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Zero patterns in multi-way binary contingency tables with uniform margins

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ABSTRACT

We study the problem of transforming a multi-way contingency table into an equivalent table with uniform margins and same dependence structure. This is an old question which relates to recent advances in copula modeling for discrete random vectors. In this work, we focus on multi-way binary tables and develop novel theory to show how the zero patterns affect the existence of the transformation as well as its statistical interpretability in terms of dependence structure. The implementation of the theory relies on combinatorial and linear programming techniques, which can also be applied to arbitrary multi-way tables. In addition, we investigate which odds ratios characterize the unique solution in relation to specific zero patterns. Several examples are described to illustrate the approach and point to interesting future research directions.

1. Introduction

Largely employed across numerous domains such as healthcare, biology, and social sciences, contingency tables serve to display data in tabular format. Contingency tables have been extensively analyzed within the field of statistics, primarily with the objective of developing methods to understand the dependence between variables (see, for example, [1]). Recent work presented in [2] highlights fascinating connections between the analysis of two-way contingency tables and copulas. The essence of copula theory is centered on distinguishing between the influence of separate variables and their mutual dependency within the model. This separation facilitates the use of *ad hoc* dependence modeling techniques by transforming the initial joint probability distribution into one with uniform margins on $[0, 1]$, known as the copula. When the marginal distributions are continuous, the copula associated with the original distribution is uniquely defined ([3]). For discrete random variables, it is not possible to transform marginal distributions into uniform distributions using the Probability Integral Transform (PIT). Sklar's theorem identifies the copula solely within a specific subdomain. As a result, numerous copula models align with this specific subdomain. The adaptation of copula theory to utilize an analogous notion for establishing a margin-free model within a discrete framework has been investigated in [2,4]. In those studies and the referenced literature, the authors explore the concept of transforming a given two-way contingency table into a new one that has uniform margins. This type of transformation clarifies the underlying relationships in the table, which could be obscured by notably uneven margins, as explained in the example below.

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Table 1
Sheffield smallpox epidemic reported in [5]. The values of \bar{p} are rounded to 3 decimal places.

Vaccination (X_1)	Recovery (X_2)	\bar{n}	\bar{p}
no	no	274	0.058
no	yes	278	0.059
yes	no	200	0.043
yes	yes	3951	0.840

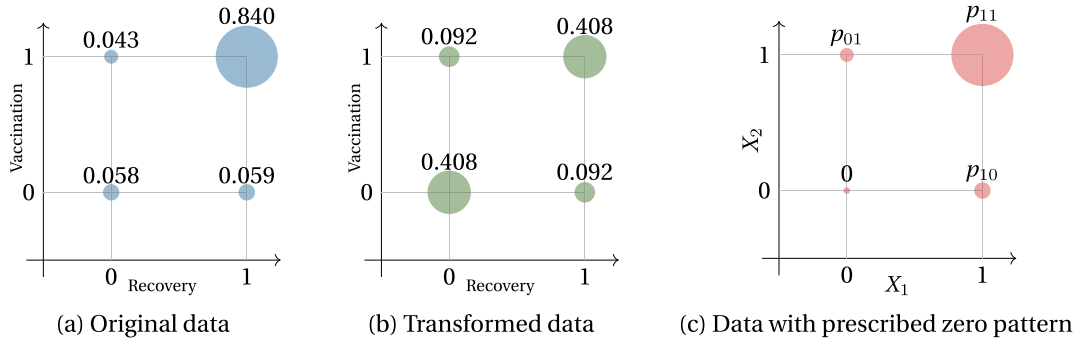


Fig. 1. Bubble plot of original data (a) and transformed data (b) for the Sheffield smallpox epidemic data in Table 1. Part (c) represents a possible zero pattern in the observed table that motivates the investigations in this paper.

Motivating example. For 2×2 tables, the process entails converting the original table into a new one in which each marginal probability equals $1/2$, indicating a uniform distribution across the subdomain. In Table 1, we provide a classic instance from [5] that demonstrates smallpox cases documented at Sheffield Hospital. The dataset categorizes 4703 patients based on their vaccination status (yes or no) and their recovery outcome (yes or no). The odds ratio, frequently used to evaluate associations in contingency table analysis, is notable with a value of 19.47. Despite this, the unevenness of the marginals might obscure the link within the original dataset. The connection becomes apparent once the data is altered to show marginal probabilities of $1/2$, as illustrated in Fig. 1 (b), while maintaining an odds ratio of 19.47.

The transformed table also has an interpretation in terms of the information projection (I-projection) of the original probability table on the space of tables with uniform margins and prescribed support (see, e.g., [2,4]). In fact, this is the closest element to the original table with respect to the Kullback-Leibler divergence, and as such it is unique [6]. The uniqueness of the transformation is guaranteed only if a table with fixed margins and zero pattern exists. However, this might not be the case when the original table contains zero entries. To clarify this, we consider a modification of the above example where the probability mass p_{00} is zero. A generic table with this structure is represented in Fig. 1 (c). It is straightforward to check that a table that preserves such a zero-structure and has uniform margins does not exist. Indeed, if such a table would exist, it would be the solution of the following system of equations

$$\begin{cases} p_{00} + p_{01} + p_{10} + p_{11} = 1 \\ p_{00} + p_{01} - p_{10} - p_{11} = 0 \\ p_{00} - p_{01} + p_{10} - p_{11} = 0 \\ p_{00} = 0 \end{cases} \quad (1)$$

However, the system in Eq. (1) has no solutions unless p_{11} is also set to zero, which means the original zero pattern is not maintained.

Research problem and paper’s contribution. The situation described in Fig. 1 (c) is not artificial as zero entries are often observed in real datasets. Being an issue in applications, the problem of zero entries in contingency table analysis has caught the attention of researchers, especially in Algebraic Statistics, see for instance [7, Chap. 9]. When working with sampling distributions, zeros can appear both as structural zeros and sampling zeros, a far more common situation than the structural zeros: As the number of cells increases in multi-way tables, so does the probability of sampling zeros even when the sample size is moderate or large. In both cases, some of the conditional odds ratios become zero or undefined, leading to the removal of the corresponding odds ratio equation in the transformation. As a consequence, conditional odds ratios become uninformative of the relationship between the variables and new constraints on higher order combinations of the conditional odds ratios must be added to characterize the transformed table that preserves the original odds ratio structure.

In this work, we further develop the initial investigations of [8,9] to address the case of zeros in binary multi-way contingency tables. Our *problem statement* is the following: Given a table T (a probability table or a contingency table of observed frequencies), find a table \tilde{T} with uniform margins and the same odds ratios structure as T . It is known that such a table \tilde{T} is unique and can be found through scaling algorithms if and only if there exists a table with same zero pattern of T and uniform margins (e.g., [6]). However, a characterization of the existence of \tilde{T} in terms of possible zero patterns is not available in dimension $d > 2$. In this paper,

we provide conditions to ensure the existence of such a \tilde{T} . Under existence, we further investigate which combinations of conditional odds ratios are required to derive the unique solution in relation to the corresponding zero pattern.

The paper is organized as follows: In Section 2, we describe the mathematical context of this work, introduce the notation, and connect our research to the state-of-the-art. Section 3 presents novel theoretical results on the existence of a transformed table with certain zero patterns. In Section 4, we show that in some degenerate cases, there might be a wider class of tables that satisfy the conditional odds ratio constraints and have uniform margins. Therefore, higher order combinations of the primary conditional odds ratios are needed to obtain the unique transformation. We conclude the paper with a discussion in Section 5.

2. Background, notation, and relevance to the state-of-the-art

In this work, we consider the case of d -dimensional multi-way binary contingency tables with zero entries and study how the presence of zeros affects the possibility of transforming a given table into one with uniform margins. In particular, we analyze all possible zero patterns, where a zero pattern represents the set of the table cells whose corresponding frequencies are zero.

Here, we consider d binary factors, X_1, \dots, X_d , i.e., a d -dimensional random vector (X_1, \dots, X_d) . We refer to a specific cell of a table T with the binary vector $\alpha = (\alpha_1, \dots, \alpha_d) \in \{0, 1\}^d$. We assume the set $\{0, 1\}^d$ in lexicographic order and then we can refer to the k -th cell of T , $k = 1, \dots, 2^d$. We observe that the k -th cell of a table is the one corresponding to $\alpha_k = ((\alpha_k)_1, \dots, (\alpha_k)_d)$ such that $\sum_{j=1}^d (\alpha_k)_j 2^{d-j} = k - 1$, $k = 1, \dots, 2^d$, i.e., α_k is the binary representation of $k - 1$. For each cell α , $\alpha \in \{0, 1\}^d$, we define p_α , the relative frequency of the cell. Thus, a table T is described by the 2^d -vector $p = (p_\alpha, \alpha \in \{0, 1\}^d)$. In the d -dimensional case, there are 2^{2^d} possible zero patterns, including the 2^d -zero pattern that results in a trivial all-zero table. We can represent each zero pattern \mathcal{Z} with a binary 2^d vector, i.e., $\mathcal{Z} = (z_1, \dots, z_{2^d})$, where $z_i = 0$ ($z_i = 1$) indicates that the corresponding cell α_i has $p_{\alpha_i} = 0$ ($p_{\alpha_i} > 0$, respectively). We write that a zero pattern \mathcal{Z} is a k -zero pattern if the number of zeros in \mathcal{Z} is k , with $k = 0, \dots, 2^d$. Finally, we say that a table T with uniform margin is \mathcal{Z} -compatible if the corresponding probability mass function (pmf) p satisfies that $p_{\alpha_i} = 0$ ($p_{\alpha_i} > 0$) when $z_i = 0$ ($z_i = 1$, respectively), $i = 1, \dots, 2^d$.

