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On the uniqueness of correspondence analysis solutions

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In correspondence analysis (CA), the rows and columns of a contingency table are optimally represented in a k-dimensional approximation, where it is common to set $k = 3$ (which includes a so-called trivial dimension). Since CA is a dimension reduction technique, we might expect that the k-dimensional approximation is not unique, i.e. there exist several contingency tables with the same k-dimensional approximation. Interestingly, Van de Velden et al. [17] find in their computational experiments that 3-dimensional CA solutions are unique up to rotation, which leads to the question whether this is always the case. We show that k-dimensional CA solutions are not necessarily unique. That is, two distinct contingency tables may have the same k-dimensional approximation. We present necessary and sufficient conditions for the non-uniqueness of CA solutions, which hold for any value of k. Based on our sufficient conditions, we present a procedure to generate contingency tables with the same k-dimensional solution. Finally, we note that it is difficult to satisfy the necessary conditions, which suggests that CA solutions are most likely unique in practice.

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1. Introduction

Correspondence analysis (CA) is a multivariate statistical technique [1]. The aim of CA is to project the rows and columns of a two-way contingency table, which contains the frequencies of co-occurrences of two categorical variables, onto a low-dimensional space. This k-dimensional solution is often visualised in a plane by setting $k = 3$ and excluding the first dimension, which contains the scaled row and column sums. CA is applied on a multitude of applications, see for instance Greenacre [7,8] and the references therein.

Since CA projects two-way contingency tables in a low-dimensional space, we might expect that the low-dimensional solution is not unique. By unique, we mean that there exists only one table that yields, up to orthogonal rotation, the given low-dimensional CA solution. Van de Velden et al. [17] perform an extensive computational study, in which they investigate the uniqueness of 3-dimensional CA solutions. In their experiments, they never find two tables with the same 3-dimensional CA solution, which leads to the hypothesis that CA solutions are unique. In this paper, we demonstrate that k-dimensional CA solutions are not necessarily unique, for any value of k.

The contribution of this paper is as follows. First, we provide necessary conditions that a contingency table must satisfy for its CA solution to be non-unique. Afterwards, we provide sufficient conditions on the non-uniqueness of k-dimensional CA solutions. Secondly, based on the sufficient conditions, we present a procedure to generate contingency tables that have the same k-dimensional CA solution.

Our sufficient conditions imply that contingency tables with a non-unique CA solution exist for any given value of k. Furthermore, from the necessary conditions it follows that two tables with the same low-dimensional CA solution, are uniquely related through a linear transformation matrix. Finally, based on the difficulty of satisfying the necessary conditions, we deduce that CA solutions are likely to be unique in practice, which is in line with the experiments of Van de Velden et al. [17].

In the literature, integer matrices with given row and column sums and their properties have been studied by, amongst others, Brualdi [3], Brualdi and Michael [5], Brualdi and Dahl [4] and Chen [6]. One of the properties of such an integer matrix is the lonesum property. An integer matrix is called lonesum if it can be uniquely reconstructed from its row and column sums. Ryser [13,14] prove that a binary matrix (each entry is 0 or 1) is lonesum if and only if its 2×2 submatrices satisfy a certain condition. Brewbaker [2] exploits this result to compute the number of binary lonesum matrices for a given dimension. The results of Ryser [13,14] and Brewbaker [2] are generalised by Kim et al. [11] and Lee [12]. Kim et al. [11] present results for general integer matrices and Lee [12] extends these results to integer matrices in a multidimensional space. In general, two-dimensional integer matrices are not expected to be lonesum, i.e. there are multiple matrices with the same marginals. In this paper, we show that integer matrices can often be uniquely reconstructed when a k-dimensional CA solution is known (where the first dimension includes the scaled row and column sums). We contribute to the literature by providing necessary and sufficient conditions for an integer matrix to have a non-unique CA solution. Moreover, our main theorems can also be applied to non-integer matrices, and the results are therefore more generally applicable.

The remainder of this paper is structured as follows. We present CA notation and stylised examples of (non-)unique CA solutions in Section 2. In Section 3, we describe a linear relationship between contingency tables and its low-dimensional solution. Next, we derive necessary conditions of non-unique CA solutions in Section 4. In Section 5, we provide sufficient conditions and introduce a method to generate contingency tables with a non-unique CA solution. We discuss the implications of the main results and conclude in Sections 6 and 7, respectively.

2. Problem description

In this section, we present CA, where we use similar notation as Van de Velden et al. [17]. Let $\mathbf{F}$ be an $n_r \times n_c$ matrix, where f_{ij} denotes the number of times each observation i, j occurs. We assume without loss of generality $n_r \leq n_c$. We denote the total number of observations as $s = \sum_i \sum_j f_{ij} = \mathbf{1}_{n_r}^\top \mathbf{F} \mathbf{1}_{n_c}$, where $\mathbf{1}_n$ is a vector containing ones of length n. The row and column totals are defined as $\mathbf{r}$ and $\mathbf{c}$, respectively. We denote the diagonal matrix containing the row and column totals by $\mathbf{D}_r$ and $\mathbf{D}_c$, such that $\mathbf{r} = \mathbf{F}\mathbf{1}_{n_c} = \mathbf{D}_r \mathbf{1}_{n_r}$ and $\mathbf{c} = \mathbf{F}^\top \mathbf{1}_{n_r} = \mathbf{D}_c \mathbf{1}_{n_c}$.

Consider the singular value decomposition (SVD) of the standardised matrix $\tilde{\mathbf{F}} = \mathbf{D}_r^{-\frac{1}{2}} \mathbf{F} \mathbf{D}_c^{-\frac{1}{2}}$, that is,

$$\tilde{\mathbf{F}} = \tilde{\mathbf{U}} \tilde{\mathbf{\Lambda}} \tilde{\mathbf{V}}^\top,$$

where $\tilde{\mathbf{U}}$ and $\tilde{\mathbf{V}}$ are orthonormal, $\tilde{\mathbf{\Lambda}}$ is a diagonal matrix of singular values in non-increasing order and $\tilde{\boldsymbol{\lambda}} = \tilde{\mathbf{\Lambda}} \mathbf{1}_{n_r}$ is a vector of singular values. Due to the standardisation all singular values lie in the interval $[0, 1]$. The largest singular value is 1, which we refer to as the trivial solution, and the corresponding columns of $\tilde{\mathbf{U}}$ and $\tilde{\mathbf{V}}$ are $\frac{1}{\sqrt{s}} \mathbf{D}_r^{1/2} \mathbf{1}_{n_r}$ and $\frac{1}{\sqrt{s}} \mathbf{D}_c^{1/2} \mathbf{1}_{n_c}$, see for example Van de Velden and Neudecker [16].

The k-dimensional approximation is determined by selecting the first k singular values (including the trivial solution) of $\tilde{\mathbf{\Lambda}}$ and the corresponding columns of $\tilde{\mathbf{U}}$ and $\tilde{\mathbf{V}}$, where we assume without loss of generality that $k \leq n_r \leq n_c$. We can partition the matrices as

$$\tilde{\mathbf{U}} = \begin{pmatrix} \tilde{\mathbf{U}}_k & \tilde{\mathbf{U}}_c \end{pmatrix}, \; \tilde{\mathbf{V}} = \begin{pmatrix} \tilde{\mathbf{V}}_k & \tilde{\mathbf{V}}_c \end{pmatrix} \text{ and } \tilde{\mathbf{\Lambda}} = \begin{pmatrix} \tilde{\mathbf{\Lambda}}_k & \\ & \tilde{\mathbf{\Lambda}}_c \end{pmatrix}.$$

We rewrite the SVD on the standardised matrix $\tilde{\mathbf{F}}$ to obtain

$$\begin{aligned} \tilde{\mathbf{F}} &= \tilde{\mathbf{U}} \tilde{\mathbf{\Lambda}} \tilde{\mathbf{V}}^\top \\ &= \begin{pmatrix} \tilde{\mathbf{U}}_k & \tilde{\mathbf{U}}_c \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{\Lambda}}_k & \\ & \tilde{\mathbf{\Lambda}}_c \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{V}}_k^\top \\ \tilde{\mathbf{V}}_c^\top \end{pmatrix} \end{aligned}$$

$$= \mathbf{H} + \tilde{\mathbf{U}}_c \tilde{\mathbf{\Lambda}}_c \tilde{\mathbf{V}}_c^\top,$$

where $\mathbf{H} = \tilde{\mathbf{U}}_k \tilde{\mathbf{\Lambda}}_k \tilde{\mathbf{V}}_k^\top$ is the k-dimensional approximation of $\tilde{\mathbf{F}}$ and $\tilde{\mathbf{U}}_c \tilde{\mathbf{\Lambda}}_c \tilde{\mathbf{V}}_c^\top$ is the remainder. The matrix $\mathbf{F}$ can be expressed in terms of the k-dimensional approximation and the remainder, resulting in

$$\mathbf{F} = \mathbf{D}_r^{\frac{1}{2}} (\mathbf{H} + \tilde{\mathbf{U}}_c \tilde{\mathbf{\Lambda}}_c \tilde{\mathbf{V}}_c^\top) \mathbf{D}_c^{\frac{1}{2}}. \tag{1}$$

In CA, it is common to set $k = 3$ and discard the trivial solution, such that the k-dimensional approximation can be visualised in the plane using the so-called row and column coordinate matrices

$$\mathbf{R}_k = \mathbf{D}_r^{-\frac{1}{2}} \tilde{\mathbf{U}}_k \tilde{\mathbf{\Lambda}}_k^{\alpha}, \tag{2}$$

$$\mathbf{C}_k = \mathbf{D}_c^{-\frac{1}{2}} \tilde{\mathbf{V}}_k \tilde{\mathbf{\Lambda}}_k^{1-\alpha}, \tag{3}$$

where the parameter α is often set to the values 0 or 1 [15,8]. Throughout this paper, we assume without loss of generality that $\alpha = 1$. We consider Assumption 2.1, which states that the k-th singular value is strictly larger than the $k+1$-th singular value of $\tilde{\mathbf{F}}$, such that the k-dimensional approximation is uniquely determined and hence the k-dimensional approximation is well-defined.

