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n-Way Metrics

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Abstract: We study a family of n-way metrics that generalize the usual two-way metric. The n-way metrics are totally symmetric maps from E^n into $\mathbb{R}_{\geq 0}$. The three-way metrics introduced by Joly and Le Calvé (1995) and Heiser and Bennani (1997) and the n-way metrics studied in Deza and Rosenberg (2000) belong to this family. It is shown how the n-way metrics and n-way distance measures are related to $(n-1)$-way metrics, respectively, $(n-1)$-way distance measures.

Keywords. n-Way distance measure; Triangle inequality; Tetrahedron inequality; Polyhedron inequality; Parametrized inequality.

1. Introduction

Dissimilarity functions are important tools in many domains of data analysis. Most dissimilarity analysis has however been limited to the two-way case. Multi-way dissimilarities may be used to evaluate complex relationships between three or more objects (see, e.g., Diatta 2006, 2007; Warrens 2009a). For various data analysis techniques in the two-way case, metric spaces are the basic tool (Deza and Deza 2006). Several authors, among whom Bennani-Dosse (1993), Joly and Le Calvé (1995), Heiser and Bennani (1997), Chepoi and Fichet (2007) and Warrens (2008a), have studied metricity for the three-way case. Furthermore, Deza and Rosenberg (2000, 2005) studied n-way metrics for the general multi-way case that extend the three-way and four-way metrics considered in Warrens (2008a).

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This paper is devoted to multi-way metricity. There are several ways for introducing n-way metricity. We introduce a family of n-way metrics that are totally symmetric maps from E^n into $\mathbb{R}_{\geq 0}$. The three-way metrics introduced by Joly and Le Calvé (1995) and Heiser and Bennani (1997) and the n-way metrics studied in Deza and Rosenberg (2000, 2005) are in the family. Each inequality that defines a metric is linear in the sense that we have a single, possibly weighted, distance measure, which is equal or smaller than an unweighted sum of distance measures. The inequalities extend the usual triangle inequality.

In Section 2 we define n-way distance measures and n-way metrics. In Sections 4 and 5 we study how n-way distance measures may be related to $(n-1)$-way distances measures. First definitions and properties of a n-way distance with two identical objects are presented in Section 3. Bounds of n-way distance measures in terms of $(n-1)$-way distance measures are investigated in Section 4. Section 5 is used to study what $(n-1)$-way metrics are implied by n-way metrics. In Section 6 we consider various examples that satisfy the polyhedron inequality (4). Section 7 contains a discussion.

2. Definitions

Let $\mathbb{R}_{\geq 0}$ denote the set of nonnegative real numbers. A metric is a pair (E, d) where E is a nonempty set and $d : E^2 \to \mathbb{R}_{\geq 0}$ satisfies for all $x, y, z \in E$ (Deza and Deza 2006, p. 3):

$$
\begin{aligned}
&d(x,y) = 0 \Leftrightarrow x = y && \text{(minimality)}\\
&d(x,y) = d(y,x) && \text{(symmetry)}\\
&d(x,y) \leq d(x,z) + d(y,z) && \text{(triangle inequality).}
\end{aligned}
$$

All the dissimilarity functions occurring in this paper are defined on the set E. The dissimilarity measure d may be constructed from the observed data. Warrens (2008a) discusses several axiom systems for three-way and four-way distance measures.

In this paper we study a family of n-way metrics that generalize the two-way metric. Let $x_{1,n}$ denote the n-tuple $(x_1, x_2, ..., x_n)$ and let $x_{1,n}^{-i}$ denote the $(n-1)$-tuple $(x_1, ..., x_{i-1}, x_{i+1}, ..., x_n)$ where the minus in the superscript of $x_{1,n}^{-i}$ is used to indicate that the element x_i drops out. In the following the elements of tuple $x_{1,n}$ will be referred to as objects. In addition it is assumed that the equations throughout the paper hold for all objects in E that are involved in a definition.

A distance measure $d_n : E^n \to \mathbb{R}_{\geq 0}$ is totally symmetric if for all $x_1, ..., x_n \in E$ and every permutation π of $\{1, 2, ..., n\}$

$$d_n(x_{\pi(1)}, ...x_{\pi(n)}) = d_n(x_1, ..., x_n).$$

This property captures the fact that the value of $d_n(x_{1,n})$ is independent of the order of $x_1, ..., x_n$. Furthermore, as a generalization of minimality we define $d_n(x_1, ..., x_1) = 0$.

Joly and Le Calvé (1995), Deza and Rosenberg (2000, 2005) and Heiser and Bennani (1997) consider, respectively, the following three-way generalizations of the triangle inequality:

$$d_3(x_{1,3}) \leq d_3(x_{2,4}) + d_3(x_{1,4}^{-2}) \tag{1}$$

$$d_3(x_{1,3}) \leq d_3(x_{2,4}) + d_3(x_{1,4}^{-2}) + d_3(x_{1,4}^{-3}) \quad \text{(tetrahedron inequality)}$$

$$2d_3(x_{1,3}) \leq d_3(x_{2,4}) + d_3(x_{1,4}^{-2}) + d_3(x_{1,4}^{-3}). \tag{2}$$

Inequalities (1) and (2) are called respectively weak and strong metrics in Chepoi and Fichet (2007). The tetrahedron inequality can also be found in Deza and Deza (2006, p. 36). Interpreting $d_3(x_{1,3})$ as the area of the triangle with vertices x_1, x_2 and x_3, the tetrahedron inequality specifies that the area of each triangle face of the tetrahedron formed by x_1, x_2, x_3 and x_4 does not exceed the sum of the areas of the remaining faces.

