



## Connectivity for $3 \times 3 \times K$ contingency tables

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**Abstract.** We consider an exact sequential conditional test for three-way conditional test of no interaction. At each time  $\tau$ , the test uses as the conditional inference frame the set  $\mathcal{F}(H_\tau)$  of tables with the same three two-way marginal tables as the obtained table  $H_\tau$ . For  $3 \times 3 \times K$  tables, we propose a method to construct  $\mathcal{F}(H_\tau)$  from  $\mathcal{F}(H_{\tau-1})$ . This enables us to perform efficiently the sequential exact conditional test. The subset  $\mathcal{S}_\tau$  of  $\mathcal{F}(H_\tau)$  consisting of  $s + H_\tau - H_{\tau-1}$  for  $s \in \mathcal{F}(H_{\tau-1})$  contains  $H_\tau$ , where the operations  $+$  and  $-$  are defined elementwise. Our argument is based on the minimal Markov basis for  $3 \times 3 \times K$  contingency tables and we give a minimal subset  $\mathcal{M}$  of some Markov basis which has the property that  $\mathcal{F}(H_\tau) = \{s - m \mid s \in \mathcal{S}_\tau, m \in \mathcal{M}\}$ .

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### 1. Introduction

An  $I \times J \times K$  contingency table is denoted by

$$(t_{ijk})_{1 \leq i \leq I, 1 \leq j \leq J, 1 \leq k \leq K}$$

where  $t_{ijk}$  is a nonnegative integer which is the count of events at the  $(i, j, k)$  level of considered three factors. The object of the statistical analysis of contingency tables is to understand the factor effects and their interaction effects. For such an analysis, the conditional inference is often applied where the set of contingency tables with fixed marginals is used as the frame of conditional inference.

Now we define some terminology. We denote by  $\Omega(I, J, K)$  the set of all  $I \times J \times K$  contingency tables. The marginal of  $I$ -direction is a  $J \times K$  matrix

$$\left( \sum_{i=1}^I t_{ijk} \right)_{1 \leq j \leq J, 1 \leq k \leq K}.$$

The marginals of  $J$ -direction and  $K$ -direction are similarly defined. For an  $I \times J \times K$  contingency table  $t$ , let  $\mathcal{F}(t)$  be the set of  $I \times J \times K$  contingency tables with the same

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marginals as those of  $t$ . A table with all zero marginals is called a *move*. A *Markov basis* is defined as a set of moves connecting all elements of  $\mathcal{F}(t)$  for any contingency table  $t$ . Diaconis and Sturmfels [12, 6] studied an algebraic algorithm for sampling from conditional distributions by using the concept of Markov basis.

In the sequential conditional test, we consider the sequence of conditional frames

$$\mathcal{F}(H_1) \rightarrow \mathcal{F}(H_2) \rightarrow \cdots \rightarrow \mathcal{F}(H_{\tau-1}) \rightarrow \mathcal{F}(H_\tau) \rightarrow \cdots,$$

where  $H_\tau$  is a contingency table obtained from  $H_{\tau-1}$  by adding one data point.

The Markov chain Monte Carlo (MCMC) method is often used to perform the exact conditional test of no three-way interaction [1], which is based on Markov bases. Markov bases are known for  $\Omega(I, J, 2)$  and  $\Omega(3, 3, K)$  [12, 3], however, determining a Markov basis is NP hard in general [7].

The object of this paper is to propose a method to obtain  $\mathcal{F}(H_\tau)$  from  $\mathcal{F}(H_{\tau-1})$  and to prove several neighborhood theorems which are foundations for performing the sequential conditional test. The sequential conditional test proceeds as follows. For a given table  $H_{\tau-1}$  at the stage  $\tau - 1$ , we perform the conditional test by calculating the p-value of the table  $H_{\tau-1}$ . If the p-value is small enough we reject the null hypothesis and stop the sequential test. Otherwise we take one more data point with a new table  $H_\tau$  and repeat the process up to the predetermined stage. The difference of our method and the MCMC method is how to get the p-value. Our method calculates the p-value exactly by generating all tables of  $\mathcal{F}(H_\tau)$  by using the previous frame  $\mathcal{F}(H_{\tau-1})$  in  $\Omega(I, J, K)$  (see Theorem 1). On the other hand, the MCMC method estimates the p-value by a random sample of size  $n$  from the null distribution over the set  $\mathcal{F}(H_\tau)$ , without using any information about  $\mathcal{F}(H_{\tau-1})$ . To take one random sample from the null distribution we run a Markov chain of length  $\ell$  by Metropolis-Hastings' trick [8, 9] which converges to the null distribution in the limit. Note that for convergence to the null distribution, a length  $\ell$  of Markov chain must be large (for example, [6, 5]). Therefore for cases that  $|\mathcal{F}(H_\tau)|$ , the cardinality of  $\mathcal{F}(H_\tau)$ , is moderate, it is expected that our exact calculation method has better performance than the MCMC method. Moreover note that our method performs the exact calculation of the p-value though the MCMC method only estimate the p-value.

We describe the simulation result in Table 1, whose entries are the average of 5000 trials of our method of the sequential conditional test for  $\Omega(3, 3, 3)$  with 50 data points by the software R on a personal computer (Linux 2.6, Intel Xeon CPU E5420 2.5GHz, R version 2.11.1). The significance level at each stage was set as 5% and then  $r$  denotes the rejected stage. The simulation of the MCMC method spends longer than one month in the same environment. Therefore we only estimated the spending time from the result on  $\ell = 100$ . That is, since the time to estimate the p-value by Metropolis-Hastings' algorithm grows linearly with respect to each of  $n$ ,  $\ell$  and  $r$ , we estimated that the spending time is 12549 seconds on average for  $n = 10000$  and  $\ell = 1000$ . It is much longer than 0.95034 seconds with our method. The time in our method depends on  $|\mathcal{F}(t)|$  and is spent mainly to remove duplications.

This article is organized as follows. We summarize our methods and main results in Section 2. We define a set  $\mathfrak{N}(i_0, j_0, k_0)$  of contingency tables obtained from a set of

Table 1: Sequential conditional test by our method

Ave. stages $r$	times (sec.)	Max. times	Ave. $ \mathcal{F}(H_r) $	Max. $ \mathcal{F}(H_r) $	Rejection rate
29.2154	0.95034	39.29	132.5364	5682	0.905

moves. The set determines whether  $\mathcal{F}(t)$  has a contingency table  $t'$  with  $t'_{i_0j_0k_0} > 0$  for a  $3 \times 3 \times K$  contingency table  $t$  with  $t_{i_0j_0k_0} = 0$  (see Theorem 2). In Sections 3–6, we study  $3 \times 3 \times K$  contingency tables of  $\mathfrak{N}(i_0, j_0, k_0)$  for  $K = 2, 3, 4, 5$ , respectively, which are minimal among contingency tables  $t$  with  $t_{i_0j_0k_0} = 0$  such that  $\mathcal{F}(t)$  has a contingency table  $t'$  with  $t'_{i_0j_0k_0} > 0$ . In the last section, we prove the main theorems.

## 2. A method and main results

In this section, we fix integers  $i_0, j_0$  and  $k_0$ . For two  $I \times J \times K$  tables  $s = (s_{ijk})$  and  $t = (t_{ijk})$ , we define the elementwise addition and subtraction by  $(s + t)_{ijk} = s_{ijk} + t_{ijk}$  and  $(s - t)_{ijk} = s_{ijk} - t_{ijk}$ , respectively. We call an element of a Markov basis a *basis move*. A Markov basis has the property that for any contingency table  $t$ , two distinct tables  $s_1$  and  $s_2$  of  $\mathcal{F}(t)$  are connected, that is, there are an integer  $r \geq 1$  and basis moves  $m_1, m_2, \dots, m_r$  such that all of

$$s_1 + m_1, s_1 + m_1 + m_2, \dots, s_1 + m_1 + \dots + m_r$$

are elements of  $\mathcal{F}(t)$  and  $s_2 = s_1 + m_1 + \dots + m_r$ . The sequence  $m_1, m_2, \dots, m_r$  is called a path connecting from  $s_1$  to  $s_2$  of length  $r$ .

For two matrices  $M$  and  $N$  with the same size, if all elements of  $M - N$  are nonnegative, we say that  $M$  is larger than or equal to  $N$  elementwise, and denote the relation as  $M \geq N$ . Similarly for two tables  $t$  and  $s$ , if all elements of  $t - s$  are nonnegative, we say  $t \geq s$ .

Suppose that an  $I \times J \times K$  contingency table  $H_\tau$  is obtained from  $H_{\tau-1}$  simply by adding one at  $(i_0, j_0, k_0)$ . Let  $\varphi: \mathcal{F}(H_{\tau-1}) \rightarrow \mathcal{F}(H_\tau)$  be an injective map given by increasing  $(i_0, j_0, k_0)$  by one. Then,  $\varphi(s) = s + H_\tau - H_{\tau-1}$  and in particular,  $\varphi(H_{\tau-1}) = H_\tau$ . We want to obtain every element of  $\mathcal{F}(H_\tau)$ . The subset  $\varphi(\mathcal{F}(H_{\tau-1}))$  of  $\mathcal{F}(H_\tau)$  is a set consisting of all tables  $t = (t_{ijk})$  of  $\mathcal{F}(H_\tau)$  with  $t_{i_0j_0k_0} > 0$ . To obtain every table  $t$  of  $\mathcal{F}(H_\tau)$  with  $t_{i_0j_0k_0} = 0$ , we need to consider a sequence of basis moves from  $t$  to some table  $t' = (t'_{ijk})$  with  $t'_{i_0j_0k_0} > 0$ . Fixing a Markov basis, for a table  $t$ , a table  $s \in \mathcal{F}(t)$  is called in an  $r$ -neighbourhood of  $t$  if there is a path of length less than or equal to  $r$  which connects from  $t$  to  $s$  in  $\mathcal{F}(t)$ . Since a Markov basis connects between any two elements of  $\mathcal{F}(t)$ , all elements of  $\mathcal{F}(t)$  are in an  $m$ -neighbourhood of  $t$  for a sufficiently large integer  $m$ . In [11], we studied the minimal integer  $n$  such that all elements of  $\mathcal{F}(H_\tau)$  are in an  $n$ -neighbourhood of  $t$  for some  $t \in \varphi(\mathcal{F}(H_{\tau-1}))$  and proved mathematically that  $n = 1$  for  $I \times J \times 2$  contingency tables, and computationally that  $n = 2$  for  $3 \times 3 \times 3$  contingency tables with respect to the minimal Markov basis given by Aoki and Takemura [3, 2]. In this paper we show  $n = 3$  mathematically for any  $3 \times 3 \times K$  contingency table with  $K \geq 4$  with respect to the minimal Markov basis [3, 2].

In the case when  $K = 1$ , Sakata and Sawae [10] developed the sequential conditional test for contingency two-way tables. In the case when  $H_\tau$  is an  $I \times J \times 2$  contingency table, the set  $\mathcal{F}(H_\tau) \setminus \varphi(\mathcal{F}(H_{\tau-1}))$  is covered by the set consisting of tables  $s + m$  for all  $s \in \varphi(\mathcal{F}(H_{\tau-1}))$  with  $s_{i_0 j_0 k_0} = 1$  and all basis moves  $m$  with  $m_{i_0 j_0 k_0} = -1$  [see 11, in detail]. In the case when  $H_\tau$  is a  $3 \times 3 \times 3$  contingency table, the set  $\mathcal{F}(H_\tau) \setminus \varphi(\mathcal{F}(H_{\tau-1}))$  is covered by the set consisting of tables  $s + m_2$  and  $s + m_1 + m_2$  for all  $s \in \varphi(\mathcal{F}(H_{\tau-1}))$  with  $s_{i_0 j_0 k_0} = 1$  and all basis moves  $m_1$  with  $(m_1)_{i_0 j_0 k_0} = 0$  and  $m_2$  with  $(m_2)_{i_0 j_0 k_0} = -1$ . There are duplications. Hence, all  $m_1$  and  $m_2$  are not needed and then we obtained some pairs  $(m_1, m_2)$ .