We now introduce the notion of conditional odds ratios, which is key to this work. In particular, we define the conditional odds ratios constraints on each 2×2 sub-tables by fixing $d - 2$ variables. When $d = 2$, there is only one odds ratio given by

$$\omega^{12} = \frac{p_{11}p_{00}}{p_{10}p_{01}}.$$

In the case $d = 3$ there are six conditional odds ratios given by

$$\begin{aligned} \omega_0^{23} &= \frac{p_{000}p_{011}}{p_{001}p_{010}} & \omega_1^{23} &= \frac{p_{100}p_{111}}{p_{101}p_{110}} \\ \omega_0^{13} &= \frac{p_{000}p_{101}}{p_{001}p_{100}} & \omega_1^{13} &= \frac{p_{010}p_{111}}{p_{011}p_{110}} \\ \omega_0^{12} &= \frac{p_{000}p_{110}}{p_{010}p_{100}} & \omega_1^{12} &= \frac{p_{001}p_{111}}{p_{011}p_{101}} \end{aligned} \tag{2}$$

The notation ω_0^{23} denotes the conditional odds ratio for the variables X_2 and X_3 given the value 0 for X_1 . The conditions in Eq. (2) are not independent, and only four of them are independent.

In arbitrary dimension $d > 3$, the generic conditional odds ratio is defined in the same way: for each pair of variables X_i and X_j we consider the conditional odds ratio for given values of the other $(d - 2)$ variables. If we denote with $\alpha' \in \{0, 1\}^{d-2}$ the values of the fixed $(d - 2)$ variables, the conditional odds ratio is denoted as $\omega_{\alpha'}^{ij}$ and defined by:

$$\omega_{\alpha'}^{ij} = \frac{p_{\alpha_1} p_{\alpha_2}}{p_{\alpha_3} p_{\alpha_4}}, \tag{3}$$

where $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ are equal to $\alpha' \in \{0, 1\}^{d-2}$ in the entries $\{1, \dots, d\} - \{i, j\}$ and are equal to $(1, 1), (0, 0), (1, 0), (0, 1)$ respectively in the entries (i, j) . An example in $d = 4$ is

$$\omega_{01}^{13} = \frac{p_{0001}p_{1011}}{p_{0011}p_{1001}}.$$

In the d -way case there are $\binom{d}{2} 2^{d-2}$ equations, which are not independent. In the remainder of the paper, we refer to the conditional odds ratios defined in Eq. (3) simply as *odds ratios*. In the following, we draw connections with previous research on discrete copulas and classical results for log-linear models.

2.1. Table transformations and discrete copulas

In this section, we relate our research problems to the theory of discrete copulas. For the sake of clarity, we first restrict to the two-dimensional case. In this paper, we define a discrete copula as a subcopula restricted on a discrete domain [10]. This is in line with previous work on the topic, namely, see [11–13] and references therein. We consider $R \in \mathbb{Z}_{>0}$ and denote $I_R = \{0, 1/R, \dots, (R - 1)/R, 1\}$, $[R] = \{1, \dots, R\}$, and $\langle R \rangle = \{0, \dots, R\}$. Given R and S as positive integers, we define $U_R = \{u_0 = 0, u_1, \dots, u_{R-1}, u_R = 1\}$, with $u_0 < \dots < u_R$, and $V_S = \{v_0 = 0, v_1, \dots, v_{S-1}, v_S = 1\}$, with $v_0 < \dots < v_S$, as two discrete grid partitions over the unit interval.

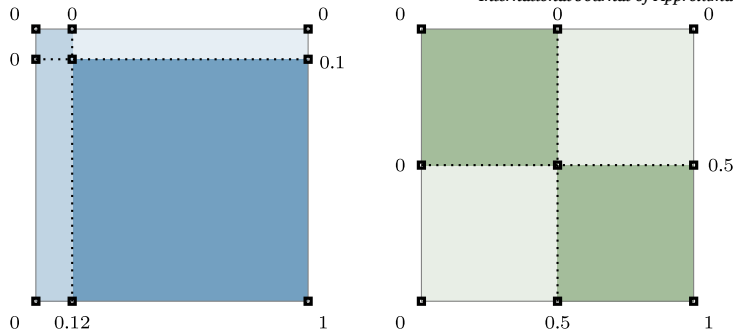


Fig. 2. Left: A representation of the grid domain $U_2 \times V_2$, support of the discrete copula C_1 . Right: The grid support $I_2 \times I_2$ of the discrete copula \tilde{C}_1 with the same dependence structure of C_1 . The colors represent a heatmap of the corresponding probabilities.

In this framework, a discrete copula C_{U_R, V_S} is then defined on the set $U_R \times V_S$ and retains the characteristic properties of a copula function over the grid domain $U_R \times V_S$.

As noted in [12,13], interesting relationships exist between the domain of discrete copulas and certain convex polytopes known as *transportation polytopes*, i.e., convex sets of nonnegative matrices with prescribed row and column sums defined by linear constraints. These convex sets also appear in the analysis of contingency tables, where one seeks a nonnegative table with specified row and column sums, known as *margins* [14]. Specifically, given two positive vectors $\tilde{u} = (\tilde{u}_1, \dots, \tilde{u}_R) \in \mathbb{R}_{>0}^R$ and $\tilde{v} = (\tilde{v}_1, \dots, \tilde{v}_S) \in \mathbb{R}_{>0}^S$, the *transportation polytope* $\mathcal{T}(\tilde{u}, \tilde{v})$ is the set of nonnegative $R \times S$ matrices $(x_{i,j})$ satisfying:

$$x_{i,j} \geq 0, \quad \sum_{h=1}^S x_{i,h} = \tilde{u}_i, \quad \sum_{\ell=1}^R x_{\ell,j} = \tilde{v}_j,$$

for all $i \in [R], j \in [S]$. The vectors \tilde{u} and \tilde{v} define the row and column sums, or margins, of the table.

According to [11], each discrete copula C_{U_R, V_S} is associated with a matrix in a transportation polytope $\mathcal{T}(\tilde{u}, \tilde{v})$, and conversely. The transportation matrix is connected to the probability mass function of the discrete random vector, whereas the associated discrete copula corresponds to the cumulative distribution function. We now show how to derive the discrete copula associated with a given contingency table. We consider the motivating example presented in Table 1. There, we get $N = 4703$ total observations. In this example, $R = S = 2$, the vectors \tilde{u} and \tilde{v} are the margins of the contingency table, i.e., $\tilde{u} = (552, 4151)$ and $\tilde{v} = (474, 4229)$, while the defining grids of the corresponding discrete copula are $U_2 = \frac{1}{N} \{0, \tilde{u}_1, \tilde{u}_1 + \tilde{u}_2\} = \{0, 0.12, 1\}$ and $V_2 = \{0, 0.1, 1\}$. The entries of the discrete copula $C_1 = C_{U_2, V_2} = (c_{i,j})$, $i \in [2]$ and $j \in [2]$ are computed from the entries of the contingency table $(x_{i,j})$ by summing up and normalizing, i.e., $c_{i,j} = \frac{1}{N} \sum_{\ell=1}^i \sum_{h=1}^j x_{\ell,h}$, while $c_{0,0} = c_{i,0} = c_{0,j} = 0$, for $i \in [2]$ and $j \in [2]$. Namely, C_1 is as follows, and its non-uniform grid domain is depicted in Fig. 2 (left):

$$C_1 = \begin{pmatrix} 0 & 0.00 & 0.00 \\ 0 & 0.058 & 0.1 \\ 0 & 0.12 & 1.00 \end{pmatrix}.$$

As discussed in the introduction, in [2], the author emphasizes the challenge of inferring dependence from tables with non-uniform margins, such as Table 1.

In line with copula theory for continuous random variables, the author proposes finding a representative $\tilde{\mathbf{p}}$ for all $(R \times S)$ probability distributions that (i) maintains the inter-dependencies in a contingency table using odds ratios, and (ii) has uniform margins of $1/R$ on the first dimension and $1/S$ on the second dimension. In discrete copulas terms, this corresponds to finding a discrete copula defined on the rectangular grid $I_R \times I_S$ that maintains the dependence structure of the initial discrete copula derived from a specific contingency table. In the example above, the problem is to identify a discrete copula \tilde{C}_1 with its domain on $I_2 \times I_2$ and margins I_2 , which is somehow compatible with the original discrete copula C_1 . A depiction of the domain of such a representative is depicted in Fig. 2(right).