Deza and Rosenberg (2000, p. 803) generalize the tetrahedron inequality to

$$d_n(x_{1,n}) \leq \sum_{i=1}^{n} d_n(x_{1,n+1}^{-i}). \tag{3}$$

Inequality (3) is called the $(n-1)$-simplex inequality in Deza and Deza (2006, p. 36). De Rooij (2001, p. 128) noted that inequality (2) can be generalized to the polyhedron inequality

$$(n-1) \cdot d_n(x_{1,n}) \leq \sum_{i=1}^{n} d_n(x_{1,n+1}^{-i}). \tag{4}$$

Examples of distance measures that satisfy this interesting inequality are presented in Example 2 and Section 6. We may generalize (3) and (4) to

$$k \cdot d_n(x_{1,n}) \leq \sum_{i=1}^{n} d_n(x_{1,n+1}^{-i}), \tag{5}$$

where $k \in (0, n)$ (a positive real number smaller than n). We can further generalize (5) to

$$k \cdot d_n(x_{1,n}) \leq \sum_{i=1}^{m} d_n(x_{1,n+1}^{-i}), \tag{6}$$

where $m \in \{2, 3, ..., n\}$ is a positive integer. For (6) we require that $k \in (0, m)$ (a positive real number smaller than m). Note that the number of linear terms on the right-hand side of (5) is determined by n, whereas the number of linear terms on the right-hand side of (6) is determined by m.

Clearly, if $k^{'} \in (0, k)$ (a positive real number smaller than k), then (6) implies

$$k^{'} \cdot d_n(x_{1,n}) \leq \sum_{i=1}^{m} d_n(x_{1,n+1}^{-i}).$$

Furthermore, if $m \leq m^{'}$, then (6) implies

$$k \cdot d_n(x_{1,n}) \leq \sum_{i=1}^{m^{'}} d_n(x_{1,n+1}^{-i}).$$

Moreover, for $k = 1$ and $n = 1$, adding the two inequalities

$$d_n(x_{1,n}) \leq d_n(x_{2,n+1}) + d_n(x_{1,n+1}^{-2})$$

and

$$d_n(x_{2,n+1}) \leq d_n(x_{1,n}) + d_n(x_{1,n+1}^{-2})$$

shows that distance measure $d_n(x_{1,n}) \geq 0$. In addition, we have the following property.

Theorem 1. *For* $k \in (0, m)$, (6) *implies*

$$(k-1) \cdot d_n(x_{1,n}) \leq \sum_{i=2}^{m} d_n(x_{1,n+1}^{-i}). \tag{7}$$

Proof: Interchanging the roles of x_1 and x_{n+1} in (6) and dividing the result by k, we obtain

$$d_n(x_{2,n+1}) \leq \frac{1}{k}\, d_n(x_{1,n}) + \frac{1}{k} \sum_{i=2}^{m} d_n(x_{1,n+1}^{-i}). \tag{8}$$

Adding (8) to (6) we obtain

$$\frac{k^2-1}{k} \cdot d_n(x_{1,n}) \leq \frac{k+1}{k} \sum_{i=2}^{m} d_n(x_{1,n+1}^{-i}). \tag{9}$$

Using $k^2 - 1 = (k+1)(k-1)$, multiplication of (9) by $k/(k+1)$ yields (7).

■

3. Two Identical Objects

In the remainder of the paper we are interested in how distance measure d_n is related to d_{n-1}. In Section 4 we consider lower and upper bounds of d_n in terms of d_{n-1}. Furthermore, in Section 5 we study what $(n-1)$-way metrics are implied by (6). Apart from minimality, symmetry and (6), we discuss below several additional requirements that specify how d_n and d_{n-1} are related when two objects of d_n are identical.

A first requirement is the following condition. Following Heiser and Bennani (1997) for the three-way case and Deza and Rosenberg (2000) for the n-way case, we require that, if two objects are identical then d_n should remain invariant regardless which two objects are the same, i.e.,

$$d_n(x_1, x_{1,n-1}) = d_n(x_{1,2}, x_{2,n-1}) = ... = d_n(x_{1,n-1}, x_{n-1}). \tag{10}$$

In view of the total symmetry, (10) implies that $d_n(x_1, ..., x_n)$ only depends on the h-element set $\{x_{i_1}, ..., x_{i_h}\}$ such that $\{x_1, ..., x_n\} = \{x_{i_1}, ..., x_{i_h}\}$ where $1 \leq i_1 \leq i_h \leq n$.

Deza and Rosenberg (2000, p. 803) introduced the n-way extension of the three-way star distance discussed in Joly and Le Calvé (1995). In Example 1, $|\{x_1, ..., x_n\}|$ denotes the cardinality of set $\{x_1, ..., x_n\}$.