We denote by  $\Phi(I, J, K; i_0, j_0, k_0)$  the set of  $I \times J \times K$  contingency tables  $t$  such that  $t_{i_0 j_0 k_0} = 0$  and  $t$  can be transformed to a contingency table  $s$  with  $s_{i_0 j_0 k_0} > 0$  by a sequence of basis moves. In other words,  $\Phi(I, J, K; i_0, j_0, k_0)$  is the set of  $I \times J \times K$  contingency tables  $t$  with  $t_{i_0 j_0 k_0} = 0$  such that  $\mathcal{F}(t)$  has a table  $s$  with  $s_{i_0 j_0 k_0} > 0$ . If a sequence of moves  $m_1, m_2, \dots, m_r$  transforms  $t$  to  $s$ , then the sequence of moves  $-m_r, -m_{r-1}, \dots, -m_1$  inversely transforms  $s$  to  $t$ . To obtain  $\mathcal{F}(H_\tau)$  from  $\mathcal{F}(H_{\tau-1})$ , we prove that there exists a unique minimal set  $\mathcal{S}$  of contingency tables having the property that for  $t \in \Phi(3, 3, K; i_0, j_0, k_0)$  there is  $s \in \mathcal{S}$  with  $t \geq s$ . Note that hereafter we describe a  $3 \times 3 \times K$  table  $(t_{ijk})$  as follows.

$$\begin{matrix} t_{111} & t_{121} & t_{131} & t_{112} & t_{122} & t_{132} & & t_{11K} & t_{12K} & t_{13K} \\ t_{211} & t_{221} & t_{231} & t_{212} & t_{222} & t_{232} & \cdots & t_{21K} & t_{22K} & t_{23K} \\ t_{311} & t_{321} & t_{331} & t_{312} & t_{322} & t_{332} & & t_{31K} & t_{32K} & t_{33K} \end{matrix}$$

For  $I \geq I', J \geq J'$  and  $K \geq K'$ , an  $I' \times J' \times K'$  contingency table  $t = (t_{ijk})$  is regarded as an  $I \times J \times K$  contingency table  $t' = (t'_{ijk})$  given by

$$t'_{ijk} = \begin{cases} t_{ijk} & \text{if } i \leq I', j \leq J', \text{ and } k \leq K', \\ 0 & \text{otherwise.} \end{cases}$$

We introduce elements of the unique minimal Markov basis given by [3] for  $3 \times 3 \times K$  contingency tables.  $222_4(i_1 i_2, j_1 j_2, k_1 k_2)$  is a table whose elements at  $(i_1, j_1, k_1), (i_2, j_2, k_1), (i_1, j_2, k_2), (i_2, j_1, k_2)$  have a value 1, elements at  $(i_1, j_2, k_1), (i_2, j_1, k_1), (i_1, j_1, k_2), (i_2, j_2, k_2)$  have a value  $-1$ , and the other elements have a value 0, and  $332_6(i_1 i_2 i_3, j_1 j_2 j_3, k_1 k_2)$  is a table whose elements at  $(i_1, j_1, k_1), (i_2, j_2, k_1), (i_3, j_3, k_1), (i_1, j_2, k_2), (i_2, j_3, k_2), (i_3, j_1, k_2)$  have a value 1, elements at  $(i_1, j_2, k_1), (i_2, j_3, k_1), (i_3, j_1, k_1), (i_1, j_1, k_2), (i_2, j_2, k_2), (i_3, j_3, k_2)$  have a value  $-1$ , and the other elements have a value 0. They are denoted respectively by  $M_4(i_1 i_2, j_1 j_2, k_1 k_2)$  and  $M_6^K(i_1 i_2 i_3, j_1 j_2 j_3, k_1 k_2)$  in [3]. Both are illustrated in Table 2.

Table 2: Markov moves with size  $2 \times 2 \times 2$  or  $3 \times 3 \times 2$

$$\begin{matrix} 1 & -1 & -1 & 1 & & 1 & -1 & 0 & -1 & 1 & 0 \\ -1 & 1 & & 1 & -1 & & 0 & 1 & -1 & 0 & -1 & 1 \\ & & & & & -1 & 0 & 1 & & 1 & 0 & -1 \\ 222_4(12, 12, 12) & & & & & 332_6(123, 123, 12) & & & & & & \end{matrix}$$

The basis moves  $233_6(i_1 i_2, j_1 j_2 j_3, k_1 k_2 k_3)$  and  $323_6(i_1 i_2 i_3, j_1 j_2, k_1 k_2 k_3)$  are defined similarly as  $332_6(i_1 i_2 i_3, j_1 j_2 j_3, k_1 k_2)$ . They are denoted respectively by  $M_6^I(i_1 i_2, j_1 j_2 j_3, k_1 k_2 k_3)$

and  $M_6^J(i_1i_2i_3, j_1j_2, k_1k_2k_3)$  in [3]. The basis move  $m = 334(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4)$  which is denoted by  $M_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4)$  in [3] is defined as

$$\begin{aligned} m_{i_1j_1k_1} &= m_{i_1j_2k_2} = m_{i_2j_1k_3} = m_{i_2j_2k_1} = m_{i_2j_3k_4} = m_{i_3j_1k_2} = m_{i_3j_2k_4} = m_{i_3j_3k_3} = 1, \\ m_{i_1j_1k_2} &= m_{i_1j_2k_1} = m_{i_2j_1k_1} = m_{i_2j_2k_4} = m_{i_2j_3k_3} = m_{i_3j_1k_3} = m_{i_3j_2k_2} = m_{i_3j_3k_4} = -1, \end{aligned}$$

and all the other elements are zero, and  $m = 335(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4k_5)$  which is denoted by  $M_{10}(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4k_5)$  in [3] is defined as

$$\begin{aligned} m_{i_1j_1k_1} &= m_{i_1j_2k_2} = m_{i_1j_2k_5} = m_{i_1j_3k_4} = m_{i_2j_1k_3} = m_{i_2j_2k_1} \\ &= m_{i_2j_3k_5} = m_{i_3j_1k_2} = m_{i_3j_2k_4} = m_{i_3j_3k_3} = 1, \\ m_{i_1j_1k_2} &= m_{i_1j_2k_1} = m_{i_1j_2k_4} = m_{i_1j_3k_5} = m_{i_2j_1k_1} = m_{i_2j_2k_5} \\ &= m_{i_2j_3k_3} = m_{i_3j_1k_3} = m_{i_3j_2k_2} = m_{i_3j_3k_4} = -1, \end{aligned}$$

and all the other elements are zero.

Furthermore, we denote by  $\mathfrak{M}(i_0, j_0, k_0)$  the set of all the following moves whose element at  $(i_0, j_0, k_0)$  has a value 1, where all moves are sums of elements of the minimal Markov basis, integers  $i_2$  and  $i_3$  are all positive, distinct and different from  $i_0$ , and for the integers  $j_r, r = 2, 3$  and  $k_r, r = 2, \dots, 5$  we assume the same convention.

$$\begin{aligned} &222_4(i_0i_2, j_0j_2, k_0k_2), \quad 332_6(i_0i_3i_2, j_0j_2j_3, k_0k_2), \quad 233_6(i_0i_2, j_0j_3j_2, k_0k_2k_3), \\ &323_6(i_0i_3i_2, j_0j_2, k_0k_2k_3), \quad 334_8(i_0i_2i_3, j_0j_2j_3, k_0k_2k_4k_3), \quad 334_8(i_2i_0i_3, j_2j_0j_3, k_0k_4k_3k_2), \\ &334_8(i_3i_0i_2, j_0j_3j_2, k_2k_4k_0k_3), \quad 334_8(i_3i_0i_2, j_3j_2j_0, k_3k_4k_2k_0), \\ &222_4(i_2i_3, j_2j_3, k_2k_3) + 222_4(i_0i_2, j_0j_2, k_0k_2), \quad 222_4(i_0i_3, j_0j_3, k_3k_2) + 222_4(i_0i_2, j_0j_2, k_0k_3), \\ &222_4(i_0i_3, j_2j_3, k_3k_0) + 222_4(i_0i_2, j_0j_3, k_0k_2), \quad 222_4(i_2i_3, j_0j_3, k_3k_0) + 222_4(i_0i_3, j_0j_2, k_0k_2), \\ &222_4(i_0i_3, j_0j_3, k_3k_2) + 332_6(i_0i_2i_3, j_2j_0j_3, k_3k_0), \\ &222_4(i_0i_3, j_0j_2, k_3k_2) + 233_6(i_0i_2, j_0j_3j_2, k_0k_3k_4), \\ &222_4(i_2i_3, j_0j_2, k_4k_3) + 233_6(i_0i_2, j_0j_3j_2, k_0k_2k_3), \\ &222_4(i_2i_3, j_0j_3, k_4k_0) + 233_6(i_0i_3, j_0j_3j_2, k_0k_2k_3), \\ &233_6(i_0i_3, j_0j_2j_3, k_4k_3k_0) + 222_4(i_0i_2, j_0j_3, k_0k_2), \\ &222_4(i_0i_3, j_0j_3, k_3k_2) + 222_4(i_2i_3, j_2j_3, k_3k_4) + 222_4(i_0i_2, j_0j_2, k_0k_3), \\ &222_4(i_0i_2, j_2j_3, k_3k_0) + 222_4(i_2i_3, j_0j_2, k_4k_0) + 222_4(i_0i_3, j_0j_3, k_0k_2), \\ &335_{10}(i_0i_2i_3, j_3j_0j_2, k_2k_4k_5k_3k_0), \quad 335_{10}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_5k_3k_4), \\ &335_{10}(i_2i_0i_3, j_2j_0j_3, k_0k_5k_3k_4k_2), \quad 335_{10}(i_2i_0i_3, j_3j_2j_0, k_3k_5k_2k_4k_0), \\ &335_{10}(i_3i_0i_2, j_0j_3j_2, k_2k_5k_0k_4k_3) \end{aligned}$$

Then, we establish the following theorems.

**Theorem 1.** Let  $\varphi: \Omega(3, 3, K) \rightarrow \Omega(3, 3, K)$  be a map given by increasing  $(i_\tau, j_\tau, k_\tau)$  by one and let  $H_{\tau-1}$  and  $H_\tau$  be  $3 \times 3 \times K$  contingency tables such that  $\varphi(H_{\tau-1}) = H_\tau$ . Then

$$\mathcal{F}(H_\tau) = \varphi(\mathcal{F}(H_{\tau-1})) \cup \{s - m \mid s \in \varphi(\mathcal{F}(H_{\tau-1})), m \in \mathfrak{M}(i_\tau, j_\tau, k_\tau)\} \cap \Omega(3, 3, K).$$

For an integer  $n$ , we put  $n^+ := \max(n, 0)$  and  $n^- := \max(-n, 0)$ . It is clear that  $n = n^+ - n^-$  and  $n^- = (-n)^+$ . Further we put  $m^+ = (t_{ijk}^+)$  and  $m^- = (t_{ijk}^-)$  for a table  $(t_{ijk})$  and

$$\mathfrak{N}(i_0, j_0, k_0) = \{m^- \mid m \in \mathfrak{M}(i_0, j_0, k_0)\}.$$

**Lemma 1.** *Let  $m$  be an  $I \times J \times K$  move. For an  $I \times J \times K$  contingency table  $t$ , if  $t \geq m^-$ , then  $t + m$  is a contingency table.*

*Proof.* This is obvious. □

Note that a minimal Markov basis for  $3 \times 3 \times K$  contingency tables consists of indispensable moves, where a move  $m$  with  $m_{i_0j_0k_0} > 0$  is said to be *indispensable* if  $\mathcal{F}(m^+) = \mathcal{F}(m^-) = \{m^+, m^-\}$  [3, 4]. For a contingency table  $t$ , we put  $\mathcal{F}_{i_0j_0k_0}^+(t) = \{s \in \mathcal{F}(t) \mid s_{i_0j_0k_0} > 0\}$  and  $\mathcal{F}_{i_0j_0k_0}^0(t) = \{s \in \mathcal{F}(t) \mid s_{i_0j_0k_0} = 0\}$ . In this paper, we use the same terminology in a slightly different way. We call a contingency table  $t$  an *indispensable table for the  $(i_0, j_0, k_0)$ -element*, if  $t_{i_0j_0k_0} = 0$ ,  $\mathcal{F}_{i_0j_0k_0}^+(t) \neq \emptyset$  and  $\mathcal{F}_{i_0j_0k_0}^+(t') = \emptyset$  for any contingency table  $t'$  such that  $t' \leq t$  and  $t' \neq t$ .