A natural question that arises is whether or not such an element exists. If it exists, it is unique in line with the theory of I-projections [6]. For two-dimensional tables, the answer to this question is provided by a theorem presented in [2], which we summarize below in a simplified version. The theorem examines the structure of the given zero pattern in terms of the *rectangular sets* it contains, establishing conditions based on their “size”.

Theorem 2.1. *Let \mathbf{p} be in the set $\mathcal{P}_{R \times S}$ of all $(R \times S)$ probability distributions. We define $\text{Supp}(\mathbf{p}) = \{(i, j) \in [R] \times [S] \text{ s.t. } p_{i,j} > 0\}$, the support of \mathbf{p} , and $N(\mathbf{p}) = \{v_{X_1} \times v_{X_2} : v_{X_1} \subset [R], v_{X_2} \subset [S] \text{ s.t. } \sum_{(i,j) \in v_{X_1} \times v_{X_2}} p_{i,j} = 0\}$, the set of rectangular subsets of $[R] \times [S]$ where \mathbf{p} is null. The cardinality of a set A is denoted by $|A|$.*

1. Suppose that for all $v_{X_1} \times v_{X_2} \in N(\mathbf{p})$, $\frac{|v_{X_1}|}{R} + \frac{|v_{X_2}|}{S} < 1$, then there exists a unique $\bar{\mathbf{p}}$ with uniform margins associated with a discrete copula $C_{I_R \times I_S}$.
2. Suppose that for all $v_{X_1} \times v_{X_2} \in N(\mathbf{p})$, $\frac{|v_{X_1}|}{R} + \frac{|v_{X_2}|}{S} \leq 1$ with $\frac{|\bar{v}_{X_1}|}{R} + \frac{|\bar{v}_{X_2}|}{S} = 1$ for some $\bar{v}_{X_1} \times \bar{v}_{X_2} \in N(\mathbf{p})$.
 - (i) If, for all $\bar{v}_{X_1} \times \bar{v}_{X_2} \in N(\mathbf{p})$ such that $\frac{|\bar{v}_{X_1}|}{R} + \frac{|\bar{v}_{X_2}|}{S} = 1$, $[R] \setminus \bar{v}_{X_1} \times [S] \setminus \bar{v}_{X_2} \in N(\mathbf{p})$, then there exists a unique $\bar{\mathbf{p}}$ with uniform margins associated with a discrete copula $C_{I_R \times I_S}$.
 - (ii) If, there exists $\bar{v}_{X_1}^* \times \bar{v}_{X_2}^* \in N(\mathbf{p})$ such that $\frac{|\bar{v}_{X_1}^*|}{R} + \frac{|\bar{v}_{X_2}^*|}{S} = 1$, and $[R] \setminus \bar{v}_{X_1}^* \times [S] \setminus \bar{v}_{X_2}^* \notin N(\mathbf{p})$, then there is no element $\bar{\mathbf{p}}$ with uniform margins and same support of the original table, but there is one element $\bar{\mathbf{p}}$ with support strictly contained in that of \mathbf{p} , $\text{Supp}(\bar{\mathbf{p}}) \subset \text{Supp}(\mathbf{p})$, and uniform margins.
3. Suppose that there exists $\bar{v}_{X_1} \times \bar{v}_{X_2} \in N(\mathbf{p})$ such that $\frac{|\bar{v}_{X_1}|}{R} + \frac{|\bar{v}_{X_2}|}{S} > 1$. Then there is no element $\bar{\mathbf{p}}$ with uniform margins such that it has same odds ratio structure of \mathbf{p} and is associated with a discrete copula $C_{I_R \times I_S}$, not even with a modified support.

We can interpret the example of Table 1 in light of Theorem 2.1. For a broader discussion of the two-dimensional binary case, we refer the reader to [2]. The case reported in Table 1 does not show any zero pattern, since all entries are strictly positive. Therefore, the transformed table exists and is unique in agreement with Part 1 of Theorem 2.1. We now analyze the situation depicted in Fig. 1 (c) where one entry is zero while the others are non-zero. This case falls under point 2 (ii) of Theorem 2.1.

Specifically, $N(\mathbf{p}) = v_{X_1} \times v_{X_2}$ with $v_{X_1} = v_{X_2} = \{1\}$. Letting $\bar{v}_{X_1}^* = v_{X_1}$ and $\bar{v}_{X_2}^* = v_{X_2}$ we get $|\bar{v}_{X_1}^*| = |\bar{v}_{X_2}^*| = 1$, $\frac{|\bar{v}_{X_1}^*|}{2} + \frac{|\bar{v}_{X_2}^*|}{2} = 1$ and $[R] \setminus \bar{v}_{X_1}^* \times [S] \setminus \bar{v}_{X_2}^* = \{2\} \times \{2\} \notin N(\mathbf{p})$. Then a solution with exactly the same support does not exist in agreement with the conclusion of the introduction. If we move to the boundary of the probability space by adding an extra zero in the zero pattern (that is, allowing p_{11} to be set equal to zero), a solution exists. When it exists, the element $\bar{\mathbf{p}}$ can be obtained using the Iterative Proportional Fitting Procedure (IPFP), which is a standard method in contingency table analysis for a meaningful comparison of tables with different margins and same dependence structure in terms of corresponding odds ratios and their higher order combinations [1,2]. We consider an $R \times S$ table T and a probability distribution $p = (p_{ij} : i = 1, \dots, R, j = 1, \dots, S)$ defined over T . Without loss of generality, we assume all marginals $p_{i+} = \sum_{j=1}^S p_{ij}$ and $p_{+j} = \sum_{i=1}^R p_{ij}$ to be nonzero, $i = 1, \dots, R, j = 1, \dots, S$. At the k -th iteration, $k = 1, \dots, N_{\max}$, the IPFP algorithm performs the following row and column transformations:

$$p_{ij}^{(k+1)} = \frac{1/R}{p_{i+}^{(k)}} p_{ij}^{(k)}, \quad i = 1, \dots, R, j = 1, \dots, S \tag{4}$$

$$p_{ij}^{(k+1)} = \frac{1/S}{p_{+j}^{(k+1)}} p_{ij}^{(k+1)}, \quad i = 1, \dots, R, j = 1, \dots, S, \tag{5}$$

where $p_{ij}^{(1)} = p_{ij}$ and N_{\max} is a predefined maximum number of iterations. The output of the algorithm is a new table T' with pmf $p_{ij}^{(N_{\max})}$ that, under the conditions of Theorem 2.1, has uniform margins. For further details, particularly regarding the extension to d -way tables, we refer the interested reader to [15]. It should be noted that IPFP preserves the support and odds ratio structure in terms of the odds ratio matrix, i.e., the matrix of all conditional odds ratios, and the higher order interactions of the odds ratio of the initial table across the iterations. If there are no zeros in the support, the odds ratio matrix gives sufficient constraints to identify the transformed table. With an example, we now show that if zeros are present in the table, the conditional odds ratios alone do not determine the table, and higher order combinations of the odds ratios must be considered. We examine the following 3×3 table with three zeros on the main diagonal:

$$\begin{pmatrix} 0 & p_{12} & p_{13} \\ p_{21} & 0 & p_{23} \\ p_{31} & p_{32} & 0 \end{pmatrix}. \tag{6}$$

This table falls within the existence case of Theorem 2.1. Nevertheless, the odds-ratios defined on 2×2 sub-tables are not enough to identify the equivalent table. In fact, no odds ratio on 2×2 sub-tables is well defined, and to identify the transformed table we need to fix also the quantity

$$\frac{p_{12}p_{23}p_{31}}{p_{13}p_{21}p_{32}}, \tag{7}$$

which arises as the symbolic product

$$\frac{p_{12}p_{23}}{p_{13}p_{22}} \cdot \frac{p_{22}p_{31}}{p_{21}p_{32}}. \tag{8}$$

The quantity reported in Eq. (7) is well known in Algebraic Statistics for tables with structural zeros: It arises from elimination theory, which provides a formal and rigorous justification for the symbolic cancellation in Eq. (8). For more details, see, e.g. [16]. In Sec. 4, we analyze similar examples in dimension three.

A formal introduction to elimination theory is beyond the scope of this paper. However, the construction of the odds ratio in Eq. (7) from those in Eq. (2) illustrates a generalizable procedure: Given a system of polynomial equations, one can systematically eliminate the variables corresponding to zero entries and derive polynomial relations that hold on the projection, i.e., involving only

the non-zero probabilities. Further directions for a systematic treatment of zero patterns via elimination methods are discussed in the final section.

The table in Eq. (6) illustrates that the specification of the constrained support, while informative, is in general insufficient to ensure the uniqueness of the representative discrete copula. Indeed, in that example, there exist infinitely many discrete copulas on $I_3 \times I_3$ compatible with the given zero pattern that satisfy the conditional odds ratio constraints, as these constraints are not well defined due to the support. However, only one discrete copula satisfies the higher-order constraints imposed by the odds ratios derived from the original contingency table. This underscores that, despite the information conveyed by the support and undefined odds ratios, uniqueness requires consideration of these higher-order conditions. In the following, we further discuss how our problem relates to standard theory in log-linear models.

