Minimal basis for connected Markov chain over $3 \times 3 \times K$ contingency tables with fixed two-dimensional marginals

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SUMMARY

We consider connected Markov chain for sampling $3 \times 3 \times K$ contingency tables having fixed two-dimensional marginal totals. Such sampling arises in performing various tests of the hypothesis of no three-factor interactions. Markov chain algorithm is a valuable tool for evaluating p values, especially for sparse data sets where large-sample theory does not work well. For constructing a connected Markov chain over high dimensional contingency tables with fixed marginals, algebraic algorithms were proposed by Diaconis and Sturmfels (1998). Their algorithms involve computations in polynomial rings using Gröbner bases. However, algorithms based on Gröbner bases do not incorporate symmetry among variables and are very time consuming when the size of contingency tables is large. We construct a minimal basis for connected Markov chain over $3 \times 3 \times K$ contingency tables. Some numerical examples are also given to illustrate the practicality of our algorithms.

Keywords: Conditional inference, Contingency tables, Markov chain Monte Carlo.

1 Introduction

Markov chain over three-way contingency tables with fixed two-dimensional marginals arises in carrying out various tests for the hypothesis that there is no three-factor interaction in the log-linear model expressed as

$$p_{ijk} = \psi_{ij}\phi_{jk}\omega_{ik},$$

where p_{ijk} is a cell probability. By elementary arguments, we give an explicit form of a minimal basis for connected Markov chain over $3 \times 3 \times K$ contingency tables. Although our results are restricted to the $3 \times 3 \times K$ case, they have merits because at the present no general theory or algorithm seems to be known for obtaining a minimal basis.

For illustrating the problem, first consider a simpler case of generating two-way contingency tables with fixed row and column totals. Let $\mathbb{N} = \{0, 1, 2, \ldots\}$ and let $\boldsymbol{X}$ be an $I \times J$ contingency table with entries $x_{ij} \in \mathbb{N},\ i = 1, \ldots, I,\ j = 1, \ldots, J$. Let

$$\mathcal{F}(\{x_{i\cdot}, x_{\cdot j}\}) = \left\{ \boldsymbol{Y} \ \middle|\ \sum_{j=1}^{J} y_{ij} = x_{i\cdot}, \sum_{i=1}^{I} y_{ij} = x_{\cdot j},\ y_{ij} \in \mathbb{N} \right\}$$

denote the reference set of all $I \times J$ contingency tables with the same marginal totals as $\boldsymbol{X}$. Under the hypothesis of statistical independence (i.e. $p_{ij} = p_{i\cdot}p_{\cdot j}$), the sufficient statistics are the row and column sums, $x_{i\cdot}, x_{\cdot j},\ i = 1, \dots, I,\ j = 1, \dots, J$. The hypergeometric distribution on $\mathcal{F}(\{x_{i\cdot}, x_{\cdot j}\})$

$$H(\boldsymbol{X}) = \prod_{j=1}^{J} \binom{x_{\cdot j}}{x_{1j}, \dots, x_{Ij}} \Big/ \binom{x_{\cdot\cdot}}{x_{1\cdot}, \dots, x_{I\cdot}}$$

is the conditional distribution of X, given the sufficient statistics (for details, see Plackett, 1981, or Agresti, 1990, for examples). To test the hypothesis of independence, one approach is to generate samples from $H(\boldsymbol{X})$ and calculate the null distribution of various test statistics. If a connected Markov chain on $\mathcal{F}(\{x_{i\cdot}, x_{\cdot j}\})$ is constructed, the chain can be modified to give a connected and aperiodic Markov chain with stationary distribution $H(\boldsymbol{X})$ by the usual Metropolis procedure (Hastings, 1970, for example). In the cases of two-dimensional tables, a connected Markov chain on $\mathcal{F}(\{x_{i\cdot}, x_{\cdot j}\})$ is easily constructed as follows. Let $\boldsymbol{X}$ be the current state in $\mathcal{F}(\{x_{i\cdot}, x_{\cdot j}\})$. The next state is selected by choosing a pair of rows and a pair of columns at random, and modifying $\boldsymbol{X}$ at the four entries where the selected rows and columns intersect as

$$\begin{matrix} + & - \\ - & + \end{matrix} \quad \text{or} \quad \begin{matrix} - & + \\ + & - \end{matrix} \quad \text{with probability } \frac{1}{2} \text{ each.} \tag{1}$$

The modification adds or subtracts 1 from each of the four entries, keeping the row and column sums. If the modification forces negative entries, discard it and continue by choosing a new pairs of rows and columns. Hereafter we call $\begin{matrix} + & - \\ - & + \end{matrix}$ (two-dimensional) *rectangles* or rectangular moves. We give a precise definition of rectangles in Section 3.

Extending the above approach, now consider the three-way case. Let $\boldsymbol{X}$ be an $I \times J \times K$ contingency table with entries $x_{ijk} \in \mathbb{N},\ i = 1, \dots, I,\ j = 1, \dots, J,\ k = 1, \dots, K$. The reference set is now defined as

$$\mathcal{F}(\{x_{ij\cdot}, x_{i\cdot k}, x_{\cdot jk}\}) = \left\{ \boldsymbol{Y} \;\middle|\; \sum_{k=1}^{K} y_{ijk} = x_{ij\cdot},\ \sum_{j=1}^{J} y_{ijk} = x_{i\cdot k},\ \sum_{i=I}^{J} y_{ijk} = x_{\cdot jk},\ y_{ijk} \in \mathbb{N} \right\}$$

and our aim is to construct a connected Markov chain over $\mathcal{F}(\{x_{ij\cdot}, x_{i\cdot k}, x_{\cdot jk}\})$. The simple analogue of rectangles in (1) is the eight entries move:

$$\begin{array}{ccc} \multicolumn{3}{l}{i = i_1} \\ j \backslash k & k_1 & k_2 \\ j_1 & +1 & -1 \\ j_2 & -1 & +1 \end{array} \qquad \begin{array}{ccc} \multicolumn{3}{l}{i = i_2} \\ j \backslash k & k_1 & k_2 \\ j_1 & -1 & +1 \\ j_2 & +1 & -1 \end{array} \tag{2}$$

However, a chain constructed from this type of moves is known to be not connected. As an example, consider $3 \times 3 \times 3$ contingency tables having two-dimensional marginals as

$$x_{ij\cdot} = x_{i\cdot k} = x_{\cdot jk} = 2 \quad \text{for all } \ 1 \le i, j, k \le 3.$$

There are 132 states in $\mathcal{F}(\{x_{ij\cdot}, x_{i\cdot k}, x_{\cdot jk}\})$ in this case, but states such as

$$\boxed{\begin{matrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{matrix}} \qquad \boxed{\begin{matrix} 0 & 2 & 0 \\ 0 & 0 & 2 \\ 2 & 0 & 0 \end{matrix}} \qquad \boxed{\begin{matrix} 0 & 0 & 2 \\ 2 & 0 & 0 \\ 0 & 2 & 0 \end{matrix}}$$

are not connected to any other states in $\mathcal{F}(\{x_{ij\cdot}, x_{i\cdot k}, x_{\cdot jk}\})$ by the eight entries moves described in (2), i.e., none of the eight entry moves can be added to this table without causing negative entries.

Markov chain Monte Carlo approach is extensively used in various two-way settings, for example, Besag and Clifford (1989) for performing significance tests for the Ising model (two-way binary tables); Smith *et al.* (1996) for tests of independence, quasi-independence and quasi-symmetry for square two-way contingency tables; Guo and Thompson (1992) for exact tests of Hardy-Weinberg proportions (triangular two-way contingency tables). There are also many works that discuss the convergence of the chain, for example, Diaconis and Saloff-Coste (1995) for two-way contingency tables; Hernek (1998), Dyer and Greenhill (2000) for $2 \times J$ contingency tables. On the other hand, there are only a few works dealing with high dimensional tables except for the simple case of 2^d tables, for example, Forster *et al.* (1996).

Diaconis and Sturmfels (1998) proposed algebraic algorithms for finding a set of moves for constructing a connected Markov chain over higher dimensional contingency tables in the framework of general discrete exponential families. Their algorithms involve computations in polynomial rings using Gröbner bases. However, algorithms based on Gröbner bases do not incorporate symmetry among variables and are very time consuming when the size of contingency tables is large. For example, their algorithm involves computation of polynomials of 54 variables for $3 \times 3 \times 3$ case, and of 112 variables for $4 \times 4 \times 4$ case. Moreover, many superfluous outputs are produced by their algorithm. In their paper they reported that the reduced Gröbner basis for the $3 \times 3 \times 3$ case contains moves of the form

$$\boxed{\begin{array}{ccc} 0 & 0 & 0 \\ 0 & -1 & +1 \\ 0 & +1 & -1 \end{array}} \quad \boxed{\begin{array}{ccc} +1 & 0 & -1 \\ -1 & +1 & 0 \\ 0 & -1 & +1 \end{array}} \quad \boxed{\begin{array}{ccc} -1 & 0 & +1 \\ +1 & 0 & -1 \\ 0 & 0 & 0 \end{array}} \tag{3}$$

and

$$\boxed{\begin{array}{ccc} -2 & +1 & +1 \\ +1 & 0 & -1 \\ +1 & -1 & 0 \end{array}} \quad \boxed{\begin{array}{ccc} +1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & +1 \end{array}} \quad \boxed{\begin{array}{ccc} +1 & -1 & 0 \\ -1 & 0 & +1 \\ 0 & +1 & -1 \end{array}} \ . \tag{4}$$

However, as remarked by Diaconis and Sturmfels, the moves of the above types are not essential in view of the connectedness of the chain. This corresponds to the notion of minimality of Markov basis as defined below. We will discuss these moves after Theorem 1 in Section 2.2.

