Distance and dissimilarities

Contents


```
knitr::opts_chunk$set(echo = TRUE)
```

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:

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

* A1A2 ae onbvious. * The proof of A3 is provided below.

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.

Manhattan distance vs Euclidean distance Graph

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

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

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

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

```
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 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.

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

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

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

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

Exercice 2

- 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:

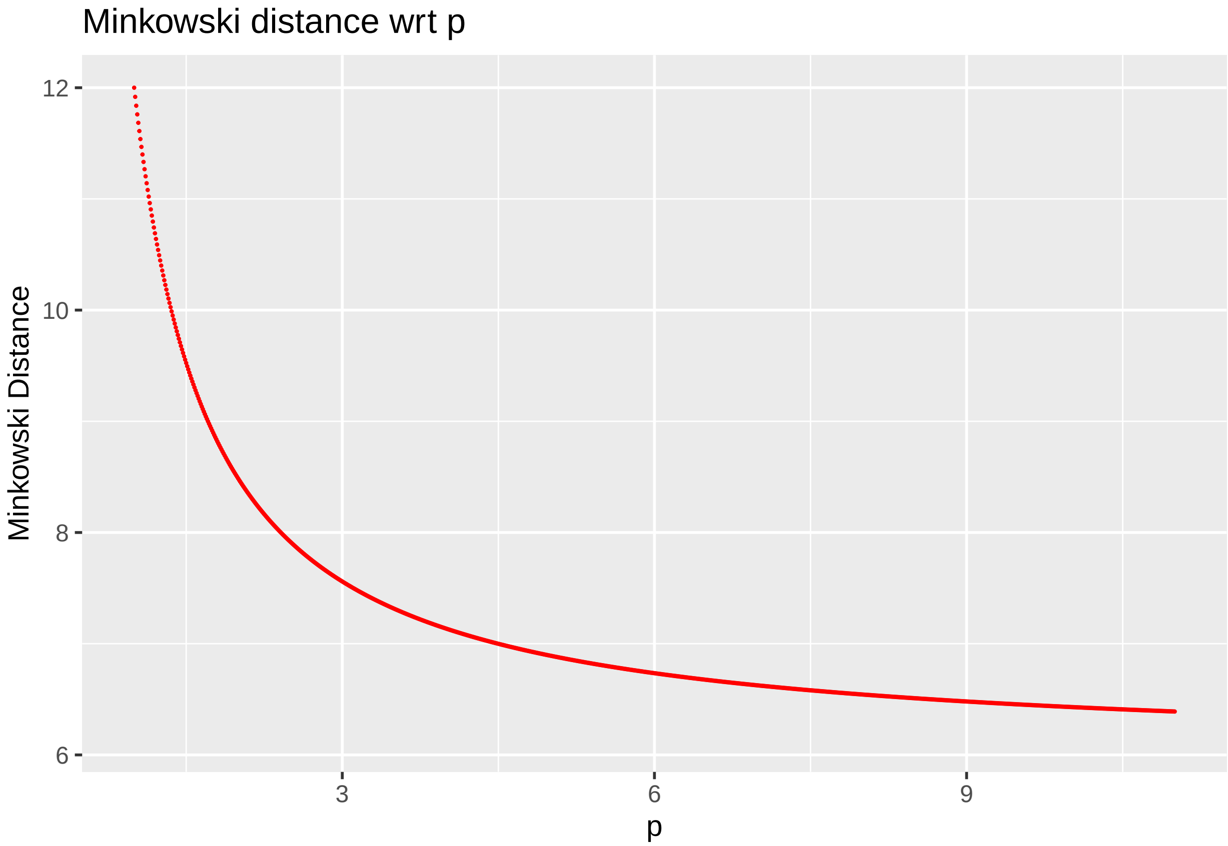
$$\|\mathbf{x}\|_p = d(\mathbf{x}, \mathbf{0}),$$

  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(size
```

```
## 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 $\text{sign}(\cdot)$ 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 measured characters.
- *The presence of the character or type is coded 1 and the absence by 0.
- We have have at our disposal two vectors.
- $\mathbf{x}$ is observed for first indiviual (or object).
- $\mathbf{y}$ is observed for a second individual.
- We can then calculate the following 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 $(0, 1)$).
- 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

- We are using a data set 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", "I
```

- We are comparing the records for Ilan with Talia.

```
x=data["Ilan",]
y=data["Talia",]
```

- We make up a table like (16) which yields a = 1, b = 3, c = 1, and d = 5.
- Note that interchanging Ilan and Talia would permute b and c (while leaving a and d unchanged), so a good similarity or dissimilarity coefficient must treat b and c in the same way in order to satisfy (D3) or (S3). At this point a cruc
- A list of some of the similarity measures that have been suggested for binary data is shown in Table 3.3; a more extensive list can be found in Gower and Legendre (1986).

Measure	Formula
Matching coefficient	$(a + d)/(a + b + c + d)$

Measure	Formula
Jaccard coefficient	$a/(a+b+c)$
Rogers and Tanimoto (1960)	$(a+d)/[a+2(b+c)+d]$
Gower and Legendre (1986)	$(a+d)/[a+\frac{1}{2}(b+c)+d]$
Gower and Legendre (1986)	$a/[a+\frac{1}{2}(b+c)]$

- 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 in Table 3.2).
- 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.

Distance matrix computation

- We'll use a subset of the data USArrests
- We'll use only a by taking 15 random rows among the 50 rows in the data set.
- Next, we standardize the data using the function scale():

```
install.packages("FactoMineR")
```

```
## Installing package into '/home/rstudio-user/R/x86_64-pc-linux-gnu-library/4.0'
## (as 'lib' is unspecified)
```

```
library("FactoMineR")
data("USArrests") # Loading
head(USArrests, 3) # Print the first 3 rows
```

```
##         Murder Assault UrbanPop Rape
## Alabama   13.2     236       58 21.2
## Alaska    10.0     263       48 44.5
## Arizona    8.1     294       80 31.0
```

```
set.seed(123)
ss <- sample(1:50, 15) # Take 15 random rows
df <- USArrests[ss, ] # Subset the 15 rows
df.scaled <- scale(df) # Standardize the variables
```

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

Figure 1: KAUFMANBinarydata