2.2. Relations with the classical theory of log-linear models

In log-linear models, there is a well-established link between IPFP and Maximum Likelihood Estimation (MLE). The use of IPFP to find MLE in complete tables dates back to [17] (see also [18]). IPFP works in log-linear models as follows: First, define a table satisfying all the desired independence and/or conditional independence statements, and then, run the IPFP to adjust the table with respect to the relevant marginal distributions of the sufficient statistic. When there are zeros in the table, the existence of the MLE is generally not guaranteed. Important developments in this case have been achieved with the use of Algebraic Statistics: In most cases there are criteria to identify zero patterns which preserve the existence of the MLE, see [19]. In large classes of statistical models, including hierarchical log-linear models and staged trees, recent results have been introduced in [20]. Despite these connections, our problem is different because the margins are constrained to be uniform, while in log-linear models the margins are determined by suitable margins of the observed table. To clarify this key difference, we can refer again to the example depicted in Fig. 1 (c). In that situation, it is clear that there is no table with uniform margins and the prescribed support. However, if we start with unbalanced margins, i.e., $(1/3, 2/3)$, and relax the constraints of uniform margins, we can easily obtain tables that maintain the zero pattern.

3. Impact of zeros in the existence of the transformed multi-way table

As mentioned in the previous sections, the presence of zeros in the table affects the construction of a table with uniform margins in different ways. First, some odds ratio equations in Eq. (3) become meaningless and can thus be removed from the system. Additionally, the presence of zeros reduces the support of the probability distribution, reducing the number of free probabilities in the table.

As a prototype, let us consider again the 2×2 case. Given a 2×2 contingency table $(\tilde{n}_{ij}, i, j = 0, 1)$ let $N = \tilde{n}_{00} + \tilde{n}_{11} + \tilde{n}_{01} + \tilde{n}_{10}$ be the grand total and $\omega^{12} = \frac{\tilde{n}_{00}\tilde{n}_{11}}{\tilde{n}_{01}\tilde{n}_{10}}$ the odds ratio. We examine the table in terms of the relative frequencies $\tilde{p}_{ij} = \frac{\tilde{n}_{ij}}{N}$ rather than the counts \tilde{n}_{ij} . As shown in the motivating example in Sect. 1, the goal is to determine a new table $(p_{ij} \geq 0, i, j = 0, 1)$ such that the marginals are still $1/2$ and the original table's odds ratio ω^{12} is maintained. Such a table can be obtained by solving the following system of equations:

$$\begin{cases} \frac{p_{00}p_{11}}{p_{01}p_{10}} = \omega^{12} \\ p_{00} + p_{01} + p_{10} + p_{11} = 1 \\ p_{00} + p_{01} - p_{10} - p_{11} = 0 \\ p_{00} - p_{01} + p_{10} - p_{11} = 0 \end{cases}, \tag{9}$$

whose unique solution is given as follows:

$$p_{00} = p_{11} = \frac{\sqrt{\omega^{12}}}{2(1 + \sqrt{\omega^{12}})}, \quad p_{01} = p_{10} = \frac{1}{2(1 + \sqrt{\omega^{12}})}. \tag{10}$$

In the described 2^2 scenario, addressing the issue of zeros in the table is straightforward, with two possible situations: (a) The table is entirely filled, or (b) The table might contain one or more zero entries. As discussed in Sec. 2, if the table is complete, there exists a unique table with identical odds ratios and uniform margins, obtainable through the IPFP. Referring again to [2], in scenario (b), odds ratios are absent, simplifying the task of identifying a table with the same support as the original and uniform margins. This scenario is only achievable when there are two zeros located at $(0, 0), (1, 1)$ or $(1, 0), (0, 1)$. In an intermediate scenario with a single zero present in the table as in Fig. 1 (c), the IPFP leads to a boundary solution, resulting in another cell probability approaching zero. In this case, there are no tables which are zero-compatible with the original table and also have uniform margins. In the next section, we provide existence results for arbitrary dimensions and zero patterns.

3.1. d -way binary tables

We now move to the general d -way binary case. We denote $\{0, 1\}^k$ by $V_k, k = 1, \dots, d$. To simplify the notation, sometimes we write D instead of $V_d = \{0, 1\}^d$. Here, we are interested in tables with uniform margins. More specifically, there are d margins $m_i, i = 1, \dots, d$ defined as

$$m_i = (m_{i,0}, m_{i,1}) = \left(\sum_{\alpha \in D, \alpha_i=0} p_\alpha, \sum_{\alpha \in D, \alpha_i=1} p_\alpha \right),$$

where $D = \{0, 1\}^d$. We observe that $m_{i,1} = E[X_i]$ and $m_{i,0} + m_{i,1} = 1, i = 1, \dots, d$. To obtain uniform margins, the pmf of the table must satisfy the following constraints

$$m_{i,0} = m_{i,1} = \frac{1}{2}, i = 1, \dots, d.$$

The next Proposition 3.1 states a general result on the structure of the tables with uniform margins that are compatible with a class of zero patterns.

Proposition 3.1. *Let us consider a table T , with relative frequencies $p = (p_\alpha, \alpha \in V_d)$ and uniform margins. Let us suppose that, given $i_1, i_2 \in \{1, \dots, d\}, i_1 \neq i_2$, and $y_{i_1}, y_{i_2} \in \{0, 1\}, p_\alpha = 0$ for $\alpha \in \{(\alpha_1, \dots, \alpha_d) \in V_d : \alpha_{i_1} = y_{i_1}, \alpha_{i_2} = y_{i_2}\}$. Then $p_\alpha = 0$ for $\alpha \in \{(\alpha_1, \dots, \alpha_d) \in V_d : \alpha_{i_1} = 1 - y_{i_1}, \alpha_{i_2} = 1 - y_{i_2}\}$.*

Proof. Without loss of generality, we can take $i_1 = 1, i_2 = 2, y_{i_1} = y_{i_2} = 0$. The hypothesis on p can be written as $p_{00\alpha} = 0, \alpha \in V_{d-2}$. We compute $m_{1,0}$, the first component of the first margin:

$$m_{1,0} = \sum_{\alpha' \in V_{d-1}} p_{0\alpha'} = \sum_{\alpha'' \in V_{d-2}} p_{00\alpha''} + \sum_{\alpha'' \in V_{d-2}} p_{01\alpha''} = \sum_{\alpha'' \in V_{d-2}} p_{01\alpha''}.$$

The last equality in the above equation follows by $p_{00\alpha} = 0, \alpha \in V_{d-2}$. The table has uniform margins, in particular $m_{1,0} = \frac{1}{2}$, and as a consequence,

$$\sum_{\alpha'' \in V_{d-2}} p_{01\alpha''} = \frac{1}{2}.$$

Let us now consider the second component of the second margin, $m_{2,1}$. The table T has uniform margins and then $m_{2,1} = \frac{1}{2}$. Thus, we obtain the following chain of equalities:

$$m_{2,1} = \sum_{\alpha_1 \in \{0,1\}, \alpha'' \in V_{d-2}} p_{\alpha_1,1,\alpha''} = \sum_{\alpha'' \in V_{d-2}} p_{01\alpha''} + \sum_{\alpha'' \in V_{d-2}} p_{11\alpha''} = \frac{1}{2} + \sum_{\alpha'' \in V_{d-2}} p_{11\alpha''}.$$

Consequently, we obtain $\sum_{\alpha'' \in V_{d-2}} p_{11\alpha''} = 0$, that is $p_{11\alpha''} = 0, \alpha'' \in V_{d-2}$. \square

We observe that if the zero pattern is one of those expressed by the condition of Proposition 3.1, e.g., by choosing $i_1 = 1, i_2 = 2, y_{i_1} = 0, y_{i_2} = 0$ that means

$$p_\alpha = \begin{cases} 0 & \alpha = (0, 0, \alpha'') \text{ or } \alpha = (1, 1, \alpha''), \alpha'' \in V_{d-2} \\ > 0 & \text{elsewhere} \end{cases},$$

we can build a compatible table T with uniform margins. Namely, we define

$$p_\alpha = \begin{cases} 0 & \alpha = (0, 0, \alpha'') \text{ or } \alpha = (1, 1, \alpha''), \alpha'' \in V_{d-2} \\ \frac{1}{2^{d-1}} & \text{elsewhere} \end{cases}.$$

Since all margins have a similar structure, it is enough to compute $m_{1,0}$ and $m_{3,0}$, which are:

$$m_{1,0} = \sum_{\alpha'' \in V_{d-2}} p_{01\alpha''} = \sum_{\alpha'' \in V_{d-2}} \frac{1}{2^{d-1}} = \frac{2^{d-2}}{2^{d-1}} = \frac{1}{2},$$

$$m_{3,0} = \sum_{\alpha \in D, \alpha_3=0} p_\alpha = \sum_{\alpha \in V_{d-3}} p_{010\alpha} + \sum_{\alpha \in V_{d-3}} p_{100\alpha} = \frac{1}{2^{d-1}} 2^{d-3} + \frac{1}{2^{d-1}} 2^{d-3} = \frac{1}{2}.$$

Finally, the condition $\sum_{\alpha \in D} p_\alpha = 1$ can be verified by observing, for example, that

$$\sum_{\alpha \in D} p_\alpha = m_{1,0} + m_{1,1} = \frac{1}{2} + \frac{1}{2} = 1.$$

To further explore the existence of a table with uniform margins, we use the following lemma. The lemma is based on a rewriting of the multidimensional case Th. 3 in [21], and an adaptation of the notation to binary tables.