**Lemma 2.** *Let  $\mathcal{S}$  be a set of contingency tables  $s$  of  $\Phi(I, J, K; i_0, j_0, k_0)$  with  $s_{i_0j_0k_0} = 0$  having the property that for  $s' \in \Omega(I, J, K)$  with  $s'_{i_0j_0k_0} = 0$ ,  $s' \in \Phi(I, J, K; i_0, j_0, k_0)$  if and only if there is  $s \in \mathcal{S}$  with  $s' \geq s$ . Then any indispensable table for the  $(i_0, j_0, k_0)$ -element lies in  $\mathcal{S}$ . Furthermore, if there exists a unique minimal Markov basis  $\mathfrak{B}$ , then for any  $m \in \mathfrak{B}$  with  $m_{i_0j_0k_0} > 0$ ,  $m^-$  is an indispensable table for the  $(i_0, j_0, k_0)$ -element and in particular  $m^- \in \mathcal{S}$ .*

*Proof.* It follows from the definition that an indispensable table for the  $(i_0, j_0, k_0)$ -element lies in  $\mathcal{S}$ . Let  $m \in \mathfrak{B}$  with  $m_{i_0j_0k_0} > 0$ . Since  $m^- \in \Phi(I, J, K; i_0, j_0, k_0)$ , take a table  $s \in \mathcal{S}(i_0, j_0, k_0)$  with  $m^- \geq s$ . Note that  $s \in \Phi(I, J, K; i_0, j_0, k_0)$ . Take a sequence of basis moves  $m_1, \dots, m_r$  such that  $s_1 := s + m_1$ ,  $s_2 := s_1 + m_2$ ,  $\dots$ ,  $s_r := s_{r-1} + m_r$  belong to  $\Omega(I, J, K)$  and  $(s_r)_{i_0j_0k_0} > 0$ . Suppose to the contrary that  $s \neq m^-$ . Then the sum of all entries of  $s$  is less than one for  $m^-$ . Since the sums of all entries of  $s_a$  for  $a = 1, \dots, r$  are same,  $s_a \neq m^-$  for any  $a = 1, \dots, r$ . Thus the basis move  $m$  is removable from the Markov basis. However it contradicts to the minimality of the Markov basis. Therefore,  $s = m^-$  and  $m^- \in \mathcal{S}(i_0, j_0, k_0)$ . □

For any indispensable move  $m$  with  $m_{i_0j_0k_0} > 0$ ,  $m^-$  is an indispensable table for the  $(i_0, j_0, k_0)$ -element.

**Theorem 2.** *Let  $t \in \Omega(3, 3, K)$ . Then  $t \in \Phi(3, 3, K; i_0, j_0, k_0)$  if and only if there exists a table  $s \in \mathfrak{N}(i_0, j_0, k_0) \cap \Omega(3, 3, K)$  such that  $t \geq s$ .*

**Theorem 3.** *The set  $\mathfrak{N}(i_0, j_0, k_0) \cap \Omega(3, 3, K)$  is a minimal and unique set for  $3 \times 3 \times K$  contingency tables having the properties as Theorems 1 and 2.*

For an  $I \times J \times K$  table  $t = (t_{ijk})$ , we denote by  $t_{..k}$  the  $k$ -th  $K$ -face of  $t$  and write  $t$  as  $(t_{..1}; t_{..2}; \dots; t_{..K})$ . For an  $I \times J \times K$  contingency table  $t$  and an  $I \times J \times K'$  contingency table

$t'$ ,  $t$  is said to be  $K$ -subordinate to  $t'$  if  $t_{\cdot k_0} \leq t'_{\cdot k_0}$ , and there is a number  $\ell$  ( $1 \leq \ell \leq K'$ ) such that  $t_{\cdot k} \leq t'_{\cdot \ell}$  for each  $k$  with  $1 \leq k \leq K$  and  $k \neq k_0$ .

Let  $S_n$  be the set of permutations on  $1, 2, \dots, n$  and put  $S_n(m) = \{\sigma \in S_n \mid \sigma(1) = m\}$  for  $1 \leq m \leq n$ . Let  $\sigma_I \in S_I(i_0)$ ,  $\sigma_J \in S_J(j_0)$ , and  $\sigma_K \in S_K(k_0)$ . For an  $I \times J \times K$  contingency table  $t = (t_{ijk})$ , we have a new  $I \times J \times K$  contingency table  $(\sigma_I, \sigma_J, \sigma_K) \cdot t = (t'_{ijk})$  given by  $t'_{ijk} = t_{\sigma_I(i)\sigma_J(j)\sigma_K(k)}$ . The bijection map  $(\sigma_I, \sigma_J, \sigma_K)$  from  $\Omega(I, J, K)$  to itself induces a bijection from  $\Phi(I, J, K; 1, 1, 1)$  to  $\Phi(I, J, K; i_0, j_0, k_0)$ .

**Theorem 4.** *Let  $t \in \Omega(3, 3, K)$  and  $u = \max_{i,j,k} t_{ijk}$ . If  $t \notin \Phi(3, 3, K; i_0, j_0, k_0)$  then  $\sum_{i=1}^3 t_{ij_0k_0} = 0$ ,  $\sum_{j=1}^3 t_{i_0jk_0} = 0$ ,  $\sum_{k=1}^K t_{i_0j_0k} = 0$ , or  $t$  is  $K$ -subordinate to  $(\sigma_I, \sigma_J, \sigma_K) \cdot h$  for some  $\sigma_I \in S_I(i_0)$ ,  $\sigma_J \in S_J(j_0)$ ,  $\sigma_K \in S_K(k_0)$  and some table  $h$  of the following tables.*

$0u0 \quad uuu$ $uuu \quad u0u$ , $0u0 \quad uuu$	$0uu \quad uuu$ $uuu \quad u00$ , $uuu \quad u00$	$0uu \quad uuu$ $uuu \quad u00$ , $0uu \quad uuu$	$0u0 \quad uuu$ $uuu \quad u0u$ , $uuu \quad u0u$
$0u0 \quad uuu \quad uu0$ $uuu \quad u0u \quad u00$ , $0uu \quad 00u \quad uuu$	$0u0 \quad uuu \quad 0uu$ $uuu \quad u0u \quad 00u$ , $uu0 \quad u00 \quad uuu$	$0uu \quad uuu \quad 00u$ $uuu \quad u00 \quad u0u$ , $0u0 \quad uu0 \quad uuu$	
$0u0 \quad uuu \quad 0uu$ $uu0 \quad u00 \quad uuu$ , $uuu \quad u0u \quad 00u$	$0uu \quad uuu \quad 0u0$ $uuu \quad u00 \quad uu0$ $00u \quad u0u \quad uuu$		

Proofs of the above theorems are based on the mathematical proof for  $3 \times 3 \times 3$  contingency tables in [13].

### 3. $3 \times 3 \times 2$ contingency tables

The minimal Markov basis for  $3 \times 3 \times 2$  contingency tables is the set consisting of  $222_4(i_1i_2, j_1j_2, k_1k_2)$  and  $332_6(i_1i_2i_3, j_1j_2j_3, k_1k_2)$ .

**Theorem 5.** *A contingency table  $t \in \Phi(3, 3, 2; i_0, j_0, k_0)$  can be transformed to a contingency table  $t'$  with  $t'_{i_0j_0k_0} = 1$  by  $222_4(i_0i_2, j_0j_2, k_0k_2)$  or  $332_6(i_0i_3i_2, j_0j_2j_3, k_0k_2)$ .*

*Proof.* Every tables  $t \in \Phi(I, J, 2; i_0, j_0, k_0)$  can be moved to some table  $t'$  with  $t'_{i_0j_0k_0} = 1$  by one basis move [11]. Thus  $t$  is moved to  $t'$  by  $222_4(i_0i_2, j_0j_2, k_0k_2)$  or  $332_6(i_0i_2i_3, j_2j_0j_3, k_0k_2)$  if  $I = J = 3$ . □

We put

$$ct_4(i_0i_2, j_0j_2, k_0k_2) = 222_4(i_0i_2, j_0j_2, k_2k_0)^-$$

and

$$ct_6^K(i_0i_2i_3, j_0j_2j_3, k_0k_2) = 332_6(i_0i_3i_2, j_0j_2j_3, k_0k_2)^-$$

Then  $ct_4(i_0i_2, j_0j_2, k_0k_2)$  is a table of  $\Phi(3, 3, K; i_0, j_0, k_0)$  whose four elements at  $(i_0, j_2, k_0)$ ,  $(i_0, j_2, k_0)$ ,  $(i_0, j_0, k_2)$ , and  $(i_2, j_2, k_2)$  have a value 1 and the other elements have a value 0, and  $ct_6^K(i_0i_2i_3, j_0j_2j_3, k_0k_2)$  is a table of  $\Phi(3, 3, K; i_0, j_0, k_0)$  whose six elements at

Table 3: Contingency  $3 \times 3 \times 2$  tables

$\begin{matrix} 010 & 100 \\ 100 & 010 \\ 000 & 000 \end{matrix}$	$\begin{matrix} 010 & 100 \\ 100 & 001 \\ 001 & 010 \end{matrix}$
$ct_4(12, 12, 12)$	$ct_6^K(123, 123, 12)$

$(i_0, j_2, k_0), (i_2, j_0, k_0), (i_3, j_3, k_0), (i_0, j_0, k_2), (i_2, j_3, k_2),$  and  $(i_3, j_2, k_2)$  have a value 1 and the other elements have a value 0.

Further, we put

$$\mathfrak{N}_2(i_0, j_0, k_0) = \{ct_4(i_0i_2, j_0j_2, k_0k_2), ct_6^K(i_0i_2i_3, j_0j_2j_3, k_0k_2) \mid i_2, i_3, j_2, j_3, k_2\}.$$

The set  $\mathfrak{N}_2(i_0, j_0, k_0) \cap \Omega(3, 3, K)$  consists of  $6(K - 1)$  tables. Thus, Theorem 5 and Lemma 2 imply the following proposition.

**Proposition 1.** *Theorems 2–4 hold for  $K = 2$ .*

A contingency table  $t$  is called *isolated* if there exists no basis move transforming  $t$ . It is easy to see directly that  $3 \times 2 \times 2$  tables

$$\begin{matrix} 0* & ** \\ ** & *0 \\ 0* & ** \end{matrix} \quad \text{and} \quad \begin{matrix} 0* & ** \\ ** & *0 \\ ** & *0 \end{matrix}$$

are isolated. Then Proposition 1 implies the following corollary.