Assumption 2.1. Let $\tilde{\lambda}_k$ and $\tilde{\lambda}_{k+1}$ be the k-th and $k+1$-th singular values, we assume that $\tilde{\lambda}_k > \tilde{\lambda}_{k+1}$.

Using the previous assumptions and definitions we state a first definition of a k-dimensional CA solution.

Definition 2.2 *(A k-dimensional CA solution in terms of coordinate matrices).* A k-dimensional CA solution of a matrix $\mathbf{F}$ consists of matrices $\mathbf{R}_k, \mathbf{C}_k, \mathbf{D}_r$ and $\mathbf{D}_c$.

In CA, it is common to visualise only matrices $\mathbf{R}_k$ and $\mathbf{C}_k$ in a two-dimensional figure. We assume in Definition 2.2 that the marginals $\mathbf{D}_r$ and $\mathbf{D}_c$ are known. The row and column coordinate matrices can be rotated to improve interpretability [15]. Given any invertible $\mathbf{A}$ of appropriate size, multiplying $\mathbf{R}_k$ and $\mathbf{C}_k$ by $\mathbf{A}$ and $\mathbf{A}^{-1}$, respectively, results in a rotated solution. When considering such pairs of rotations the coordinate matrices $\mathbf{R}_k$ and $\mathbf{C}_k$ are not unique. In this paper, we investigate the uniqueness of CA solutions without rotations. While Definition 2.2 is often used in practice to visualise CA solutions, for our purposes it is more convenient to make use of an alternative CA definition, namely Definition 2.3, which is equivalent, as matrices $\mathbf{R}_k$ and $\mathbf{C}_k$ can be obtained from $\mathbf{H}$ and vice versa [17].

Definition 2.3 *(A k-dimensional CA solution).* A k-dimensional CA solution of $\mathbf{F}$ consists of the matrices $\mathbf{H}, \mathbf{D}_r$ and $\mathbf{D}_c$.

Let $h(\mathbf{F})$ denote a function that maps a matrix $\mathbf{F}$ to its k-dimensional approximation $\mathbf{H}$, which is unique under Assumption 2.1. The first aim of this paper is to determine under which conditions there exist matrices with the same marginals as $\mathbf{F}$ that have the same CA solution. Or using the introduced notation: under which conditions are there different matrices $\mathbf{F}^o$ and $\mathbf{F}^a$ with the same marginals such that $h(\mathbf{F}^o) = h(\mathbf{F}^a)$? As a second question, can we systematically generate matrices with the same k-dimensional approximation?

The examples below illustrate that the number of matrices with the same k-dimensional solution is instance dependent. We consider a 3-dimensional approximation and we denote $diag(\mathbf{A})$ as the diagonal elements of a matrix $\mathbf{A}$. We present two examples where either one or three matrices have the same CA solution. The example containing a unique CA solution can be verified by enumerating the matrices satisfying the row and column marginals, which is possible since the given examples are relatively small, while the example containing three matrices with the same k-dimensional solution can be verified by computing the corresponding CA solutions.

Example 2.4. Consider the matrix $\mathbf{F}^o$ and its (rounded) singular values $\tilde{\boldsymbol{\lambda}}^o$ shown below. We can verify by enumeration that there is no other matrix having the same CA solution (based on Definition 2.3).

$$\mathbf{F}^o = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 3 & 5 & 1 & 1 \\ 4 & 6 & 1 & 1 \end{pmatrix}$$

$$\tilde{\boldsymbol{\lambda}}^o = \begin{pmatrix} 1 & 0.33 & 0.14 & 0.00 \end{pmatrix}^\top$$

Example 2.5. Consider the matrix $\mathbf{F}^o$ below and its (rounded) singular values $\tilde{\boldsymbol{\lambda}}^o$. It can be verified that $h(\mathbf{F}^o) = h(\mathbf{F}_1^a) = h(\mathbf{F}_2^a)$. That is, matrices $\mathbf{F}^o$, $\mathbf{F}_1^a$ and $\mathbf{F}_2^a$ have the same $k = 3$-dimensional solution.

$$\mathbf{F}^o = \begin{pmatrix} 11 & 0 & 0 & 0 \\ 0 & 10 & 0 & 0 \\ 0 & 0 & 8 & 3 \\ 0 & 0 & 3 & 8 \end{pmatrix} \qquad \mathbf{F}_1^a = \begin{pmatrix} 11 & 0 & 0 & 0 \\ 0 & 10 & 0 & 0 \\ 0 & 0 & 7 & 4 \\ 0 & 0 & 4 & 7 \end{pmatrix} \qquad \mathbf{F}_2^a = \begin{pmatrix} 11 & 0 & 0 & 0 \\ 0 & 10 & 0 & 0 \\ 0 & 0 & 6 & 5 \\ 0 & 0 & 5 & 6 \end{pmatrix}$$

$$\tilde{\boldsymbol{\lambda}}^o = \begin{pmatrix} 1 & 0.71 & 0.69 & 0.38 \end{pmatrix}^\top \qquad \tilde{\boldsymbol{\lambda}}_1^a = \begin{pmatrix} 1 & 0.71 & 0.69 & 0.23 \end{pmatrix}^\top \qquad \tilde{\boldsymbol{\lambda}}_2^a = \begin{pmatrix} 1 & 0.71 & 0.69 & 0.08 \end{pmatrix}^\top$$

3. Relation to inverse correspondence analysis

We consider a k-dimensional CA solution of $\mathbf{F}$ to be unique, if there is no other matrix $\hat{\mathbf{F}}$ with the same k-dimensional approximation. Van de Velden et al. [17] are interested in retrieving a matrix $\mathbf{F}$ that satisfies a given k-dimensional CA solution, which is known as the inverse correspondence analysis problem. They show, in a computational study consisting of thousands of randomly generated tables, that 3-dimensional CA solutions of a contingency table are always unique up to rotation [15]. To see whether this holds theoretically, we investigate if we can identify conditions under which there exist different matrices $\mathbf{F}$ and $\hat{\mathbf{F}}$ that have the same k-dimensional CA solution.

If we can retrieve two matrices $\mathbf{F}$ and $\hat{\mathbf{F}}$ that satisfy (1) and have the same k-dimensional CA solution, we have a pair of matrices such that $h(\mathbf{F}) = h(\hat{\mathbf{F}})$. However, finding a matrix that satisfies (1) for a given $\mathbf{H}$ is a non-linear problem, since matrices $\tilde{\mathbf{U}}_c$, $\tilde{\mathbf{\Lambda}}_c$ and $\tilde{\mathbf{V}}_c$ are unknown. Groenen and Van de Velden [9] show that it is possible to rewrite this to a linear problem, which provides a necessary condition for satisfying (1). In this section, we present this linear relationship between a matrix $\mathbf{F}$ and its k-dimensional CA solution. This means that if another matrix $\hat{\mathbf{F}}$ has the same k-dimensional CA solution as $\mathbf{F}$, then both matrices satisfy the same linear relationship.

To verify that a k-dimensional CA solution is unique we can use the known matrices shown in Definition 2.3, where $\mathbf{H}$ can be decomposed into the matrices $\tilde{\mathbf{U}}_k$, $\tilde{\mathbf{V}}_k$ and $\tilde{\mathbf{\Lambda}}_k$. On the other hand, the matrices $\tilde{\mathbf{U}}_c$, $\tilde{\mathbf{V}}_c$ and $\tilde{\mathbf{\Lambda}}_c$ are unknown. Matrices $\tilde{\mathbf{U}}$ and $\tilde{\mathbf{V}}$ are orthonormal, which means that each column of $\tilde{\mathbf{U}}_\mathbf{c}$ and $\tilde{\mathbf{V}}_\mathbf{c}$ is orthogonal to each column of $\tilde{\mathbf{U}}_k$ and $\tilde{\mathbf{V}}_k$, respectively. Let $\tilde{\mathbf{U}}_0$ and $\tilde{\mathbf{V}}_0$ denote the null space of $\tilde{\mathbf{U}}_k$ and $\tilde{\mathbf{V}}_k$, respectively, which can be obtained using

$$\begin{aligned}\tilde{\mathbf{U}}_k^\top \tilde{\mathbf{U}}_0 &= \mathbf{0}_{(k,n_r-k)},\\ \tilde{\mathbf{V}}_k^\top \tilde{\mathbf{V}}_0 &= \mathbf{0}_{(k,n_c-k)},\end{aligned}$$

where $\mathbf{0}_{m,n}$ is a zero matrix of size $m \times n$. There exist orthonormal matrices $\mathbf{W}$ and $\mathbf{Q}$ such that

$$\tilde{\mathbf{U}}_c = \tilde{\mathbf{U}}_0 \mathbf{W}, \tag{4}$$

$$\tilde{\mathbf{V}}_c = \tilde{\mathbf{V}}_0 \mathbf{Q}, \tag{5}$$

which shows that the unknown matrices $\tilde{\mathbf{U}}_c$ and $\tilde{\mathbf{V}}_c$ can be obtained up to rotation.

We define $\mathbf{G} = \mathbf{W}\tilde{\mathbf{\Lambda}}_c\mathbf{Q}^\top$ and substitute (4) and (5) into the SVD of $\tilde{\mathbf{F}}$ to obtain

$$\begin{aligned}\tilde{\mathbf{F}} &= \mathbf{H} + \tilde{\mathbf{U}}_c\tilde{\mathbf{\Lambda}}_c\tilde{\mathbf{V}}_c^\top\\ &= \mathbf{H} + \tilde{\mathbf{U}}_0\mathbf{W}\tilde{\mathbf{\Lambda}}_c\mathbf{Q}^\top\tilde{\mathbf{V}}_0^\top\\ &= \mathbf{H} + \tilde{\mathbf{U}}_0\mathbf{G}\tilde{\mathbf{V}}_0^\top.\end{aligned} \tag{6}$$

Since $\tilde{\mathbf{F}} = \mathbf{D}_r^{-\frac{1}{2}}\mathbf{F}\mathbf{D}_c^{-\frac{1}{2}}$, we know that any integer matrix $\mathbf{F}_{rec}$, which has $\mathbf{H}$ as its k-dimensional approximation, satisfies the following linear relationship, called the recovery equation

$$\mathbf{F}_{rec} = \mathbf{D}_r^{\frac{1}{2}}(\mathbf{H} + \tilde{\mathbf{U}}_0\mathbf{G}\tilde{\mathbf{V}}_0^\top)\mathbf{D}_c^{\frac{1}{2}}. \tag{7}$$

The inverse correspondence analysis problem is formally stated as: given a k-dimensional CA solution consisting of matrices $\mathbf{H}$, $\mathbf{D}_r$ and $\mathbf{D}_c$, can we find an integer matrix that satisfies the recovery equation [9]. Note that both matrices $\tilde{\mathbf{U}}_0$ and $\tilde{\mathbf{V}}_0$ are not unique. When $\mathbf{F}_{rec}$ is a solution to the recovery equation, it remains a solution even after rotating $\tilde{\mathbf{U}}_0$ (or $\tilde{\mathbf{V}}_0$), since both $\mathbf{F}_{rec}$ and $\tilde{\mathbf{\Lambda}}_c$ remain unchanged when considering the standardised decomposition in (6).