Here we give a definition of *Markov basis* and its *minimality* as introduced in Diaconis and Sturmfels (1998). Let $\mathcal{F}_0$ be the set of $I \times J \times K$ contingency tables with zero two-way marginal totals

$$\mathcal{F}_0 = \left\{ \boldsymbol{Y} \;\middle|\; \sum_{k=1}^{K} y_{ijk} = \sum_{j=1}^{J} y_{ijk} = \sum_{i=I}^{J} y_{ijk} = 0, \; y_{ijk} \in \mathbb{Z} \right\},$$

where $\mathbb{Z}$ denotes the set of integers. We call elements of $\mathcal{F}_0$ *moves.*

Definition 1 *A Markov basis is a set $\mathcal{B} = \{\boldsymbol{B}_1, \ldots, \boldsymbol{B}_L\}$ of $I \times J \times K$ contingency tables $\boldsymbol{B}_i \in \mathcal{F}_0$, $i = 1 \ldots, L$, such that, for any $\{x_{ij\cdot}, x_{i\cdot k}, x_{\cdot jk}\}$ and $\boldsymbol{X}, \boldsymbol{X}' \in \mathcal{F}(\{x_{ij\cdot}, x_{i\cdot k}, x_{\cdot jk}\})$, there exist $A > 0$, $(\varepsilon_1, \boldsymbol{B}_{t_1}), \ldots, (\varepsilon_A, \boldsymbol{B}_{t_A})$ with $\varepsilon_s = \pm 1$, such that*

$$\boldsymbol{X}' = \boldsymbol{X} + \sum_{s=1}^{A} \varepsilon_s \boldsymbol{B}_{t_s} \quad \textit{and} \quad \boldsymbol{X} + \sum_{s=1}^{a} \varepsilon_s \boldsymbol{B}_{t_s} \in \mathcal{F}(\{x_{ij\cdot}, x_{i\cdot k}, x_{\cdot jk}\}) \;\; \textit{for} \; 1 \le a \le A.$$

A Markov basis $\mathcal{B}$ is minimal if no proper subset of $\mathcal{B}$ is a Markov basis.

If a Markov basis is obtained, a connected Markov chain over $\mathcal{F}(\{x_{ij\cdot}, x_{i\cdot k}, x_{\cdot jk}\})$ is easily constructed. For general $I \times J \times K$ case, a closed form expression of Markov basis is very complicated, except for the case of $\min(I, J, K) = 2$ (see section 4 of Diaconis and Sturmfels, 1998). In this paper, as the next simplest case, we consider the case of $I = J = 3$. Our main contribution in this paper is to give a closed form expressions of a minimal Markov basis for $3 \times 3 \times K$ contingency tables.

The construction of this paper is as follows. Section 2 describes main results. Section 3 provides proofs of the theorems. Some numerical examples are given to illustrate the practicality of our algorithms in Section 4. In Section 5 we give some discussions and considerations of higher order tables.

2 Representation of a minimal Markov basis for $3 \times 3 \times K$ tables

In this section, we derive a closed form expression of a minimal Markov basis for $3 \times 3 \times K$ tables. Theorem 1 gives a minimal basis for the $3 \times 3 \times 3$ case. Theorem 2 is for the $3 \times 3 \times 4$ case, Theorem 3 is for the $3 \times 3 \times 5$ case, and finally our main result in Theorem 4 gives a a minimal basis for the $3 \times 3 \times K$ case. Proofs of these theorems are postponed to the next section.

We define the *degree* of $\boldsymbol{B} \in \mathcal{F}_0$ in the following sense according to Diaconis and Sturmfels (1998). Write $\boldsymbol{B} = \boldsymbol{B}^+ - \boldsymbol{B}^-$ where $\boldsymbol{B}^+$ and $\boldsymbol{B}^-$ are the positive and the negative part of $\boldsymbol{B}$ having the elements

$$b_{ijk}^+ = \max(b_{ijk}, 0), \quad b_{ijk}^- = \max(-b_{ijk}, 0)$$

and define

$$\deg \boldsymbol{B} = \sum_{i,j,k} b_{ijk}^+ = \sum_{i,j,k} b_{ijk}^-.$$

For an $I \times J \times K$ contingency table $\boldsymbol{Y} = \{y_{ijk}\}$, *i-slice* (or $i = i_0$ slice) of $\boldsymbol{Y}$ is the two-dimensional slice $\{y_{i_0 jk}\}_{1 \le j \le J,\ 1 \le k \le K}$, where $i = i_0$ is fixed. We similarly define j-slice and k-slice. To display $3 \times 3 \times K$ contingency tables, we write three i-slices of size $3 \times K$ as follows:

$$
\begin{array}{ll}
i=1 & \\
j \backslash k & 1 \ \cdots \ K \\
1 & \\
2 & \\
3 &
\end{array}
\qquad
\begin{array}{ll}
i=2 & \\
j \backslash k & 1 \ \cdots \ K \\
1 & \\
2 & \\
3 &
\end{array}
\qquad
\begin{array}{ll}
i=3 & \\
j \backslash k & 1 \ \cdots \ K \\
1 & \\
2 & \\
3 &
\end{array}
$$

In the following, we assume that the level indices $i_1, i_2, \ldots,\ j_1, j_2, \ldots$ and $k_1, k_2, \ldots,$ are all distinct, i.e.,

$$i_m \neq i_n,\ j_m \neq j_n,\ k_m \neq k_n,\ \text{for all } m \neq n.$$

2.1 Moves of degree 4 (basic moves)

First we define the most elemental eight entries move that is already discussed in (2).

Definition 2 *A move of degree 4 is a* $3\times3\times K$ *contingency table* $\boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_2) \in \mathcal{F}_0,\ 1 \le i_1, i_2, j_1, j_2 \le 3,\ 1 \le k_1, k_2 \le K$*, where* $\boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_2)$ *has the elements*

$$m_{i_1j_1k_1} = m_{i_1j_2k_2} = m_{i_2j_1k_2} = m_{i_2j_2k_1} = 1,$$

$$m_{i_1j_1k_2} = m_{i_1j_2k_1} = m_{i_2j_1k_1} = m_{i_2j_2k_2} = -1,$$

and all the other elements are zero.

We call this move *basic move*. For example,

$$\boxed{\begin{array}{cccc} +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}} \qquad \boxed{\begin{array}{cccc} -1 & +1 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}} \qquad \boxed{\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}}$$

is a basic move expressed as $\boldsymbol{M}_4(12, 12, 12)$ for the $3\times3\times4$ case. Figure 1 gives a 3-dimensional view of the basic move.

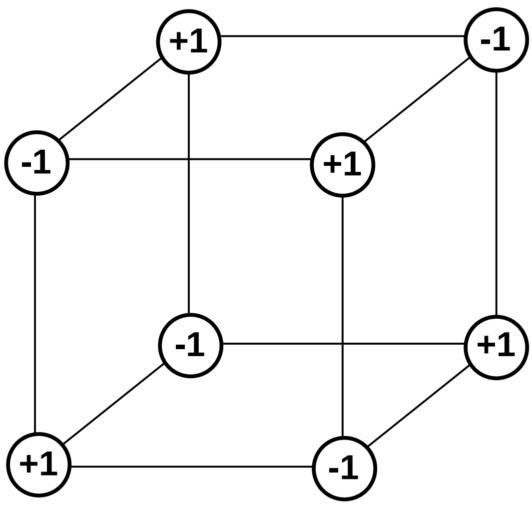

Figure 1: Basic move

From the definition,

$$M_4(i_1i_2, j_1j_2, k_1k_2) = M_4(i_1i_2, j_2j_1, k_2k_1) = M_4(i_2i_1, j_1j_2, k_2k_1)$$

and

$$M_4(i_1i_2, j_1j_2, k_1k_2) = -M_4(i_2i_1, j_1j_2, k_1k_2)$$

are derived. Using these relations repeatedly, we see that eight expressions;

$$\begin{array}{cccc} M_4(i_1i_2, j_1j_2, k_1k_2), & M_4(i_1i_2, j_2j_1, k_2k_1), & M_4(i_2i_1, j_1j_2, k_2k_1), & M_4(i_2i_1, j_2j_1, k_1k_2), \\ -M_4(i_2i_1, j_1j_2, k_1k_2), & -M_4(i_1i_2, j_2j_1, k_1k_2), & -M_4(i_1i_2, j_1j_2, k_2k_1), & -M_4(i_2i_1, j_2j_1, k_2k_1) \end{array}$$

are equivalent. Hence, for $3 \times 3 \times K$ case, there are

$$\binom{3}{2}\binom{3}{2}\binom{K}{2} = 9\binom{K}{2}$$

different basic moves, if the signs are ignored (i.e. we identify $-\boldsymbol{M}_4(12,12,12)$ with $\boldsymbol{M}_4(12,12,12)$).

The moves of degree 4 are the most elemental moves in the sense that all the other moves of larger degree in $\mathcal{F}_0$ are written as linear combinations of degree 4 moves with integral coefficients.