**Corollary 1.** *The following  $3 \times 3 \times 2$  contingency tables can not be transformed to a contingency table  $t$  with  $t_{111} = 1$ . The former two tables are isolated.*

$$\begin{matrix} 0*0 & *** \\ *** & *0* \\ 0*0 & *** \end{matrix}, \quad \begin{matrix} 0** & *** \\ *** & *00 \\ *** & *00 \end{matrix}, \quad \begin{matrix} 0** & *** \\ *** & *00 \\ 0** & *** \end{matrix}, \quad \begin{matrix} 0*0 & *** \\ *** & *0* \\ *** & *0* \end{matrix}$$

(2a)                      (2b)                      (2c)                      (2d)

**Theorem 6.** *Let  $t$  be a  $3 \times 3 \times 2$  contingency table with  $t_{121}, t_{211}, t_{112} > 0$  and  $t_{111} = 0$ . The table  $t$  belongs to  $\Phi(3, 3, 2; 1, 1, 1)$  if and only if it is not  $K$ -subordinate to any table in Corollary 1.*

*Proof.* If  $t$  is  $K$ -subordinate to a table  $h$  in Corollary 1, then  $t \notin \Phi(3, 3, 2; 1, 1, 1)$  since  $h \notin \Phi(3, 3, 2; 1, 1, 1)$  by Corollary 1. Suppose that  $t$  is not  $K$ -subordinate to any table in Corollary 1. If  $t_{222} > 0$ , then  $t \in \Phi(3, 3, 2; 1, 1, 1)$  by  $ct_4(12, 12, 12)$  and so suppose that  $t_{222} = 0$ . Now suppose that  $t_{131} = 0$ . Then  $t_{322} > 0$  since  $t$  is not  $K$ -subordinate to a table of type (2d). If  $t_{311} > 0$  then  $t \in \Phi(3, 3, 2; 1, 1, 1)$  by  $ct_4(13, 12, 12)$  and so let suppose  $t_{311} = 0$ . Then  $t_{232} > 0$  since  $t$  is not  $K$ -subordinate to a table of type (2c). It holds that  $t_{331} > 0$  since  $t$  is not  $K$ -subordinate to a table of type (2a). Then we have  $t \in \Phi(3, 3, 2; 1, 1, 1)$  by  $ct_6^K(123, 123, 12)$ . Similarly we obtain the assertion if  $t_{311} = 0$ . So, finally suppose that  $t_{131}, t_{311} > 0$ . Since  $t$  is not  $K$ -subordinate to a table of type (2b) there are integers  $a$  and  $b$  such that  $t_{ab} > 0$  and  $2 \leq a, b \leq 3$ . Thus  $t \in \Phi(3, 3, 2; 1, 1, 1)$  by  $ct_4(1a, 1b, 12)$ . □



### 4. $3 \times 3 \times 3$ contingency tables

The minimal Markov basis of  $3 \times 3 \times 3$  contingency tables consists of moves of four types:

$$222_4(i_1i_2, j_1j_2, k_1k_2), 332_6(i_1i_2i_3, j_1j_2j_3, k_1k_2), 233_6(i_1i_2, j_1j_2j_3, k_1k_2k_3), \text{ and } 323_6(i_1i_2, j_1j_2, k_1k_2k_3).$$

We put

$$ct_6^I(i_0i_2, j_0j_2j_3, k_0k_2k_3) = 233_6(i_0i_2, j_0j_3j_2, k_0k_2k_3)^- \text{ and } ct_6^J(i_0i_2i_3, j_0j_2, k_0k_2k_3) = 323_6(i_0i_3i_2, j_0j_2, k_0k_2k_3)^-.$$

$ct_6^I(i_0i_2, j_0j_2j_3, k_0k_2k_3)$  has 1 at  $(i_0, j_2, k_0), (i_2, j_0, k_0), (i_0, j_0, k_2), (i_2, j_3, k_2), (i_0, j_3, k_3), (i_2, j_2, k_3)$  and 0 at the other  $(i, j, k)$ , and  $ct_6^J(i_0i_2i_3, j_0j_2, k_0k_2k_3)$  has 1 at  $(i_0, j_2, k_0), (i_2, j_0, k_0), (i_0, j_0, k_2), (i_3, j_2, k_2), (i_2, j_2, k_3), (i_3, j_0, k_3)$  and 0 at the other  $(i, j, k)$ . Moreover, we put

$$\begin{aligned} ct_{44}^{(1)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3) &= (222_4(i_2i_3, j_2j_3, k_2k_3) + 222_4(i_0i_2, j_0j_2, k_0k_2))^- , \\ ct_{44}^{(2)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3) &= (222_4(i_0i_3, j_0j_3, k_3k_2) + 222_4(i_0i_2, j_0j_2, k_0k_3))^- , \\ ct_{44}^{(3)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3) &= (222_4(i_0i_3, j_2j_3, k_3k_0) + 222_4(i_0i_2, j_0j_3, k_0k_2))^- , \\ ct_{44}^{(4)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3) &= (222_4(i_2i_3, j_0j_3, k_3k_0) + 222_4(i_0i_3, j_0j_2, k_0k_2))^- , \text{ and } \\ ct_{46}^K(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3) &= (222_4(i_0i_3, j_0j_3, k_3k_2) + 332_6(i_0i_2i_3, j_2j_0j_3, k_3k_0))^- . \end{aligned}$$

Table 4: Contingency  $3 \times 3 \times 3$  tables

$\begin{matrix} 010 & 100 & 001 \\ 100 & 001 & 010 \\ 000 & 000 & 000 \end{matrix}$	$\begin{matrix} 010 & 100 & 000 \\ 100 & 000 & 010 \\ 000 & 010 & 100 \end{matrix}$	$\begin{matrix} 010 & 100 & 000 \\ 100 & 001 & 010 \\ 000 & 010 & 001 \end{matrix}$	$\begin{matrix} 010 & 100 & 001 \\ 100 & 000 & 010 \\ 000 & 001 & 100 \end{matrix}$
$ct_6^I(12, 123, 123)$	$ct_6^J(123, 12, 123)$	$ct_{44}^{(1)}(123, 123, 123)$	$ct_{44}^{(2)}(123, 123, 123)$
$\begin{matrix} 010 & 100 & 001 \\ 100 & 001 & 000 \\ 001 & 000 & 010 \end{matrix}$	$\begin{matrix} 010 & 100 & 000 \\ 100 & 000 & 001 \\ 001 & 010 & 100 \end{matrix}$	$\begin{matrix} 010 & 100 & 001 \\ 100 & 000 & 001 \\ 001 & 001 & 110 \end{matrix}$	
$ct_{44}^{(3)}(123, 123, 123)$	$ct_{44}^{(4)}(123, 123, 123)$	$ct_{46}^K(123, 123, 123)$	

Then every contingency table described above as  $(m_1 + m_2)^-$  is transformed to a table  $h = (m_1 + m_2)^+$  with  $h_{i_0j_0k_0} = 1$  by a transformation by the sequence  $m_1, m_2$ . Therefore all these tables belong to  $\Phi(3, 3, 3; i_0, j_0, k_0)$ . Let  $\mathfrak{N}_3(i_0, j_0, k_0)$  be the set of all these tables.  $\mathfrak{N}_3(i_0, j_0, k_0) \cap \Omega(3, 3, K)$  consists of  $14(K - 1)(K - 2)$  tables.

**Theorem 7** ([13, Theorem C]). *Theorem 2 is true for  $K = 3$ .*

We define the  $K$ -transposed table of  $t$  as a  $J \times I \times K$  table  $(t_{\cdot 1}^T; t_{\cdot 2}^T; \dots; t_{\cdot K}^T)$  where  $t_{\cdot k}^T$  is transposed of  $t_{\cdot k}$  as a matrix.

We have the following lemma whose proof is straightforward.

**Lemma 3.** *The following contingency tables are isolated. In particular they do not belong to  $\Phi(3, 3, 3; 1, 1, 1)$ .*

$$\begin{array}{ccc}
 0*0 & *** & **0 \\
 *** & *0* & *00 \\
 0** & 00* & ***
 \end{array}, \quad
 \begin{array}{ccc}
 0*0 & *** & 0** \\
 *** & *0* & 00* \\
 **0 & *00 & ***
 \end{array}, \quad
 \begin{array}{ccc}
 0** & *** & 00* \\
 *** & *00 & *0* \\
 0*0 & **0 & ***
 \end{array},$$

(3a)                      (3b)                      (3c)

$$\begin{array}{ccc}
 0*0 & *** & 0** \\
 **0 & *00 & *** \\
 *** & *0* & 00*
 \end{array}, \quad
 \begin{array}{ccc}
 0** & *** & 0*0 \\
 *** & *00 & **0 \\
 00* & *0* & ***
 \end{array}$$

(3d)                      (3e)

*Proof.* (3a) is isolated, since any  $3 \times 3 \times 2$  basis move can not be applied. (3e) is obtained by exchanging 2 and 3 columns in (3c), (3d) is obtained by exchanging 2 and 3 rows in (3b), (3c) is a  $K$ -transposed table of (3b), and (3b) is obtained by exchanging 1 and 3 columns in (3a). Therefore (3b)–(3e) are also isolated.  $\square$

### 5. $3 \times 3 \times 4$ contingency tables

The minimal Markov basis of  $3 \times 3 \times 4$  contingency tables consists of moves

$$334_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4)$$

in addition to the minimal Markov basis of  $3 \times 3 \times 3$  contingency tables. We put

$$\begin{aligned}
 ct_8^{(1)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4) &= 334_8(i_0i_2i_3, j_0j_2j_3, k_0k_2k_4k_3)^-, \\
 ct_8^{(2)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4) &= 334_8(i_2i_0i_3, j_2j_0j_3, k_0k_4k_3k_2)^-, \\
 ct_8^{(3)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4) &= 334_8(i_3i_0i_2, j_0j_3j_2, k_2k_4k_0k_3)^-, \text{ and} \\
 ct_8^{(4)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4) &= 334_8(i_3i_0i_2, j_3j_2j_0, k_3k_4k_2k_0)^-.
 \end{aligned}$$

Table 5: Contingency  $3 \times 3 \times 4$  tables I

010	100	000	000	010	100	001	000	010	100	001	000
100	000	010	001	100	000	000	010	100	000	010	001
000	010	001	100	000	001	010	100	000	001	000	100
$ct_8^{(1)}(123, 123, 1234)$				$ct_8^{(2)}(123, 123, 1234)$				$ct_8^{(3)}(123, 123, 1234)$			
010	100	001	000								
100	001	000	010								
000	000	010	001								
$ct_8^{(4)}(123, 123, 1234)$											

Furthermore, we put

$$\begin{aligned}
 ct_{46}^{(1)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4) &= (222_4(i_0i_3, j_0j_2, k_3k_2) + 233_6(i_0i_2, j_0j_3j_2, k_0k_3k_4))^- , \\
 ct_{46}^{(2)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4) &= (222_4(i_2i_3, j_0j_2, k_4k_3) + 233_6(i_0i_2, j_0j_3j_2, k_0k_2k_3))^- , \\
 ct_{46}^{(3)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4) &= (222_4(i_2i_3, j_0j_3, k_4k_0) + 233_6(i_0i_3, j_0j_3j_2, k_0k_2k_3))^- , \\
 ct_{64}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4) &= (233_6(i_0i_3, j_0j_2j_3, k_4k_3k_0) + 222_4(i_0i_2, j_0j_3, k_0k_2))^- , \\
 ct_{444}^{(1)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4) &= (222_4(i_0i_3, j_0j_3, k_3k_2) + 222_4(i_2i_3, j_2j_3, k_3k_4) \\
 &\quad + 222_4(i_0i_2, j_0j_2, k_0k_3))^- , \text{ and} \\
 ct_{444}^{(2)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4) &= (222_4(i_0i_2, j_2j_3, k_3k_0) + 222_4(i_2i_3, j_0j_2, k_4k_0) \\
 &\quad + 222_4(i_0i_3, j_0j_3, k_0k_2))^- .
 \end{aligned}$$

Then every contingency table described above as  $(m_1 + m_2)^-$  (resp.  $(m_1 + m_2 + m_3)^-$ ) is transformed to a table  $h = (m_1 + m_2)^+$  (resp.  $h = (m_1 + m_2 + m_3)^+$ ) with  $h_{i_0j_0k_0} = 1$  by a transformation by the sequence  $m_1, m_2$  (resp.  $m_1, m_2, m_3$ ).