Example 1. *Let $\alpha : E \to \mathbb{R}_{\geq 0}$ and $n \geq 3$. The star n-distance $d_n^\alpha : E^n \to \mathbb{R}_{\geq 0}$ is defined as follows. Let $x_1, ..., x_n \in E$ and let $0 \leq i_1 \leq ... \leq i_h \leq n$ be such that $|\{x_1, ..., x_n\}| = |\{x_{i_1}, ..., x_{i_h}\}| = h$. Set*

$$d_n^\alpha(x_{1,n}) = \begin{cases} \sum_{j=1}^{h} \alpha(x_{i_j}) & \text{if } h > 1, \\ 0 & \text{if } h = 1. \end{cases}$$

Deza and Rosenberg (2000, p. 803) showed that the star n-distance d_n^α satisfies (10).

Condition (10) is perhaps not an intuitive requirement, because the condition may not hold for certain distance measures.

Example 2. *The perimeter distance gives a geometrical interpretation of the concept "average distance" between objects. Heiser and Bennani (1997) and De Rooij and Gower (2003) study the three-way perimeter distance function*

$$d_3^p(x_{1,3}) = d(x_1, x_2) + d(x_1, x_3) + d(x_2, x_3). \tag{11}$$

A possible n-way extension of (11) is

$$d_n^p(x_{1,n}) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} d(x_i, x_j). \tag{12}$$

Perimeter distance d_n^p is the sum of all pairwise distances between the objects involved. It may be verified that d_n^p does not satisfy (10) for $n \geq 4$. We will show that (12) satisfies polyhedron inequality (4) if and only if $d(x_i, x_j)$ satisfies the triangle inequality.

Proposition 1. *Measure* (12) *satisfies polyhedron inequality* (4) *if and only if $d(x_i, x_j)$ satisfies the triangle inequality.*

Proof: Let $d(x, x) = 0$. Using (12) in (4) we obtain

$$(n-1)\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(x_i, x_j) \leq$$
$$(n-2)\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(x_i, x_j) + (n-1)\sum_{i=1}^{n} d(x_i, x_{n+1}). \tag{13}$$

Inequality (13) can be written as

$$\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(x_i, x_j) \leq (n-1)\sum_{i=1}^{n} d(x_i, x_{n+1}). \tag{14}$$

Supplying (14) with the $(n+1)$-tuple $(x_1, x_2, x_3, ..., x_3)$ we obtain $d(x_1, x_2) \leq d(x_2, x_3) + d(x_1, x_3)$. Conversely, inequality (14) follows from adding the $n(n-1)/2$ triangle inequalities formed between all pairs in $\{x_1, x_2, ..., x_n\}$ and x_{n+1}, e.g., $d(x_1, x_2) \leq d(x_2, x_{n+1}) + d(x_1, x_{n+1})$.
■

In the remainder of this paper it is assumed that $d_n(x_{1,n})$ satisfies (10).

To relate a n-way distance measure d_n to a $(n-1)$-way distance measure d_{n-1}, we study two additional restrictions. Let $p \in \mathbb{R}_{>0}$ be a real positive number. Suppose that, if two objects of the n-way distance measure are identical, d_n and d_{n-1} are equal up to multiplication by a factor p, i.e.,

$$d_{n-1}(x_{1,n-1}) = \frac{1}{p}\, d_n(x_1, x_{1,n-1}). \tag{15}$$

The value of p in (15) may depend on the particular distance model or function that is used.

Example 3. *Joly and Le Calvé (1995) introduce the three-way semi-perimeter distance*

$$d_3^{sp}(x_{1,3}) = \frac{d(x_1, x_2) + d(x_1, x_3) + d(x_2, x_3)}{2}. \tag{16}$$

Supplying (11) with tuple (x_1, x_1, x_2) we obtain $d_3^p(x_1, x_1, x_2) = 2d(x_1, x_2)$. However, supplying (16) with tuple (x_1, x_1, x_2) we obtain $d_3^{sp}(x_1, x_1, x_2) = d(x_1, x_2)$.

For generality we let p in (15) be a positive real number. Of course, it may be argued that $p \geq 1$. The bounds studied in the Section 4 depend on the value of p. The bounds of d_n in terms of the d_{n-1} therefore depend on the distance function that is used to relate the n-way distance measure and $(n-1)$-way distance measure. The results in Section 5 however, do not depend on the value of p.

The final requirement we discuss in this section is given by

$$d_n(x_1, x_{1,n-1}) \leq d_n(x_{1,n}). \tag{17}$$

In (17), the n-way distance measure without identical objects is equal or larger than the n-way distance measure with two identical objects (Heiser and Bennani 1997). Condition (17) seems to be a natural requirement for a multi-way distance measure. Combining (15) and (17) we obtain

$$p \cdot d_{n-1}(x_{1,n-1}) \leq d_n(x_{1,n}). \tag{18}$$

4. Bounds

In this section we study the lower and upper bounds of distance measure d_n in terms of the d_{n-1}. We first turn our attention to the lower bound of n-way distance measure $d_n(x_{1,n})$ that satisfies minimality, total symmetry, and (10).

