sum_{i=1}^{n} w_i \delta(x_i, y_i)}{\sum_{i=1}^{n} w_i}.$$

- The wheight w_i is put equal to 1 when both measurements x_i and y_i are nonmissing,
- The number $\delta(x_i, y_i)$ is the contribution of the ith measure or variable to the dissimilarity measure.
- It the ith measure is nominal, we take

$$\delta(x_i, y_i) \equiv \begin{cases} 0, & \text{if } x_i = y_i; \\ 1, & \text{if } x_i \neq y_i. \end{cases}$$

- If the ith measure is interval-scaled, we take instead:

$$\delta(x_i, y_i) \equiv \frac{|x_i - y_i|}{R_i},$$

  where R_i is the range of variable i over the available data.
- Consider the following data set:

	variable							
object	1	2	3	4	5	6	7	8
Begonia	0	1	1	4	3	15	25	15
Broom	1	0	0	2	1	3	150	50
Camellia	0	1	0	3	3	1	150	50
Dahlia	0	0	1	4	2	16	125	50
Forget-me-not	0	1	0	5	2	2	20	15
Fuchsia	0	1	0	4	3	12	50	40
Geranium	0	0	0	4	3	13	40	20
Gladiolus	0	0	1	2	2	7	100	15
Heather	1	1	0	3	1	4	25	15
Hydrangea	1	1	0	5	2	14	100	60
Iris	1	1	1	5	3	8	45	10
Lily	1	1	1	1	2	9	90	25
Lily-of-the-valley	1	1	0	1	2	6	20	10
Peony	1	1	1	4	2	11	80	30
Pink Carnation	1	0	0	3	2	10	40	20
Red Rose	1	0	0	4	2	18	200	60
Scotch Rose	1	0	0	2	2	17	150	60
Tulip	0	0	1	2	1	5	25	10

Table 1: Flower dataset.

Data

from: Struyf, A., Hubert, M., & Rousseeuw, P. (1997). Clustering in an object-oriented environment. Journal of Statistical Software*, 1(4), 1-30.*

- The dataset contains 18 flowers and 8 characteristics:

1. Winters: binary, indicates whether the plant may be left in the garden when it freezes.
2. Shadow: binary, shows whether the plant needs to stand in the shadow.
3. Tubers (Tubercule): asymmetric binary, distinguishes between plants with tubers and plants that grow in any other way.
4. Color: nominal, specifies the flower's color (1=white, 2=yellow, 3= pink, 4=red, 5= blue).
5. Soil: ordinal, indicates whether the plant grows in dry (1), normal (2), or wet (3) soil.
6. Preference: ordinal, someone's preference ranking, going from 1 to 18.
7. Height: interval scaled, the plant's height in centimeters.
8. Distance: interval scaled, the distance in centimeters that should be left between the plants.

- The dissimilarity between Begonia and Broom (Genêt) can be calculated as follows:

Begonia
Genêt

```
library(cluster)
library(dplyr)
```

```
##
## Attaching package: 'dplyr'
```

```
## The following objects are masked from 'package:stats':
##
##     filter, lag
```

```
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```
data <-flower %>%
rename(Winters=V1,Shadow=V2,Tubers=V3,Color=V4,Soil=V5,Preference=V6,Height=V7,Distance=V8) %>%
mutate(Winters=recode(Winters,"1"="Yes","0"="No"),
      Shadow=recode(Shadow,"1"="Yes","0"="No"),
      Tubers=recode(Tubers,"1"="Yes","0"="No"),
      Color=recode(Color,"1"="white", "2"="yellow", "3"= "pink", "4"="red", "5"="blue"),
      Soil=recode(Soil,"1"="dry", "2"="normal", "3"= "wet")
      )
```

```
res=lapply(data,class)
res=as.data.frame(res)
res[1,] %>%
```

```r
knitr::kable()
```

Winters	Shadow	Tubers	Color	Soil	Preference	Height	Distance
factor	factor	factor	factor	ordered	ordered	numeric	numeric

```r
flower[1:2,]
```

```
##   V1 V2 V3 V4 V5 V6  V7 V8
## 1  0  1  1  4  3 15  25 15
## 2  1  0  0  2  1  3 150 50
```

```r
max(data$Height)-min(data$Height)
```

```
## [1] 180
```

```r
max(data$Distance)-min(data$Distance)
```

```
## [1] 50
```

$$\frac{|1-0|+|0-1|+|0-1|+1+|1-3|/2+|3-15|/17+|150-25|/180+|50-15|/50}{8} \approx 0.8875408$$

`daisy`	*Dissimilarity Matrix Calculation*

Description

Compute all the pairwise dissimilarities (distances) between observations in the data set. The original variables may be of mixed types. In that case, or whenever `metric = "gower"` is set, a generalization of Gower's formula is used, see 'Details' below.