Table 6: Contingency  $3 \times 3 \times 4$  tables II

010 100 010 001	010 100 001 000	010 100 001 000
100 000 001 010	100 001 100 010	100 000 001 010
000 010 100 000	000 000 010 100	001 001 010 100
$ct_{46}^{(1)}(123, 123, 1234)$	$ct_{46}^{(2)}(123, 123, 1234)$	$ct_{46}^{(3)}(123, 123, 1234)$
010 100 100 001	010 100 001 000	010 100 001 000
100 001 000 000	100 000 001 010	101 000 010 010
001 000 010 100	000 001 110 001	010 001 000 100
$ct_{64}(123, 123, 1234)$	$ct_{444}^{(1)}(123, 123, 1234)$	$ct_{444}^{(2)}(123, 123, 1234)$

Therefore all these tables belong to  $\Phi(3, 3, 4; i_0, j_0, k_0)$ . Let  $\mathfrak{N}_4(i_0, j_0, k_0)$  be the set of all these tables.  $\mathfrak{N}_4(i_0, j_0, k_0) \cap \Omega(3, 3, K)$  consists of  $20(K - 1)(K - 2)(K - 3)/3$  tables. Note that

$$\begin{aligned}
 &222_4(i_0i_3, j_0j_2, k_3k_2) + 233_6(i_0i_2, j_0j_3j_2, k_0k_3k_4) \\
 &\quad = 222_4(i_0i_2, j_2j_3, k_4k_3) + 323_6(i_0i_2i_3, j_2j_0, k_2k_0k_3), \\
 &222_4(i_2i_3, j_0j_2, k_4k_3) + 233_6(i_0i_2, j_0j_3j_2, k_0k_2k_3) \\
 &\quad = 222_4(i_0i_2, j_0j_3, k_3k_2) + 323_6(i_0i_3i_2, j_0j_2, k_0k_3k_4), \\
 &222_4(i_2i_3, j_0j_3, k_4k_0) + 233_6(i_0i_3, j_0j_3j_2, k_0k_2k_3) \\
 &\quad = 222_4(i_0i_3, j_2j_3, k_3k_0) + 323_6(i_0i_3i_2, j_0j_3, k_0k_2k_4), \text{ and} \\
 &233_6(i_0i_3, j_0j_2j_3, k_4k_3k_0) + 222_4(i_0i_2, j_0j_3, k_0k_2) \\
 &\quad = 323_6(i_0i_2i_3, j_0j_3, k_4k_2k_0) + 222_4(i_0i_3, j_0j_2, k_0k_3).
 \end{aligned}$$

### 6. $3 \times 3 \times 5$ contingency tables

The minimal Markov basis of  $3 \times 3 \times 5$  contingency tables consists of moves

$$335_{10}(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4k_5)$$

in addition to the minimal Markov basis of  $3 \times 3 \times 4$  contingency tables. We put

$$\begin{aligned}
 ct_{10}^{(1)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4k_5) &= 335_{10}(i_0i_2i_3, j_3j_0j_2, k_2k_4k_5k_3k_0)^-, \\
 ct_{10}^{(2)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4k_5) &= 335_{10}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_5k_3k_4)^-, \\
 ct_{10}^{(3)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4k_5) &= 335_{10}(i_2i_0i_3, j_2j_0j_3, k_0k_5k_3k_4k_2)^-, \\
 ct_{10}^{(4)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4k_5) &= 335_{10}(i_2i_0i_3, j_3j_2j_0, k_3k_5k_2k_4k_0)^-, \text{ and} \\
 ct_{10}^{(5)}(i_0i_2i_3, j_0j_2j_3, k_0k_2k_3k_4k_5) &= 335_{10}(i_3i_0i_2, j_0j_3j_2, k_2k_5k_0k_4k_3)^-.
 \end{aligned}$$

Table 7: Contingency  $3 \times 3 \times 5$  tables

$  \begin{array}{ccccc}  010 & 100 & 100 & 001 & 000 \\  100 & 001 & 000 & 000 & 010 \\  000 & 000 & 010 & 100 & 001 \\  ct_{10}^{(1)}(123, 123, 12345)  \end{array}  $	$  \begin{array}{ccccc}  010 & 100 & 010 & 001 & 000 \\  100 & 000 & 000 & 010 & 001 \\  000 & 010 & 001 & 000 & 100 \\  ct_{10}^{(2)}(123, 123, 12345)  \end{array}  $
$  \begin{array}{ccccc}  010 & 100 & 001 & 000 & 000 \\  100 & 001 & 000 & 100 & 010 \\  000 & 000 & 010 & 001 & 100 \\  ct_{10}^{(3)}(123, 123, 12345)  \end{array}  $	$  \begin{array}{ccccc}  010 & 100 & 001 & 000 & 000 \\  100 & 000 & 010 & 010 & 001 \\  000 & 001 & 000 & 100 & 010 \\  ct_{10}^{(4)}(123, 123, 12345)  \end{array}  $
$  \begin{array}{ccccc}  010 & 100 & 001 & 000 & 000 \\  100 & 000 & 000 & 010 & 001 \\  000 & 001 & 010 & 001 & 100 \\  ct_{10}^{(5)}(123, 123, 12345)  \end{array}  $	

All these tables belong to  $\Phi(3, 3, 5; i_0, j_0, k_0)$ . Let  $\mathfrak{N}_5(i_0, j_0, k_0)$  be the set of all these tables.  $\mathfrak{N}_5(i_0, j_0, k_0) \cap \Omega(3, 3, K)$  consists of  $5(K-1)(K-2)(K-3)(K-4)/6$  tables. Then

$$\mathfrak{N}(i_0, j_0, k_0) = \mathfrak{N}_2(i_0, j_0, k_0) \cup \mathfrak{N}_3(i_0, j_0, k_0) \cup \mathfrak{N}_4(i_0, j_0, k_0) \cup \mathfrak{N}_5(i_0, j_0, k_0).$$

### 7. Proof of main theorems

In this section we give a proof for Theorems 1–4 respectively. We prepare lemmas.

**Lemma 4.** *Let  $t$  and  $t'$  be  $I \times J \times K$  contingency tables with  $t_{i_0j_0k_0} = t'_{i_0j_0k_0} = 0$ . If  $t' \geq t$  and  $t \in \Phi(I, J, K; i_0, j_0, k_0)$  then  $t' \in \Phi(I, J, K; i_0, j_0, k_0)$ .*

*Proof.* A sequence of basis moves which connects  $t$  with a contingency table  $h$  with  $h_{i_0j_0k_0} > 0$  connects also  $t'$  with a contingency table  $h' = h + (t' - t)$  with  $h'_{i_0j_0k_0} > 0$ .  $\square$

We denote a positive element by  $+$ . The next two lemmas apply to  $3 \times 3 \times 4$  contingency tables.

**Lemma 5.** *Let*

$$t' = \begin{matrix} 0+0 & +\cdot\cdot & +\cdot 0 \\ +\cdot\cdot & \cdot 0+ & \cdot 00 \\ 0\cdot+ & 00\cdot & \cdot+\cdot \end{matrix}$$

*be a  $3 \times 3 \times 3$  contingency table and  $M$  a  $3 \times 3$  matrix. Put  $t = (t'; M)$  which is a  $3 \times 3 \times 4$  contingency table. If there is no table  $N \in \mathfrak{N}(1, 1, 1)$  such that  $t \geq N$  then the  $3 \times 3 \times 4$  table  $t$  is  $K$ -subordinate to a table of type (3a).*

*Proof.* We show the claim by dividing into two cases whether some element is positive or 0 step by step. If  $t_{134} > 0$  then  $t_{314} = t_{224} = t_{324} = 0$  by  $ct_{64}(123, 123, 1234)$ ,  $ct_6^I(12, 123, 124)$  and  $ct_{44}^{(3)}(123, 123, 124)$ , and thus the table is  $K$ -subordinate to a table of type (3a). Therefore  $t_{134} = 0$ . If  $t_{224} > 0$  it holds that  $t_{314} = t_{114} = 0$  by  $ct_6^J(123, 12, 134)$  and  $ct_4(12, 12, 14)$ , and then the table is  $K$ -subordinate to a table of type (3a). Therefore  $t_{224} = 0$ . If  $t_{234} = 0$  the table is  $K$ -subordinate to a table of type (3a). Then  $t_{234} > 0$ .  $ct_{44}^{(4)}(123, 123, 134)$  implies  $t_{314} = 0$ . If  $t_{114} = 0$  the table is  $K$ -subordinate to a table of type (3a) and otherwise,  $t_{324} = 0$  by  $ct_6^K(123, 123, 14)$  and then the table is  $K$ -subordinate to a table of type (3a).  $\square$

**Lemma 6.** *Let*

$$t' = \begin{matrix} 0+0 & +\cdot\cdot & 0\cdot+ \\ +\cdot\cdot & \cdot 0+ & 00\cdot \\ +\cdot 0 & \cdot 00 & \cdot+\cdot \end{matrix}$$

*be a  $3 \times 3 \times 3$  contingency table and  $M$  a  $3 \times 3$  matrix. For the  $3 \times 3 \times 4$  table  $t = (t'; M)$ , if there is no table  $N \in \mathfrak{N}(1, 1, 1)$  such that  $t \geq N$ , then  $t$  is  $K$ -subordinate to a table of type (3b).*

*Proof.* If  $t_{114} > 0$  it holds that  $t_{224} = t_{324} = t_{334} = 0$  by  $ct_4(12, 12, 14)$ ,  $ct_4(13, 12, 14)$  and  $ct_6^I(13, 123, 143)$ , and then  $t$  is  $K$ -subordinate to a table of type (3b) since  $t$  has of form

$$\begin{matrix} 0+0 & +\cdot\cdot & 0\cdot+ & +\cdot\cdot \\ +\cdot\cdot & \cdot 0+ & 00\cdot & \cdot 0\cdot \\ +\cdot 0 & \cdot 00 & \cdot+\cdot & \cdot 00 \end{matrix}$$

Therefore  $t_{114} = 0$ . If  $t_{224} > 0$  then  $t_{334} = t_{134} = 0$  by  $ct_8^{(4)}(123, 123, 1234)$  and  $ct_6^I(12, 123, 124)$  and thus  $t$  is  $K$ -subordinate to a table of type (3b). Therefore  $t_{224} = 0$ . If  $t_{214} = 0$  then  $t$  is  $K$ -subordinate to a table of type (3b). Thus let  $t_{214} > 0$ .  $ct_8^{(3)}(132, 123, 1234)$  implies  $t_{334} = 0$ . Now the table  $t$  is of form

$$\begin{matrix} 0+0 & +\cdot\cdot & 0\cdot+ & 0\cdot\cdot \\ +\cdot\cdot & \cdot 0+ & 00\cdot & +0\cdot \\ +\cdot 0 & \cdot 00 & \cdot+\cdot & \cdot\cdot 0 \end{matrix}$$

If  $t_{134} = 0$  then  $t$  is  $K$ -subordinate to a table of type (3b), and otherwise  $t_{324} = 0$  by  $ct_{44}^{(2)}(132, 123, 124)$  and thus  $t$  is  $K$ -subordinate to a table of type (3b).  $\square$

The next three lemmas apply to  $3 \times 3 \times 5$  contingency tables.

**Lemma 7.** *Let*

$$t' = \begin{matrix} 0+0 & +\cdot\cdot & +\cdot 0 & 0\cdot 0 \\ +\cdot\cdot & \cdot 0+ & \cdot 00 & \cdot +\cdot \\ 0\cdot 0 & 00\cdot & \cdot +\cdot & 0\cdot + \end{matrix}$$

*be a  $3 \times 3 \times 4$  contingency table and  $M$  a  $3 \times 3$  matrix. For the  $3 \times 3 \times 5$  table  $t = (t'; M)$ , if there is no table  $N \in \mathfrak{N}(1, 1, 1)$  such that  $t \geq N$ , then  $t$  is  $K$ -subordinate to a table of type (3a).*

*Proof.* If  $t_{135} > 0$  then  $t_{315} = t_{225} = t_{325} = 0$  by  $ct_{10}^{(1)}(123, 123, 12354)$ ,  $ct_6^I(12, 123, 125)$  and  $ct_8^{(4)}(123, 123, 1254)$ , and thus  $t$  is  $K$ -subordinate to a table of type (3a). Therefore  $t_{135} = 0$ . If  $t_{225} > 0$  then  $t_{315} = t_{115} = 0$  by  $ct_6^J(123, 12, 135)$  and  $ct_4(12, 12, 15)$ , and hence  $t$  is  $K$ -subordinate to a table of type (3a). Therefore  $t_{225} = 0$ . If  $t_{235} = 0$  then  $t$  is  $K$ -subordinate to a table of type (3a). Thus  $t_{235} > 0$ .  $ct_8^{(1)}(123, 123, 1345)$  implies  $t_{315} = 0$ . If  $t_{115} = 0$  then  $t$  is  $K$ -subordinate to a table of type (3a), and otherwise  $t_{325} = 0$  by  $ct_{44}^{(1)}(123, 123, 154)$ , which implies that  $t$  is  $K$ -subordinate to a table of type (3a).  $\square$

**Lemma 8.** *Let*

$$t' = \begin{matrix} 0+0 & +\cdot\cdot & 0\cdot + & 0\cdot 0 \\ +\cdot\cdot & \cdot 0+ & 00\cdot & \cdot +\cdot \\ 0\cdot 0 & \cdot 00 & \cdot +\cdot & +\cdot 0 \end{matrix}$$

*be a  $3 \times 3 \times 4$  contingency table and  $M$  a  $3 \times 3$  matrix. For the  $3 \times 3 \times 5$  table  $t = (t'; M)$ , if there is no table  $N \in \mathfrak{N}(1, 1, 1)$  such that  $t \geq N$ , then  $t$  is  $K$ -subordinate to a table of type (3b).*