2.2 Moves of degree 6

As we have seen in Section 1, a connected Markov chain cannot be constructed by the set of basic moves alone for the case of $\min(I,J,K) \geq 3$. Here we consider patterns of moves that are composed of two basic moves.

As preparations, we provide a complete list of the patterns that are obtained by the sum of two overlapping basic moves. For two basic moves, $\boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_2)$, $\boldsymbol{M}_4(i'_1i'_2, j'_1j'_2, k'_1k'_2)$, we define

$$\begin{aligned}
\delta_I &= \delta_{i_1i'_1} + \delta_{i_1i'_2} + \delta_{i_2i'_1} + \delta_{i_2i'_2},\\
\delta_J &= \delta_{j_1j'_1} + \delta_{j_1j'_2} + \delta_{j_2j'_1} + \delta_{j_2j'_2},\\
\delta_K &= \delta_{k_1k'_1} + \delta_{k_1k'_2} + \delta_{k_2k'_1} + \delta_{k_2k'_2},\\
\delta &= \delta_I + \delta_J + \delta_K.
\end{aligned}$$

Since two moves are overlapping we have $\delta_I, \delta_J, \delta_K \geq 1$. Furthermore $\delta_I \leq 2$, because $i_1 \neq i_2$, $i'_1 \neq i'_2$. Similarly $\delta_J, \delta_K \leq 2$. Therefore $\delta \in \{3,4,5,6\}$. Corresponding to the values of δ, all the patterns are classified as follows.

- Case of $\delta = 3$:
  $\boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_2)$ and $\boldsymbol{M}_4(i'_1i'_2, j'_1j'_2, k'_1k'_2)$ overlap at one nonzero entry. We call this case *combination of type 1* or *type 1 combination*. If the signs of this overlapped cell are opposite, a move of degree 7 is obtained. Figure 2 gives a 3-dimensional view of this type of move. Note that (3) in Section 1 is this type of move.

- Case of $\delta = 4$:
  $\boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_2)$ and $\boldsymbol{M}_4(i'_1i'_2, j'_1j'_2, k'_1k'_2)$ overlap at two nonzero entries. We call this case *combination of type 2* or *type 2 combination*. If the pairs of signs of these two cells are opposite, a move of degree 6 is obtained. Figure 3 gives a 3-dimensional view of this type of move.

- Case of $\delta = 5$:
  $\boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_2)$ and $\boldsymbol{M}_4(i'_1i'_2, j'_1j'_2, k'_1k'_2)$ overlap at four nonzero entries along a two-dimensional rectangle. If all the pairs of signs are canceled, a basic move is obtained again as

$$\left.\begin{aligned}
\boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_2) &= \boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_3) + \boldsymbol{M}_4(i_1i_2, j_1j_2, k_3k_2)\\
&= \boldsymbol{M}_4(i_1i_2, j_1j_3, k_1k_2) + \boldsymbol{M}_4(i_1i_2, j_3j_2, k_1k_2)\\
&= \boldsymbol{M}_4(i_1i_3, j_1j_2, k_1k_2) + \boldsymbol{M}_4(i_3i_2, j_1j_2, k_1k_2).
\end{aligned}\right\} \quad (5)$$

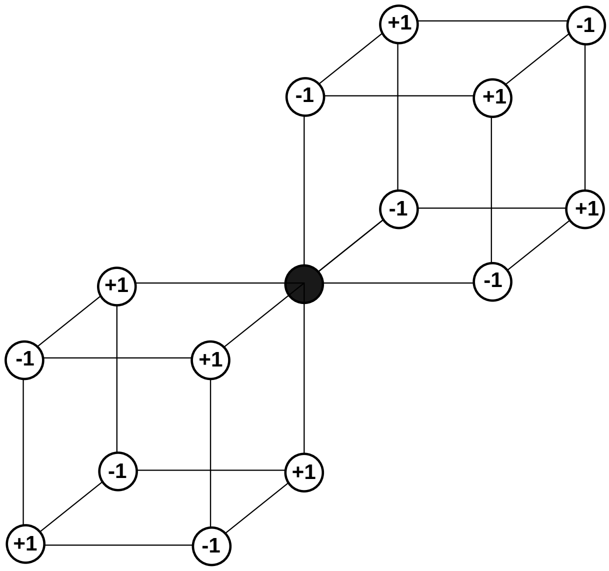

Figure 2: $3 \times 3 \times 3$ move of degree 7

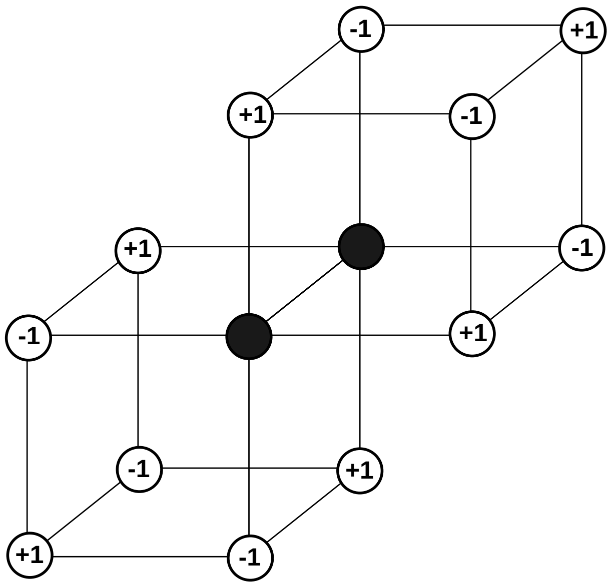

Figure 3: $2 \times 3 \times 3$ move of degree 6

- Case of $\delta = 6$:
  $\boldsymbol{M}_4(i_1 i_2, j_1 j_2, k_1 k_2)$ and $\boldsymbol{M}_4(i'_1 i'_2, j'_1 j'_2, k'_1 k'_2)$ overlap completely.

The relation (5) suggests the difficulty of the concept of decomposing a larger move into several basic moves. If we call a move of degree 6 or 7 as a "two step move", it means that *at least two* basic moves are needed to construct these moves. Among the above list, combination of type 2 is the most important case from the viewpoint of a connected Markov chain. We discuss it in the next definition and in Theorem 1 below.

Definition 3 *A move of degree 6 is a* $3 \times 3 \times K$ *contingency table* $\boldsymbol{M}_6^I(i_1 i_2, j_1 j_2 j_3, k_1 k_2 k_3) \in \mathcal{F}_0,\ 1 \le i_1, i_2, i_3, j_1, j_2, j_3 \le 3,\ 1 \le k_1, k_2, k_3 \le K$ *with elements*

$$
\begin{aligned}
m_{i_1 j_1 k_1} = m_{i_1 j_2 k_2} = m_{i_1 j_3 k_3} = m_{i_2 j_1 k_2} = m_{i_2 j_2 k_3} = m_{i_2 j_3 k_1} = 1, \\
m_{i_1 j_1 k_2} = m_{i_1 j_2 k_3} = m_{i_1 j_3 k_1} = m_{i_2 j_1 k_1} = m_{i_2 j_2 k_2} = m_{i_2 j_3 k_3} = -1,
\end{aligned}
$$

and all the other elements are zero. $\boldsymbol{M}_6^J(i_1 i_2 i_3, j_1 j_2, k_1 k_2 k_3)$ *and* $\boldsymbol{M}_6^K(i_1 i_2 i_3, j_1 j_2 j_3, k_1 k_2)$ *are defined similarly.*

Examples for the $3 \times 3 \times 4$ case are displayed as follows.

$$
\boldsymbol{M}_6^I(12, 123, 123): \quad
\begin{array}{|cccc|}\hline +1 & -1 & 0 & 0 \\ 0 & +1 & -1 & 0 \\ -1 & 0 & +1 & 0 \\ \hline\end{array}
\quad
\begin{array}{|cccc|}\hline -1 & +1 & 0 & 0 \\ 0 & -1 & +1 & 0 \\ +1 & 0 & -1 & 0 \\ \hline\end{array}
\quad
\begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array}
$$

$$
\boldsymbol{M}_6^J(123, 12, 123): \quad
\begin{array}{|cccc|}\hline +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array}
\quad
\begin{array}{|cccc|}\hline 0 & +1 & -1 & 0 \\ 0 & -1 & +1 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array}
\quad
\begin{array}{|cccc|}\hline -1 & 0 & +1 & 0 \\ +1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array}
$$

$$
\boldsymbol{M}_6^K(123, 123, 12): \quad
\begin{array}{|cccc|}\hline +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array}
\quad
\begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ \hline\end{array}
\quad
\begin{array}{|cccc|}\hline -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ \hline\end{array}
$$

