Robinson cubes

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Abstract. A square similarity matrix is called a Robinson matrix if the highest entries within each row and column are on the main diagonal and if, when moving away from this diagonal, the entries never increase. This paper formulates Robinson cubes as three-way generalizations of Robinson matrices. The first definition involves only those entries that are in a row, column or tube with an entry of the main diagonal. A stronger definition, called a regular Robinson cube, involves all entries. Several examples of the definitions are presented.

1 Introduction

Let $\mathbf{A} = \{a_{ij}\}$ be a $m \times m$ matrix. A similarity matrix $\mathbf{A}$ is called a *Robinson matrix* if the highest entries within each row and column of $\mathbf{A}$ are on the main diagonal (elements a_{ii}) and if the entries never increase when moving away from the diagonal. If $\mathbf{A}$ is a dissimilarity matrix, then $\mathbf{A}$ is called a Robinson matrix if the lowest entries are on the main diagonal and if the entries never increase when moving away from this diagonal in any direction (in this case Hubert et al. (1998) speak of an anti-Robinson matrix). Since an object i has usually 0 dissimilarity with itself, this main diagonal consists of 0s in the latter case. If the $\mathbf{A}$ is symmetric, that is, $a_{ij} = a_{ji}$, then $\mathbf{A}$ is a Robinson matrix if we have

$$1 \leq i < j \leq m \Rightarrow a_{ij} \leq a_{i+1j} \quad \text{and} \quad 1 \leq j \leq i < m \Rightarrow a_{ij} \geq a_{i+1j}$$

for similarities, and

$$1 \leq i < j \leq m \Rightarrow a_{ij} \geq a_{i+1j} \quad \text{and} \quad 1 \leq j \leq i < m \Rightarrow a_{ij} \leq a_{i+1j}$$

for dissimilarities.

The Robinson property of a (dis)similarity matrix reflects an ordering of the objects, but also constitutes a clustering system with overlapping clusters. Such ordered clustering systems were introduced under the name *pyramids* by Diday (1984, 1986) and under the name *pseudo-hierarchies* by Fichet (1984, 1986). The CAP algorithm to find an ordered clustering structure was described in Diday (1986) and Diday and Bertrand (1986), and later extended to deal with symbolic data by Brito (1991) and with missing data by Gaul

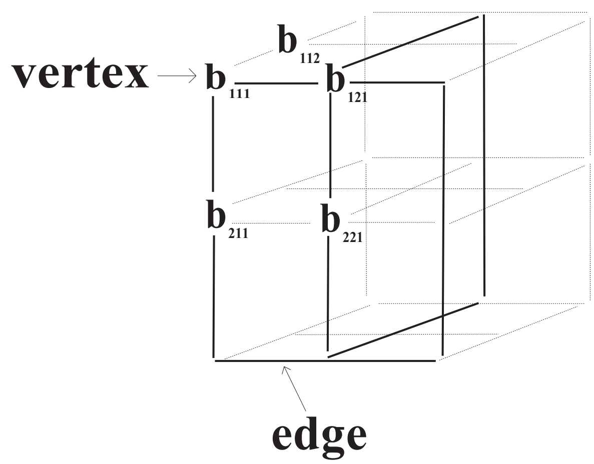

Fig. 1. Some aspects of a cube.

and Schader (1994). Chepoi and Fichet (1997) describe several circumstances in which Robinson matrices are encountered. For an in-depth review of overlapping clustering systems we refer to Barthélemy et al. (2004).

Let $\mathbf{B} = \{b_{ijk}\}$ be a $m \times m \times m$ array. In the present paper the concept of a Robinson matrix is extended to a three-way (dis)similarity cube $\mathbf{B}$, which will be called a *Robinson cube*. Whereas a matrix is characterized by rows and columns, a cube consists of rows, columns and *tubes*. The eight elements of $\mathbf{B}$ characterized by

$$b_{ijk} \quad \text{for } i, j, k = 1 \text{ or } m$$

are called the *vertices* of the cube. The twelve rows, columns and tubes containing two vertices are called the *edges* of $\mathbf{B}$. Some aspects of a cube are demonstrated in Figure 1.

The remainder of the paper looks as follows. Several definitions and some properties of a Robinson cube are presented in the next section. Various examples are presented in Section 3. Section 4 contains the discussion.