Several approaches have been proposed to solve the inverse correspondence analysis problem. Groenen and Van de Velden [9] solve inverse correspondence analysis using a full enumeration approach. Van de Velden et al. [17] note that the inverse correspondence analysis problem can be modelled as a mixed-integer programming formulation, which leads to a more efficient algorithm.

Even though the recovery equation describes a linear relationship, it only provides a necessary condition for answering our research question. Van de Velden et al. [17] sometimes retrieve a matrix $\hat{\mathbf{F}}$ that satisfies the recovery equation (7), but the k largest singular values of $\mathbf{F}$ and $\hat{\mathbf{F}}$ differ. Moreover, inverse correspondence analysis is an algorithmic approach to verify the uniqueness of a given CA solution. To structurally find matrices that have the same k-dimensional approximation an analytical approach is needed.

We classify the possible input integer matrices $\mathbf{F}_{rec}$ that satisfy the recovery equation, associated with an original matrix $\mathbf{F}^o$, into three groups: original, admissible and non-admissible input matrices. Clearly, the original input $\mathbf{F}^o$ satisfies the recovery equation. Admissible matrices satisfy the recovery equation, and the k largest singular values are the same as those corresponding to the original $\mathbf{F}^o$. Note that in the inverse correspondence analysis problem the original matrix is not known, therefore, it is not possible to determine whether the k-dimensional solution belongs to matrix $\mathbf{F}^o$ or an admissible matrix $\mathbf{F}^a$. Non-admissible input matrices do satisfy the recovery equation, however, one of its k largest singular values differs from those corresponding to the original $\mathbf{F}^o$. In order to determine under which conditions it is possible have $h(\mathbf{F}^o) = h(\mathbf{F}^a)$, it is important to understand how one can construct admissible input matrices. To do so, consider the following definition.

Definition 3.1 *(Admissible input matrix).* A matrix $\mathbf{F}^a \neq \mathbf{F}^o$ is an admissible input matrix of $\mathbf{F}^o$ if the following three conditions are satisfied.

C1. $\mathbf{F}^o$ and $\mathbf{F}^a$ have the same marginals, i.e. $\mathbf{D}_r^o = \mathbf{D}_r^a$ and $\mathbf{D}_c^o = \mathbf{D}_c^a$.
C2. $\mathbf{F}^a$ is a solution to the recovery equation (7) with $\mathbf{H} = h(\mathbf{F}^o)$.
C3. $\mathbf{F}^o$ and $\mathbf{F}^a$ have the same first k singular values, sorted in a non-increasing order.

Note that Definition 3.1 describes a symmetric relation in the sense that $\mathbf{F}^o$ is an admissible input matrix of $\mathbf{F}^a$ if and only if $\mathbf{F}^a$ is an admissible input matrix of $\mathbf{F}^o$. Also, note that if we only satisfy C1 and C2, while C3 is violated, we have obtained a non-admissible input matrix. In Section 4, we investigate the structural properties of admissible matrices. We exploit these properties to systematically construct admissible input matrices in Section 5.

4. Structural properties of correspondence analysis solutions

We prove that when an original matrix $\mathbf{F}^o$ and an admissible matrix $\mathbf{F}^a$ are given, i.e. $h(\mathbf{F}^o) = h(\mathbf{F}^a)$, then $\mathbf{F}^o$ and $\mathbf{F}^a$ are uniquely related with a linear transformation matrix $\mathbf{T}$. We show several properties of matrix $\mathbf{T}$, which are necessary conditions for the existence of an admissible matrix.

Consider $n_r \times n_c$ matrices $\mathbf{F}^o$ and $\mathbf{F}^a$. Suppose that $\mathbf{F}^a$ is an admissible matrix of $\mathbf{F}^o$, then by Definition 3.1 it holds that their k-dimensional approximations are the same

$$\begin{aligned}\mathbf{F}^o &= \mathbf{U}^o\mathbf{\Lambda}^o\mathbf{V}^{o\top}\\ &= \mathbf{U}_k\mathbf{\Lambda}_k\mathbf{V}_k^\top + \mathbf{U}_c^o\mathbf{\Lambda}_c^o\mathbf{V}_c^{o\top},\\ \mathbf{F}^a &= \mathbf{U}^a\mathbf{\Lambda}^a\mathbf{V}^{a\top}\\ &= \mathbf{U}_k\mathbf{\Lambda}_k\mathbf{V}_k^\top + \mathbf{U}_c^a\mathbf{\Lambda}_c^a\mathbf{V}_c^{a\top},\end{aligned}$$

which implies that

$$\begin{aligned}\mathbf{U}_k^\top\mathbf{U}_c^o &= \mathbf{0},\\ \mathbf{U}_k^\top\mathbf{U}_c^a &= \mathbf{0}.\end{aligned}$$

This means that $\mathbf{U}_c^o$ and $\mathbf{V}_c^o$ can be obtained from $\mathbf{U}_c^a$ and $\mathbf{V}_c^a$, respectively, using an orthonormal transformation

$$\begin{aligned}\mathbf{U}_c^o &= \mathbf{U}_c^a\mathbf{W}^*,\\ \mathbf{V}_c^o &= \mathbf{V}_c^a\mathbf{Q}^*,\end{aligned}$$

where $\mathbf{W}^*$ and $\mathbf{Q}^*$ are orthonormal. Let

$$\mathbf{W} = \begin{pmatrix}\mathbf{I} & \\ & \mathbf{W}^*\end{pmatrix}, \mathbf{Q} = \begin{pmatrix}\mathbf{I} & \\ & \mathbf{Q}^*\end{pmatrix}.$$

Thus, $\mathbf{U}^o$ and $\mathbf{V}^o$ can be obtained from $\mathbf{U}^a$ and $\mathbf{V}^a$ using an orthonormal transformation

$$\begin{aligned}\mathbf{U}^o &= \mathbf{U}^a\mathbf{W},\\ \mathbf{V}^o &= \mathbf{V}^a\mathbf{Q}.\end{aligned}$$

Next, we present a lemma on the right Moore–Penrose inverse, which is a generalised inverse satisfying specific properties, see for instance Horn and Johnson [10].

Lemma 4.1. *The Moore-Penrose inverse of a matrix* $\mathbf{F}$ *is unique. If matrix* $\mathbf{F}$ *has linearly independent rows, then the Moore–Penrose inverse is defined as* $\mathbf{F}^+ = \mathbf{F}^\top(\mathbf{F}\mathbf{F}^\top)^{-1}$. *This is a right inverse, because* $\mathbf{F}\mathbf{F}^+ = \mathbf{I}$.

Consider the following three partitioned matrices

$$\mathbf{F}^o = \begin{pmatrix}\mathbf{U}_k & \mathbf{U}_c^o\end{pmatrix}\begin{pmatrix}\mathbf{\Lambda}_k & \\ & \mathbf{\Lambda}_c^o\end{pmatrix}\begin{pmatrix}\mathbf{V}_k^\top \\ \mathbf{V}_c^{o\top}\end{pmatrix}, \tag{8}$$

$$\mathbf{F}^{o+} = \begin{pmatrix}\mathbf{V}_k & \mathbf{V}_c^o\end{pmatrix}\begin{pmatrix}\mathbf{\Lambda}_k^{-1} & \\ & \mathbf{\Lambda}_c^{o-1}\end{pmatrix}\begin{pmatrix}\mathbf{U}_k^\top \\ \mathbf{U}_c^{o\top}\end{pmatrix}, \tag{9}$$

$$\mathbf{F}^a = \begin{pmatrix}\mathbf{U}_k & \mathbf{U}_c^a\end{pmatrix}\begin{pmatrix}\mathbf{\Lambda}_k & \\ & \mathbf{\Lambda}_c^a\end{pmatrix}\begin{pmatrix}\mathbf{V}_k^\top \\ \mathbf{V}_c^{a\top}\end{pmatrix}, \tag{10}$$

where $\mathbf{F}^{o+}$ denotes the Moore-Penrose inverse of $\mathbf{F}^o$ if it exists. Note that we can verify that $\mathbf{F}^o\mathbf{F}^{o+} = \mathbf{I}$, because for square orthonormal matrices $\mathbf{U}^{-1} = \mathbf{U}^\top$.

The following theorem states that the original and admissible matrix are uniquely related through a linear transformation.

Theorem 4.2. *Given an admissible matrix* $\mathbf{F}^a$ *of* $\mathbf{F}^o$ *as shown in (10) and (8), where the singular values of matrix* $\mathbf{F}^o$ *are non-zero, then there exists a unique* $\mathbf{T}$ *such that* $\mathbf{T}\mathbf{F}^o = \mathbf{F}^a$.

Proof. We define $\mathbf{T} = \mathbf{F}^a\mathbf{F}^{o+}$ and show that it has the desired properties. By assumption all singular values of matrix $\mathbf{F}^o$ are non-zero and the rank of $\mathbf{F}^o$ equals the number of non-zero singular values. The rank equals the number of linearly independent rows, so $\mathbf{F}^o$ has linearly independent rows. From Lemma 4.1 it follows that the right Moore-Penrose inverse $\mathbf{F}^{o+}$ exists. Since the Moore-Penrose is unique, $\mathbf{T} = \mathbf{F}^a\mathbf{F}^{o+}$ is unique as well.