Similar to the basic move, the relations

$$
\boldsymbol{M}_6^I(i_1 i_2, j_1 j_2 j_3, k_1 k_2 k_3) = \boldsymbol{M}_6^I(i_1 i_2, j_2 j_3 j_1, k_2 k_3 k_1) = \boldsymbol{M}_6^I(i_2 i_1, j_1 j_3 j_2, k_2 k_1 k_3),
$$

$$
\boldsymbol{M}_6^I(i_1 i_2, j_1 j_2 j_3, k_1 k_2 k_3) = -\boldsymbol{M}_6^I(i_2 i_1, j_1 j_2 j_3, k_1 k_2 k_3),
$$

and similar relations for $\boldsymbol{M}_6^J(i_1 i_2 i_3, j_1 j_2, k_1 k_2 k_3)$ and $\boldsymbol{M}_6^K(i_1 i_2 i_3, j_1 j_2 j_3, k_1 k_2)$ are derived from the definition. Using these relations repeatedly, we see that the 12 expressions,

$$
\begin{array}{ccc}
\boldsymbol{M}_6^I(i_1 i_2, j_1 j_2 j_3, k_1 k_2 k_3), & \boldsymbol{M}_6^I(i_1 i_2, j_2 j_3 j_1, k_2 k_3 k_1), & \boldsymbol{M}_6^I(i_1 i_2, j_3 j_1 j_2, k_3 k_1 k_2), \\
\boldsymbol{M}_6^I(i_2 i_1, j_1 j_3 j_2, k_2 k_1 k_3), & \boldsymbol{M}_6^I(i_2 i_1, j_2 j_1 j_3, k_3 k_2 k_1), & \boldsymbol{M}_6^I(i_2 i_1, j_3 j_2 j_1, k_1 k_3 k_2), \\
-\boldsymbol{M}_6^I(i_2 i_1, j_1 j_2 j_3, k_1 k_2 k_3), & -\boldsymbol{M}_6^I(i_2 i_1, j_2 j_3 j_1, k_2 k_3 k_1), & -\boldsymbol{M}_6^I(i_2 i_1, j_3 j_1 j_2, k_3 k_1 k_2), \\
-\boldsymbol{M}_6^I(i_1 i_2, j_1 j_3 j_2, k_2 k_1 k_3), & -\boldsymbol{M}_6^I(i_1 i_2, j_2 j_1 j_3, k_3 k_2 k_1), & -\boldsymbol{M}_6^I(i_1 i_2, j_3 j_2 j_1, k_1 k_3 k_2)
\end{array}
$$

are equivalent, for example. Hence for $3 \times 3 \times K$ case, there are

$$
\left\{ \binom{3}{2}\binom{3}{3}\binom{K}{3} + \binom{3}{3}\binom{3}{2}\binom{K}{3} + \binom{3}{3}\binom{3}{3}\binom{K}{2} \right\} \times 3! = 3K(K-1)(2K-3)
$$

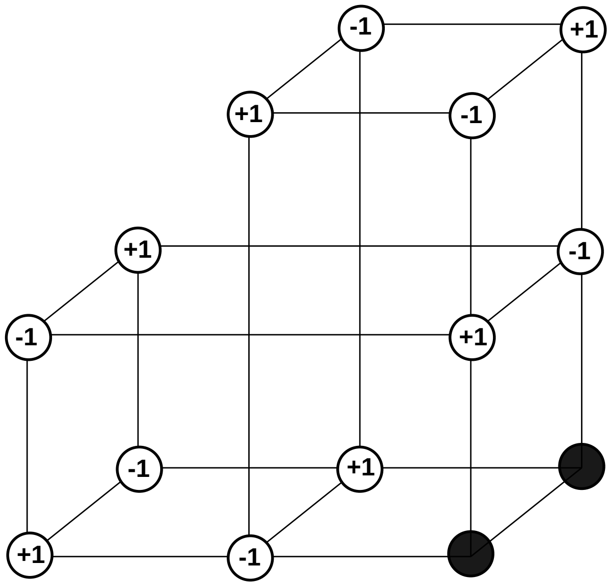

Figure 4: $2 \times 3 \times 3$ move of degree 6 (as another combination of type 2)

different moves of degree 6.

The expression of the move of degree 6 as the type 2 combination of two basic moves is not unique. Figure 4 illustrates the same move of degree 6 shown in Figure 3, but the overlapped cells of two basic moves are different. The following relations constitute a complete list of the decomposition of the move $\boldsymbol{M}_6^I(i_1i_2, j_1j_2j_3, k_1k_2k_3)$ into basic moves, with the configurations of the overlapped cells.

$$
\begin{aligned}
&\boldsymbol{M}_6^I(i_1i_2, j_1j_2j_3, k_1k_2k_3) \\
&\quad = \boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_2) + \boldsymbol{M}_4(i_1i_2, j_2j_3, k_1k_3) \quad \cdots \quad (i_1, j_2, k_1), (i_2, j_2, k_1) \\
&\quad = \boldsymbol{M}_4(i_1i_2, j_1j_2, k_3k_2) + \boldsymbol{M}_4(i_1i_2, j_1j_3, k_1k_3) \quad \cdots \quad (i_1, j_1, k_3), (i_2, j_1, k_3) \\
&\quad = \boldsymbol{M}_4(i_1i_2, j_1j_3, k_1k_2) + \boldsymbol{M}_4(i_1i_2, j_2j_3, k_2k_3) \quad \cdots \quad (i_1, j_3, k_2), (i_2, j_3, k_2).
\end{aligned}
$$

Similar decompositions can be written down for $\boldsymbol{M}_6^J(i_1i_2i_3, j_1j_2, k_1k_2k_3)$ and $\boldsymbol{M}_6^K(i_1i_2i_3, j_1j_2j_3, k_1k_2)$ by symmetry between axes.

We now give a minimal basis for connected Markov chain over $3 \times 3 \times 3$ tables.

Theorem 1 *A set of basic moves* $\boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_2)$ *and moves of degree* 6, $\boldsymbol{M}_6^I(i_1i_2, j_1j_2j_3, k_1k_2k_3)$, $\boldsymbol{M}_6^J(i_1i_2i_3, j_1j_2, k_1k_2k_3), \boldsymbol{M}_6^K(i_1i_2i_3, j_1j_2j_3, k_1k_2)$, $1 \le i_1, i_2, i_3, j_1, j_2, j_3, k_1, k_2, k_3 \le 3$ *constitute a minimal Markov basis for* $3 \times 3 \times 3$ *tables.*

This theorem shows that the move of degree 7 is not necessary to construct a connected Markov chain. To see this, consider the following two $3 \times 3 \times 3$ contingency tables.

$$
\boldsymbol{X}: \quad \begin{array}{|ccc|}\hline 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ \hline \end{array} \qquad \begin{array}{|ccc|}\hline 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccc|}\hline 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ \hline \end{array}
$$

$$
\boldsymbol{Y}: \quad \begin{array}{|ccc|}\hline 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \\ \hline\end{array}
$$

These two contingency tables are the negative part and the positive part of the move of degree 7 in (3) and mutually accessible by the move of degree 7. However, instead of adding (3) to $\boldsymbol{X}$, we can add $\boldsymbol{M}_4(23, 12, 13)$ to $\boldsymbol{X}$, and then, add $\boldsymbol{M}_4(12, 23, 32)$ to $\boldsymbol{X} + \boldsymbol{M}_4(23, 12, 13)$, to obtain $\boldsymbol{Y}$. Note that the move (3) is type 1 combination of $\boldsymbol{M}_4(23, 12, 13)$ and $\boldsymbol{M}_4(12, 23, 32)$, and $\boldsymbol{X} + \boldsymbol{M}_4(23, 12, 13)$ does not contain a negative cell, while $\boldsymbol{X} + \boldsymbol{M}_4(12, 23, 32)$ contains a negative cell $(2, 2, 3)$. Note also that $\boldsymbol{M}_4(23, 12, 13)$ and $\boldsymbol{M}_4(12, 23, 32)$ overlap at this cell. Because the two basic moves are canceling at this cell, it is obvious that at least one of these basic moves (that has $+1$ at this cell) can be added without causing negative cells.

On the other hand, because the type 2 combination has two overlapped cells, it cannot be avoided that one of these two cells becomes negative in adding basic moves one by one. For this reason, the type 2 combination is essential.

Concerning the move (4) of Section 1, it can be written as type 1 combination of a basic move and a move of degree 6

$$
\boldsymbol{M}_4(12, 13, 31) + \boldsymbol{M}_6^I(31, 132, 123)
$$

and hence is not needed by the same reason as the degree 7 move.

2.3 Moves of degree 8

The next essential move is a *three step move*. For the case of general $I \times J \times K$ contingency table, there is two types of such move. One is a $2 \times 4 \times 4$ move of degree 8 already discussed in equation (4.6) of Diaconis and Sturmfels (1998). For $3 \times 3 \times K$ case, another type of move is needed.

Definition 4 *A move of degree 8 is a $3 \times 3 \times K$ contingency table $\boldsymbol{M}_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4) \in \mathcal{F}_0$, $1 \le i_1, i_2, i_3, j_1, j_2, j_3 \le 3$, $1 \le k_1, k_2, k_3, k_4 \le K$, with the elements*

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

and all the other elements are zero.

For example, $\boldsymbol{M}_8(123, 123, 1234)$ is displayed as follows.

$$
\begin{array}{|cccc|}\hline +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline -1 & 0 & +1 & 0 \\ +1 & 0 & 0 & -1 \\ 0 & 0 & -1 & +1 \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0 & +1 & -1 & 0 \\ 0 & -1 & 0 & +1 \\ 0 & 0 & +1 & -1 \\ \hline\end{array}
$$

Figure 5 gives a 3-dimensional view of this type of move.