2 Definitions and properties

Before defining a Robinson cube we turn our attention to two natural requirements for cubes. Similar to a matrix **A** a cube **B** may satisfy *three-way symmetry*:

$$b_{ijk} = b_{ikj} = b_{jik} = b_{jki} = b_{kij} = b_{kji} \quad \text{for all } i, j \text{ and } k.$$

Another natural requirement for a cube **B** is the restriction

$$b_{iji} = b_{ijj} \quad \text{for all } i \text{ and } j.$$

The latter requirement is called *diagonal-plane equality* (Heiser and Bennani, 1997, p. 191) because it requires equality of the three matrices $\{b_{iij}\}$, $\{b_{iji}\}$ and $\{b_{ijj}\}$, which are formed by cutting the cube diagonally, starting at one of the three edges joining at the vertex b_{111}. A weak extension of the Robinson matrix is the following definition.

Definition 1. A (dis)similarity cube **B** is called a *Robinson cube* if the highest (lowest) entries within each row, column and tube of **B** are on the main diagonal (elements b_{iii}) and moving away from this diagonal, the entries never increase (decrease).

From Definition 1 it follows that a similarity cube **B** is a Robinson cube if we have

$$1 \le i < j \le m \Rightarrow \begin{cases} b_{ijj} \le b_{i+1jj} \\ b_{jij} \le b_{ji+1j} \\ b_{jji} \le b_{jji+1} \end{cases} \quad \text{and} \quad 1 \le j \le i < m \Rightarrow \begin{cases} b_{ijj} \ge b_{i+1jj} \\ b_{jij} \ge b_{ji+1j} \\ b_{jji} \ge b_{jji+1}. \end{cases}$$

The inequalities for a dissimilarity cube are obtained by interchanging $\le$ and $\ge$ in the right parts of both equations. If the similarity cube **B** satisfies the diagonal-plane equality, then **B** is a Robinson cube if we have

$$1 \le i < j \le m \Rightarrow \begin{cases} b_{ijj} \le b_{i+1jj} \\ b_{jij} \le b_{ji+1j} \end{cases} \quad \text{and} \quad 1 \le j \le i < m \Rightarrow \begin{cases} b_{ijj} \ge b_{i+1jj} \\ b_{jij} \ge b_{ji+1j}. \end{cases}$$

Moreover, if the similarity cube **B** satisfies three-way symmetry, then **B** is a Robinson cube if we have

$$1 \le i < j \le m \Rightarrow b_{ijj} \le b_{i+1jj} \quad \text{and} \quad 1 \le j \le i < m \Rightarrow b_{ijj} \ge b_{i+1jj}.$$

Note that, although this is perhaps suggested in the above argument, a Robinson cube that satisfies three-way symmetry does not necessarily satisfy the diagonal-plane equality.

Note that not all entries of **B** are involved in Definition 1. More precisely, only those entries that are in a row, column or tube with an entry of the main diagonal are involved in Definition 1. A stronger definition compared to Definition 1 is the following.

Definition 2. A cube **B** is called a *regular Robinson cube* if

1. **B** is a Robinson cube (Definition 1)
2. all matrices, which are formed by cutting the cube perpendicularly, where for each matrix **A** entry a_{11} is an element of one of the three edges joining at the vertex b_{111} (with $a_{11} = b_{111}$ if **A** is one of the three faces joining at the vertex b_{111}), are Robinson matrices.

An example of a regular Robinson cube is the bottom cube in Figure 2. A regular Robinson cube has some interesting features. For example, if **B** is a regular Robinson cube then it satisfies both three-way symmetry and the diagonal-plane equality. These properties become clear from the following result on the composition of a regular Robinson cube.