Moreover, using (8) and (9) we can show that

$$\begin{aligned}\mathbf{F}^{o+}\mathbf{F}^o &= \mathbf{V}^o\mathbf{V}^{o\top} \\ &= \mathbf{V}^a\mathbf{Q}\mathbf{Q}^\top\mathbf{V}^{a\top} \\ &= \mathbf{V}^a\mathbf{V}^{a\top}.\end{aligned} \tag{11}$$

Using (11)

$$\begin{aligned}\mathbf{T}\mathbf{F}^o &= \mathbf{F}^a\mathbf{F}^{o+}\mathbf{F}^o \\ &= \mathbf{U}^a\mathbf{\Lambda}^a\mathbf{V}^{a\top}\mathbf{V}^a\mathbf{V}^{a\top} \\ &= \mathbf{U}^a\mathbf{\Lambda}^a\mathbf{V}^{a\top} \\ &= \mathbf{F}^a.\end{aligned}$$

To conclude, there exists a unique $\mathbf{T}$ such that $\mathbf{F}^a = \mathbf{T}\mathbf{F}^o$. $\square$

Below we give a closed form expression for this unique $\mathbf{T}$.

$$\begin{aligned}
\mathbf{T} &= \mathbf{F}^a\mathbf{F}^{o+} \\
&= \begin{pmatrix}\mathbf{U}_k & \mathbf{U}_c^a\end{pmatrix}\begin{pmatrix}\boldsymbol{\Lambda}_k & \\ & \boldsymbol{\Lambda}_c^a\end{pmatrix}\begin{pmatrix}\mathbf{V}_k^\top \\ \mathbf{V}_c^{a\top}\end{pmatrix}\begin{pmatrix}\mathbf{V}_k & \mathbf{V}_c^o\end{pmatrix}\begin{pmatrix}\boldsymbol{\Lambda}_k^{-1} & \\ & \boldsymbol{\Lambda}_c^{o-1}\end{pmatrix}\begin{pmatrix}\mathbf{U}_k^\top \\ \mathbf{U}_c^{o\top}\end{pmatrix} \\
&= \begin{pmatrix}\mathbf{U}_k & \mathbf{U}_c^a\end{pmatrix}\begin{pmatrix}\boldsymbol{\Lambda}_k & \\ & \boldsymbol{\Lambda}_c^a\end{pmatrix}\begin{pmatrix}\mathbf{I} & \mathbf{V}_k^\top\mathbf{V}_c^o \\ \mathbf{V}_c^{a\top}\mathbf{V}_k & \mathbf{V}_c^{a\top}\mathbf{V}_c^o\end{pmatrix}\begin{pmatrix}\boldsymbol{\Lambda}_k^{-1} & \\ & \boldsymbol{\Lambda}_c^{o-1}\end{pmatrix}\begin{pmatrix}\mathbf{U}_k^\top \\ \mathbf{U}_c^{o\top}\end{pmatrix} \\
&= \begin{pmatrix}\mathbf{U}_k & \mathbf{U}_c^a\end{pmatrix}\begin{pmatrix}\boldsymbol{\Lambda}_k & \\ & \boldsymbol{\Lambda}_c^a\end{pmatrix}\begin{pmatrix}\mathbf{I} & \\ & \mathbf{V}_c^{a\top}\mathbf{V}_c^o\end{pmatrix}\begin{pmatrix}\boldsymbol{\Lambda}_k^{-1} & \\ & \boldsymbol{\Lambda}_c^{o-1}\end{pmatrix}\begin{pmatrix}\mathbf{U}_k^\top \\ \mathbf{U}_c^{o\top}\end{pmatrix} \\
&= \begin{pmatrix}\mathbf{U}_k & \mathbf{U}_c^a\end{pmatrix}\begin{pmatrix}\mathbf{I} & \\ & \boldsymbol{\Lambda}_c^a\mathbf{V}_c^{a\top}\mathbf{V}_c^o\boldsymbol{\Lambda}_c^{o-1}\end{pmatrix}\begin{pmatrix}\mathbf{U}_k^\top \\ \mathbf{U}_c^{o\top}\end{pmatrix} \\
&= \mathbf{U}_k\mathbf{U}_k^\top + \mathbf{U}_c^a\boldsymbol{\Lambda}_c^a\mathbf{V}_c^{a\top}\mathbf{V}_c^o\boldsymbol{\Lambda}_c^{o-1}\mathbf{U}_c^{o\top}.
\end{aligned}$$

In the lemma below we state what properties are satisfied by $\mathbf{T}$.

Lemma 4.3. *Given an admissible matrix* $\mathbf{F}^a$ *of* $\mathbf{F}^o$ *as shown in (10) and (8) and* $\mathbf{T} = \mathbf{F}^a\mathbf{F}^{o+}$, *then* $\mathbf{T}\mathbf{r} = \mathbf{r}$ *and* $\mathbf{1}_{n_r}^\top\mathbf{T} = \mathbf{1}_{n_r}^\top$.

Proof. Recall that the row and column totals are the same for $\mathbf{F}^o$ and $\mathbf{F}^a$ due to Definition 3.1. The first property can be derived using the row total of $\mathbf{F}^o$ and $\mathbf{F}^a$

$$\begin{aligned}
\mathbf{r} &= \mathbf{F}^a\mathbf{1}_{n_c} \\
&= \mathbf{T}\mathbf{F}^o\mathbf{1}_{n_c} \\
&= \mathbf{T}\mathbf{r},
\end{aligned}$$

where we used that $\mathbf{F}^o\mathbf{1}_{n_c} = \mathbf{r}$.

Similarly, the second property can be derived based on the column total

$$\begin{aligned}
\mathbf{1}_{n_r}^\top\mathbf{F}^{\mathrm{o}} &= \mathbf{c}^\top \\
&= \mathbf{1}_{n_r}^\top\mathbf{F}^{\mathrm{a}} \\
&= \mathbf{1}_{n_r}^\top\mathbf{T}\mathbf{F}^{\mathrm{o}}.
\end{aligned}$$

Post-multiplying by $\mathbf{F}^{o+}$ on both sides results in

$$\begin{aligned}
\mathbf{1}_{n_r}^\top\mathbf{F}^{\mathrm{o}}\mathbf{F}^{o+} &= \mathbf{1}_{n_r}^\top\mathbf{T}\mathbf{F}^{\mathrm{o}}\mathbf{F}^{o+} \implies \\
\mathbf{1}_{n_r}^\top &= \mathbf{1}_{n_r}^\top\mathbf{T}. \quad \square
\end{aligned}$$

In this section, we have shown that when $\mathbf{F}^a$ is an admissible matrix of $\mathbf{F}^o$, i.e. $h(\mathbf{F}^o) = h(\mathbf{F}^a)$, then there exists a unique $\mathbf{T}$ satisfying the relation $\mathbf{T}\mathbf{F}^o = \mathbf{F}^a$. We have shown what properties are satisfied by $\mathbf{T}$, which are necessary conditions for an admissible matrix to exist. These conditions are summarised in the theorem below.

Theorem 4.4. *Given an admissible matrix $\mathbf{F}^a$ of $\mathbf{F}^o$ as shown in (10) and (8), where the singular values of matrix $\mathbf{F}^o$ are non-zero. Then there exists a unique linear transformation matrix $\mathbf{T} = \mathbf{F}^a\mathbf{F}^{o+}$, which satisfies $\mathbf{T}\mathbf{r} = \mathbf{r}$ and $\mathbf{1}_{n_r}^\top \mathbf{T} = \mathbf{1}_{n_r}^\top$.*

In the upcoming section, we establish sufficient conditions for having admissible matrices using symmetric matrices $\mathbf{T}$.

5. Generating admissible matrices

In this section, we describe a method to generate a class of matrices for which an admissible matrix exists. First, we show what conditions the original matrix $\mathbf{F}^o$ and a specific linear transformation matrix $\mathbf{T}$ must satisfy, such that an admissible matrix $\mathbf{F}^a$ exists. Afterwards, we show how to generate such a pair of matrices $\mathbf{F}^o$ and $\mathbf{F}^a$, which therefore satisfy $h(\mathbf{F}^o) = h(\mathbf{F}^a)$.

5.1. A class of candidate matrices

We prove several general lemmas, which are used to obtain sufficient conditions under which candidate matrices exist.

Consider an $n_r \times n_c$ matrix $\mathbf{F}$ and an $n_r \times n_r$ matrix $\mathbf{T}$ and their respective SVDs, where the singular values $\mathbf{\Lambda}_\mathrm{T}$ are unsorted.

$$\begin{aligned}\mathbf{F} &= \mathbf{U}\mathbf{\Lambda}\mathbf{V}^\top \\ &= \begin{pmatrix}\mathbf{U}_k & \mathbf{U}_c\end{pmatrix}\begin{pmatrix}\mathbf{\Lambda}_k & \\ & \mathbf{\Lambda}_c\end{pmatrix}\begin{pmatrix}\mathbf{V}_k^\top \\ \mathbf{V}_c^\top\end{pmatrix}, \end{aligned} \tag{12}$$

$$\begin{aligned}\mathbf{T} &= \mathbf{U}_\mathrm{T}\mathbf{\Lambda}_\mathrm{T}\mathbf{U}_\mathrm{T}^\top \\ &= \begin{pmatrix}\mathbf{U}_\mathrm{kT} & \mathbf{U}_\mathrm{cT}\end{pmatrix}\begin{pmatrix}\mathbf{\Lambda}_\mathrm{kT} & \\ & \mathbf{\Lambda}_\mathrm{cT}\end{pmatrix}\begin{pmatrix}\mathbf{U}_\mathrm{kT}^\top \\ \mathbf{U}_\mathrm{cT}^\top\end{pmatrix}. \end{aligned} \tag{13}$$

The next theorem states that when the last c singular vectors of matrix $\mathbf{F}$ are equal to a set of c singular vectors of $\mathbf{T}$ and the remaining k singular values of $\mathbf{T}$ are all equal to 1, then a QR decomposition of $\mathbf{T}\mathbf{U}$ can be written as $\mathbf{U}\mathbf{\Lambda}_\mathrm{T}$.