Proposition 2. *Suppose* (15) *and* (17) *hold. Then for n-way distance measure $d_n(x_{1,n})$ we have*

$$\frac{p}{n}\sum_{i=1}^{n} d_{n-1}(x_{1,n}^{-i}) \leq d_n(x_{1,n}). \tag{19}$$

Proof: For given n, there are n variants of $d_{n-1}(x_{1,n-1})$, which are given by $d_{n-1}(x_{1,n}^{-i})$ for $i \in \{1, 2, ..., n\}$. We obtain n variants of (18) by substituting $d_{n-1}(x_{1,n-1})$ on the left-hand side of (18) by one of its variants. Adding up all n variants of (18), i.e., adding the inequalities

$$\begin{aligned}
p \cdot d_{n-1}(x_{1,n}^{-n}) &\leq d_n(x_{1,n}) \\
p \cdot d_{n-1}(x_{1,n}^{-(n-1)}) &\leq d_n(x_{1,n}) \\
&\vdots \\
p \cdot d_{n-1}(x_{1,n}^{-3}) &\leq d_n(x_{1,n}) \\
p \cdot d_{n-1}(x_{1,n}^{-2}) &\leq d_n(x_{1,n}) \\
p \cdot d_{n-1}(x_{2,n}) &\leq d_n(x_{1,n})
\end{aligned}$$

followed by division by n, we obtain (19).

■

For $p = 1$, lower bound (19) is equivalent to the arithmetic mean of the $(n-1)$-way distance measures $d_{n-1}(x_{1,n}^{-i})$.

For the case $(k - m + 2) > 0$ we have the following lower bound for a n-way distance (i.e., $d_n(x_{1,n})$ satisfies minimality, total symmetry, (6) and (10)). In contrast to Proposition 2, we only require validity of (15), not (17), for this lower bound.

Theorem 2. *Suppose* (15) *holds,* $k \in (0, m)$ *and* $m < k + 2$. *Then for* n*-way distance measure* $d_n(x_{1,n})$*, we have*

$$\frac{p(k-m+2)}{2n} \sum_{i=1}^{n} d_{n-1}(x_{1,n}^{-i}) \leq d_n(x_{1,n}). \tag{20}$$

Proof: Supplying (6) with $(n+1)$-tuple $(x_1, x_1, x_3, ..., x_{n+1})$, and replacing x_{n+1} by x_2 in the result, we obtain

$$p\,k \cdot d_{n-1}(x_{1,n}^{-2}) \leq 2d_n(x_{1,n}) + p \sum_{i=3}^{m} d_{n-1}(x_1, x_2, x_{3,n}^{-i}) \tag{21}$$

for $m \geq 3$, and

$$p\,k \cdot d_{n-1}(x_{1,n}^{-2}) \leq 2d_n(x_{1,n}) \tag{22}$$

for $m = 2$. We have n variants of d_{n-1} for given n, e.g. $d_{n-1}(x_{1,n}^{-2})$ in the left-hand side of (22). We may obtain n variants of (22) by replacing $d_{n-1}(x_{1,n}^{-2})$ by one of the other $(n-1)$ variants. Adding up all n variants of (22), followed by division by $2n$, we obtain

$$\frac{p\,k}{2n} \sum_{i=1}^{n} d_{n-1}(x_{1,n}^{-i}) \leq d_n(x_{1,n}),$$

which is the inequality that is obtained by using $m = 2$ in (20).

We may obtain n variants of (21) by replacing $d_{n-1}(x_{1,n}^{-2})$ in the left-hand side of (21) by one of the other $(n-1)$ variants. Considering all n variants of (21), the n variants of d_{n-1} on the right-hand side each occur a total of $(m-2)$ times. Adding up all n variants of (21), followed by division by $2n$, we obtain (20).
■

Example 4. *If (15) and (4) hold, then* $d_n(x_{1,n})$ *has a lower bound*

$$\frac{p}{2n} \sum_{i=1}^{n} d_{n-1}(x_{1,n}^{-i}) \leq d_n(x_{1,n}). \tag{23}$$

We obtain (23) by using $k = n - 1$ *and* $m = n$ *in (20). For* $p = 2$ *the lower bound of* $d_n(x_{1,n})$ *is equivalent to the arithmetic mean of the* $(n-1)$*-way* *distance measures $d_{n-1}(x_{1,n}^{-i})$. If not only (15) but also (17) is valid, then (19) is the lower bound of $d_n(x_{1,n})$. Note that (19) is sharper than (23).*

Next, we focus on the upper bound of n-way distance $d_n(x_{1,n})$.

Theorem 3. *If* (15) *holds, then for n-way distance $d_n(x_{1,n})$ we have*

$$d_n(x_{1,n}) \leq \frac{mp}{nk} \sum_{i=1}^{n} d_{n-1}(x_{1,n}^{-i}) \tag{24}$$

for $m \in \{2, 3, ..., n-1\}$, and

$$d_n(x_{1,n}) \leq \frac{(n-1)p}{n(k-1)} \sum_{i=1}^{n} d_{n-1}(x_{1,n}^{-i}) \tag{25}$$

for $m = n$.