Proposition 1. Let $q = \min(i, j, k)$ and $r = \max(i, j, k)$. If **B** is a regular Robinson cube, then its entries b_{ijk} equal

$$b_{qrs} = b_{rqs} = b_{qsr} = b_{rsq} = b_{sqr} = b_{srq} \quad \text{for } s = q, ..., r.$$

Proof. The idea for the proof is depicted in Figure 1. First, let **A** be the front face of the cube, where $a_{11} = b_{111}$. Since b_{221} is a diagonal element of **A**, **A** is a Robinson matrix if $b_{121} \leq b_{221}$. Next, let **A** be the cutting perpendicular on the front face of the cube, with $a_{11} = b_{121}$. Since b_{121} is a diagonal element of **A**, the latter is a Robinson matrix if $b_{121} \geq b_{221}$. Thus, if **B** is a regular Robinson cube, then $b_{121} = b_{221}$ $(= b_{211} = b_{212} = b_{112} = b_{122})$. □

3 Examples

The most popular functions for triadic dissimilarities used in classification literature are the symmetric L_p-transforms:

$$b_{ijk} = (a_{ij}^p + a_{ik}^p + a_{jk}^p)^{1/p}.$$

For example, for $p = 1$ we have the perimeter function, for $p = 2$ the generalized Euclidean function, and for $p = \infty$ the generalized dominance function, that is, $b_{ijk} = \max(a_{ij}, a_{ik}, a_{jk})$. An alternative function for dissimilarities is the variance function, defined by

$$b_{ijk}^2 = \text{var}(a_{ij}, a_{ik}, a_{jk}) \;=\; (a_{ij}^2 + a_{ik}^2 + a_{jk}^2) - \frac{1}{3}(a_{ij} + a_{ik} + a_{jk})^2$$

which is also symmetric in i, j and k (De Rooij and Gower, 2003, p. 188).

Proposition 2. Let **A** and **B** be respectively a dissimilarity matrix and cube. Suppose b_{ijk} is defined as a L_p-transform or the variance function. Then **B** is a Robinson cube if and only if **A** is a Robinson matrix.

Proof. For $1 \leq i < j \leq m$ we have

$$b_{ijj} = (2a_{ij}^p)^{1/p} \geq (2a_{i+1j}^p)^{1/p} = b_{i+1jj} \quad \text{if and only if} \quad a_{ij} \geq a_{i+1j}$$

for a L_p-transform of a_{ij}, a_{ik} and a_{jk}, and

$$b_{ijj}^2 = 2a_{ij}^2 - \frac{1}{3}(2a_{ij})^2 \geq 2a_{i+1j}^2 - \frac{1}{3}(2a_{i+1j})^2 = b_{i+1jj}^2$$

if and only if

$$\frac{2}{3}a_{ij}^2 \geq \frac{2}{3}a_{i+1j}^2 \quad \text{if and only if} \quad a_{ij} \geq a_{i+1j}$$

for the variance function of a_{ij}, a_{ik} and a_{jk}. A similar property holds for $b_{ijj} \leq b_{i+1jj}$ for $1 \leq j \leq i < m$. □

A stronger property holds for the dominance function for dissimilarities, or equivalently the minimum function $b_{ijk} = \min(a_{ij}, a_{ik}, a_{jk})$ for similarities.

Proposition 3. Let **A** and **B** be respectively a similarity matrix and cube. If $b_{ijk} = \min(a_{ij}, a_{ik}, a_{jk})$, then **B** is a regular Robinson cube if and only if **A** is a Robinson matrix.

Proof. If **A** is a Robinson matrix then the minimum function has the property

$$1 \leq i \leq j \leq k \leq m \quad \Rightarrow \quad b_{ijk} = \min(a_{ij}, a_{ik}, a_{jk}) = a_{ik}$$

which fulfills the second requirement in Definition 2. Moreover, we have

$$\begin{aligned} 1 \leq i < j \leq m &\Rightarrow b_{ijj} = a_{ij} \leq a_{i+1j} = b_{i+1jj} \quad \text{and} \\ 1 \leq j \leq i < m &\Rightarrow b_{ijj} = a_{ij} \geq a_{i+1j} = b_{i+1jj} \end{aligned}$$

which shows the first requirement of Definition 2. □

Suppose the data at hand are binary (0/1) scores and that there are n records of i, j and k. Denote by

$$\begin{aligned} n_i &= \text{the number of 1s in } i \\ n_{ij} &= \text{the number of 1s common in } i \text{ and } j \\ n_{ijk} &= \text{the number of 1s common in } i, j \text{ and } k. \end{aligned}$$

In the remainder of this paper we assume that all matrices and cubes are of the similarity kind. However, the properties below could also have been formulated for dissimilarities.