Theorem 5.1. *Consider (12) and (13). If $\mathbf{U}_c = \mathbf{U}_{cT}$ and $\mathbf{\Lambda}_{kT} = \mathbf{I}$, then $\mathbf{T}\mathbf{U} = \mathbf{U}\mathbf{\Lambda}_T$.*

Proof. Since $\mathbf{U}$ is orthonormal, it follows that

$$\begin{aligned}\mathbf{U}_k^\top \mathbf{U}_c &= \mathbf{0} \\ &= \mathbf{U}_{\mathrm{kT}}^\top \mathbf{U}_{\mathrm{cT}} \\ &= \mathbf{U}_{\mathrm{kT}}^\top \mathbf{U}_{\mathrm{c}},\end{aligned}$$

where we use that $\mathbf{U}_c = \mathbf{U}_{\mathrm{cT}}$. This implies that $\mathbf{U}_k$ can be obtained from $\mathbf{U}_{\mathrm{kT}}$ by applying an orthonormal transformation

$$\mathbf{U}_k = \mathbf{U}_{\mathrm{kT}} \mathbf{W}^*, \tag{14}$$

where $\mathbf{W}^*$ is an orthonormal $k \times k$ matrix. Therefore, the following matrix is also orthonormal

$$\mathbf{W} = \begin{pmatrix} \mathbf{W}^* & \\ & \mathbf{I} \end{pmatrix}.$$

Using (14) and $\mathbf{U}_c = \mathbf{U}_{\mathrm{cT}}$, we observe that $\mathbf{U}$ can be obtained from $\mathbf{U}_{\mathrm{T}}$ by applying another orthonormal transformation

$$\begin{aligned}\mathbf{U} &= \begin{pmatrix} \mathbf{U}_{\mathrm{k}} & \mathbf{U}_{\mathrm{c}} \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{U}_{\mathrm{kT}} & \mathbf{U}_{\mathrm{cT}} \end{pmatrix} \begin{pmatrix} \mathbf{W}^* & \\ & \mathbf{I} \end{pmatrix} \\ &= \mathbf{U}_{\mathrm{T}} \mathbf{W}.\end{aligned} \tag{15}$$

Starting with the SVD of $\mathbf{T}$, we obtain the following expression by post-multiplying by $\mathbf{U}_{\mathrm{T}}$ and $\mathbf{W}$ and applying (15)

$$\begin{aligned}\mathbf{T} &= \mathbf{U}_{\mathrm{T}} \mathbf{\Lambda}_{\mathrm{T}} \mathbf{U}_{\mathrm{T}}^\top \implies \\ \mathbf{T}\mathbf{U}_{\mathrm{T}} &= \mathbf{U}_{\mathrm{T}} \mathbf{\Lambda}_{\mathrm{T}} \mathbf{U}_{\mathrm{T}}^\top \mathbf{U}_{\mathrm{T}} \implies \\ \mathbf{T}\mathbf{U}_{\mathrm{T}} &= \mathbf{U}_{\mathrm{T}} \mathbf{\Lambda}_{\mathrm{T}} \implies \\ \mathbf{T}\mathbf{U}_{\mathrm{T}}\mathbf{W} &= \mathbf{U}_{\mathrm{T}} \mathbf{\Lambda}_{\mathrm{T}} \mathbf{W} \implies \\ \mathbf{T}\mathbf{U} &= \mathbf{U}_{\mathrm{T}} \mathbf{\Lambda}_{\mathrm{T}} \mathbf{W}.\end{aligned} \tag{16}$$

Since $\mathbf{\Lambda}_{\mathrm{kT}} = \mathbf{I}$, it follows that

$$\mathbf{\Lambda}_{\mathrm{T}} \mathbf{W} = \begin{pmatrix} \mathbf{I} & \\ & \mathbf{\Lambda}_{\mathrm{cT}} \end{pmatrix} \begin{pmatrix} \mathbf{W}^* & \\ & \mathbf{I} \end{pmatrix}$$

$$
\begin{aligned}
&= \begin{pmatrix} \mathbf{W}^* & \\ & \mathbf{\Lambda}_{\mathrm{cT}} \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{W}^* & \\ & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \\ & \mathbf{\Lambda}_{\mathrm{cT}} \end{pmatrix} \\
&= \mathbf{W}\mathbf{\Lambda}_{\mathrm{T}}. \qquad (17)
\end{aligned}
$$

By applying (17) on (16), we obtain

$$
\begin{aligned}
\mathbf{TU} &= \mathbf{U}_{\mathrm{T}}\mathbf{\Lambda}_{\mathrm{T}}\mathbf{W} \\
&= \mathbf{U}_{\mathrm{T}}\mathbf{W}\mathbf{\Lambda}_{\mathrm{T}} \\
&= \mathbf{U}\mathbf{\Lambda}_{\mathrm{T}}.
\end{aligned}
$$

To conclude, we have shown that $\mathbf{TU} = \mathbf{U}\mathbf{\Lambda}_{\mathrm{T}}$ holds. Since $\mathbf{U}$ is orthonormal and $\mathbf{\Lambda}_{\mathrm{T}}$ is diagonal (and hence upper triangular), this implies that $\mathbf{U}\mathbf{\Lambda}_{\mathrm{T}}$ is indeed a QR decomposition of $\mathbf{TU}$. □

From now on we restrict ourselves to a symmetric $\mathbf{T}$. Instead of analysing whether the standardised relation $\mathbf{T}\tilde{\mathbf{F}}^o = \tilde{\mathbf{F}}^a$ holds, we can verify $\mathbf{TF}^o = \mathbf{F}^a$, where $\tilde{\mathbf{F}}$ is the standardised version of $\mathbf{F}$. This implies we can use non-standardised matrices to make the proofs and derivations more tractable.

Lemma 5.2. *Given a symmetric matrix $\mathbf{T}$, (standardised) matrices $\mathbf{F}^a = \mathbf{D}_r^{\frac{1}{2}}\tilde{\mathbf{F}}^a\mathbf{D}_c^{\frac{1}{2}}$ and $\mathbf{F}^o = \mathbf{D}_r^{\frac{1}{2}}\tilde{\mathbf{F}}^o\mathbf{D}_c^{\frac{1}{2}}$, such that $\mathbf{D}_r^o = \mathbf{D}_r^a = \mathbf{D}_r$ and $\mathbf{D}_c^o = \mathbf{D}_c^a = \mathbf{D}_c$. The standardised relation $\mathbf{T}\tilde{\mathbf{F}}^o = \tilde{\mathbf{F}}^a$ holds if and only if $\mathbf{TF}^o = \mathbf{F}^a$.*

Proof. We prove this statement in both directions.

$\Longrightarrow$ Assume that $\mathbf{T}\tilde{\mathbf{F}}^o = \tilde{\mathbf{F}}^a$ holds. We start with the definition of matrix $\mathbf{F}^a$:

$$
\begin{aligned}
\mathbf{F}^a &= \mathbf{D}_r^{\frac{1}{2}}\tilde{\mathbf{F}}^a\mathbf{D}_c^{\frac{1}{2}} \\
&= \mathbf{D}_r^{\frac{1}{2}}\mathbf{T}\tilde{\mathbf{F}}^o\mathbf{D}_c^{\frac{1}{2}} \\
&= \mathbf{T}\mathbf{D}_r^{\frac{1}{2}}\tilde{\mathbf{F}}^o\mathbf{D}_c^{\frac{1}{2}} \\
&= \mathbf{TF}^o,
\end{aligned}
$$

where we use that $\mathbf{T}$, $\mathbf{D}_r^{\frac{1}{2}}$ and $\mathbf{TD}_r^{\frac{1}{2}}$ are symmetric matrices.

$\Longleftarrow$ Assuming that $\mathbf{TF}^o = \mathbf{F}^a$

$$
\begin{aligned}
\mathbf{D}_r^{\frac{1}{2}}\tilde{\mathbf{F}}^a\mathbf{D}_c^{\frac{1}{2}} &= \mathbf{F}^a \\
&= \mathbf{TF}^o
\end{aligned}
$$

$$
\begin{aligned}
&= \mathbf{T}\mathbf{D}_r^{\frac{1}{2}}\tilde{\mathbf{F}}^o\mathbf{D}_c^{\frac{1}{2}} \\
&= \mathbf{D}_r^{\frac{1}{2}}\mathbf{T}\tilde{\mathbf{F}}^o\mathbf{D}_c^{\frac{1}{2}} \implies \\
\tilde{\mathbf{F}}^a &= \mathbf{T}\tilde{\mathbf{F}}^o. \quad \square
\end{aligned}
$$

In the next lemma, we state under which conditions on $\mathbf{T}$, the row and column marginals of $\mathbf{F}^o$ and $\mathbf{F}^a$ are equal to each other.

Lemma 5.3. *If* $\mathbf{T}\mathbf{F}^o = \mathbf{F}^a$ *holds, where* $\mathbf{T}$ *satisfies* $\mathbf{T}\mathbf{r} = \mathbf{r}$ *and* $\mathbf{1}_{n_r}^\top \mathbf{T} = \mathbf{1}_{n_r}^\top$*, then* $\mathbf{D}_r^o = \mathbf{D}_r^a = \mathbf{D}_r$ *and* $\mathbf{D}_c^o = \mathbf{D}_c^a = \mathbf{D}_c$*.*

Proof. Starting with the row marginals $\mathbf{r}$ of $\mathbf{F}^o$, we have

$$
\begin{aligned}
\mathbf{F}^o\mathbf{1}_{n_c} &= \mathbf{r} \implies \\
\mathbf{T}\mathbf{F}^o\mathbf{1}_{n_c} &= \mathbf{T}\mathbf{r} \implies \\
\mathbf{F}^a\mathbf{1}_{n_c} &= \mathbf{r}.
\end{aligned}
$$

So the row marginals are indeed the same for $\mathbf{F}^o$ and $\mathbf{F}^a$. Likewise, with $\mathbf{1}_{n_r}^\top \mathbf{F}^o = \mathbf{c}^\top$, we have

$$
\begin{aligned}
\mathbf{1}_{n_r}^\top \mathbf{T} &= \mathbf{1}_{n_r}^\top \implies \\
\mathbf{1}_{n_r}^\top \mathbf{T}\mathbf{F}^o &= \mathbf{1}_{n_r}^\top \mathbf{F}^o \implies \\
\mathbf{1}_{n_r}^\top \mathbf{F}^a &= \mathbf{c}^\top,
\end{aligned}
$$

which shows that the column marginals are also the same for $\mathbf{F}^o$ and $\mathbf{F}^a$. $\square$

Using Theorem 5.1 and Lemmas 5.2-5.3, we derive sufficient conditions for the existence of admissible matrices. Let $\boldsymbol{\delta}$ be a vector of length c, with elements satisfying

$$
\delta_j = \frac{\tilde{\lambda}_k^o}{\tilde{\lambda}_{k+j}^o} \text{ for } j = 1, \ldots, c.
$$

We impose an additional restriction on the singular values of $\mathbf{T}$, namely that $\boldsymbol{\lambda}_{c\mathrm{T}} < \boldsymbol{\delta}$, where $\mathbf{a} < \mathbf{b}$ states that the entries of vector $\mathbf{a}$ are strictly smaller than the entries of vector $\mathbf{b}$. Since $\tilde{\lambda}_k^o > \tilde{\lambda}_{k+1}^o$ by Assumption 2.1, it holds that $\mathbf{1}_c < \boldsymbol{\delta}$ is always a valid lower bound.