Proof: Supplying (6) with $(n+1)$-tuple $(x_1, ..., x_n, x_n)$ we obtain

$$k \cdot d_n(x_{1,n}) \leq p \sum_{i=1}^{m} d_{n-1}(x_{1,n}^{-i}) \tag{26}$$

for $m \in \{2, 3, ..., n-1\}$, and

$$(k-1) \cdot d_n(x_{1,n}) \leq p \sum_{i=1}^{n-1} d_{n-1}(x_{1,n}^{-i}) \tag{27}$$

for $m = n$. We have n variants of $d_{n-1}(x_{1,n}^{-i})$ in (26) and (27). Considering all n variants of (26) and (27), each $d_{n-1}(x_{1,n}^{-i})$ occurs a total of m times. Adding up all n variants of (26) and (27), followed by division by nk, respectively $n(k-1)$, we obtain (24) and (25).
■

5. $(n-1)$-Way metrics Implied by n-Way Metrics

In this section we study what $(n-1)$-way metrics are implied by the family of n-way metrics defined in (6). Again n-way distance measure $d_n(x_{1,n})$ satisfies minimality, total symmetry, and (10). It is interesting to note that, although we use condition (15) throughout this section, the results do not depend on the value of p in (15). Unless stated otherwise we use $n \geq 3$ throughout this section.

Proposition 3. *If* (15) *and* (17) *hold, then* (6) *implies*

$$k \cdot d_{n-1}(x_{1,n-1}) \leq \sum_{i=1}^{m} d_{n-1}(x_{1,n}^{-i}) \tag{28}$$

for $m \in \{2, 3, ..., n-1\}$, *and*

$$(k-1) \cdot d_{n-1}(x_{1,n-1}) \leq \sum_{i=1}^{n-1} d_{n-1}(x_{1,n}^{-i}) \tag{29}$$

for $m = n$ *and* $k \in (1, m)$.

Proof: Inequalities (28) and (29) are obtained from combining (18) with (26), respectively (27).
■

As it turns out, condition (17) is not required to obtain (28). We first show that if (15) holds, then (6) implies (28) for $n \geq 4$ and $m \in \{2, 3, ..., n-2\}$.

Proposition 4. *If* (15) *holds, then* (6) *implies* (28) *for* $n \geq 4$ *and* $m \in \{2, 3, ..., n-2\}$.

Proof: Supplying (6) with $(n+1)$-tuple $(x_1, ..., x_{n-1}, x_{n-1}, x_n)$, we obtain (28).
■

Proposition 4 suggests that the metrics characterized by $m = n - 1$ and $m = n$ have somewhat different properties. These two cases are considered in the remainder of this section.

Using $m = n-1$ in (6) we obtain

$$k \cdot d_n(x_{1,n}) \leq \sum_{i=1}^{n-1} d_n(x_{1,n+1}^{-i}). \tag{30}$$

Using $m = n-1$ in (28) we obtain

$$k \cdot d_{n-1}(x_{1,n-1}) \leq \sum_{i=1}^{n-1} d_{n-1}(x_{1,n}^{-i}). \tag{31}$$

In Theorem 4, we show that if (15) holds, then inequality (30) does not imply (31), but the weaker parametrized inequality

$$k \cdot d_{n-1}(x_{1,n-1}) \leq \left[\frac{(n-2)(k+1)+1}{(n-1)k}\right] \sum_{i=1}^{n-1} d_{n-1}(x_{1,n}^{-i}). \tag{32}$$

Let us first show that that inequality (32) is weaker than (31).

Proposition 5. *Let* $k \in (0, n-1)$. *Inequality* (31) *implies* (32).

Proof: It must be shown that

$$\frac{(n-2)(k+1)+1}{(n-1)k} > 1. \tag{33}$$

We have (33) if and only

$$\begin{gathered}(n-2)(k+1)+1 > (n-1)k \\ \Updownarrow \\ n-1 > k.\end{gathered} \tag{34}$$

Inequality (34) is true under the conditions of the assertion.
■

Theorem 4. *Suppose* (15) *holds and let* $k \in (0, n-1)$. *Then* (30) *implies* (32).

Proof: Supplying (30) with $(n+1)$-tuple $(x_1, ..., x_{n-1}, x_{n-1}, x_{n+1})$ and replacing x_{n+1} by x_n in the result, we obtain

$$p\,k \cdot d_{n-1}(x_{1,n-1}) \leq p \sum_{i=1}^{n-2} d_{n-1}(x_{1,n}^{-i}) + d_n(x_{1,n}). \tag{35}$$

Using $m = n-1$ in (26) we obtain

$$k \cdot d_n(x_{1,n}) \leq p \sum_{i=1}^{n-1} d_{n-1}(x_{1,n}^{-i}). \tag{36}$$

Adding (36) to $k \times (35)$ yields

$$k^2 \cdot d_{n-1}(x_{1,n-1}) \leq (k+1) \sum_{i=1}^{n-2} d_{n-1}(x_{1,n}^{-i}) + d_{n-1}(x_{1,n}^{-(n-1)}). \tag{37}$$