Proposition 4. Let the Jaccard similarity coefficient be defined as

$$a_{ij} = \frac{n_{ij}}{n_i + n_j - n_{ij}} \qquad \text{for pairs of objects, and}$$

$$b_{ijk} = \frac{n_{ijk}}{n_i + n_j + n_k - (n_{ij} + n_{ik} + n_{jk}) + n_{ijk}} \quad \text{for triples of objects.}$$

(The latter definition comes from Heiser and Bennani, 1997, p. 196). Then **B** is a Robinson cube if and only if **A** is a Robinson matrix.

Proof. The result follows from the fact that

$$a_{ij} = \frac{n_{ij}}{n_i + n_j - n_{ij}} = b_{ijj}. \quad \square$$

Proposition 5. If $a_{ij} = n_{ij}$ and $b_{ijk} = n_{ijk}$, then the following statements are equivalent:

1. **A** is a Robinson matrix
2. **B** is a regular Robinson cube
3. $b_{ijk} = \min(a_{ij}, a_{ik}, a_{jk})$.

Proof. The result follows from the fact that $n_{ijj} = n_{ij}$, and if **A** is a Robinson matrix, then n_{ijk} has the property

$$1 \leq i \leq j \leq k \leq m \quad \Rightarrow \quad n_{ijk} = \min(n_{ij}, n_{ik}, n_{jk}) = n_{ik}. \quad \square$$

The result in Proposition 5 applies to the Russel-Rao similarity coefficient which is defined as n_{ij}/n for pairs of objects and n_{ijk}/n for triples of objects (Heiser and Bennani, 1997, p. 197). A sufficient condition for **A** with elements $a_{ij} = n_{ij}$ to be a Robinson matrix can be found in Hodson et al. (1971, p. 279). Let the binary scores be in a $n \times m$ table **X**, for example

$$\mathbf{X} = \begin{bmatrix} 1\,0\,0 \\ 1\,1\,0 \\ 0\,1\,0 \\ 1\,1\,1 \\ 0\,1\,1 \\ 0\,0\,1 \end{bmatrix}$$

where the objects i, j and k identify the columns of **X**. Suppose that the columns of **X** are ordered such that in each row the 1s are bunched together: **X** is said to posses the *consecutive 1s* property (see, for example, Hubert, 1974, p. 977 or Heiser, 1981, p. 73). If the rows of **X** contain consecutive 1s, then **A** with elements $a_{ij} = n_{ij}$ is a Robinson matrix. It follows from Proposition 5 that this condition is then also sufficient for **B** with elements $b_{ijk} = n_{ijk}$ to be a Robinson cube. Alternatively, it is also possible to generalize the original proof in Hodson et al. (1971) for a matrix to a cube.

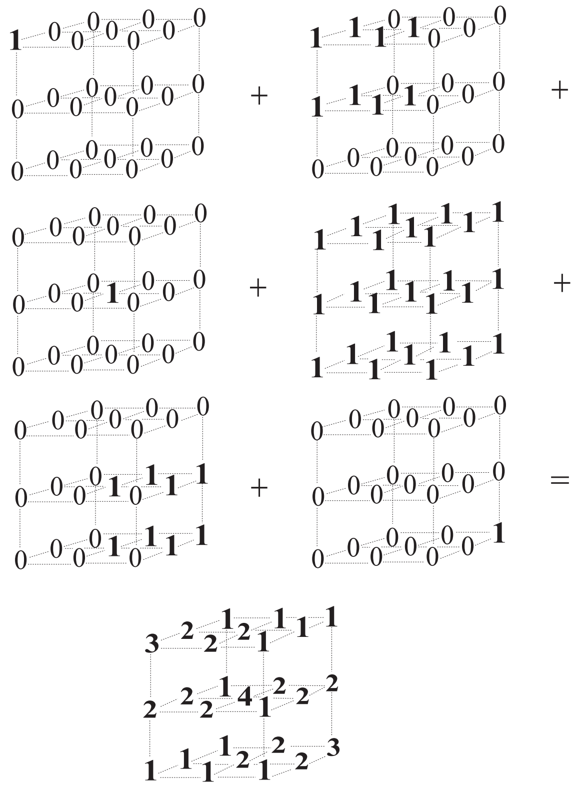

Fig. 2. The sum of regular Robinson cubes is a regular Robinson cube.