*Proof.*  $ct_6^J(123, 12, 134)$  implies  $t_{113} = 0$ . If  $t_{115} > 0$  then  $t_{225} = t_{335} = t_{325} = 0$  by  $ct_4(12, 12, 15)$ ,  $ct_8^{(2)}(123, 123, 1534)$  and  $ct_6^J(123, 12, 154)$ , and thus  $t$  is  $K$ -subordinate to a table of type (3b). Therefore  $t_{115} = 0$ . If  $t_{225} > 0$  then  $t_{335} = t_{135} = 0$  by  $ct_8^{(4)}(123, 123, 1235)$  and  $ct_6^I(12, 123, 125)$ , and thus  $t$  is  $K$ -subordinate to a table of type (3b). Therefore  $t_{225} = 0$ . It holds that  $t_{215} > 0$  since, if not,  $t$  is  $K$ -subordinate to a table of type (3b). Then  $ct_{10}^{(3)}(123, 123, 12354)$  implies  $t_{335} = 0$ . If  $t_{135} = 0$  then  $t$  is  $K$ -subordinate to a table of type (3b) and otherwise  $t_{325} = 0$  by  $ct_{46}^{(2)}(123, 123, 1254)$ , which implies that  $t$  is  $K$ -subordinate to a table of type (3b).  $\square$

**Lemma 9.** *Let*

$$t' = \begin{matrix} 0+0 & +\cdot\cdot & 0\cdot + & 0\cdot 0 \\ +\cdot\cdot & \cdot 00 & \cdot +\cdot & \cdot +0 \\ 0\cdot 0 & \cdot 0+ & 00\cdot & +\cdot\cdot \end{matrix}$$

*be a  $3 \times 3 \times 4$  contingency table and  $M$  a  $3 \times 3$  matrix. For the  $3 \times 3 \times 5$  table  $t = (t'; M)$ , if there is no table  $N \in \mathfrak{N}(1, 1, 1)$  such that  $t \geq N$ , then  $t$  is  $K$ -subordinate to a table of type (3d) or (3e). Furthermore, if  $t_{321} > 0$  then  $t$  is  $K$ -subordinate to a table of type (3d), if  $t_{231} > 0$  then  $t$  is  $K$ -subordinate to a table of type (3e), and if  $t_{231} = t_{321} = 0$  then  $t$  is  $K$ -subordinate to a table of both type (3d) and (3e).*

*Proof.* If  $t_{231} > 0$  then  $t$  is not subordinate to any table of type (3d) and if  $t_{321} > 0$  then  $t$  is not subordinate to any table of type (3e). Furthermore, if  $t_{231} = t_{321} = 0$  and  $t$

is subordinate to a table of type (3d) or (3e), then  $t$  is subordinate to both of a table of type (3d) and a table of type (3e). Therefore, it suffices to show that if  $t_{231} = 0$  (resp.  $t_{321} = 0$ ) then  $t$  is not subordinate to any table of type (3d) (resp. (3e)).

First we divide into two cases when  $t_{115} > 0$  and  $t_{115} = 0$ . Suppose  $t_{115} > 0$ . It holds that  $t_{225} = t_{235} = t_{325} = 0$  by  $ct_4(12, 12, 15)$ ,  $ct_6^I(12, 123, 153)$  and  $ct_6^J(123, 12, 154)$ . If  $t_{231} = 0$  then  $t$  is  $K$ -subordinate to a table of type (3d) and otherwise  $t_{321} = 0$  by  $ct_{444}^{(2)}(123, 123, 1234)$ , which implies that  $t$  is  $K$ -subordinate to a table of type (3e). Suppose  $t_{115} = 0$ . Now  $t$  has the following type.

$$\begin{matrix} 0+0 & +\cdot\cdot & 0\cdot+ & 0\cdot0 & 0\cdot\cdot \\ +\cdot\cdot & \cdot00 & \cdot+\cdot & \cdot+0 & \cdot\cdot\cdot \\ 0\cdot0 & \cdot0+ & 00\cdot & +\cdot\cdot & \cdot\cdot\cdot \end{matrix}$$

We divide into two cases when  $t_{235} > 0$  and  $t_{235} = 0$ .

Suppose  $t_{235} > 0$ .  $ct_{10}^{(4)}(123, 123, 12345)$  implies  $t_{325} = 0$  and  $ct_8^{(3)}(123, 123, 1235)$  implies  $t_{315} = 0$ . If  $t_{231} = 0$  then  $t$  is  $K$ -subordinate to a table of type (3d), and otherwise  $t_{321} = 0$  by  $ct_{444}^{(2)}(123, 123, 1234)$  and thus  $t$  is  $K$ -subordinate to a table of type (3e). We are done in the case when  $t_{235} > 0$ .

Next suppose  $t_{235} = 0$ . We divide into two cases when  $t_{135} = 0$  and  $t_{135} > 0$ . Suppose  $t_{135} = 0$ . If  $t_{231} = 0$  then  $t$  is  $K$ -subordinate to a table of type (3d) and otherwise  $t_{321} = 0$  by  $ct_{444}^{(2)}(123, 123, 1234)$ , which implies that  $t$  is  $K$ -subordinate to a table of type (3e). Next suppose  $t_{135} > 0$ . Then  $ct_8^{(2)}(123, 123, 1254)$  implies  $t_{325} = 0$ . If  $t_{225} = 0$  and  $t_{231} = 0$ , then  $t$  is  $K$ -subordinate to a table of type (3d). If  $t_{225} = 0$  and  $t_{231} > 0$  then  $ct_{444}^{(2)}(123, 123, 1234)$  implies  $t_{321} = 0$  and thus  $t$  is  $K$ -subordinate to a table of type (3e). Therefore we suppose  $t_{225} > 0$ . Then  $ct_{44}^{(2)}(123, 123, 125)$  implies  $t_{315} = 0$ . If  $t_{231} = 0$  then  $t$  is  $K$ -subordinate to a table of type (3d), and otherwise  $t_{321} = 0$  by  $ct_{444}^{(2)}(123, 123, 1234)$ , which implies that  $t$  is  $K$ -subordinate to a table of type (3e).  $\square$

Let  $t$  be a  $3 \times 3 \times K$  table. Put  $S_0 = \{k \mid t_{11k} = 0\}$  and  $S_+ = \{k \mid t_{11k} > 0\}$ . It is clear that if  $S_+$  is empty then  $t \notin \Phi(3, 3, K; 1, 1, 1)$ .

**Theorem 8.** *Let  $K \geq 2$  and  $t \in \Omega(3, 3, K)$ . Suppose that  $t_{111} = 0$ ,  $t_{121}, t_{211} > 0$  and  $S_+ \neq \emptyset$ . If there is no table  $N \in \mathfrak{N}(1, 1, 1)$  such that  $t \geq N$ , then  $t$  is  $K$ -subordinate to a table of type (2a)–(3e).*

*Proof.* Suppose that there is no table  $N \in \mathfrak{N}(1, 1, 1)$  such that  $t \geq N$ . If  $t_{..k} = \begin{matrix} +\cdot\cdot \\ \cdot00 \\ \cdot00 \end{matrix}$  for all  $k \in S_+$ , then  $t$  is  $K$ -subordinate to a table of type (2b). So, assume that there is

$k_2 \in S_+$  such that  $t_{..k_2} \neq \begin{matrix} +\cdot\cdot \\ \cdot00 \\ \cdot00 \end{matrix}$ .

We divide into five cases:

$$t_{..1} = \begin{matrix} 0++ & 0+0 & 0++ & 0+0 & 0+0 \\ +\cdot\cdot & +\cdot\cdot & 0\cdot\cdot & 0\cdot+ & 0\cdot0 \end{matrix}.$$

(1) If  $t_{..1} = \begin{matrix} 0++ \\ +\cdot\cdot \\ +\cdot\cdot \end{matrix}$  then  $t_{..k} = \begin{matrix} +\cdot\cdot \\ \cdot00 \\ \cdot00 \end{matrix}$  for any  $k \in S_+$ , which is a contradiction, since  $(t_{..1}; t_{..k}) \not\geq ct_4(1i_2, 1j_2, 12)$  for  $i_2, j_2 = 2, 3$ .

(2) Second, suppose that  $t_{..1} = \begin{matrix} 0+0 \\ +\cdot\cdot \\ +\cdot\cdot \end{matrix}$ .  $(t_{..1}; t_{..k}) \notin \Phi(3, 3, 2; 1, 1, 1)$  for each  $k \in S_+$  implies that  $t_{..k} = \begin{matrix} +\cdot\cdot \\ \cdot 0+ \\ \cdot 0\cdot \end{matrix}$  or  $\begin{matrix} +\cdot\cdot \\ \cdot 0\cdot \\ \cdot 0+ \end{matrix}$ . If  $S_0 = \{1\}$  then  $t$  is  $K$ -subordinate to a table of type (2d). If  $t_{22k} > 0$  or  $t_{32k} > 0$  implies  $t_{13k} = 0$  for each  $k \in S_0$ , then  $t$  is  $K$ -subordinate to a table of type (2d). So, we are done when  $K = 2$  and we may assume that  $K \geq 3$  and that there is  $k_3 \in S_0$  such that  $t_{..k_3} = \begin{matrix} 0\cdot+ \\ \cdot\cdot\cdot \\ \cdot\cdot\cdot \end{matrix}$  and  $t_{22k_3} > 0$  or  $t_{32k_3} > 0$ . We may assume that

$$(t_{..1}; t_{..k_2}; t_{..k_3}) = \begin{matrix} 0+0 & +\cdot\cdot & 0\cdot+ \\ +\cdot\cdot & \cdot 0+ & \cdot\cdot\cdot \\ +\cdot\cdot & \cdot 0\cdot & \cdot\cdot\cdot \end{matrix},$$

since if not we can apply this by exchanging 2 and 3 in the  $I$ -coordinate. It holds that  $t_{22k_3} = 0$  by  $ct_6^I(12, 123, 1k_2k_3)$  and then  $t_{32k_3} > 0$ . Thus  $t_{331} = t_{33k_2} = t_{21k_3} = 0$  by  $ct_{44}^{(3)}(123, 123, 1k_2k_3)$ ,  $ct_6^I(13, 123, 1k_2k_3)$  and  $ct_{44}^{(2)}(132, 123, 1k_2k_3)$  respectively. Therefore,  $(t_{..1}; t_{..k_2}; t_{..k_3})$  is a table of type (3b) and not  $K$ -subordinate to a table of the other types.

$$(t_{..1}; t_{..k_2}; t_{..k_3}) = \begin{matrix} 0+0 & +\cdot\cdot & 0\cdot+ \\ +\cdot\cdot & \cdot 0+ & 00\cdot \\ +\cdot 0 & \cdot 00 & \cdot +\cdot \end{matrix}.$$

Therefore, we are done when  $K = 3$ , and if  $K \geq 4$  then since  $(t_{..1}; t_{..k_2}; t_{..k_3}; t_{..k}) \notin \Phi(3, 3, 4; 1, 1, 1)$ , it is  $K$ -subordinate to a table of type (3b) by Lemma 6, which means that  $t$  is also  $K$ -subordinate to a table of type (3b).

(3) The third case when  $t_{..1} = \begin{matrix} 0++ \\ +\cdot\cdot \\ 0\cdot\cdot \end{matrix}$  is similar as the second case by  $K$ -transposing of  $t$ .

(4) Fourth, suppose that  $t_{..1} = \begin{matrix} 0+0 \\ +\cdot\cdot \\ 0\cdot+ \end{matrix}$ . Note that  $t_{22k} = 0$  for any  $k \in S_+$  by  $ct_4(12, 12, 1k)$ . We divide into four cases (4.1)–(4.4).