Apart from variant $d_{n-1}(x_{1,n-1})$ on the left-hand side of (37), there are $(n-1)$ variants of d_{n-1}, e.g., variant $d_{n-1}(x_{1,n}^{-(n-1)})$, on the right-hand side of (37). We have $(n-1)$ variants of (37) by varying all $(n-1)$ variants of d_{n-1} on the right-hand side of (37). Adding up all $(n-1)$ variants of (37), followed by division by $(n-1)k$, yields (32).
■

Using $m = n$ in (6) we obtain (5). From Proposition 3 we know that if both (15) and (17) hold, then (5) implies (29). If only (15) is valid, (5) implies the parametrized inequality

$$(k-1)\cdot d_{n-1}(x_{1,n-1}) \leq \left[1+\frac{n-k}{(n-1)k}\right]\sum_{i=1}^{n-1} d_{n-1}(x_{1,n}^{-i}). \tag{38}$$

Note that the inequality (38) is weaker than (29) because $n > k$, and the quantity

$$1+\frac{n-k}{(n-1)k} \tag{39}$$

on the right-hand side in (38) is > 1.

Theorem 5. *If* (15) *holds, then for* $k \in (1, n)$, (5) *implies* (38).

Proof: Supplying (5) with $(n+1)$-tuple $(x_1, ..., x_{n-1}, x_{n-1}, x_{n+1})$ and replacing x_{n+1} by x_n in the result, we obtain

$$p\,k\cdot d_{n-1}(x_{1,n-1}) \leq p\sum_{i=1}^{n-2} d_{n-1}(x_{1,n}^{-i}) + 2d_n(x_{1,n}). \tag{40}$$

Adding $2\times(27)$ to $(k-1)\times(40)$ we obtain

$$k(k-1)\cdot d_{n-1}(x_{1,n-1}) \leq (k+1)\sum_{i=1}^{n-2} d_{n-1}(x_{1,n}^{-i}) + 2d_{n-1}(x_{1,n}^{-(n-1)}). \tag{41}$$

Apart from variant $d_{n-1}(x_{1,n-1})$ on the left-hand side of (41), there are $(n-1)$ variants of d_{n-1} on the right-hand side of (41). We have $(n-1)$ variants of (41) by varying all $(n-1)$ variants of d_{n-1} on the right-hand side of (41). Adding up these $(n-1)$ variants of (41), followed by division by $(n-1)k$, yields (38).
■

With respect to the quantity (39), we have the limit

$$\lim_{n\to\infty}\left[1+\frac{n-k}{(n-1)k}\right] = 1+\frac{1}{k}.$$

Because of this limit, it may be argued that inequality (38) is more interesting for small n and k.

Using $k = n-1$ in (5) we obtain the polyhedron inequality (4).

Example 5. *If (15) holds, then for* $n \geq 3$ *the polyhedron inequality (4) implies*

$$(n-2)\cdot d_{n-1}(x_{1,n-1}) \leq \left[1+\frac{1}{(n-1)^2}\right]\sum_{i=1}^{n-1} d_{n-1}(x_{1,n}^{-i}). \tag{42}$$

We obtain (42) by using $k = n - 1$ in (38) and noting that $n^2 - 2n + 2 = (n-1)^2 + 1$. The quantity

$$1 + \frac{1}{(n-1)^2}$$

on the right-hand side in (42) with limit

$$\lim_{n\to\infty}\left[1 + \frac{1}{(n-1)^2}\right] = 1,$$

approximates 1 rapidly as n increases. As shown in Heiser and Bennani (1997, p. 192), if (15) holds then the strong tetrahedron inequality (2) does not imply the triangle inequality, but the weaker parametrized triangle inequality

$$d(x_1, x_2) \leq \frac{5}{4}\left[d(x_2, x_3) + d(x_1, x_3)\right].$$

Furthermore, if (15) holds, then

$$3d_4(x_{1,4}) \leq d_4(x_{2,5}) + d_4(x_{1,5}^{-2}) + d_4(x_{1,5}^{-3}) + d_4(x_{1,5}^{-4})$$

does not imply inequality (2), but the weaker parametrized inequality

$$2d_3(x_{1,3}) \leq \frac{10}{9}\left[d_3(x_{2,4}) + d_3(x_{1,4}^{-2}) + d_3(x_{1,4}^{-3})\right].$$

6. Bennani-Heiser Dissimilarity Coefficients

In Example 2 we showed that the n-way perimeter distance satisfies the strong polyhedron inequality (4) if the triangle inequality holds. In this section we consider additional examples that satisfy (4). The distance measures are the complements of n-way similarity coefficients that may be used to assess the resemblance of n binary (0,1) sequences at a time (Warrens 2009a). These measures extend similarity coefficients for two binary sequences or 2×2 tables (see, e.g., Warrens 2008b,c,d,e).