Lemma 3.2. *Let $T_1 = (p_\alpha)$ and $T_2 = (q_\alpha)$ be two d -dimensional binary probability tables with the same zero pattern, and assume that T_2 has uniform margins. Then there exist positive vectors $w_1 = (w_{10}, w_{11}), \dots, w_d = (w_{d0}, w_{d1})$ such that the table T_3 with generic element*

$$\tilde{p}_{\alpha_1 \dots \alpha_d} = p_{\alpha_1 \dots \alpha_d} w_{1\alpha_1} \dots w_{d\alpha_d}$$

Table 2
Extreme pmfs with uniform margins $d = 3$.

α_1	α_2	α_3	r_1	r_2	r_3	r_4	r_5	r_6
0	0	0	$\frac{1}{2}$	0	0	0	$\frac{1}{4}$	0
1	0	0	0	$\frac{1}{2}$	0	0	0	$\frac{1}{4}$
0	1	0	0	0	$\frac{1}{2}$	0	0	$\frac{1}{4}$
1	1	0	0	0	0	$\frac{1}{2}$	$\frac{1}{4}$	0
0	0	1	0	0	0	$\frac{1}{2}$	0	$\frac{1}{4}$
1	0	1	0	0	$\frac{1}{2}$	0	$\frac{1}{4}$	0
0	1	1	0	$\frac{1}{2}$	0	0	$\frac{1}{4}$	0
1	1	1	$\frac{1}{2}$	0	0	0	0	$\frac{1}{4}$

has uniform margins.

First of all we point out that the transformation in Lemma 3.2 preserves the zero pattern and the odds ratio structure of the table. We now highlight two key points on the use of Lemma 3.2. First, for the existence of a solution to our problem, it is enough to check the conditions on margins, since the conditions on the odds ratios and their higher order combinations are automatically adjusted by the IPPF. Second, it is enough to prove the existence of a table with the same zero pattern and uniform margins, and it is not even necessary to actually determine such a table.

To do this, we propose two methods. The first method is based on combinatorial objects, while the second method is based on integer programming.

We point out that to have uniform margins the pmf p of a table T must satisfy the following constraints

$$m_{i0} = m_{i1} = \frac{1}{2} \Leftrightarrow m_{i0} - m_{i1} = 0 \Leftrightarrow \sum_{\alpha \in D, \alpha_i=0} p_\alpha - \sum_{\alpha \in D, \alpha_i=1} p_\alpha = 0, \quad i = 1, \dots, d$$

that can be rewritten as

$$(1_{\{\alpha \in D, \alpha_i=0\}} - 1_{\{\alpha \in D, \alpha_i=1\}})^T p = 0, \quad i = 1, \dots, d, \tag{11}$$

where 1_A is the indicator vector of A , b^T denotes the transpose of b , and p is the vector $p = (p_\alpha, \alpha \in D)$. Eq. (11) can be rewritten in compact form by denoting as H_d its matrix of coefficients. Namely, Eq. (11) becomes:

$$H_d p = 0. \tag{12}$$

For example, for $d = 3$ we obtain

$$H_3 p = \begin{pmatrix} 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \end{pmatrix} p = 0.$$

The extreme rays of the system defined by $H_d y = 0$ with $y = (y_\alpha, \alpha \in D, y_\alpha \geq 0)$ can be computed using software for commutative algebra. We used 4ti2, [22]. Then the corresponding extreme pmfs are computed by simple normalization $p_\alpha = \frac{y_\alpha}{\sum_{\alpha \in D} y_\alpha}$. For the 3-dimensional case we obtain the extreme pmfs that are shown in Table 2.

It is worth noting that, given the extreme pmfs $r_i, i = 1, \dots, n_d$ where n_d depends on the dimension d of the multi-way table (e.g., for the three-dimensional case we have $n_3 = 6$) any pmf p with uniform margins can be written as $p = \sum_{i=1}^{n_d} \lambda_i r_i$ with $\lambda_i \geq 0, i = 1, \dots, n_d$ and $\sum_{i=1}^{n_d} \lambda_i = 1$. In Theorem 3.3, we provide conditions that a zero pattern must satisfy to be compatible with the existence of a table with uniform margins.

Theorem 3.3. Let Z be a zero pattern with $Z = (z_i, i = 1, \dots, 2^d)$. Let us denote by \mathcal{A} the set of indices corresponding to zero cells, $\mathcal{A} = \{i \in \{0, \dots, 2^d\} : z_i = 0\}$ and $\bar{\mathcal{A}}$ the set of the indices corresponding to non-zero cells, $\bar{\mathcal{A}} = \{i \in \{0, \dots, 2^d\} : z_i = 1\}$. Let $\{r_i : i = 1, \dots, n_d\}$ be the set of extreme pmfs of the polytope defined by $H_d p = 0$.

Let S_1 be the subset of $\{1, \dots, n_d\}$ defined as $S_1 = \{k \in \{1, \dots, n_d\} : r_k(\alpha_i) = 0, i \in \mathcal{A}\}$. If S_1 is not empty we consider the set $S_2 \subseteq \bar{\mathcal{A}}$ that contains all $i \in \bar{\mathcal{A}}$ such that $\sum_{j \in S_1} r_j(\alpha_i) > 0$.

If $S_2 = \bar{\mathcal{A}}$ then $p = \sum_{i \in S_1} \frac{1}{|S_1|} r_i$ is a pmf of a Z -compatible table with uniform margins. If $S_1 = \emptyset$ or $S_2 \subset \bar{\mathcal{A}}$ no Z -compatible table with uniform margins exists.

Proof. We know that any p associated with a table T with uniform margins can be represented as $p = \sum_{k=1}^{n_d} \lambda_k r_k$ where $\lambda_k \geq 0, \sum_{k=1}^{n_d} \lambda_k = 1$, and $r_k, k = 1, \dots, n_d$ are the extreme pmfs of the polytope defined by $H_d p = 0$. We must have

$$p(\alpha_i) = \sum_{k=1}^{n_d} \lambda_k r_k(\alpha_i) = 0, \quad i \in \mathcal{A}.$$

Table 3
 $d = 3$: Extreme pmfs with uniform margins and four zero patterns.

α_1	α_2	α_3	r_1	r_2	r_3	r_4	r_5	r_6	\mathcal{Z}_1	\mathcal{Z}_2	\mathcal{Z}_3	\mathcal{Z}_4
0	0	0	$\frac{1}{2}$	0	0	0	$\frac{1}{4}$	0	1	1	0	0
1	0	0	0	$\frac{1}{2}$	0	0	0	$\frac{1}{4}$	0	1	1	1
0	1	0	0	0	$\frac{1}{2}$	0	0	$\frac{1}{4}$	0	0	0	0
1	1	0	0	0	0	$\frac{1}{2}$	$\frac{1}{4}$	0	0	0	1	1
0	0	1	0	0	0	$\frac{1}{2}$	0	$\frac{1}{4}$	0	0	1	1
1	0	1	0	0	$\frac{1}{2}$	0	$\frac{1}{4}$	0	0	0	1	0
0	1	1	0	$\frac{1}{2}$	0	0	$\frac{1}{4}$	0	0	0	1	1
1	1	1	$\frac{1}{2}$	0	0	0	0	$\frac{1}{4}$	0	0	1	0

We can choose a strictly positive value for λ_k only if the extreme pmf r_k satisfies the condition $r_k(\alpha_i) = 0, i \in \mathcal{A}$. If S_1 is empty, no \mathcal{Z} -compatible pmf can be built. If S_1 is not empty, we have

$$p = \sum_{k \in S_1} \lambda_k r_k, \lambda_k \geq 0, \sum_{k \in S_1} \lambda_k = 1.$$

The pmf p must be positive for $\alpha_i, i \in \bar{\mathcal{A}}$:

$$p(\alpha_i) = \sum_{k \in S_1} \lambda_k r_k(\alpha_i) > 0, i \in \bar{\mathcal{A}}.$$

The coefficients $\lambda_k, k \in S_1$ are positive or zero. Then we can consider $\sum_{k \in S_1} r_k(\alpha_i)$. If $S_2 = \bar{\mathcal{A}}$ it would be enough to choose $\lambda_k = \frac{1}{|\bar{\mathcal{A}}|}$: the pmf $p = \sum_{k \in \bar{\mathcal{A}}} \frac{1}{|\bar{\mathcal{A}}|} r_k$ has uniform margins and is \mathcal{Z} -compatible by construction. If S_2 is a proper subset of $\bar{\mathcal{A}}, S_2 \subset \bar{\mathcal{A}}$ no \mathcal{Z} -compatible pmf can be built. \square

Corollary 3.4. Let \mathcal{Z} be a zero pattern with $\mathcal{Z} = (z_i, i = 1, \dots, 2^d)$. If S_1 is empty then no \mathcal{Z}' -compatible table with uniform margins exists for any $\mathcal{Z}' \leq \mathcal{Z}$, where $\mathcal{Z}' \leq \mathcal{Z}$ means $z'_i \leq z_i, i = 1, \dots, 2^d, \mathcal{Z}' = (z'_1, \dots, z'_{2^d})$.