(4.1) Suppose that there are  $k_3, k_4 \in S_+$  such that  $t_{..k_3} = \begin{matrix} +\cdot\cdot \\ \cdot 0+ \\ \cdot\cdot\cdot \end{matrix}$  and  $t_{..k_4} = \begin{matrix} +\cdot\cdot \\ \cdot 0\cdot \\ \cdot +\cdot \end{matrix}$ . Since  $(t_{..1}; t_{..k_3}) \notin \Phi(3, 3, 2; 1, 1, 1)$ , it holds that  $k_3 \neq k_4$  by  $ct_6^K(123, 123, 1k_3)$ .

$$(t_{..1}; t_{..k_3}; t_{..k_4}) = \begin{matrix} 0+0 & +\cdot\cdot & +\cdot\cdot \\ +\cdot\cdot & \cdot 0+ & \cdot 0\cdot \\ 0\cdot+ & \cdot\cdot\cdot & \cdot +\cdot \end{matrix}.$$

It holds that  $t_{31k_3} = t_{32k_3} = t_{23k_4} = t_{13k_4} = 0$  by  $ct_{44}^{(4)}(123, 123, 1k_4k_3)$ ,  $ct_6^K(123, 123, 1k_3)$ ,  $ct_6^K(123, 123, 1k_4)$  and  $ct_{44}^{(3)}(123, 123, 1k_3k_4)$  respectively. Then the type of  $(t_{..1}; t_{..k_3}; t_{..k_4})$  is uniquely (3a). Thus  $t$  is  $K$ -subordinate to a table of type (3a) by Lemma 5.

(4.2) Suppose that there is  $k_3 \in S_+$  such that  $t_{23k_3} > 0$  and that  $t_{32k} = 0$  for each  $k \in S_+$  with  $k \neq k_3$ . Then  $t_{32k_3} = 0$  by  $ct_6^K(123, 123, 1k_3)$  and thus  $t_{22k} = t_{32k} = 0$



for any  $k \in S_+$ . For each  $k \in S_0$  such that  $t_{13k} > 0$  we see that  $t_{22k} = t_{32k} = 0$  by  $ct_6^I(12, 123, 1k_3k)$  and  $ct_{44}^{(3)}(123, 123, 1k_3k)$  respectively. Therefore  $t$  is  $K$ -subordinate to a table of type (2d).

(4.3) Suppose that there is  $k_3 \in S_+$  such that  $t_{32k_3} > 0$  and  $t_{23k} = 0$  for each  $k \in S_+$  with  $k \neq k_3$ . This case is similar as (4.2) by  $K$ -transposing of  $t$ .

(4.4) Suppose that  $t_{23k} = t_{32k} = 0$  for each  $k \in S_+$ :

$$t_{..k} = \begin{matrix} + \cdot \cdot \\ \cdot 00 \\ \cdot 0 \cdot \end{matrix}, \quad k \in S_+.$$

If  $t_{13k} = 0$  or  $t_{22k} = t_{32k} = 0$  for each  $k \in S_0$  then  $t$  is  $K$ -subordinate to a table of type (2d). If  $t_{31k} = 0$  or  $t_{22k} = t_{23k} = 0$  for each  $k \in S_0$  then  $t$  is  $K$ -subordinate to a table of type (2c). Now suppose that there are  $k_3, k_4 \in S_+$  such that  $t_{..k_3} = \begin{matrix} 0 \cdot + \\ \cdot \cdot \cdot \\ \cdot \cdot \cdot \end{matrix}$  and  $t_{22k_3} > 0$  or

$t_{32k_3} > 0$ , and  $t_{..k_4} = \begin{matrix} 0 \cdot \cdot \\ \cdot \cdot \cdot \\ + \cdot \cdot \end{matrix}$  and  $t_{22k_4} > 0$  or  $t_{23k_4} > 0$ . First show that  $k_3 \neq k_4$ . Assume that  $k_3 = k_4$ .

$$(t_{..1}; t_{..k_2}; t_{..k_3}) = \begin{matrix} 0+0 & + \cdot \cdot & 0 \cdot + \\ + \cdot \cdot & \cdot 00 & \cdot \cdot \cdot \\ 0 \cdot + & \cdot 0+ & + \cdot \cdot \end{matrix}.$$

It holds that  $t_{22k_3} = 0$  by  $ct_{44}^{(2)}(123, 123, 1k_2k_3)$  and then  $t_{23k_3}, t_{32k_3} > 0$ . Thus the contingency table  $(t_{..1}; t_{..k_2}; t_{..k_3}) \in \Phi(3, 3, 3; 1, 1, 1)$  by  $ct_{46}^K(123, 123, 1k_2k_3)$ , which is a contradiction. Thus  $k_3 \neq k_4$ . We show that  $t_{31k_3} = t_{13k_4} = 0$ . Let  $t_{31k_3} > 0$ . Then  $t_{22k_3} = 0$  by  $ct_{44}^{(2)}(123, 123, 1k_2k_3)$  and thus  $t_{32k_3} > 0$ . It contradicts to  $(t_1; t_{k_2}; t_{k_3}) \notin \Phi(3, 3, 3; 1, 1, 1)$  by  $ct_{46}^K(123, 123, 1k_2k_3)$ . Therefore,  $t_{31k_3} = 0$ . Similarly we see that  $t_{13k_4} = 0$ .

Now, we show that  $t_{22k_3}, t_{22k_4} > 0$ . First suppose that  $t_{22k_3} = t_{22k_4} = 0$ . By assumption,  $t_{32k_3}, t_{23k_4} > 0$  and then the contingency table  $(t_{..1}; t_{..k_2}; t_{..k_3}; t_{..k_4})$  lies in  $\Phi(3, 3, 4; 1, 1, 1)$  by  $ct_{46}^{(3)}(123, 123, 1k_2k_3k_4)$ , which is a contradiction. Next, suppose that  $t_{22k_3} > 0$  and  $t_{22k_4} = 0$ . Noting that  $t_{23k_4} > 0$ ,  $(t_{..1}; t_{..k_2}; t_{..k_3}; t_{..k_4})$  lies in  $\Phi(3, 3, 4; 1, 1, 1)$  by  $ct_8^{(3)}(123, 123, 1k_2k_3k_4)$ , which is a contradiction. Similarly, if  $t_{22k_4} > 0$  and  $t_{22k_3} = 0$  then  $(t_{..1}; t_{..k_2}; t_{..k_3}; t_{..k_4})$  lies in  $\Phi(3, 3, 4; 1, 1, 1)$  by  $ct_8^{(2)}(123, 123, 1k_2k_4k_3)$ , which is a contradiction. Therefore we conclude that  $t_{22k_3}, t_{22k_4} > 0$ . It holds that  $t_{32k_3} = t_{23k_4} = 0$  by  $ct_8^{(2)}(123, 123, 1k_2k_3k_4)$  and  $ct_8^{(3)}(123, 123, 1k_2k_3k_4)$ . Furthermore, it holds that  $t_{231} = 0$  or  $t_{321} = 0$ , by  $ct_{444}^{(2)}(123, 123, 1k_2k_3k_4)$ , and thus

$$(t_{..1}; t_{..k_2}; t_{..k_3}; t_{..k_4}) = \begin{matrix} 0+0 & + \cdot \cdot & 0 \cdot + & 0 \cdot 0 \\ + \cdot \cdot & \cdot 00 & \cdot + \cdot & \cdot +0 \\ 0 \cdot + & \cdot 0+ & 00 \cdot & + \cdot \cdot \end{matrix}.$$

is  $K$ -subordinate to a table of type (3d) or (3e). By Lemma 9, the table  $t$  is also  $K$ -subordinate to a table of type (3d) or (3e).

(5) Fifth, suppose that  $t_{..1} = \begin{matrix} 0+0 \\ +\cdot\cdot \\ 0\cdot0 \end{matrix}$ . Note that  $t_{22k} = 0$  for any  $k \in S_+$ . If  $t_{13k} = t_{31k} = t_{33k} = 0$  for any  $k \in S_0$  then  $t$  is  $K$ -subordinate to a table of type (2a). Suppose that there is  $k_5 \in S_0$  such that  $t_{22k_5} > 0$  and at least one of  $t_{13k_5}$ ,  $t_{31k_5}$ , and  $t_{33k_5}$  is nonzero. We divide into four cases.

(5.1) In the first case, suppose that there are numbers  $k_3, k_4 \in S_+$  such that  $t_{..k_3} = \begin{matrix} +\cdot\cdot \\ \cdot0+ \\ \cdot\cdot\cdot \end{matrix}$  and  $t_{..k_4} = \begin{matrix} +\cdot\cdot \\ \cdot0\cdot \\ \cdot+\cdot \end{matrix}$ . First we show that  $k_3 \neq k_4$ . If  $k_3 = k_4$  then  $t_{13k_5} = t_{31k_5} = t_{33k_5} = 0$  by  $ct_6^I(12, 123, 1k_3k_5)$ ,  $ct_6^J(12, 123, 1k_3k_5)$  and  $ct_{44}^{(1)}(123, 123, 1k_3k_5)$ , since  $(t_{..1}; t_{..k_3}; t_{..k_5}) \notin \Phi(3, 3, 3; 1, 1, 1)$ , which is a contradiction. Thus  $k_3 \neq k_4$ . We see the table  $(t_{..1}; t_{..k_3}; t_{..k_4}; t_{..k_5})$ . We have  $t_{13k_5} = t_{31k_5} = 0$  by  $ct_6^I(12, 123, 1k_3k_5)$  and  $ct_6^J(123, 12, 1k_4k_5)$  and then  $t_{33k_5} > 0$ . Furthermore,  $t_{31k_3} = 0$  by  $ct_8^I(123, 123, 1k_4k_5k_3)$ ,  $t_{13k_4} = 0$  by  $ct_8^{(4)}(123, 123, 1k_3k_4k_5)$ , and  $t_{32k_3} = t_{23k_4} = 0$  by  $ct_{44}^{(1)}(123, 123, 1k_3k_5)$ ,  $ct_{44}^{(1)}(123, 123, 1k_4k_5)$ . The table  $(t_{..1}; t_{..k_3}; t_{..k_4}; t_{..k_5})$  is  $K$ -subordinate to a table of type (3a) uniquely and thus  $t$  is  $K$ -subordinate to a table of type (3a) by Lemma 7.

(5.2) As the second case, suppose that there is  $k_3 \in S_+$  such that  $t_{23k_3} > 0$  and that  $t_{32k} = 0$  for all  $k \in S_+$ . If there is no  $k \in S_0$  such that  $t_{13k} > 0$  then  $t$  is  $K$ -subordinate to a table of type (2d). Suppose that there is  $k_4 \in S_0$  such that  $t_{13k_4} > 0$ . Further suppose that  $t_{22k_4} > 0$  or  $t_{32k_4} > 0$ , since if there is no such a  $k_4$  then  $t$  is  $K$ -subordinate to a table of type (2d).  $(t_{..1}; t_{..k_3}; t_{..k_4}) \notin \Phi(3, 3, 4; 1, 1, 1)$  implies that  $t_{22k_4} = 0$  by  $ct_6^I(12, 123, 1k_3k_4)$  and then  $t_{32k_4} > 0$ . We consider the following table

$$(t_{..1}; t_{..k_3}; t_{..k_4}; t_{..k_5}) = \begin{matrix} 0+0 & +\cdot\cdot & 0\cdot+ & 0\cdot\cdot \\ +\cdot\cdot & \cdot0+ & \cdot0\cdot & \cdot+\cdot \\ 0\cdot0 & \cdot0\cdot & \cdot+\cdot & \cdot\cdot\cdot \end{matrix} \notin \Phi(3, 3, 4; 1, 1, 1).$$

It holds that  $t_{13k_5} = t_{33k_5} = 0$  by  $ct_6^I(12, 123, 1k_3k_5)$  and  $ct_8^{(4)}(123, 123, 1k_3k_4k_5)$  respectively. Then  $t_{31k_5} > 0$  by assumption on  $t_{..k_5}$ . Furthermore, it holds that  $t_{33k_3} = t_{21k_4} = 0$  by  $ct_8^{(2)}(123, 123, 1k_3k_4k_5)$  and  $ct_{46}^{(2)}(123, 123, 1k_3k_4k_5)$  respectively. Thus, the table  $(t_{..1}; t_{..k_3}; t_{..k_4}; t_{..k_5})$  is  $K$ -subordinate to a table of type (3b), which implies that  $t$  is also  $K$ -subordinate to a table of type (3b) by Lemma 8.

(5.3) The third case is one that there is  $k_4 \in S_+$  such that  $t_{32k_4} > 0$  and  $t_{23k} = 0$  for all  $k \in S_+$ . This case is similar as the second case (5.2).

(5.4) The fourth case is one that  $t_{23k} = t_{32k} = 0$  for all  $k \in S_+$ . That is, it holds that  $t_{..k} = \begin{matrix} +\cdot\cdot \\ \cdot00 \\ \cdot0\cdot \end{matrix}$  for each  $k \in S_+$ . In particular,  $t_{..k_2} = \begin{matrix} +\cdot\cdot \\ \cdot00 \\ \cdot0+ \end{matrix}$ .