From the definition, the relations

$$
\boldsymbol{M}_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4) = \boldsymbol{M}_8(i_1i_3i_2, j_2j_1j_3, k_2k_1k_4k_3) = -\boldsymbol{M}_8(i_1i_3i_2, j_1j_2j_3, k_2k_1k_3k_4)
$$

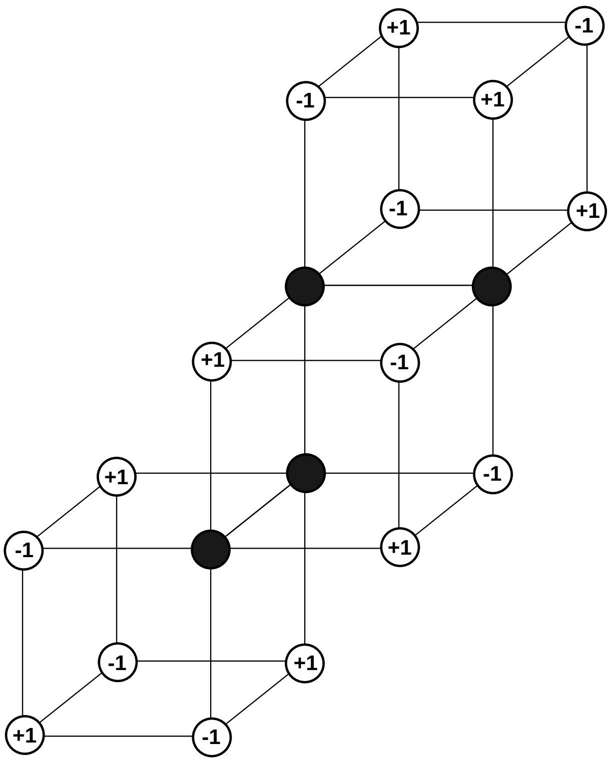

Figure 5: $3 \times 3 \times 4$ move of degree 8

are derived. Using the above relations, it follows that the four expressions

$$\begin{array}{ll} M_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4), & M_8(i_1i_3i_2, j_2j_1j_3, k_2k_1k_4k_3), \\ -M_8(i_1i_3i_2, j_1j_2j_3, k_2k_1k_3k_4), & -M_8(i_1i_2i_3, j_2j_1j_3, k_1k_2k_4k_3) \end{array}$$

are all equivalent. For example, a move

$$\begin{array}{|cccc|} \hline 0 & +1 & 0 & -1 \\ 0 & 0 & -1 & +1 \\ 0 & -1 & +1 & 0 \\ \hline \end{array} \qquad \begin{array}{|cccc|} \hline 0 & -1 & 0 & +1 \\ +1 & 0 & 0 & -1 \\ -1 & +1 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|cccc|} \hline 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 \\ +1 & 0 & -1 & 0 \\ \hline \end{array}$$

is expressed as $\boldsymbol{M}_8(312, 231, 3142)$, $\boldsymbol{M}_8(321, 321, 1324)$, $-\boldsymbol{M}_8(321, 231, 1342)$ or $-\boldsymbol{M}_8(312, 321, 3124)$. For $3 \times 3 \times K$ case, there are

$$3! \times 3! \times {}_KP_4/4 = 9K(K-1)(K-2)(K-3)$$

different moves of degree 8.

Before considering the decomposition of the move of degree 8, we state a theorem for the $3 \times 3 \times 4$ case.

Theorem 2 *A set of basic moves $\boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_2)$, moves of degree 6, $\boldsymbol{M}_6^I(i_1i_2, j_1j_2j_3, k_1k_2k_3)$, $\boldsymbol{M}_6^J(i_1i_2i_3, j_1j_2, k_1k_2k_3)$, $\boldsymbol{M}_6^K(i_1i_2i_3, j_1j_2j_3, k_1k_2)$ and moves of degree 8, $\boldsymbol{M}_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4)$), $1 \leq i_1, i_2, i_3, j_1, j_2, j_3 \leq 3, 1 \leq k_1, k_2, k_3, k_4 \leq 4$ constitute a minimal Markov basis for $3 \times 3 \times 4$ tables.*

Now consider the decomposition of the move $\boldsymbol{M}_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4)$. If this move is expressed as a sum of a basic move and the other, there are two cases:

(i) The type 2 combination of a basic move and a move of degree 6

(ii) The type 3 combination of a basic move and a move of degree 7.

Here the term *type 3 combination* means that two moves overlap in three cells. Note that the above theorem implies that the move of degree 8 cannot be expressed as the type 1 combination of a basic move and another move in view of the minimality. As we have seen the move of degree 7 is not essential. Hence we only consider (i) in this paper.

The basic move that we consider, i.e., the basic move that overlaps the move of degree 6 in two cells, has six cells in common with the move of degree 8. These six cells are two 2×2 rectangles that intersect at the right angle. In $\boldsymbol{M}_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4)$, there are six 2×2 rectangles

$$\begin{array}{l}
(i_1,j_1,k_1),(i_1,j_1,k_2),(i_1,j_2,k_2),(i_1,j_2,k_2)\\
(i_1,j_1,k_1),(i_2,j_1,k_1),(i_2,j_2,k_1),(i_1,j_2,k_1)\\
(i_1,j_2,k_2),(i_1,j_1,k_2),(i_3,j_1,k_2),(i_3,j_2,k_2)\\
(i_2,j_1,k_3),(i_2,j_3,k_3),(i_3,j_3,k_3),(i_3,j_1,k_3)\\
(i_2,j_3,k_4),(i_2,j_2,k_4),(i_3,j_2,k_4),(i_3,j_3,k_4)\\
(i_2,j_3,k_4),(i_2,j_3,k_3),(i_3,j_3,k_3),(i_3,j_3,k_4),
\end{array}$$

and among these, four pairs

$$\begin{array}{lcl}
(i_1,j_1,k_1),(i_1,j_1,k_2),(i_1,j_2,k_2),(i_1,j_2,k_2) & \perp & (i_1,j_1,k_1),(i_2,j_1,k_1),(i_2,j_2,k_1),(i_1,j_2,k_1)\\
(i_1,j_1,k_1),(i_1,j_1,k_2),(i_1,j_2,k_2),(i_1,j_2,k_2) & \perp & (i_1,j_2,k_2),(i_1,j_1,k_2),(i_3,j_1,k_2),(i_3,j_2,k_2)\\
(i_2,j_1,k_3),(i_2,j_3,k_3),(i_3,j_3,k_3),(i_3,j_1,k_3) & \perp & (i_2,j_3,k_4),(i_2,j_3,k_3),(i_3,j_3,k_3),(i_3,j_3,k_4)\\
(i_2,j_3,k_4),(i_2,j_2,k_4),(i_3,j_2,k_4),(i_3,j_3,k_4) & \perp & (i_2,j_3,k_4),(i_2,j_3,k_3),(i_3,j_3,k_3),(i_3,j_3,k_4)
\end{array}$$

intersect at the right angle. Corresponding to the above pairs, the expressions of the type 2 combinations of a basic move and a move of degree 6, with the configurations of the overlapped cells, are summarized as

$$\begin{array}{rlcl}
\multicolumn{2}{l}{M_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4)} & & \\
= & M_4(i_1i_2, j_1j_2, k_1k_2) + M_6^I(i_2i_3, j_1j_2j_3, k_3k_2k_4) & \cdots & (i_2,j_1,k_2),(i_2,j_2,k_2)\\
= & M_4(i_1i_3, j_1j_2, k_1k_2) + M_6^I(i_2i_3, j_1j_2j_3, k_3k_1k_4) & \cdots & (i_3,j_1,k_1),(i_3,j_2,k_1)\\
= & M_4(i_2i_3, j_2j_3, k_3k_4) + M_6^J(i_1i_3i_2, j_1j_2, k_1k_2k_3) & \cdots & (i_2,j_2,k_3),(i_3,j_2,k_4)\\
= & M_4(i_2i_3, j_1j_3, k_3k_4) + M_6^J(i_1i_3i_2, j_1j_2, k_1k_2k_4) & \cdots & (i_2,j_1,k_4),(i_3,j_1,k_4).
\end{array}$$

2.4 Moves of degree 10

Continuing the above discussion, next we consider a *four step move.* For the case of $3 \times 3 \times K$ contingency table, only the move of the following type needs to be considered.

Definition 5 *A move of degree 10 is a* $3 \times 3 \times K$ *contingency table* $\boldsymbol{M}_{10}(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4k_5) \in \mathcal{F}_0,\ 1 \leq i_1, i_2, i_3, j_1, j_2, j_3 \leq 3,\ 1 \leq k_1, k_2, k_3, k_4, k_5 \leq K$ *with the elements*

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

and all the other elements are zero.

For example, $\boldsymbol{M}_{10}(123, 123, 12345)$ is displayed as follows.

$$\begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ -1 & +1 & 0 & -1 & +1 \\ 0 & 0 & 0 & +1 & -1 \\ \hline \end{array} \qquad \begin{array}{|ccccc|}\hline -1 & 0 & +1 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & +1 \\ \hline \end{array} \qquad \begin{array}{|ccccc|}\hline 0 & +1 & -1 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & +1 & -1 & 0 \\ \hline \end{array}$$

Figure 6 gives a 3-dimensional view of this type of move.