Usage

```r
daisy(x, metric = c("euclidean", "manhattan", "gower"),
      stand = FALSE, type = list(), weights = rep.int(1, p),
      warnBin = warnType, warnAsym = warnType, warnConst = warnType,
      warnType = TRUE)
```

```r
library(cluster)
(abs(1-0)+abs(0-1)+abs(0-1)+1+abs(1-3)/2+abs(3-15)/17+abs(150-25)/180+abs(50-15)/50)/8
```

```
## [1] 0.8875408
```

```r
daisy(data[,1:8],metric = "Gower")
```

```
## Warning in daisy(data[, 1:8], metric = "Gower"): with mixed variables, metric
## "gower" is used automatically

## Dissimilarities :
##           1         2         3         4         5         6         7
## 2 0.8875408
```

```
## 3  0.5272467 0.5147059
## 4  0.3517974 0.5504493 0.5651552
## 5  0.4115605 0.6226307 0.3726307 0.6383578
## 6  0.2269199 0.6606209 0.3003268 0.4189951 0.3443627
## 7  0.2876225 0.5999183 0.4896242 0.3435866 0.4197712 0.1892974
## 8  0.4234069 0.4641340 0.6038399 0.2960376 0.4673203 0.5714869 0.4107843
## 9  0.5808824 0.4316585 0.4463644 0.8076797 0.3306781 0.5136846 0.5890931
## 10 0.6094363 0.4531046 0.4678105 0.5570670 0.3812908 0.4119281 0.5865196
## 11 0.3278595 0.7096814 0.5993873 0.6518791 0.3864788 0.4828840 0.5652369
## 12 0.4267565 0.5857843 0.6004902 0.5132761 0.5000817 0.5248366 0.6391340
## 13 0.5196487 0.5248366 0.5395425 0.7464461 0.2919118 0.4524510 0.5278595
## 14 0.2926062 0.5949346 0.6096405 0.3680147 0.5203431 0.3656863 0.5049837
## 15 0.6221814 0.3903595 0.5300654 0.5531454 0.4602124 0.5091503 0.3345588
## 16 0.6935866 0.3575163 0.6222222 0.3417892 0.7301471 0.5107843 0.4353758
## 17 0.7765114 0.1904412 0.5801471 0.4247141 0.6880719 0.5937092 0.5183007
## 18 0.4610294 0.4515114 0.7162173 0.4378268 0.4755310 0.6438317 0.4692402
##            8         9        10        11        12        13        14
## 2
## 3
## 4
## 5
## 6
## 7
## 8
## 9  0.6366422
## 10 0.6639706 0.4256127
## 11 0.4955474 0.4308007 0.3948121
## 12 0.4216503 0.4194036 0.3812092 0.2636029
## 13 0.5754085 0.2181781 0.3643791 0.3445670 0.2331699
## 14 0.4558007 0.4396650 0.3609477 0.2838644 0.1591503 0.3784314
## 15 0.4512255 0.2545343 0.4210784 0.4806781 0.4295752 0.3183007 0.4351307
## 16 0.6378268 0.6494690 0.3488562 0.7436683 0.6050654 0.5882353 0.4598039
## 17 0.4707516 0.6073938 0.3067810 0.7015931 0.5629902 0.5461601 0.5427288
## 18 0.1417892 0.5198529 0.8057598 0.5359477 0.5495507 0.5733252 0.5698121
##           15        16        17
## 2
## 3
## 4
## 5
## 6
## 7
## 8
## 9
## 10
## 11
## 12
## 13
## 14
## 15
## 16 0.3949346
## 17 0.3528595 0.1670752
## 18 0.5096814 0.7796160 0.6125408
##
## Metric :  mixed ;  Types = N, N, N, N, O, O, I, I
```

```
## Number of objects : 18
```