If  $t_{13k} = 0$  or  $t_{22k} = t_{32k} = 0$  for each  $k \in S_0$  then  $t$  is  $K$ -subordinate to a table of type (2d). If  $t_{31k} = 0$  or  $t_{22k} = t_{23k} = 0$  for each  $k \in S_0$  then  $t$  is  $K$ -subordinate to a table of type (2c). Thus we may suppose that there are  $k_3, k_4 \in S_+$  such that  $t_{13k_3}, t_{22k_3} > 0$  or  $t_{13k_3}, t_{32k_3} > 0$  and  $t_{31k_4}, t_{22k_4} > 0$  or  $t_{31k_4}, t_{23k_4} > 0$ . Suppose to the contrary that  $k_3 = k_4$ . It holds that  $t_{22k_3} = 0$  by  $ct_{44}^{(2)}(123, 123, 1k_2k_3)$  and then  $t_{23k_3}, t_{32k_3} > 0$ .

$$(t_{..1}; t_{..k_2}; t_{..k_3}; t_{..k_5}) = \begin{matrix} 0+0 & +\cdot\cdot & 0\cdot+ & 0\cdot\cdot \\ +\cdot\cdot & \cdot00 & \cdot0+ & \cdot+\cdot \\ 0\cdot0 & \cdot0+ & ++\cdot & \cdot\cdot\cdot \end{matrix}$$

It holds that  $t_{33k_5} = 0$  by  $ct_{444}^{(1)}(123, 123, 1k_2k_3k_5)$ ,  $t_{13k_5} = 0$  by  $ct_8^{(3)}(123, 123, 1k_2k_5k_3)$ , and  $t_{31k_5} = 0$  by  $ct_8^{(2)}(123, 123, 1k_2k_3k_5)$ . This is a contradiction. Therefore  $k_3 \neq k_4$ .

Now we show that  $t_{22k_3}, t_{22k_4} > 0$ . Suppose that  $t_{22k_3} = t_{22k_4} = 0$ . Then  $k_5 \neq k_3, k_4$  and by assumption,  $t_{32k_3}, t_{23k_4} > 0$ .

$$(t_{..1}; t_{..k_2}; t_{..k_3}; t_{..k_4}; t_{..k_5}) = \begin{pmatrix} 0+0 & +\cdot\cdot & 0\cdot+ & 0\cdot\cdot & 0\cdot\cdot \\ +\cdot\cdot & \cdot 00 & \cdot 0\cdot & \cdot 0+ & \cdot +\cdot \\ 0\cdot 0 & \cdot 0+ & \cdot +\cdot & +\cdot\cdot & \cdot\cdot\cdot \end{pmatrix}.$$

It holds that  $t_{31k_5} = t_{13k_5} = t_{33k_5} = 0$  by  $ct_8^{(2)}(123, 123, 1k_2k_3k_5)$ ,  $ct_8^{(3)}(123, 123, 1k_2k_5k_4)$ , and  $ct_{10}^{(5)}(123, 123, 1k_2k_3k_5k_4)$ , which is a contradiction. Next, suppose that  $t_{22k_3} > 0$  and  $t_{22k_4} = 0$ . Then  $t_{23k_4} > 0$ , which implies that  $t \geq ct_8^{(3)}(123, 123, 1k_2k_3k_4)$ , a contradiction. Similarly, if  $t_{22k_3} = 0$  and  $t_{22k_4} > 0$  then  $t_{32k_4} = 0$  by  $ct_8^{(2)}(123, 123, 1k_2k_4k_3)$ ,  $t_{32k_3} > 0$ , and  $t \geq ct_8^{(2)}(123, 123, 1k_2k_3k_4)$ , a contradiction. Therefore we conclude that  $t_{22k_3}, t_{22k_4} > 0$ . By  $ct_{44}^{(2)}(123, 123, 1k_2k_3)$  and  $ct_{44}^{(2)}(123, 123, 1k_2k_4)$  we have  $t_{31k_3} = t_{13k_4} = 0$ . Furthermore, we have  $t_{32k_3} = t_{23k_4} = 0$  by  $ct_8^{(2)}(123, 123, 1k_2k_3k_4)$  and  $ct_8^{(3)}(123, 123, 1k_2k_3k_4)$ . Therefore, by  $ct_{444}^{(2)}(123, 123, 1k_2k_3k_4)$ ,  $t_{231} = 0$  or  $t_{321} = 0$  and thus

$$(t_{..1}; t_{..k_2}; t_{..k_3}; t_{..k_4}) = \begin{pmatrix} 0+0 & +\cdot\cdot & 0\cdot+ & 0\cdot 0 \\ +\cdot\cdot & \cdot 00 & \cdot +\cdot & \cdot +0 \\ 0\cdot 0 & \cdot 0+ & 00\cdot & +\cdot\cdot \end{pmatrix}.$$

is  $K$ -subordinate to a table of type (3d) or (3e). By Lemma 9, the table  $t$  is also  $K$ -subordinate to a table of type (3d) or (3e).  $\square$

Theorems 2 and 4 come directly as corollaries of the following theorem.

**Theorem 9.** *Let  $i_0 = j_0 = k_0 = 1$ . Let  $t$  be a  $3 \times 3 \times K$  table with  $t_{i_0j_0k_0} = 0$ . Suppose that  $t_{211}, t_{121}, t_{112} > 0$ . Then the following conditions are equivalent.*

1.  $t$  is not  $K$ -subordinate to a table of type (2a)–(3e).
2.  $t \geq N$  for some  $N \in \mathfrak{N}(i_0, j_0, k_0)$ .
3.  $t \in \Phi(3, 3, K; i_0, j_0, k_0)$ .

*Proof.* It is easy to see that (2)  $\Rightarrow$  (3) by Lemma 4. It follows from Theorem 8 that (1)  $\Rightarrow$  (2). Hence, we show that (3)  $\Rightarrow$  (1). Suppose that  $t$  is  $K$ -subordinate to a  $3 \times 3 \times K'$  table  $t'$  of type (2a)–(3e). Let  $f: \{1, 2, \dots, K\} \rightarrow \{1, 2, \dots, K'\}$  be a map such that  $f(1) = 1$  and for  $1 \leq k \leq K$ ,  $t_{..k} \leq t'_{..f(k)}$ . For a  $3 \times 3 \times K$  table  $m$ , we take a  $3 \times 3 \times K'$  table

$$g(m) = \left( \sum_{k \in f^{-1}(1)} m_{..k}; \sum_{k \in f^{-1}(2)} m_{..k}; \dots; \sum_{k \in f^{-1}(K')} m_{..k} \right),$$

where we assume that  $\sum_{k \in f^{-1}(k')} m_{..k}$  is the zero matrix if  $f^{-1}(k')$  is empty. Suppose to the contrary that there is a sequence  $m_1, m_2, \dots, m_r$  of basis moves which connects from  $t$  to  $t'' := t + m_1 + \dots + m_r \in \mathcal{F}(t)$  with  $t''_{111} > 0$ . Then the sequence  $g(m_1), \dots, g(m_r)$  of moves is a path connecting from  $g(t)$  to  $g(t'') \in \mathcal{F}(g(t))$  with  $g(t'')_{111} > 0$  and hence  $g(t) \in \Phi(3, 3, K'; 1, 1, 1)$ . It is a contradiction by Corollary 1 and Lemma 3, since  $g(t)$  is a table of type (2a)–(3e). Therefore,  $t \notin \Phi(3, 3, K; 1, 1, 1)$ .  $\square$

*Proof of Theorem 3.* The set  $\mathfrak{N}(i_0, j_0, k_0)$  is obtained from  $\mathfrak{N}(1, 1, 1)$ , if necessary, by exchanging  $1 \leftrightarrow i_0$ ,  $1 \leftrightarrow j_0$ , and  $1 \leftrightarrow k_0$ . Then it suffices to show the claim for  $\mathfrak{N}(1, 1, 1)$ .

Let  $N \in \mathfrak{N}(1, 1, 1)$ . If  $N = m^-$  for a move  $m$  of a minimal Markov basis, then  $N$  is an indispensable table for the  $(1, 1, 1)$ -element by Lemma 2. Suppose that  $N$  is the other type. Let  $t = t(i, j, k)$  be a table made from  $N$  by changing the value of one positive  $(p, q, r)$ -element of  $N$  to 0. We straightforwardly see that  $\sum_{i=1}^3 t_{i11} = 0$ ,  $\sum_{j=1}^3 t_{1j1} = 0$ ,  $\sum_{k=1}^K t_{11k} = 0$ , or  $t$  is  $K$ -subordinate to a table of type (2a)–(3e). Thus if  $N \geq t$  and  $N \neq t$  then  $t \notin \Phi(3, 3, K; 1, 1, 1)$  and so  $N$  is an indispensable table for the  $(1, 1, 1)$ -element. Therefore  $\mathfrak{N}(1, 1, 1)$  is minimal.

We show the uniqueness. Suppose there is another minimal set  $\mathfrak{N}'(1, 1, 1)$ . Take a table  $t \in \mathfrak{N}(1, 1, 1) \setminus \mathfrak{N}'(1, 1, 1)$ . Since  $t \in \Phi(3, 3, K; 1, 1, 1)$ , there is a table  $t' \in \mathfrak{N}'(1, 1, 1)$  such that  $t \geq t'$ . Noting  $t \neq t'$ ,  $t' \notin \Phi(3, 3, K; 1, 1, 1)$  by minimality of  $\mathfrak{N}(1, 1, 1)$ , which is a contradiction. Therefore  $\mathfrak{N}(1, 1, 1)$  is unique.  $\square$

Since every element of any table of  $\Phi(3, 3, K; i_0, j_0, k_0)$  has 0 or 1, we get the following theorem.

**Theorem 10.** *Let  $t \in \Omega(3, 3, K)$ . Let  $t'$  be a contingency table made by  $t'_{ijk} = 1$  if  $t_{ijk} > 0$  and  $t'_{ijk} = 0$  otherwise. Then  $t \in \Phi(3, 3, K; i_0, j_0, k_0)$  if and only if  $t' \in \Phi(3, 3, K; i_0, j_0, k_0)$ .*

We generalize Theorem 1 as follows.

**Theorem 11.** *Let  $K \geq 2$  and let  $s = (s_{ijk})$  and  $t = (t_{ijk})$  be  $3 \times 3 \times K$  contingency tables. Suppose that  $t$  is obtained from  $s$  simply by adding one at  $(i_0, j_0, k_0)$ . Then,  $\mathcal{F}(t) = \{u - s + t \mid u \in \mathcal{F}(s)\} \cup \{u - s + t - m \mid u \in \mathcal{F}(s) \text{ with } u_{i_0 j_0 k_0} = 0, m \in \mathfrak{M}(i_0, j_0, k_0)\}$ .*

*Proof.* Let  $\varphi: \mathcal{F}(s) \rightarrow \mathcal{F}(t)$  be a map defined as  $\varphi(u) = u - s + t$ . Then,  $\varphi(\mathcal{F}(s))$  is a subset of  $\mathcal{F}(t)$ . It suffices to see that there exist  $u \in \mathcal{F}(s)$  and  $m \in \mathfrak{M}(i_0, j_0, k_0)$  such that  $u_{i_0 j_0 k_0} = 0$  and  $\varphi(u) - m = v$  for each  $v \in \mathcal{F}(t) \setminus \varphi(\mathcal{F}(s))$ . Let  $v \in \mathcal{F}(t) \setminus \varphi(\mathcal{F}(s))$ . Then,  $v \in \Phi(3, 3, K; i_0, j_0, k_0)$  and in particular,  $v_{i_0 j_0 k_0} = 0$ . By Theorem 2 or Theorem 9, there exists a move  $m \in \mathfrak{M}(i_0, j_0, k_0)$  such that  $v \geq m^-$ . Then  $v + m = (v - m^-) + m^+ \in \Omega(3, 3, K)$  and  $v + m \in \varphi(\mathcal{F}(s))$  since  $(v + m)_{i_0 j_0 k_0} = 1$ . Therefore, putting  $u = v + m + s - t$ , we have  $\varphi(u) = v + m$  and  $u_{i_0 j_0 k_0} = 0$  follows from  $(v + m)_{i_0 j_0 k_0} = 1$ .  $\square$

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