Theorem 5.4. *Given the following matrices and conditions*

A1. *a matrix* $\mathbf{F}^o$ *and a standardised matrix* $\tilde{\mathbf{F}}^o = \mathbf{D}_r^{-\frac{1}{2}}\mathbf{F}^o\mathbf{D}_c^{-\frac{1}{2}}$*,*
A2. *a symmetric matrix* $\mathbf{T}$*, such that* $\mathbf{T}\mathbf{r} = \mathbf{r}$ *and* $\mathbf{1}_{n_r}^\top \mathbf{T} = \mathbf{1}_{n_r}^\top$*,*
A3. *a matrix* $\mathbf{F}^a \neq \mathbf{F}^o$*, such that* $\mathbf{T}\mathbf{F}^o = \mathbf{F}^a$*,*

A4. *the SVD of* $\tilde{\mathbf{F}}^o$ *and* $\mathbf{T}$ *can be partitioned as*

$$\tilde{\mathbf{F}}^o = \begin{pmatrix} \tilde{\mathbf{U}}_k^o & \tilde{\mathbf{U}}_c^o \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{\Lambda}}_k^o & \\ & \tilde{\mathbf{\Lambda}}_c^o \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{V}}_k^{o\top} \\ \tilde{\mathbf{V}}_c^{o\top} \end{pmatrix},$$

$$\mathbf{T} = \begin{pmatrix} \mathbf{U}_{kT} & \mathbf{U}_{cT} \end{pmatrix} \begin{pmatrix} \mathbf{\Lambda}_{kT} & \\ & \mathbf{\Lambda}_{cT} \end{pmatrix} \begin{pmatrix} \mathbf{U}_{kT}^\top \\ \mathbf{U}_{cT}^\top \end{pmatrix},$$

where $\tilde{\mathbf{U}}_c^o = \mathbf{U}_{cT}$*,* $\mathbf{\Lambda}_{kT} = \mathbf{I}$*.*

A5. $\boldsymbol{\lambda}_{cT} < \boldsymbol{\delta}$*.*

Then $\mathbf{F}^a$ *is an admissible matrix of* $\mathbf{F}^o$*.*

Proof. To prove that $\mathbf{F}^a$ is an admissible matrix of $\mathbf{F}^o$, we show that $\mathbf{F}^a$ satisfies the three conditions stated in Definition 3.1.

- C1, which states that $\mathbf{D}_r^o = \mathbf{D}_r^a$ and $\mathbf{D}_c^o = \mathbf{D}_c^a$, holds due to A2, A3 and Lemma 5.3.
- For C2, we have to verify whether $\mathbf{F}^a$ satisfies the recovery equation (7). Due to A3 and Lemma 5.2 we know that $\tilde{\mathbf{F}}^a = \mathbf{T}\tilde{\mathbf{F}}^o$. Using Theorem 5.1, we obtain the following SVD

$$\begin{aligned} \tilde{\mathbf{F}}^a &= \mathbf{T}\tilde{\mathbf{F}}^o \\ &= \mathbf{T}\tilde{\mathbf{U}}^o\tilde{\mathbf{\Lambda}}^o\tilde{\mathbf{V}}^{o\top} \\ &= \tilde{\mathbf{U}}^o\mathbf{\Lambda}_{\mathrm{T}}\tilde{\mathbf{\Lambda}}^o\tilde{\mathbf{V}}^{o\top} \\ &= \tilde{\mathbf{U}}_k^o\tilde{\mathbf{\Lambda}}_k^o\tilde{\mathbf{V}}_k^{o\top} + \tilde{\mathbf{U}}_c^o\mathbf{\Lambda}_{c\mathrm{T}}\tilde{\mathbf{\Lambda}}_c^o\tilde{\mathbf{V}}_c^{o\top}. \end{aligned}$$

  So, we obtain

$$\mathbf{F}^a = \mathbf{D}_r^{o\frac{1}{2}}(\tilde{\mathbf{U}}_k^o\tilde{\mathbf{\Lambda}}_k^o\tilde{\mathbf{V}}_k^{o\top} + \tilde{\mathbf{U}}_c^o\mathbf{\Lambda}_{c\mathrm{T}}\tilde{\mathbf{\Lambda}}_c^o\tilde{\mathbf{V}}_c^{o\top})\mathbf{D}_c^{o\frac{1}{2}}. \tag{18}$$

  Note that at this point we have found a solution to the recovery equation (7), however, the singular values of $\tilde{\mathbf{F}}^a$ might no longer be in a non-increasing order.
- In the next two steps we verify C3, which states that the first k singular values of $\tilde{\mathbf{F}}^o$ and $\tilde{\mathbf{F}}^a$ are the same when sorted in non-increasing order.
  - We start by showing that the first k singular values of $\tilde{\mathbf{F}}^o$ and $\tilde{\mathbf{F}}^a$ are equal to each other. From the SVD of $\mathbf{F}^a$ given in (18) it follows that

$$\tilde{\lambda}_i^a = \begin{cases} \tilde{\lambda}_i^o, & \text{if } i = 1, \dots, k, \\ \lambda_{\mathrm{T}i}\tilde{\lambda}_i^o, & \text{if } i = k+1, \dots, n_r. \end{cases}$$

    From A5 we can derive that

$$\begin{aligned}\tilde{\lambda}_i^a &= \lambda_{\mathrm{T}i}\tilde{\lambda}_i^o \\ &< \delta_{i-k}\tilde{\lambda}_i^o \\ &= \tilde{\lambda}_k^o \\ &= \tilde{\lambda}_k^a,\end{aligned}$$

for $i = k+1, \dots, n_r$. Since the standardised singular values $\tilde{\lambda}_i^a$ with indices $i = k+1, \dots, n_r$ cannot become larger than the k-th singular value, we conclude that the first k singular values of $\tilde{\mathbf{F}}^o$ and $\tilde{\mathbf{F}}^a$ are the same.

– Finally, we show that not all singular values of $\tilde{\mathbf{F}}^o$ are the same as those of $\tilde{\mathbf{F}}^a$. Assume by contradiction that $\tilde{\mathbf{F}}^o$ and $\tilde{\mathbf{F}}^a$ have the same singular values, then it must hold that $\mathbf{\Lambda}_{c\mathrm{T}} = \mathbf{I}$ and $\mathbf{T} = \mathbf{I}$, which violates A3. Thus, there exists an index $i \in \{k+1, \dots, n_r\}$ such that $\tilde{\mathbf{F}}^o$ and $\tilde{\mathbf{F}}^a$ have different singular values.

We conclude that conditions C1, C2 and C3 of Definition 3.1 are satisfied. Hence, we conclude that $\mathbf{F}^a$ is an admissible matrix of $\mathbf{F}^o$. □

In this section, we demonstrated that given a matrix $\mathbf{F}^o$ and a transformation matrix $\mathbf{T}$ fulfilling certain properties, there exists an admissible matrix $\mathbf{F}^a = \mathbf{T}\mathbf{F}^o$ where more than one singular value may differ. The main insight is in the construction of matrix $\mathbf{T}$, which shares singular vectors with the standardised matrix $\tilde{\mathbf{F}}^o$. Consequently, the structural characteristics of $\mathbf{F}^o$ and $\mathbf{T}$ are sufficient conditions for the existence of an admissible matrix $\mathbf{F}^a$.

5.2. A method to generate admissible matrices

In the previous section, we presented sufficient conditions for admissible matrices. However, it is not straightforward to construct matrices satisfying those criteria, e.g. common singular vectors for $\tilde{\mathbf{F}}^o$ and $\mathbf{T}$. In this section, we introduce a method to generate admissible matrices $\mathbf{F}^a$ of $\mathbf{F}^o$, hence, satisfying $h(\mathbf{F}^o) = h(\mathbf{F}^a)$.