Example 3.5. We consider some examples for $d = 3$ with zero patterns reported in the last columns of Table 3.

Case 1. The first case, \mathcal{Z}_1 , is a 7-zero pattern. For this case, we get $S_1 = \emptyset$ and then no table with uniform margins exists for this case.

Case 2. The second case, \mathcal{Z}_2 , is a 6-zero pattern. Here, we get $S_1 = \emptyset$. Thus, in such a case, no table with uniform margins exists. Using Corollary 3.4 we can conclude that for any zero pattern $\mathcal{Z}', z' = (z_1, z_2, 0, 0, 0, 0, 0), z_1, z_2 \in \{0, 1\}$ no \mathcal{Z}' -compatible table with uniform margins exists.

Case 3. The third case, \mathcal{Z}_3 , is a 2-zero pattern. We get $S_1 = \{2, 4\}$. In this case, $\mathcal{A} = \{1, 3\}, \bar{\mathcal{A}} = \{2, 4, 5, 6, 7, 8\}$, and $S_2 = \{2, 4, 5, 7\} \subset \bar{\mathcal{A}}$. Then no table with uniform margins exists for this case.

Case 4. The fourth case, \mathcal{Z}_4 , is a 4-zero pattern. We obtain $S_1 = \{2, 4\}$. Here, $\mathcal{A} = \{1, 3, 6, 8\}, \bar{\mathcal{A}} = \{2, 4, 5, 7\}$, and $S_2 = \{2, 4, 5, 7\} = \bar{\mathcal{A}}$. Then $p = \sum_{k \in \{2,4\}} \frac{1}{2} r_k = (0.0.25 0.25 0.25 0.25 0)$ has uniform margins and is compatible with \mathcal{Z}_4 .

As previously discussed, given the extreme pmfs $r_i, i = 1, \dots, n_d$, any pmf with uniform margins can be expressed as follows:

$$p = \sum_{i=1}^{n_d} \lambda_i r_i, \lambda_i \geq 0, \sum_{i=1}^{n_d} \lambda_i = 1.$$

As a consequence, we have that each extreme pmf r_i itself represents a table with uniform margins that is compatible with $\mathcal{Z} = (z_1, \dots, z_{2^d})$, where $z_k = 0$ (or $z_k = 1$) if $r_i(\alpha_k) = 0$ (or $r_i(\alpha_k) > 0$, respectively), for $k = 1, \dots, 2^d$ and $i = 1, \dots, n_d$. Moreover, it is possible to sample from the set of tables with uniform margins by selecting $\lambda_i, i = 1, \dots, n_d$, according to some criterion within the $(n_d - 1)$ -dimensional simplex.

On the other hand, it is important to note that the cardinality n_d of the set of extreme pmfs grows rapidly with d . For instance, when $d = 6$, there are $n_6 = 707,264$ extreme pmfs, which poses a significant computational challenge for this approach.

An alternative way to tackle our problem would be through integer programming. Since our problem reduces to linear constraints through the Lemma 3.2, we can set up a linear programming problem as follows. We start by considering the matrix C_d with dimensions $(d + 1) \times 2^d$ with: A first row of 1's; then block-wise repetitions of 1's and -1's (as in a classical full-factorial 2^d design). C_d is the matrix H_d above except for the first row. Also, let us define the vector with length $d + 1$ as $b_d = (1, 0, \dots, 0)$. For a given zero pattern \mathcal{Z} , we introduce the matrix $C_d(\mathcal{Z})$ obtained from C_d by removing the columns that belong to the cells in \mathcal{Z} . The problem of the existence of a strictly positive probability distribution with uniform margins can be stated as follows:

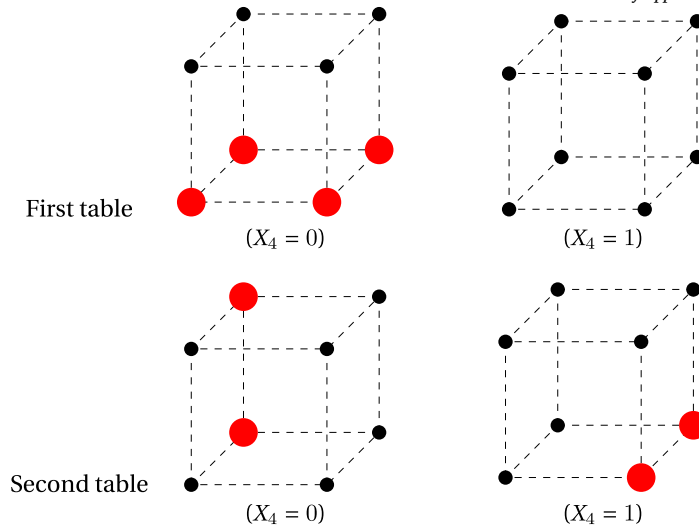


Fig. 3. Two 2^4 tables with zero patterns. The first table in the upper panel, the second table in the lower panel. The variables X_1, X_2, X_3 are the coordinates of the cubes, the variable X_4 divides the table into two cubes. Red dots denote zero probabilities. To ease readability, vertex labels are omitted.

$$\begin{aligned}
 & \max_p \delta \\
 \text{subject to} \quad & C_d(\mathcal{Z})p = b_d \\
 & p_\alpha \geq \delta, \quad \alpha \in D - \mathcal{Z}.
 \end{aligned} \tag{13}$$

If the maximum is $\delta^* = 0$, then there is no strictly positive solution. If the maximum δ^* is strictly positive, the solution exists and can be found through a standard algorithm based on the simplex method which yields a strictly positive probability table together with the value of δ^* . We do not show the output table, because the linear programming problem in Eq. (13) is only a compatibility check between the uniform margins and a given zero pattern. The algorithm above can be easily implemented with the `lpsolve` package, see [23] and [24], in R[25]. An alternative version of the optimization problem can be stated using separation theorems like the Farkas lemma, see, e.g., [26], but the refinement of the optimization problem is outside the scope of this work.

The approach via `lpsolve` is quite efficient and allows finding a solution even for large binary tables. For example, the analysis for $d = 12$ is performed in less than 1 sec. on standard hardware. For illustrative purposes, we conclude with two examples in the case $d = 4$. They are depicted in Fig. 3. In the upper panel, Fig. 3 shows a table with 4 zeros on a two-dimensional sub-table as zero pattern. According to Proposition 3.1, there is no strictly positive solution, and the linear programming algorithm yields a value of $\delta^* = 0$. In the lower panel, Fig. 3 shows a different zero pattern, which is a table with again 4 zeros but in different positions. In this case, there is a strictly positive solution, and the output of the optimization procedure is $\delta^* = 0.07143$.

In summary, a key advantage of the linear programming-based method is its computational efficiency. Conversely, the method based on extreme pmfs offers valuable insight into the structure of zero patterns that are compatible with the existence of tables with uniform margins. The computation of extreme pmfs for the class of multivariate Bernoulli distributions with given margins, particularly in high dimensions, can also benefit from recent work (e.g., see [27]). We plan to further develop this method in the future by exploring this connection further.

3.2. Examples in the 2^3 case

In this section, we show how some 2^3 tables with only a few zeros can behave differently. Specifically, we give explicit configurations where the solution does not exist or it is not determined only by the conditional odds ratios. For our goal, it is sufficient to analyze 2^3 tables with one or two zeros, leading (up to isomorphism) to four possible configurations. We recall that, in our context, two tables are isomorphic if one can be obtained from the other by permuting the levels and relabeling the variables.

1. The table in Fig. 4 (a) has one zero. In this configuration, there are still four independent equations from marginal constraints and three independent conditional odds ratios equations from the system in Eq. (2). Thus, the number of equations is equal to the number of positive probabilities.
2. The table in Fig. 4 (b) has two zero on the same edge, specifically in the entries $(0, 1, 0)$ and $(1, 1, 0)$. According to Proposition 3.1, there is no solution unless we also force the two opposite cells in $(0, 0, 1)$ and $(1, 0, 1)$ to be zero.
3. The table in Fig. 4 (c) has two zeros on the opposite cells of a face. In this configuration, there are four independent equations from marginal constraints and one independent conditional odds ratios equation from the system in Eq. (2). Since the positive probabilities are six, in this case the conditional odds-ratios in Eq. (2) are not sufficient to determine the transformed table and higher order combinations of odds ratios should be considered.