Proposition 6. If the columns of a binary table are ordered such that the rows contain consecutive 1s, then **B** with elements $b_{ijk} = n_{ijk}$ is a regular Robinson cube.

Proof. For the sake of an example consider the binary table **X**. The proof is further depicted in Figure 2. The first six cubes are the similarity cubes with elements n_{ijk} corresponding to the six rows of **X**. If a row has consecutive 1s, the similarity cube corresponding to this row, is a Robinson cube. The seventh and last cube in Figure 2, is the cube with elements n_{ijk} for the complete table **X**. Figure 2 visualizes an interesting property of regular Robinson cubes: the sum of regular Robinson cubes is again a regular Robinson cube. □

4 Discussion

A data array arranged in a cube in which rows, columns and tubes refer to the same objects has been called three-way one-mode, or triadic data. Such data have been studied in attempts to identify higher order interactions among objects (Heiser and Bennani, 1997). In this paper, we have shown that we can recognize a simple order among the objects in triadic data, by a generalization of the Robinson property for dyadic data. We have discussed a general version of the Robinson cube, and a more specific one. Studying several definitions of triadic (dis)similarities, we found that in most cases, if a dyadic (dis)similarity is Robinsonian, then the triadic (dis)similarity is Robinsonian, too. A regular Robinson cube occurs only with the Russel-Rao coefficient calculated on an attribute matrix with the consecutive 1s property, and with the dominance metric for dissimilarities.

References

BARTHÉLEMY, J.-P., BRUCKER, F. and OSSWALD, C. (2004): Combinatorial optimization and hierarchical classifications. *4OR 2, 179-219.*

BRITO, P. (1991): *Analyse de données symboliques: pyramides d'heritage.* Thèse de doctorat, Université Paris 9.

CHEPOI, V. and FICHET, B. (1997): Recognition of Robinsonian dissimilarities. *Journal of Classification 14, 311-325.*

DE ROOIJ, M. and GOWER, J. C. (2003): The geometry of triadic distances. *Journal of Classification 20, 181-220.*

DIDAY, E. (1984): *Une représentation visuelle des classes empiétantes: les pyramides.* Research report 291, INRIA.

DIDAY, E. (1986): Orders and overlapping clusters in pyramids. In: J. de Leeuw, W.J. Heiser, J.J. Meulman and F. Critchley (Eds.): *Multidimensional Data Analysis.* DSWO Press, Leiden, 201-234.

DIDAY, E. and BERTRAND, P. (1986): An extension of hierarchical clustering: the pyramidal representation. In: E.S. Gelsema and L.N. Kanal (Eds.): *Pattern Recognition in Practice II.* North-Holland, Amsterdam, 411-424.

FICHET, B. (1984): Sur une extension de la notion de hiérarchie et son équivalence avec quelques matrices de Robinson. *Actes des "Journées de statistique de la Grande Motte", 12-12.*

FICHET, B. (1986): Data analysis: geometric and algebraic structures. In: Y.A. Prohorov et al. (Eds.): *First World Congress of the Bernoulli Society Proceedings.* V.N.U. Science Press, 123-132.

GAUL, W. and SCHADER, M. (1994): Pyramidal classification based on incomplete dissimilarity data. *Journal of Classification 11, 171-193.*

HEISER, W. J. (1981): *Unfolding Analysis of Proximity Data.* Leiden University, Leiden.

HEISER, W. J. and BENNANI, M. (1997): Triadic distance models: axiomatization and least squares representation. *Journal of Mathematical Psychology 41, 189-206.*

HODSON, F. R., KENDALL, D. G. and TAUTU, P. (1971): *Mathematics in the Archaeological and Historical Sciences*. University Press, Edinburgh.

HUBERT, L. J. (1974): Problems of seriation using a subject by item response matrix. *Psychological Bulletin 81 (12), 976-983*.

HUBERT, L. J., ARABIE, P. and MEULMAN, J. J. (1998): Graph-theoretic representations for proximity matrices through strongly-anti-Robinson or circular strongly-anti-Robinson matrices. *Psychometrika 43, 81-91*.