We introduce a block structure in matrix $\mathbf{F}$. If we want to control the last $n_b - 1$ singular values, then the rows are divided into n_b blocks and the columns are divided into $n_b + 1$ blocks, where we assume that $n_b \geq 2$. The dimension of block $\mathbf{F}_{11}$ is $n_1 \times n_1$, note that we need $n_1 \geq k - 1$ when considering a k-dimensional CA solution. The rightmost $n_2 \geq 0$ columns are filled with 1's, while setting $n_2 = 0$ results in a square matrix. All blocks $\mathbf{F}_{ij}$ have size 2×2, except blocks $\mathbf{F}_{1j}$, $\mathbf{F}_{i1}$ and $\mathbf{F}_{1(n_b+1)}$. The blocks $\mathbf{F}_{ii}$ for $i = 2, \dots, n_b$ are symmetric matrices and the upper left element equals the bottom right element. The remaining blocks $\mathbf{F}_{ij}$ for $i > j$ all contain g, while the elements of blocks $\mathbf{F}_{ij}$ for $i < j$ are set to e. We leave the first block $\mathbf{F}_{11}$ unspecified, although later on we notice that the entries in that block should be large enough to influence the first k singular values. To summarise, matrix $\mathbf{F}$ has the following structure

$$\mathbf{F}=\left(\begin{array}{c|c|c|c|c}\mathbf{F}_{11} & \mathbf{F}_{12} & \dots & \mathbf{F}_{1n_b} & \mathbf{F}_{1(n_b+1)} \\ \hline \mathbf{F}_{21} & \mathbf{F}_{22} & \dots & \mathbf{F}_{2n_b} & \mathbf{F}_{2(n_b+1)} \\ \hline \vdots & \vdots & \ddots & \vdots & \vdots \\ \hline \mathbf{F}_{n_b1} & \mathbf{F}_{n_b2} & \dots & \mathbf{F}_{n_bn_b} & \mathbf{F}_{n_b(n_b+1)}\end{array}\right)=\left(\begin{array}{c|c|c|c|c}\mathbf{F}_{11} & e\mathbf{1}_{n_1,2} & \dots & e\mathbf{1}_{n_1,2} & \mathbf{1}_{n_1,n_2} \\ \hline g\mathbf{1}_{2,n_1} & \begin{matrix} c_2 & d_2 \\ d_2 & c_2 \end{matrix} & \dots & e\mathbf{1}_{2,2} & \mathbf{1}_{2,n_2} \\ \hline \vdots & \vdots & \ddots & \vdots & \vdots \\ \hline g\mathbf{1}_{2,n_1} & g\mathbf{1}_{2,2} & \dots & \begin{matrix} c_{n_b} & d_{n_b} \\ d_{n_b} & c_{n_b} \end{matrix} & \mathbf{1}_{2,n_2}\end{array}\right). \tag{19}$$

Furthermore, we construct the following block matrix $\mathbf{T}$ and corresponding partitioned vector $\mathbf{u}_i$, where the rows and columns are divided in similar blocks as matrix $\mathbf{F}$

$$\mathbf{T}=\left(\begin{array}{c|c|c|c}\mathbf{I}_{n_1} & \mathbf{0}_{n_1,2} & \dots & \mathbf{0}_{n_1,2} \\ \hline \mathbf{0}_{2,n_1} & \begin{matrix} a_2 & b_2 \\ b_2 & a_2 \end{matrix} & \dots & \mathbf{0}_{2,2} \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline \mathbf{0}_{2,n_1} & \mathbf{0}_{2,2} & \dots & \begin{matrix} a_{n_b} & b_{n_b} \\ b_{n_b} & a_{n_b} \end{matrix}\end{array}\right), \tag{20}$$

$$\mathbf{u}_i=\frac{1}{\sqrt{2}}\left(\begin{array}{c}\mathbf{0}_{n_1} \\ \hline 0 \\ 0 \\ \hline \vdots \\ \hline 1 \\ -1 \\ \hline \vdots \\ \hline 0 \\ 0\end{array}\right), \tag{21}$$

where $\mathbf{u}_i$ denotes a vector such that the i-th block contains the vector $[1 \quad -1]^\top$. In Lemma 5.5-5.7, we prove that $\mathbf{u}_i$ is a singular vector of $\mathbf{F}$, $\tilde{\mathbf{F}}$ and $\mathbf{T}$.

Lemma 5.5. *Given* $\mathbf{F}$ *and* $\mathbf{u}_i$ *for* $i = 2, \dots, n_b$ *as defined in (19) and (21). The vector* $\mathbf{u}_i$ *is a singular vector with corresponding singular value* $c_i - d_i$ *of matrix* $\mathbf{F}$.

Proof. We first show that $\mathbf{u}_i$ is an eigenvector of matrix $\mathbf{F}\mathbf{F}^\top$.

$$\begin{aligned}\mathbf{u}_i^\top \mathbf{F}\mathbf{F}^\top \mathbf{u}_i &= \left(\frac{c_i - d_i}{\sqrt{2}}\right)^2 + \left(\frac{d_i - c_i}{\sqrt{2}}\right)^2 \\ &= \frac{(c_i - d_i)^2}{2} + \frac{(c_i - d_i)^2}{2}\end{aligned}$$

$$= (c_i - d_i)^2.$$

Hence, $\mathbf{u}_i$ is an eigenvector of matrix $\mathbf{F}\mathbf{F}^\top$ with corresponding eigenvalue $(c_i - d_i)^2$. Equivalently, $\mathbf{u}_i$ is a singular vector of matrix $\mathbf{F}$ with corresponding singular value $c_i - d_i$. □

Lemma 5.6. *Given* $\mathbf{F}$ *and* $\mathbf{u}_i$ *for* $i = 2, \ldots, n_b$ *as defined in (19) and (21). The vector* $\mathbf{u}_i$ *is a singular vector of the standardised matrix* $\tilde{\mathbf{F}}$*, where* $\tilde{\mathbf{F}} = \mathbf{D}_r^{-\frac{1}{2}}\mathbf{F}\mathbf{D}_c^{-\frac{1}{2}}$.

Proof. The rows and columns corresponding to elements c_i and d_i in each block $i = 2, \ldots, n_b$ have the same row and column sum. When standardising, the values c_i and d_i are divided by the same constant. We can apply Lemma 5.5 to verify that u_i is a singular vector of $\tilde{\mathbf{F}}$. □

Lemma 5.7. *Given* $\mathbf{T}$ *and* $\mathbf{u}_i$ *for* $i = 2, \ldots, n_b$ *as defined in (20) and (21). Then* $\mathbf{u}_i$ *is a singular vector with corresponding singular value* $a_i - b_i$ *of matrix* $\mathbf{T}$.

Proof. Since $\mathbf{T}$ is a symmetric matrix it is diagonalisable, which implies that the eigenvalues of $\mathbf{T}$ are equal to its singular values. Clearly, the following relation is satisfied

$$\mathbf{T}\mathbf{u}_i = (a_i - b_i)\mathbf{u}_i,$$

which means that $\mathbf{u}_i$ is an eigenvector and $a_i - b_i$ is an eigenvalue of $\mathbf{T}$. In conclusion, $\mathbf{u}_i$ is a singular vector with corresponding singular value $a_i - b_i$ of matrix $\mathbf{T}$. □

In the upcoming lemma, we present an expression for all $n_1 + 2n_b - 2$ singular values of $\mathbf{T}$.

Lemma 5.8. *Given a matrix* $\mathbf{T}$ *as defined in (20), if*

- $a_i + b_i = 1$ *for* $i = 2, \ldots, n_b$,
- $a_i \neq b_i$ *for* $i = 2, \ldots, n_b$,
- $a_i \geq 0$ *and* $b_i \geq 0$ *for* $i = 2, \ldots, n_b$,

then matrix $\mathbf{T}$ *has singular values*

$$\lambda_i = \begin{cases} 1, i = 1, \ldots, n_1, \\ 1, i = n_1 + 1, \ldots, n_1 + n_b - 1, \\ a_i - b_i, i = n_1 + n_b, \ldots, n_1 + 2n_b - 2, \end{cases}$$

where $a_i - b_i < 1$.

Proof. Without loss of generality we can switch the rows and columns of $\mathbf{T}$ such that: $a_2 - b_2 \geq \cdots \geq a_{n_b-1} - b_{n_b-1} \geq a_{n_b} - b_{n_b}$. We can arrange the singular values of matrix $\mathbf{T}$ into the following three groups:

- The first n_1 singular values are equal to 1, which correspond to the upper left block of matrix $\mathbf{T}$.
- Using similar reasoning as in Lemma 5.7, it can be shown that $\mathbf{T}$ has singular values $a_i + b_i$ for $i = 2, \ldots, n_b$, which are all equal to 1 by assumption.
- From Lemma 5.7 it follows that the remaining singular values are $a_i - b_i$ for $i = 2, \ldots, n_b$. We can assume without loss of generality that $a_i > b_i$. Since $a_i + b_i = 1$, this implies that $1 > a_i - b_i > 0$. □

We conclude that $\mathbf{T}$ has singular values $a_i - b_i$ for $i = 2, \ldots, n_b$, and these are the smallest singular values of matrix $\mathbf{T}$. The next lemma states two other conditions that matrix $\mathbf{T}$ satisfies, which follow directly from (20).

Lemma 5.9. *Given a matrix $\mathbf{T}$ as defined in (20) and $a_i + b_i = 1$ for $i = 2, \ldots, n_b$, then $\mathbf{T}\mathbf{r} = \mathbf{r}$ and $\mathbf{1}_{n_r}^\top \mathbf{T} = \mathbf{1}_{n_r}^\top$.*

Using Theorem 5.4 and Lemmas 5.5-5.9, we prove the main result that $\mathbf{F}^a$ is an admissible matrix of $\mathbf{F}^o$.

Theorem 5.10. *Given*

B1. *a matrix $\mathbf{F}^o$, which can be partitioned as shown in (19). The values $c_i - d_i$ for $i = 2, \ldots, n_b$ are the smallest singular values of $\mathbf{F}^o$.*
B2. *a symmetric matrix $\mathbf{T} \neq \mathbf{I}$, which can be partitioned as shown in (20), the entries of $\mathbf{T}$ satisfy $a_i \geq 0$, $b_i \geq 0$, $a_i + b_i = 1$ and $a_i \neq b_i$ for $i = 2, \ldots, n_b$.*

Then $\mathbf{F}^a = \mathbf{T}\mathbf{F}^o$, implying that $h(\mathbf{F}^o) = h(\mathbf{F}^a)$.

Proof. We show that all the assumptions of Theorem 5.4 are satisfied. Assumptions A1 and A3 follow directly from the definitions of $\mathbf{F}^o$ and $\mathbf{T}$, so A2, A4 and A5 remain.

- From Lemma 5.9 it follows that $\mathbf{T}\mathbf{r} = \mathbf{r}$ and $\mathbf{1}_{n_r}^\top \mathbf{T} = \mathbf{1}_{n_r}^\top$. Thus, A2 is satisfied.
- By combining Lemma 5.6 and 5.7, we obtain that the last $n_b - 1$ singular vectors of $\tilde{\mathbf{F}}^o$ and $\mathbf{T}^o$ are the same, e.g. $\tilde{\mathbf{U}}_c = \mathbf{U}_{c\mathrm{T}}$. Furthermore, in Lemma 5.8 we have shown that $\mathbf{\Lambda}_{k\mathrm{T}} = \mathbf{I}$ and $\mathbf{\Lambda}_{c\mathrm{T}} \leq \mathbf{I}$. So, A4 holds.
- Since $\mathbf{1}_c < \boldsymbol{\delta}$ is a valid lower bound, it follows that $\boldsymbol{\lambda}_{c\mathrm{T}} \leq \mathbf{1}_c < \boldsymbol{\delta}$, so A5 is satisfied.