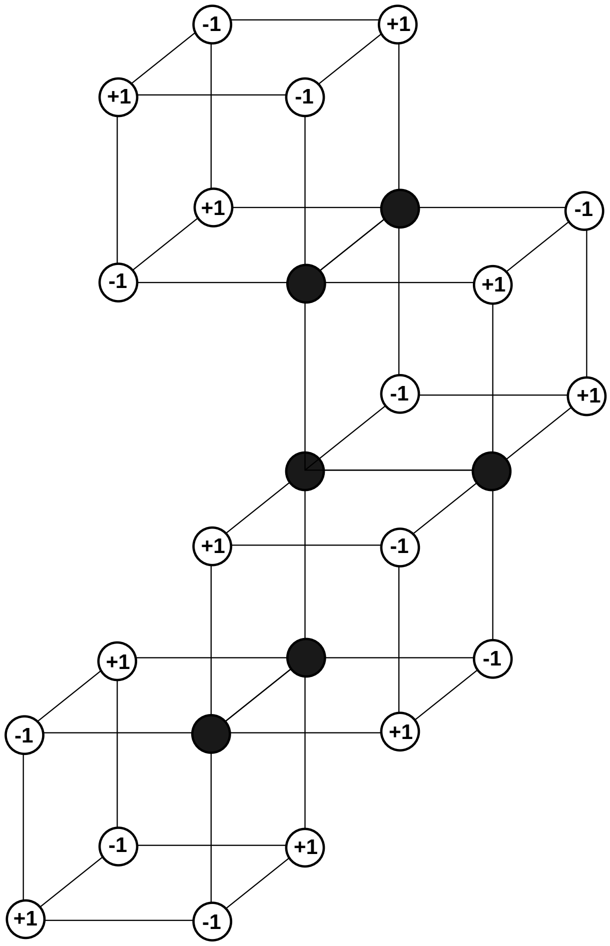

Figure 6: $3 \times 3 \times 5$ move of degree 10

From the definition, the relations

$$\boldsymbol{M}_{10}(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4k_5) = \boldsymbol{M}_{10}(i_1i_3i_2, j_3j_2j_1, k_4k_5k_3k_1k_2) = -\boldsymbol{M}_{10}(i_1i_2i_3, j_3j_2j_1, k_5k_4k_3k_2k_1)$$

are derived. It follows that the four expressions

$$\begin{array}{rr} \boldsymbol{M}_{10}(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4k_5), & \boldsymbol{M}_{10}(i_1i_3i_2, j_3j_2j_1, k_4k_5k_3k_1k_2), \\ -\boldsymbol{M}_{10}(i_1i_2i_3, j_3j_2j_1, k_5k_4k_3k_2k_1), & -\boldsymbol{M}_{10}(i_1i_3i_2, j_1j_2j_3, k_2k_1k_3k_5k_4) \end{array}$$

are all equivalent. Hence there are

$$3! \times 3! \times {}_K P_5 / 4 = 9K(K-1)(K-2)(K-3)(K-4)$$

different moves of degree 10 for $3 \times 3 \times K$ case.

As for the decomposition of this type of move, the type 2 combination of a basic move and a move of degree 8 is important for the same reason as the moves of degree 8. The result is summarized as the following eight expressions:

$$\begin{array}{lll}
M_{10}(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4k_5) & & \\
\quad = M_4(i_1i_2, j_1j_2, k_1k_2) + M_8(i_1i_2i_3, j_2j_3j_1, k_5k_4k_2k_3) & \cdots & (i_2, j_1, k_2), (i_2, j_2, k_2) \\
\quad = M_4(i_1i_3, j_1j_2, k_1k_2) + M_8(i_1i_2i_3, j_2j_3j_1, k_5k_4k_1k_3) & \cdots & (i_2, j_1, k_1), (i_2, j_2, k_1) \\
\quad = M_4(i_1i_3, j_2j_3, k_5k_4) + M_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_5) & \cdots & (i_3, j_2, k_5), (i_3, j_3, k_5) \\
\quad = M_4(i_1i_2, j_2j_3, k_5k_4) + M_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4) & \cdots & (i_2, j_2, k_4), (i_2, j_3, k_4) \\
\quad = M_4(i_1i_2, j_1j_2, k_1k_5) + M_8(i_2i_3i_1, j_1j_3j_2, k_3k_5k_2k_4) & \cdots & (i_1, j_1, k_5), (i_2, j_1, k_5) \\
\quad = M_4(i_1i_2, j_2j_3, k_5k_1) + M_8(i_2i_3i_1, j_1j_3j_2, k_3k_1k_2k_4) & \cdots & (i_1, j_3, k_1), (i_2, j_3, k_1) \\
\quad = M_4(i_1i_3, j_1j_2, k_4k_2) + M_8(i_3i_1i_2, j_1j_3j_2, k_4k_3k_1k_5) & \cdots & (i_1, j_1, k_4), (i_3, j_1, k_4) \\
\quad = M_4(i_1i_3, j_2j_3, k_2k_4) + M_8(i_3i_1i_2, j_1j_3j_2, k_2k_3k_1k_5) & \cdots & (i_1, j_3, k_2), (i_3, j_3, k_2).
\end{array}$$

As for a connected Markov chain, the next theorem holds for the $3 \times 3 \times 5$ case.

Theorem 3 *A set of basic moves* $\boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_2)$*, moves of degree* 6*,* $\boldsymbol{M}_6^I(i_1i_2, j_1j_2j_3, k_1k_2k_3)$*,* $\boldsymbol{M}_6^J(i_1i_2i_3, j_1j_2, k_1k_2k_3)$*,* $\boldsymbol{M}_6^K(i_1i_2i_3, j_1j_2j_3, k_1k_2)$*, degree* 8*,* $\boldsymbol{M}_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4))$ *and degree* 10*,* $\boldsymbol{M}_{10}(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4k_5), 1 \le i_1, i_2, i_3, j_1, j_2, j_3 \le 3, 1 \le k_1, k_2, k_3, k_4, k_5 \le 5$ *constitute a minimal Markov basis for* $3 \times 3 \times 5$ *tables.*

Finally it can be shown that for the case of $K \ge 6$, no more new moves are needed to construct a connected Markov chain. We now state the main result of this paper in the following theorem.

Theorem 4 *A set of basic moves* $\boldsymbol{M}_4(i_1i_2, j_1j_2, k_1k_2)$*, moves of degree* 6*,* $\boldsymbol{M}_6^I(i_1i_2, j_1j_2j_3, k_1k_2k_3)$*,* $\boldsymbol{M}_6^J(i_1i_2i_3, j_1j_2, k_1k_2k_3)$*,* $\boldsymbol{M}_6^K(i_1i_2i_3, j_1j_2j_3, k_1k_2)$*, degree* 8*,* $\boldsymbol{M}_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4))$ *and degree* 10*,* $\boldsymbol{M}_{10}(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4k_5), 1 \le i_1, i_2, i_3, j_1, j_2, j_3 \le 3, 1 \le k_1, k_2, k_3, k_4, k_5 \le K$ *constitute a minimal Markov basis for* $3 \times 3 \times K$ $(K \ge 5)$ *tables.*

3 Proofs of the theorems

In this section, we give proofs of the theorems in the previous section. Our proofs are based on exhaustive investigations of possible patterns and all the proofs are similar and repetitive. However we show the whole proofs without any abbreviations for the sake of completeness.

3.1 Ingredients of our proofs

Let $\boldsymbol{X}$ and $\boldsymbol{Y}$ be 3-way contingency tables of the same size with the same two-dimensional marginal totals. Note that all the marginal totals of $\boldsymbol{X} - \boldsymbol{Y}$ are zero. We also define $|\boldsymbol{X}| =$

$\sum_{i,j,k} |x_{ijk}|$. The idea of our proofs is based on the following simple observation. Suppose that a set of moves $\mathcal{B} = \{\boldsymbol{B}_1, \ldots, \boldsymbol{B}_L\}$ is given. If we make $\boldsymbol{X}$ and $\boldsymbol{Y}$ as close as possible, in other words, make $|\boldsymbol{X} - \boldsymbol{Y}|$ as small as possible, by applying moves $\boldsymbol{B}_{i_1}, \boldsymbol{B}_{i_2}, \ldots \in \mathcal{B}$ without causing negative entries on the way, then it follows that

$$|\boldsymbol{X} - \boldsymbol{Y}| \text{ can be decreased to } 0 \iff \mathcal{B} \text{ is a Markov basis.}$$

This shows that we only have to consider the patterns of $\boldsymbol{X} - \boldsymbol{Y}$, after making $|\boldsymbol{X} - \boldsymbol{Y}|$ as small as possible by applying moves from $\mathcal{B}$.

Minimality of the bases given in the theorems in the previous sections will be clear from our proofs. Our argument for the minimality is as follows. Suppose that $\mathcal{B} = \{\boldsymbol{B}_1, \ldots, \boldsymbol{B}_L\}$ is shown to be a Markov basis. To prove its minimality, it is sufficient to show that $\mathcal{B} \setminus \boldsymbol{B}_i$ is not a Markov basis for each i. Let $\boldsymbol{X} = \boldsymbol{B}_i^+$ be the positive part of $\boldsymbol{B}_i$. In our proofs it will be clear that none of $\boldsymbol{B}_j, j \neq i$, can be added to this $\boldsymbol{X}$ without causing negative entries. Therefore $\boldsymbol{X} = \boldsymbol{B}_i^+$ is not connected to any other states in $\mathcal{F}(\{x_{ij\cdot}, x_{i\cdot k}, x_{\cdot jk}\})$ by $\mathcal{B} \setminus \boldsymbol{B}_i$ and the minimality of $\mathcal{B}$ follows.

Hereafter we use the following abbreviations.