For n binary sequences, we will use the following notation. Let $p_n(x_{1,n}^1)$ denote the proportion of 1s that sequences or objects $x_1, x_2, ..., x_n$ of the same length share in the same positions. Furthermore, let $p_n(x_{1,i,n}^{1,0,1})$ denote the proportion of 1s in sequences $x_1, ..., x_n$ and 0 in sequence x_i in the same positions. Moreover, denote by $p_{n-1}(x_{1,i,n}^{1,-,1})$ the proportion of 1s that sequences $x_1, ..., x_n$ have in the same positions, but where sequence x_i drops out.

The following relation between the proportions defined above will repeatedly be used:

$$p_{n-1}(x^{1,-,1}_{1,i,n}) = p_n(x^1_{1,n}) + p_n(x^{1,0,1}_{1,i,n}). \tag{43}$$

We study the following three n-way dissimilarity coefficients:

$$d^{\mathrm{RR}}_n = 1 - p_n(x^1_{1,n}),$$
$$d^{\mathrm{SM}}_n = 1 - p_n(x^1_{1,n}) - p_n(x^0_{1,n}),$$

and

$$d^{\mathrm{J}}_n = 1 - \frac{p_n(x^1_{1,n})}{1 - p_n(x^0_{1,n})}.$$

Functions d^{RR}_n, d^{SM}_n and d^{J}_n are the complements of the n-way Russel-Rao (1940) coefficient, simple matching coefficient (Sokal and Michener 1958), and n-way Jaccard (1912) coefficient, respectively, that are studied in Warrens (2009a). Some properties of these distance measures for the two-way case can be found in Warrens (2009b). Coefficients d^{SM}_3 and d^{J}_3 were first formulated and studied in Bennani-Dosse (1993) and Heiser and Bennani (1997). It should be noted that d^{J}_n is already used in Cox, Cox and Branco (1991, p. 200) (see also Warrens 2008a). Functions d^{RR}_n, d^{SM}_n and d^{J}_n are called Bennani-Heiser coefficients in Warrens (2009a) because they can be defined using only the quantities $p_n(x^1_{1,n})$ and $p_n(x^0_{1,n})$.

Theorems 6, 7 and 8, respectively, illustrate that functions d^{RR}_n, d^{SM}_n and d^{J}_n satisfy the strong polyhedron inequality (4). For d^{SM}_n and d^{J}_n, the proofs for $n = 2$ can be found in Gower and Legendre (1986), and for $n = 3$ in Heiser and Bennani (1997, p. 197). For d^{J}_n, the proofs for $n = 3, 4$ can be found in Warrens (2008a). The proofs of Theorems 6, 7 and 8 below are generalizations of the tools presented in Heiser and Bennani (1997).

Theorem 6. *The function* d^{RR}_n *satisfies* (4).

Proof: Using d^{RR}_n in (4) we obtain

$$(n-1) - (n-1)\cdot p_n(x^1_{1,n}) \le n - \sum_{i=1}^{n} p_n(x^{1,-,1}_{1,i,n+1})$$
$$\Updownarrow$$
$$1 + (n-1)\cdot p_n(x^1_{1,n}) \ge \sum_{i=1}^{n} p_n(x^{1,-,1}_{1,i,n+1}). \tag{44}$$

Using (43), (44) becomes

$$1 + (n-1) \cdot p_{n+1}(x^1_{1,n}, x^1_{n+1}) + (n-1) \cdot p_{n+1}(x^1_{1,n}, x^0_{n+1}) \geq \\ n \cdot p_{n+1}(x^1_{1,n+1}) + \sum_{i=1}^{n} p_{n+1}(x^{1,0,1}_{1,i,n+1}),$$

which equals

$$1 + (n-1) \cdot p_{n+1}(x^1_{1,n}, x^0_{n+1}) \geq p_{n+1}(x^1_{1,n+1}) + \sum_{i=1}^{n} p_{n+1}(x^{1,0,1}_{1,i,n+1}). \quad (45)$$

All proportions on the right-hand side of (45) are different and their sum is ≤ 1. This completes the proof.
■

Theorem 7. *The function* d_n^{SM} *satisfies* (4).

Proof: Using d_n^{SM} in (4) gives

$$(n-1) - (n-1) \cdot p_n(x^1_{1,n}) - (n-1) \cdot p_n(x^0_{1,n}) \leq \\ n - \sum_{i=1}^{n} p_n(x^{1,-,1}_{1,i,n+1}) - \sum_{i=1}^{n} p_n(x^{0,-,0}_{1,i,n+1}),$$

which equals

$$1 + (n-1) \cdot p_n(x^1_{1,n}) + (n-1) \cdot p_n(x^0_{1,n}) \geq \\ \sum_{i=1}^{n} p_n(x^{1,-,1}_{1,i,n+1}) + \sum_{i=1}^{n} p_n(x^{0,-,0}_{1,i,n+1}). \quad (46)$$