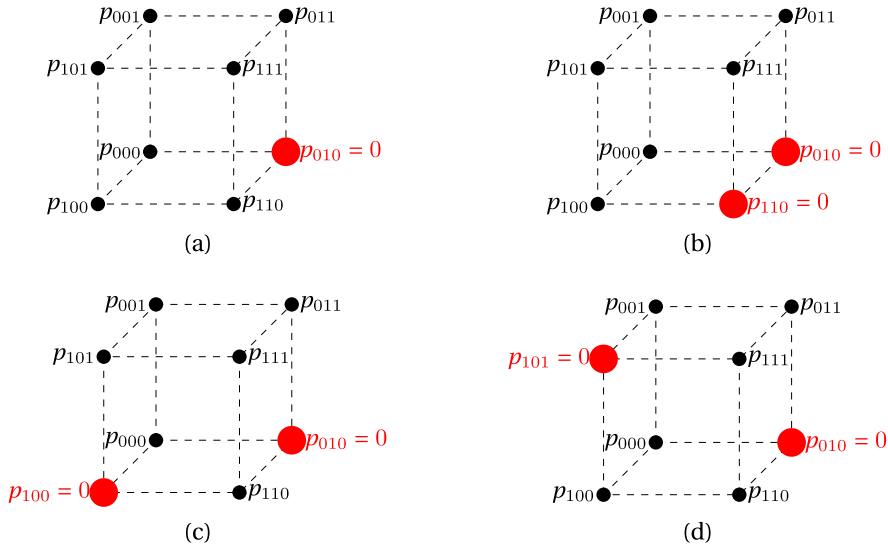


Fig. 4. Configurations with 1 or 2 zeros in the 2^3 table. Red dots denote zero probabilities. (a): one zero; (b): two zeros on the same edge; (c): two zeros in diagonal position on a face; (d): two zeros in different faces.

4. The table in Fig. 4 (d) has two zeros on two different faces. Here, there are no valid constraints on the conditional odds ratios in Eq. (2), and the number of positive probabilities is two more than the number of marginal constraints.

A discussion on cases (c) and (d) above is provided with full detail in Sect. 4.

3.3. Extension of the approach to arbitrary d -way tables

It is worth noting that both the computational methods described in Sect. 3.1 can be generalized to any d -way table, where each variable X_i takes values in $\{0, 1, \dots, x_i - 1\}$ for $x_i \geq 2$, with $i = 1, \dots, d$. For this, it is sufficient to modify H_d and C_d to express the constraints

$$m_{i,0} = \dots = m_{i,x_i-1} = \frac{1}{x_i}, \quad i = 1, \dots, d,$$

where $m_{i,j} = \sum_{\alpha \in D, \alpha_i=j} p_\alpha$, $i = 1, \dots, d$, $j = 0, \dots, x_i - 1$, and $D = \{0, \dots, x_1 - 1\} \times \dots \times \{0, \dots, x_d - 1\}$. We get

$$m_{i,0} = \dots = m_{i,x_i-1} = \frac{1}{x_i} \Leftrightarrow \begin{cases} m_{i,0} - m_{i,1} = 0 \\ \dots \\ m_{i,x_i-2} - m_{i,x_i-1} = 0 \end{cases}, \quad i = 1, \dots, d$$

that can be rewritten as follows

$$(1_{\{\alpha \in D, \alpha_i=j\}} - 1_{\{\alpha \in D, \alpha_i=j+1\}})^T p = 0, \quad i = 1, \dots, d, \quad j = 0, \dots, x_i - 2. \tag{14}$$

For example, in the case of a 3×4 table ($d = 2, x_1 = 3$, and $x_2 = 4$) the H_d matrix of Eq. (12) becomes

$$H_{x_1, x_2} = \begin{pmatrix} 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & -1 \end{pmatrix}.$$

Given a zero pattern \mathcal{Z} , we have two ways to check if a \mathcal{Z} compatible table with uniform margins exists:

1. using 4ti2 [22], we compute the rays corresponding to the matrix H_{x_1, x_2} . We obtain 96 extreme pmfs and then we proceed in a similar way as in Theorem 3.3;
2. we build the C_{x_1, x_2} matrix, by simply adding a first row of 1's to H_{x_1, x_2} and then we use the integer programming approach, as in (13).

Table 4
Marginal odds ratios of p_0 (input) and p_1 (output obtained using IPFP), all values rounded to 3 decimal places.

pmf	000	001	010	011	100	101	110	111	ω_M^{12}	ω_M^{13}	ω_M^{23}
p_0	0.1	0.05	0.3	0.2	0.1	0.05	0.15	0.05	0.4	0.64	1.111
p_1	0.09	0.09	0.14	0.18	0.16	0.16	0.11	0.07	0.357	0.714	1.033

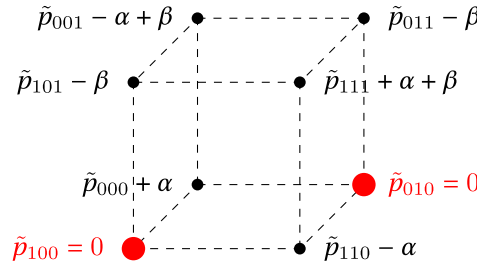


Fig. 5. The general probability table in the 2^3 case with two zeros in the diagonal of a face.

We point out that the methodology described here formally solves the problem of existence for general d -way tables. However, in the multi-dimensional setting the geometric structure of the zero patterns becomes complicated and a straightforward generalization of Theorem 2.1 is hard to obtain if not unfeasible.

4. The role of conditional odds ratios in determining the unique transformed table

In the previous section, we focused on the existence of the solution. We first investigate in which cases the set of conditional odds ratios is sufficient to describe the IPFP solution without the addition of higher order combinations of odds ratios. We start with conditional odds ratios due to their simple interpretation in terms of local dependence. Our analysis goes along the same line as the two-way table example presented in Sec. 2. Here, we analyze two scenarios in the three-dimensional case, to show that more complex equations play a role to guarantee uniqueness.

First, it is worth noting that the odds ratios considered are the *conditional* odds ratios and not the *marginal* odds ratios, which are in general not preserved by the IPFP algorithm. We show this phenomenon in Table 4 through a specific example. There, the marginal odds ratios (denoted by ω_M^{12} , ω_M^{13} , and ω_M^{23}) of p_0 (the input pmf) and p_1 (the output pmf obtained using IPFP) are different, meaning that, in general, the marginal odds ratios are not preserved in the transformation.

Let us consider a pmf p_0 with a zero pattern compatible with the existence of a table with uniform margins. Given p_0 as input, IPFP produces as output p_1 , a pmf with uniform margins that has the same odds ratio structure of p_0 . As previously discussed, it is known that p_1 is necessarily the I-projection of p_0 onto the class of d -variate Bernoulli distributions with uniform margins, and that such a I-projection is unique (Theorem 6.2 in [2] or Proposition 2.1 in [4]). In this section, we consider 3-dimensional binary tables and highlight the roles of the conditional odds ratios in determining the I-projection.

Example 4.1. We consider a 2^3 table with zeros in the entries $(0, 1, 0)$ and $(1, 0, 0)$, that is $p_{010} = p_{100} = 0$ (Fig. 4 (c)). It can be verified that this zero pattern is compatible with the existence of a table with uniform margins. In this case, we have only one non-trivial condition on the conditional odds ratio, precisely ω_1^{12} , i.e. the odds ratio of X_1, X_2 given $X_3 = 1$:

$$\omega_1^{12} = \frac{p_{001}p_{111}}{p_{011}p_{101}}. \tag{15}$$

Additionally, we have four independent conditions for the margins, $C_3(\mathcal{Z})p = b_3$ as defined in Sec. 3.1. Again using the lexicographic order for the entries, the kernel of the model matrix $C_3(\mathcal{Z})$ is generated by the two vectors:

$$(-1, 1, 0, 0, 1, -1), \quad (0, 1, -1, -1, 0, 1).$$

Given a particular solution \tilde{p} , for instance, the solution of the IPFP which is strictly positive, the general solution to the problem with fixed margins is given by

$$(p_{000} = \tilde{p}_{000} - \alpha, p_{001} = \tilde{p}_{001} + \alpha + \beta, p_{011} = \tilde{p}_{011} - \beta, p_{101} = \tilde{p}_{101} - \beta, p_{110} = \tilde{p}_{110} + \alpha, p_{111} = \tilde{p}_{111} - \alpha + \beta) \tag{16}$$

for suitable values of (α, β) , i.e. $\{(\alpha, \beta) : p_{ijk} \geq 0, i, j, k \in \{0, 1\}\}$. This distribution is shown in Fig. 5. By substitution of the generic probability distribution in Eq. (16) into the odds ratio equation in Eq. (15), we get:

$$f(\alpha, \beta) = (\tilde{p}_{111} - \tilde{p}_{001})\alpha + (\tilde{p}_{111} + \tilde{p}_{001} + \omega_1^{12}(\tilde{p}_{011} + \tilde{p}_{101}))\beta - \alpha^2 + (1 - \omega_1^{12})\beta^2 = 0. \tag{17}$$

The equation above introduces an implicit function $\beta(\alpha)$, whose explicit expression is somewhat complicated and not relevant for our application, having quadratic terms in both α and β . However, we can see that, at least locally, we have infinite solutions in a

Table 5

Conditional odds ratios of p_0 (input), p_1 (output obtained using IPFP), and p'_1 (all values rounded to 3 decimal places).