- wlog: “without loss of generality”
- wcne: “without causing negative entries”

We give the following definition for describing patterns of two-dimensional slices of $\boldsymbol{Y} - \boldsymbol{X}$.

Definition 6 *Let A be a two-dimensional matrix with elements a_{ij}. Then a rectangle is a set of four entries $(a_{i_1j_1}, a_{i_2j_1}, a_{i_2j_2}, a_{i_1j_2})$ with alternating signs. Similarly, a 6-cycle is a set of six entries $(a_{i_1j_1}, a_{i_2j_1}, a_{i_2j_2}, a_{i_3j_2}, a_{i_3j_3}, a_{i_1j_3})$ with alternating signs.*

We can easily show that any nonzero entry in a 3×3 k-slice of $\boldsymbol{Z} = \boldsymbol{Y} - \boldsymbol{X}$ has to be a member of either a rectangle or a 6-cycle in the slice by using the fact that all the marginal totals of $\boldsymbol{Z}$ are zero.

We now prove a useful lemma concerning patterns of k-slices of $\boldsymbol{Z}$.

Lemma 1 *Let $\boldsymbol{X}$ and $\boldsymbol{Y}$ be $3 \times 3 \times K$ contingency tables and let $\boldsymbol{Z} = \boldsymbol{X} - \boldsymbol{Y}$. Consider $\boldsymbol{Z}$ after minimizing $|\boldsymbol{Z}|$ by applying the basic moves and the moves of degree 6 wcne on the way. Then each (3×3) k-slice of $\boldsymbol{Z}$*

(a) *does not contain 6-cycles, and*

(b) *consist either of* (i) *one rectangle or* (ii) *three positive, three negative, and three zero elements with three zero elements occupying one row or one column.*

Proof. In this proof we display k-slices of $\boldsymbol{Z}$ instead of our usual display of i-slices.

To prove (a), suppose that wlog $k = 1$ slice of $\boldsymbol{Z}$ contains a following 6-cycle

$$\begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & * \\ 2 & - & * & + \\ 3 & * & + & - \\ \hline \end{array} .$$

Since $z_{11\cdot} = 0$, there exists at least one negative element in $z_{112}, z_{113}, ..., z_{11K}$. Let $z_{112} < 0$ wlog. As we have seen above, z_{112} has to be an element of either a rectangle or a 6-cycle in $k = 2$ slice. We consider the two cases respectively.

Case 1: z_{112} is an element of a 6-cycle
It is seen that the negative entries in the 6-cycle in the $k = 2$ slice, which includes z_{112}, can be either (i) $(z_{112}, z_{222}, z_{332})$ or (ii) $(z_{112}, z_{232}, z_{322})$. In the case of (i), we can add $\boldsymbol{M}_4(12, 12, 12)$ to $\boldsymbol{Y}$ wcne and make $|\boldsymbol{Z}|$ smaller since $y_{121}, y_{211}, y_{112}, y_{222} > 0$. On the other hand, in the case of (ii), we can add $\boldsymbol{M}_6^K(132, 123, 12)$ to $\boldsymbol{Y}$ wcne and make $|\boldsymbol{Z}|$ smaller since $y_{121}, y_{211}, y_{331}, y_{112}, y_{232}, y_{322} > 0$. These imply that Case 1 is a contradiction.

Case 2: z_{112} is an element of a rectangle
It is seen that the negative entries in the rectangle, which includes z_{112}, can be either (i) (z_{112}, z_{222}), (ii) (z_{112}, z_{232}), (iii) (z_{112}, z_{322}) or (iv) (z_{112}, z_{332}). In the case of (i), we can add $\boldsymbol{M}_4(12, 12, 12)$ to $\boldsymbol{Y}$ wcne and make $|\boldsymbol{Z}|$ smaller as we have seen in (i) of Case 1. In the case of (ii), it follows that $z_{132}, z_{212} > 0$ and we can add $\boldsymbol{M}_4(12, 13, 21)$ to $\boldsymbol{X}$ wcne and make $|\boldsymbol{Z}|$ smaller since $x_{111}, x_{231}, x_{132}, x_{212} > 0$. (iii) is the symmetric case of (ii). In the case of (iv), the two k-slices, $\{z_{ij1}\}$ and $\{z_{ij2}\}$ are represented as

$$\{z_{ij1}\} : \begin{array}{c|ccc} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & * \\ 2 & - & * & + \\ 3 & * & + & - \end{array} \qquad \{z_{ij2}\} : \begin{array}{c|ccc} i\backslash j & 1 & 2 & 3 \\ \hline 1 & - & * & + \\ 2 & * & * & * \\ 3 & + & * & - \end{array}$$

In this case, since $z_{331}, z_{332} < 0$, at least one of $z_{333}, \ldots, z_{33K}$ has to be positive. Let $z_{333} > 0$ wlog. Here, z_{333} is again an element of either a rectangle or a 6-cycle. But we have already seen in Case 1 that there cannot be another 6-cycle in the $k \neq 1$ slice. Then z_{333} has to be a member of rectangle. Moreover, for the same reason to (i)–(iii) of Case 2, the $k = 3$ slice has to be a mirror image of $k = 2$ slice:

$$\{z_{ij1}\} : \begin{array}{c|ccc} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & * \\ 2 & - & * & + \\ 3 & * & + & - \end{array} \qquad \{z_{ij2}\} : \begin{array}{c|ccc} i\backslash j & 1 & 2 & 3 \\ \hline 1 & - & * & + \\ 2 & * & * & * \\ 3 & + & * & - \end{array} \qquad \{z_{ij3}\} : \begin{array}{c|ccc} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & * & - \\ 2 & * & * & * \\ 3 & - & * & + \end{array}$$

But we can add $\boldsymbol{M}_4(13, 13, 23)$ to $\boldsymbol{X}$ or $\boldsymbol{M}_4(13, 13, 32)$ to $\boldsymbol{Y}$ wcne and make $|\boldsymbol{Z}|$ smaller, which contradicts the assumption. These imply that Case 2 also is a contradiction. From these considerations, it is seen that the 6-cycle cannot be included in any 3×3 slices and the proof of (a) is completed.

Considering the symmetry and as a consequence of (a), all the patterns of k-slices of $\boldsymbol{Z}$ have to be wlog one of the following patterns

$$\text{(i)} : \begin{array}{c|ccc} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & 0 \\ 2 & - & + & 0 \\ 3 & 0 & 0 & 0 \end{array} \qquad \text{(ii)} : \begin{array}{c|ccc} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & + \\ 2 & - & + & - \\ 3 & 0 & 0 & 0 \end{array} \qquad \text{(iii)} : \begin{array}{c|ccc} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & - \\ 2 & - & + & * \\ 3 & - & * & + \end{array}.$$

(i) and (ii) correspond to the case $z_{331} = 0$.

(iii) corresponds to the case $z_{331} \neq 0$. This case needs some explanation. First we can assume $z_{331} > 0$ wlog. One of z_{131} and z_{231} is negative and we can assume $z_{131} < 0$ wlog. One of z_{311} and z_{321} is negative. If $z_{321} < 0$ we have a 6-cycle and this is a contradiction. Therefore $z_{311} < 0$.

Note that (b) is proved if we show that (iii) is a contradiction. Therefore consider the case (iii). At least one of $z_{112}, ..., z_{11K}$ has to be negative since $z_{11\cdot} = 0$. We write $z_{112} < 0$ wlog. Since z_{112} have to be a member of the rectangle in the $k = 2$ slice, at least one of $z_{222}, z_{232}, z_{322}, z_{332}$ has to be negative. But

- if $z_{222} < 0$, we can add $\boldsymbol{M}_4(12, 12, 12)$ to $\boldsymbol{Y}$,
- if $z_{232} < 0$, we can add $\boldsymbol{M}_4(12, 13, 12)$ to $\boldsymbol{Y}$,
- if $z_{322} < 0$, we can add $\boldsymbol{M}_4(13, 12, 12)$ to $\boldsymbol{Y}$,
- if $z_{332} < 0$, we can add $\boldsymbol{M}_4(13, 13, 12)$ to $\boldsymbol{Y}$

wcne and make $|\boldsymbol{Z}|$ smaller. This is a contradiction and the proof of (b) is completed. Q.E.D.

Lemma 1 can be simply summarized as the following corollary.

Corollary 1 *Let $\boldsymbol{X}$ and $\boldsymbol{Y}$ be $3 \times 3 \times K$ contingency tables and let $\boldsymbol{Z} = \boldsymbol{X} - \boldsymbol{Y}$. Consider $\boldsymbol{Z}$ after minimizing $|\boldsymbol{Z}|$ by applying the basic moves and the moves of degree 6 wcne on the way. Then each (3×3) k-slice of $\boldsymbol{Z}$ contains at least one zero row or one zero column.*

We now carry out proofs of the theorems in the previous section using the above lemma.

3.2 Proof of Theorem 1.

We have already seen that a set of basic moves is not a Markov basis for $3 \times 3 \times 3$ case in Section 1. It is also obvious that a minimal Markov basis includes a set of basic moves. Accordingly, to prove Theorem 1, we only need to show that the elements of $\boldsymbol{Z} = \boldsymbol{X} - \boldsymbol{Y}$ have to be all zero after minimizing $|\boldsymbol{Z}|$ by applying the basic moves or the moves of degree 6 wcne on the way.