Using (43), (46) becomes

$$1 + (n-1)\left[p_{n+1}(x^1_{1,n}, x^1_{n+1}) + p_{n+1}(x^1_{1,n}, x^0_{n+1})\right] \\ +(n-1)\left[p_{n+1}(x^0_{1,n}, x^1_{n+1}) + p_{n+1}(x^0_{1,n}, x^0_{n+1})\right] \geq \\ n \cdot p_{n+1}(x^1_{1,n+1}) + \sum_{i=1}^{n} p_{n+1}(x^{1,0,1}_{1,i,n+1}) \\ + n \cdot p_{n+1}(x^0_{1,n+1}) + \sum_{i=1}^{n} p_{n+1}(x^{0,1,0}_{1,i,n+1}),$$

which equals

$$1 + (n-1)\left[p_{n+1}(x^1_{1,n}, x^0_{n+1}) + p_{n+1}(x^0_{1,n}, x^1_{n+1})\right] \geq \\ p_{n+1}(x^1_{1,n+1}) + p_{n+1}(x^0_{1,n+1}) + \sum_{i=1}^{n} p_{n+1}(x^{1,0,1}_{1,i,n+1}) + \sum_{i=1}^{n} p_{n+1}(x^{0,1,0}_{1,i,n+1}). \quad (47)$$

All proportions on the right-hand side of (47) are different and their sum is ≤ 1. This completes the proof.
■

Theorem 8 shows that function d_n^{J} satisfies polyhedron inequality (4). In the proof of Theorem 8, the following relation between n-way coefficients d_n^{SM} and d_n^{J} is used:

$$d_n^{\mathrm{SM}} = \left[1 - p_n(x_{1,n}^0)\right] \cdot d_n^{\mathrm{J}}. \tag{48}$$

Theorem 8. *The function d_n^{J} satisfies* (4).

Proof: It holds that

$$\begin{aligned} 1 \geq\ & p_{n+1}(x_{1,n+1}^1) + \sum_{i=1}^{n+1} p_{n+1}(x_{1,i,n+1}^{1,0,1}) \\ & + p_{n+1}(x_{1,n+1}^0) + \sum_{i=1}^{n+1} p_{n+1}(x_{1,i,n+1}^{0,1,0}). \end{aligned} \tag{49}$$

Note that for $n = 2$, inequality (49) becomes an equality. Adding

$$(n-1)\left[p_{n+1}(x_{1,n}^1, x_{n+1}^0) + p_{n+1}(x_{1,n}^0, x_{n+1}^1)\right]$$

to both sides of (49), we obtain

$$\begin{aligned} & \sum_{i=1}^{n} d_n^{\mathrm{SM}}(x_{1,n+1}^{-i}) - (n-1) \cdot d_n^{\mathrm{SM}}(x_{1,n}) \geq \\ & \qquad n\left[p_{n+1}(x_{1,n}^1, x_{n+1}^0) + p_{n+1}(x_{1,n}^0, x_{n+1}^1)\right]. \end{aligned} \tag{50}$$

Using (48) in (50), we obtain

$$\begin{aligned} & \left[1 - p_{n+1}(x_{1,n+1}^0)\right] \cdot \left(\sum_{i=1}^{n} d_n^{\mathrm{J}}(x_{1,n+1}^{-i}) - (n-1) \cdot d_n^{\mathrm{J}}(x_{1,n})\right) \geq \\ & n \cdot p_{n+1}(x_{1,n}^1, x_{n+1}^0) + \sum_{i=1}^{n}\left[d_n^{\mathrm{J}}(x_{1,n+1}^{-i}) \cdot p_{n+1}(x_{1,i,n+1}^{0,1,0})\right] + \\ & \qquad p_{n+1}(x_{1,n}^0, x_{n+1}^1)\left[n - (n-1) \cdot d_n^{\mathrm{J}}(x_{1,n})\right]. \end{aligned}$$

Since $1 - p_{n+1}(x_{1,n+1}^0) \geq 0$ and $d_n^{\mathrm{J}} \leq 1$, we conclude that

$$\sum_{i=1}^{n} d_n^{\mathrm{J}}(x_{1,n+1}^{-i}) - (n-1) \cdot d_n^{\mathrm{J}}(x_{1,n}) \geq 0.$$

This completes the proof.
■

7. Discussion

In this paper we studied a family of n-way metrics that extend the usual two-way metric. The three-way metrics introduced by Joly and Le Calvé (1995) and Heiser and Bennani (1997) and the n-way metrics studied in Deza and Rosenberg (2000, 2005) and Warrens (2008a) are in the family. The family gives an indication of the many possible extensions for introducing n-way metricity. We were particularly interested in how n-way metrics and n-way distance measures are related to their $(n-1)$-way counterparts. Although no well-established multi-way metric structure emerged from this study, we considered in Example 2 and Section 6, various interesting functions that satisfy the polyhedron inequality (4).

Inequality (4) generalizes the strong tetrahedron inequality proposed in Heiser and Bennani (1997). It should be noted that, although there are many cases in which the strong tetrahedron inequality (and inequality (4)) holds, the three-way data analysis models from the literature presented in, e.g., Cox et al. (1991), Heiser and Bennani (1997), Gower and De Rooij (2003) and Nakayama (2005), can be used regardless of the validity of the tetrahedron inequality. For example, the three-way multidimensional scaling methods proposed in Gower and De Rooij (2003) merely require that the underlying two-way dissimilarity measures satisfy the triangle inequality, since the scaling method uses three-way dissimilarity functions that are linear transformations of the two-way dissimilarities.

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