pmf	000	001	010	011	100	101	110	111	ω_1^{12}	$\omega_{01}^{13,23}$
p_0	0.288	0.106	0	0.106	0	0.106	0.288	0.106	1	1
p_1	0.250	0.125	0	0.125	0	0.125	0.250	0.125	1	1
p'_1	0.240	0.135	0	0.125	0	0.125	0.260	0.115	1	0.787

Table 6

$\omega_{001}^{12,13,23}$ odds ratio of p_0 (input), p_1 (output obtained using IPFP), and p'_1 (all the values are rounded to 3 decimal places).

pmf	000	001	010	011	100	101	110	111	$\omega_{001}^{12,13,23}$
p_0	0.40	0.15	0.15	0	0.15	0	0	0.15	7.111
p_1	0.225	0.137	0.137	0	0.137	0	0	0.363	7.111
p'_1	0.45	0.025	0.025	0	0.025	0	0	0.475	6156

neighborhood of the point (0, 0). The point (0, 0) is a solution because \tilde{p} is the probability distribution given by the IPFP. Since \tilde{p} is strictly positive, there is a neighborhood of (0, 0) in the strictly positive simplex of the probabilities. The local behavior of $\beta(\alpha)$ can be studied by means of the implicit functions theorem. The partial derivatives are

$$\frac{\partial f}{\partial \alpha} = \tilde{p}_{111} - \tilde{p}_{001} - 2\alpha, \quad \frac{\partial f}{\partial \beta} = \tilde{p}_{111} + \tilde{p}_{001} + \omega_1^{12}(\tilde{p}_{011} + \tilde{p}_{101}) + 2(1 - \omega_1^{12})\beta,$$

leading to

$$\beta(0) = 0, \quad \beta'(0) = -\frac{\tilde{p}_{111} - \tilde{p}_{001}}{\tilde{p}_{111} + \tilde{p}_{001} + \omega_1^{12}(\tilde{p}_{011} + \tilde{p}_{101})}.$$

A special case arises for conditional independence, i.e., $\omega_1^{12} = 1$ where the function in Eq. (17) reduces to

$$f(\alpha, \beta) = (\tilde{p}_{111} - \tilde{p}_{001})\alpha + \frac{1}{2}\beta - \alpha^2 = 0$$

from which

$$\beta(\alpha) = 2\alpha(\alpha - (\tilde{p}_{111} - \tilde{p}_{001})).$$

We consider a numerical example, shown in Table 5, where we report the original p_0 and the corresponding p_1 found using IPFP. Then, we determine one solution (α_*, β_*) of Eq. (17) and build p'_1 according to Eq. (16). We can verify that p'_1 has uniform margins and has the same value of the conditional odds ratio ω_1^{12} of p_0 and p_1 . In this case, to understand why the solution is unique we need to compute combinations of odds ratios symbolically defined as the product of two conditional odds ratios. More specifically, we consider the symbolic product of ω_0^{13} and ω_1^{23} that we denote by $\omega_{01}^{13,23}$ and obtain

$$\omega_{01}^{13,23} = \frac{p_{000}p_{111}}{p_{001}p_{110}}.$$

Looking at Table 5, we observe that $\omega_{01}^{13,23}$ of p'_1 is different to those of p_0 and p_1 . It can also be verified that by adding the condition

$$\omega_{01}^{13,23}(\alpha, \beta) = \omega_{01}^{13,23}(p_0) \Leftrightarrow \omega_{01}^{13,23}(\alpha, \beta) = 1$$

to Eq. (17), we obtain $\alpha = \beta = 0$ as the unique solution, which means that p'_1 must be chosen equal to p_1 .

Example 4.2. We consider the zero pattern $\{(0, 1, 1), (1, 0, 1), (1, 1, 0)\}$, that is $p_{011} = p_{101} = p_{110} = 0$. It can be verified that in this case, the polytope of the pmf with uniform margins is

$$\{p = \lambda r_1 + (1 - \lambda)r_6 : 0 \leq \lambda \leq 1\} \tag{18}$$

where r_1 and r_6 are the extreme pmfs defined in Table 2. We consider an initial p_0 and find p_1 as the output of IPFP. Then, taking $\lambda = .9$ for illustrative purposes, we get $p'_1 = 0.9r_1 + 0.1r_6$ (see Table 6). It is possible to verify that, in this case, all conditional odds ratios and all the products $\omega_{kk'}^{j,j'}$, which are symbolically defined as the product $\omega_k^{ij}\omega_{k'}^{i'j'}$ are trivial. In this case, to retrieve the unique solution, we need to consider three-term products of conditional odds ratios like the following

$$\omega_{001}^{12,13,23} = \frac{p_{000}^2 p_{111}}{p_{010} p_{100} p_{001}} \tag{19}$$

where $\omega_{001}^{12,13,23}$ is the symbolic product of the conditional odds ratios ω_0^{12} , ω_0^{13} , and ω_1^{23} . Considering Table 6, we observe that $\omega_{001}^{12,13,23}$ has the same value for p_0 and p_1 but not for p'_1 . In particular using Eq. (18) in Eq. (19) we obtain

Table 7
Cross classification of tables with uniform margins by N_0 and N_1 , $d = 3$.

N_0	N_1					Total
	1	2	3	4	6	
0	0	0	0	0	1	1
1	0	0	0	8	0	8
2	0	0	16	0	0	16
3	0	8	0	0	0	8
4	2	6	0	0	0	8
6	4	0	0	0	0	4
Total	6	14	16	8	1	45

$$\omega_{001}^{12,13,23} = \frac{4\lambda^2(1 + \lambda)}{(1 - \lambda)^3} \tag{20}$$

It is easy to verify that Eq. (20) is invertible for $0 \leq \lambda < 1$ and this provides a further justification of the uniqueness of p_1 for this zero pattern.

We conclude this section by considering all possible $2^{2^d} = 256$ zero patterns (of course the 8-zero pattern that results in a trivial all-zero table is excluded by the analysis). Using Theorem 3.3 and the extreme points listed in Table 3, we find 45 zero patterns compatible with the existence of a table with uniform margins. For each compatible zero pattern $\mathcal{Z} = (z_1, \dots, z_8)$ we compute the extreme rays of the polytope $\mathcal{P}_{\mathcal{Z}}$ defined by $H_3 p = 0$ and $p_{\alpha_i} = 0$ if $z_i = 0$, $i = 1, \dots, 8$. We denote by N_0 and N_1 the number of zeros in the zero pattern \mathcal{Z} and the number of extreme points of the polytope $\mathcal{P}_{\mathcal{Z}}$, respectively.

Table 7 reports the classification of the 45 compatible zero patterns by N_0 and N_1 . There are 6 cases where $N_1 = 1$. For each of these zero patterns, there is only one table with uniform margins. For the remaining 39 cases we compute the odds ratios, obtaining:

1. for the zero pattern with $N_0 \in \{0, 1, 2, 4\}$ zeros, the uniqueness of the solution is determined by the non-trivial odds ratios which are conditional odds ratios and/or products of two conditional odds ratios, like in Example 4.1;
2. for the 3-zero patterns the uniqueness of the solution is determined by non-trivial odds ratios which are the products of three conditional odds ratios, like in Example 4.2.

The analysis of 3-dimensional tables shows how conditional odds ratios and their products play a role in determining the IPFP solution when it exists.

5. Conclusions

In this paper, we provide a characterization of the zero patterns that are compatible with a transformed multi-way binary table with prescribed dependence structure in terms of odds ratios. We further study how the zero pattern impacts the relevance of conditional odds ratios in determining the unique solution of the problem. While working on this project, we identified interesting research directions for future investigations. For binary tables, the approach based on extreme rays described in Sec. 3 would benefit from a full characterization of the extreme rays to avoid the computational step. Some advances in this direction have recently been made in the context of multivariate Bernoulli distributions [27]. The possible adaptation of these results in the framework of polytopes of discrete copulas and higher order transportation polytopes is worth investigating. With these new insights, it would be possible to prove if the condition on the opposite facets of Proposition 3.1 could be generalized to multi-way tables with an arbitrary number of levels. Moreover, it would be interesting to characterize the class of solutions when conditional odds ratios are not enough to determine the transformed table in terms of the associated algebraic variety. An algebraic approach would make it possible to identify extreme tables in this variety and study if there are valuable alternatives with respect to the solution provided by the IPFP. Finally, we could investigate how the approach adapts to different dependence conditions. For instance, we might consider suitable marginal odds ratios to have a closer connection with the classical log-linear models of independence and conditional independence for multi-way contingency tables.

CRediT authorship contribution statement

Roberto Fontana: Writing – review & editing, Writing – original draft, Validation, Methodology, Investigation, Formal analysis, Conceptualization. **Elisa Perrone:** Writing – review & editing, Writing – original draft, Validation, Methodology, Investigation, Formal analysis, Conceptualization. **Fabio Rapallo:** Writing – review & editing, Writing – original draft, Validation, Methodology, Investigation, Formal analysis, Conceptualization.

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.

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Data availability

The small datasets used for illustrative purposes are reported in the manuscript.

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