Thus, if we set $\mathbf{F}^a = \mathbf{T}\mathbf{F}^o$, then $\mathbf{F}^a$ is an admissible matrix of $\mathbf{F}^o$. □

We illustrate Theorem 5.10 by means of an example.

Example 5.11. Throughout this example we consider 3-dimensional CA solutions. Suppose we have the following original matrix

$$\mathbf{F}^{o*} = \begin{pmatrix} 3 & 1 & 3 & 10 & 3 & 3 & 1 \\ 3 & 1 & 5 & 2 & 9 & 3 & 2 \\ 4 & 1 & 2 & 2 & 2 & 7 & 2 \\ 3 & 1 & 9 & 2 & 5 & 3 & 2 \\ 3 & 1 & 3 & 1 & 3 & 3 & 11 \\ 7 & 1 & 2 & 2 & 2 & 4 & 2 \end{pmatrix}.$$

At first glance we do not suspect this matrix $\mathbf{F}^{o*}$ to have an admissible matrix, since this matrix looks quite different compared to Example 2.5. However, permuting the rows and columns (which does not influence the singular values) yields

$$\mathbf{F}^{o} = \left(\begin{array}{cc|cc|cc|c} 11 & 1 & 3 & 3 & 3 & 3 & 1 \\ 1 & 10 & 3 & 3 & 3 & 3 & 1 \\ \hline 2 & 2 & 9 & 5 & 3 & 3 & 1 \\ 2 & 2 & 5 & 9 & 3 & 3 & 1 \\ \hline 2 & 2 & 2 & 2 & 7 & 4 & 1 \\ 2 & 2 & 2 & 2 & 4 & 7 & 1 \end{array}\right),$$

$$\boldsymbol{\lambda}^{o} = \begin{pmatrix} 22.52 & 9.57 & 7.95 & 5.31 & 4.00 & 3.00 \end{pmatrix}^{\top}.$$

We notice that $\mathbf{F}^{o}$ satisfies the structure defined in (19). Also, we can construct a matrix

$$\mathbf{T} = \left(\begin{array}{cc|cc|cc} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & \frac{3}{4} & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{4} & \frac{3}{4} & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & \frac{2}{3} & \frac{1}{3} \\ 0 & 0 & 0 & 0 & \frac{1}{3} & \frac{2}{3} \end{array}\right),$$

satisfying (20). It can be verified that the two conditions of Theorem 5.10 hold, which means that the matrix obtained using $\mathbf{F}^{a} = \mathbf{T}\mathbf{F}^{o}$ is an admissible matrix. We can verify that

$$\mathbf{F}^a = \left(\begin{array}{cc|cc|cc|c} 11 & 1 & 3 & 3 & 3 & 3 & 1 \\ 1 & 10 & 3 & 3 & 3 & 3 & 1 \\ \hline 2 & 2 & 8 & 6 & 3 & 3 & 1 \\ 2 & 2 & 6 & 8 & 3 & 3 & 1 \\ \hline 2 & 2 & 2 & 2 & 6 & 5 & 1 \\ 2 & 2 & 2 & 2 & 5 & 6 & 1 \end{array}\right),$$

$$\boldsymbol{\lambda}^a = \begin{pmatrix} 22.52 & 9.57 & 7.95 & 5.31 & 2.00 & 1.00 \end{pmatrix}^\top,$$

is indeed an admissible matrix. Note that in this example the last two (rounded) singular values of the original and admissible matrix are different from each other.

To summarise, this section contains a general approach to generate pairs of matrices $\mathbf{F}^o$ and $\mathbf{F}^a$ that satisfy $h(\mathbf{F}^o) = h(\mathbf{F}^a)$. The main idea is to construct matrices $\mathbf{F}^o$ and $\mathbf{T}$ as shown in (19) and (20). In addition, the assumptions of Theorem 5.10 should be satisfied, which should not be too difficult. For instance, B1 is often satisfied by choosing elements in block $\mathbf{F}_{11}$ to be much larger than the remaining blocks, such that the "singular values of block $\mathbf{F}_{11}$" are larger than the "singular values corresponding to blocks $i = 2, \ldots, n_b$".

6. Discussion

We discuss the implications of Theorems 4.4 and 5.4. Also, we provide an example which satisfies the necessary conditions, but not our sufficient conditions.

When assuming that all singular values are non-zero, the necessary conditions for the existence of an admissible matrix shown in Theorem 4.4 imply that there is a unique relationship between two matrices that have the same k-dimensional approximation. Even if other (possibly non-linear) relations between the original and admissible matrices exist, these relations can always be replaced by the linear relationship. Satisfying the necessary conditions in practice with an arbitrary contingency table is not trivial and it is unlikely that one would encounter this in an empirical setting. Thus, we expect that it is unlikely that admissible matrices are found in practice, which is in line with the experimental results from Van de Velden et al. [17], who never found an admissible matrix when generating random matrices.

Based on the sufficient conditions shown in Theorem 5.4 we are able to generate admissible matrices. This implies that there exist matrices $\mathbf{F}^1$ and $\mathbf{F}^2$ with the same k-dimensional approximation. The described procedure is flexible both in terms of k and the number of singular values that may change. Firstly, this procedure works for any value of k. Suppose we have a suitable $\mathbf{F}$ in the form of (19) for which an admissible matrix exists. If we want to find an admissible matrix for larger values of k, we can increase the size of block $\mathbf{F}_{11}$. This larger matrix is expected to satisfy the sufficient conditions, so the admissible matrix exists as well. Secondly, we can control the number of singular values that differ between $\mathbf{F}^1$ and $\mathbf{F}^2$ by adjusting the number of blocks shown in (19). In conclusion, k-dimensional CA solutions are not necessarily unique for any value of k.

In our derivations and formulations of the necessary and sufficient conditions, the integrality constraint of a contingency matrix was not used. Hence, the presented results are also applicable to non-integer matrices. Notice that when we find an admissible non-integer matrix satisfying the conditions of Theorem 5.10, we can generate infinitely many admissible matrices by slightly perturbing matrix $\mathbf{T}$.

Finally, it is important to note that the sufficient conditions in Theorem 5.4 are not the same as the necessary conditions in Theorem 4.4. In Theorem 4.4, in contrast with Theorem 5.4, we assume that all singular values are non-zero, so it is not known whether a unique matrix $\mathbf{T}$ exists when there are singular values that take the value zero. Also, Theorem 5.4 requires $\mathbf{T}$ to be symmetric and have singular values smaller or equal to 1, which is not required in Theorem 4.4. By manipulating a matrix that satisfied the sufficient conditions in Theorem 5.4 we obtain an admissible matrix that satisfies the necessary conditions, but no longer satisfies the sufficient conditions, which is shown in the next example.

Example 6.1. Consider the original matrix

$$\mathbf{F}^o = \begin{pmatrix} 100 & 1 & 1 & 1 & 1 \\ 1 & 90 & 1 & 1 & 1 \\ 1 & 1 & 80 & 1 & 1 \\ 1 & 1 & 1 & 7 & 4 \\ 1 & 1 & 1 & 5 & 1 \end{pmatrix},$$

$$\tilde{\boldsymbol{\lambda}}^o = \begin{pmatrix} 1 & 0.950 & 0.943 & 0.724 & 0.142 \end{pmatrix}^\top,$$

and admissible matrix

$$\mathbf{F}^a = \begin{pmatrix} 100 & 1 & 1 & 1 & 1 \\ 1 & 90 & 1 & 1 & 1 \\ 1 & 1 & 80 & 1 & 1 \\ 1 & 1 & 1 & 8 & 3 \\ 1 & 1 & 1 & 4 & 2 \end{pmatrix},$$

$$\tilde{\boldsymbol{\lambda}}^a = \begin{pmatrix} 1 & 0.950 & 0.943 & 0.726 & 0.043 \end{pmatrix}^\top.$$

We can verify that $\mathbf{T}\mathbf{F}^o = \mathbf{F}^a$ and $h(\mathbf{F}^o) = h(\mathbf{F}^a)$ hold for the following (rounded) linear transformation matrix

$$\mathbf{T} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ -0.004 & -0.004 & -0.005 & 0.542 & 0.843 \\ 0.004 & 0.004 & 0.005 & 0.458 & 0.157 \end{pmatrix},$$

$$\boldsymbol{\lambda}_{\mathrm{T}} = \begin{pmatrix} 1.08 & 1.00 & 1.00 & 1.00 & 0.28 \end{pmatrix}^{\top}.$$

It can be verified that $\mathbf{T}$ satisfies the necessary conditions, however, since $\mathbf{T}$ is not symmetric assumption A2 of Theorem 5.4 is violated.

It remains an open problem under which less restrictive sufficient conditions an admissible matrix exists. Hopefully, in further research the gap between the sufficient and necessary conditions can be closed.

7. Conclusion

In correspondence analysis (CA), the aim is to optimally depict the rows and columns of a contingency table in a k-dimensional space. Van de Velden et al. [17] found in their experiments that the 3-dimensional CA solution uniquely corresponds with the original contingency table up to rotation [15]. Therefore, we investigated the uniqueness of k-dimensional correspondence analysis (CA) solutions.

We presented a relationship between a contingency table and the k-dimensional solution [9]. We provided stylised examples in which two tables exist with the same k-dimensional CA solution. In the first main result, we outlined necessary conditions that must be satisfied for a non-unique CA solution to exist. In the second main result, we presented sufficient conditions for the existence of non-unique CA solutions. This is followed by a method that generates tables with a non-unique CA solution based on the sufficient conditions.

The two main results have several implications. Firstly, based on the sufficient conditions we concluded that contingency tables with a non-unique CA solution exist for any value of k. In addition, we showed that two tables with the same low-dimensional CA solution are uniquely related by a linear transformation. Lastly, based on the necessary conditions it is unlikely to find such tables in practice, thereby confirming the experimental results of Van de Velden et al. [17], who always found contingency tables with a unique CA solution.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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