Suppose $\boldsymbol{Z}$ has nonzero entries. Let $z_{111} > 0$ wlog. Since $z_{11\cdot} = z_{1\cdot 1} = z_{\cdot 11} = 0$, we can assume $z_{112}, z_{121}, z_{211} < 0$ wlog.

$$\begin{array}{|ccc|}\hline + & - & * \\ - & * & * \\ * & * & * \\ \hline\end{array} \quad \begin{array}{|ccc|}\hline - & * & * \\ * & * & * \\ * & * & * \\ \hline\end{array} \quad \begin{array}{|ccc|}\hline * & * & * \\ * & * & * \\ * & * & * \\ \hline\end{array}$$

From Lemma 1, z_{111} has to be an element of rectangles, in each of $i = 1, j = 1$ and $k = 1$ slices. We can take one of these rectangles in $i = 1$ slice as $(z_{111}, z_{112}, z_{122}, z_{121})$ wlog.

$$\begin{array}{|ccc|}\hline + & - & * \\ - & + & * \\ * & * & * \\ \hline\end{array} \quad \begin{array}{|ccc|}\hline - & * & * \\ * & * & * \\ * & * & * \\ \hline\end{array} \quad \begin{array}{|ccc|}\hline * & * & * \\ * & * & * \\ * & * & * \\ \hline\end{array}$$

Next consider $j = 1$ slice. We claim that z_{111} and z_{112} are elements of the same rectangle in $j = 1$ slice. To prove this consider the sign of z_{113}. If $z_{113} \geq 0$, the rectangle containing z_{111} in

$j=1$ slice contains z_{112}, and if $z_{113}<0$, the rectangle containing z_{112} in $j=1$ slice contains z_{111}. Therefore z_{111} and z_{112} are elements of the same rectangle in $j=1$ slice and the rectangle can be taken as $(z_{111}, z_{112}, z_{212}, z_{211})$ wlog.

$$\begin{array}{|ccc|}\hline + & - & * \\ - & + & * \\ * & * & * \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline - & + & * \\ * & * & * \\ * & * & * \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline * & * & * \\ * & * & * \\ * & * & * \\ \hline\end{array}$$

Now consider the rectangle in $k=1$ slice containing z_{111}. From the similar reason as above, this rectangle also contains z_{121}. In addition, if $z_{221}>0$, we can add $\boldsymbol{M}_4(12,12,21)$ to $\boldsymbol{X}$ wcne and make $|\boldsymbol{Z}|$ smaller, which contradicts the assumption. Hence the rectangle in $k=1$ slice including z_{111} has to be $(z_{111}, z_{121}, z_{321}, z_{311})$.

$$\begin{array}{|ccc|}\hline + & - & * \\ - & + & * \\ * & * & * \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline - & + & * \\ * & * & * \\ * & * & * \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline - & * & * \\ + & * & * \\ * & * & * \\ \hline\end{array}$$

Next consider the rectangle in the slice of $k=1$ including z_{211}. By Corollary 1 the rectangle has to be $(z_{111}, z_{121}, z_{221}, z_{211})$, which again contradicts the assumption as we have already seen.

From these considerations, a set of the basic moves and the moves of degree 6 is shown to be a Markov basis for $3\times 3\times 3$ case. The minimality is obvious as discussed in Section 3.1. This completes the proof of Theorem 1. Q.E.D.

3.3 Proof of Theorem 2.

From Theorem 1, it is also shown that a (minimal) Markov basis for $3\times 3\times 4$ case has to include a set of basic moves and moves of degree 6. In addition, if the pattern of $\boldsymbol{Z}=\boldsymbol{X}-\boldsymbol{Y}$ is expressed as

$$\begin{array}{|cccc|}\hline + & - & 0 & 0 \\ - & + & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0 & + & 0 \\ + & 0 & 0 & - \\ 0 & 0 & - & + \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0 & + & - & 0 \\ 0 & - & 0 & + \\ 0 & 0 & + & - \\ \hline\end{array},$$

it is observed that we cannot add any basic moves or moves of degree 6 to $\boldsymbol{X}$ or $\boldsymbol{Y}$ wcne. This implies that a set of basic moves and moves of degree 6 is not a Markov basis for $3\times 4\times 4$ case. Accordingly, to prove Theorem 2, we only need to show that the pattern of $\boldsymbol{Z}$ has to be of all zero entries after minimizing $|\boldsymbol{Z}|$ by adding the basic moves, the moves of degree 6 or degree 8, wcne on the way.

Suppose $\boldsymbol{Z}$ has nonzero entries. Similarly to the proof of Theorem 1, we write $z_{111}>0$ and $z_{112}, z_{121}, z_{211}<0$ wlog. Moreover, we write $z_{221}>0$ wlog since we know that z_{111} is an element of a rectangle in $k=1$ slice.

$$\begin{array}{|cccc|}\hline + & - & * & * \\ - & * & * & * \\ * & * & * & * \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & * & * & * \\ + & * & * & * \\ * & * & * & * \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ \hline\end{array}$$

Here we consider the following two cases:

- Case 1: there exists at least one rectangle in 3×4 i-slices or j-slices of $\boldsymbol{Z}$
- Case 2: there exists no rectangle in 3×4 i-slices or j-slices of $\boldsymbol{Z}$.

Case 1: We write $z_{122} > 0$ wlog to make a rectangle in the $i = 1$ slice.

$$\begin{array}{|cccc|}\hline + & - & \ast & \ast \\ - & + & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & \ast & \ast & \ast \\ + & \ast & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline \ast & \ast & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array}$$

As in the proof of Theorem 1, by considering the sign of z_{132}, we see that that z_{112}, z_{122} are members of the same rectangle in $k = 2$ slice. Then (z_{212}, z_{222}) and/or (z_{312}, z_{322}) has to be $(+, -)$. But

- if $z_{212} > 0$, we can add $\boldsymbol{M}_4(12, 12, 21)$ to $\boldsymbol{X}$ wcne and
- if $z_{222} < 0$, we can add $\boldsymbol{M}_4(12, 12, 12)$ to $\boldsymbol{Y}$ wcne

and make $|\boldsymbol{Z}|$ smaller. These imply that $z_{312} > 0, z_{322} < 0$ and $z_{212} \leq 0, z_{222} \geq 0$. Similarly,

- if $z_{311} < 0$, we can add $\boldsymbol{M}_4(13, 12, 12)$ to $\boldsymbol{Y}$ wcne and
- if $z_{321} > 0$, we can add $\boldsymbol{M}_4(13, 12, 21)$ to $\boldsymbol{X}$ wcne

and make $|\boldsymbol{Z}|$ smaller, which forces $z_{311} \geq 0$ and $z_{321} \leq 0$.

$$\begin{array}{|cccc|}\hline + & - & \ast & \ast \\ - & + & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & \ast & \ast \\ + & 0+ & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0+ & + & \ast & \ast \\ 0- & - & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array}$$

Hereafter we display non-negative elements by $0+$ and non-positive elements by $0-$. Since $z_{21\cdot} = 0$, let $z_{213} > 0$ wlog, which forces $z_{123} \leq 0$, otherwise we can add $\boldsymbol{M}_4(12, 12, 31)$ to $\boldsymbol{X}$ wcne and make $|\boldsymbol{Z}|$ smaller.

$$\begin{array}{|cccc|}\hline + & - & \ast & \ast \\ - & + & 0- & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & + & \ast \\ + & 0+ & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0+ & + & \ast & \ast \\ 0- & - & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \tag{6}$$

Since $z_{22\cdot} = 0$, at least one of z_{223} and z_{224} has to be negative. If $z_{223} < 0$, it follows $z_{113} \geq 0$, otherwise we can add $\boldsymbol{M}_4(12, 12, 13)$ wcne and make $|\boldsymbol{Z}|$ smaller. In addition, since $z_{\cdot 13} = z_{\cdot 23} = 0$, it also follows that $z_{313} < 0$ and $z_{323} > 0$.

$$\begin{array}{|cccc|}\hline + & - & 0+ & \ast \\ - & + & 0- & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & + & \ast \\ + & 0+ & - & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0+ & + & - & \ast \\ 0- & - & + & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array}$$

But then we can add $\boldsymbol{M}_6^J(132, 21, 123)$ to $\boldsymbol{X}$ (or $\boldsymbol{M}_6^J(132, 12, 123)$ to $\boldsymbol{Y}$) wcne and make $|\boldsymbol{Z}|$ smaller. This implies that $z_{223} \geq 0$ and $z_{224} < 0$ in (6).

$$\begin{array}{|cccc|}\hline + & - & \ast & \ast \\ - & + & 0- & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & + & \ast \\ + & 0+ & 0+ & - \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0+ & + & \ast & \ast \\ 0- & - & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array}$$

We then have $z_{214} \leq 0$ from symmetry (in interchanging roles of $+$ and $-$). Since $z_{2\cdot 3} = z_{2\cdot 4} = 0$, $z_{233} < 0$ and $z_{234} > 0$. It follows $z_{114} \geq 0$, otherwise we can add $\boldsymbol{M}_4(12, 12, 14)$ to $\boldsymbol{Y}$ wcne and make $|\boldsymbol{Z}|$ smaller.

$$\begin{array}{|cccc|}\hline + & - & \ast & 0+ \\ - & + & 0- & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & + & 0- \\ + & 0+ & 0+ & - \\ \ast & \ast & - & + \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0+ & + & \ast & \ast \\ 0- & - & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \tag{7}$$

Because of the symmetry between $i = 2$ slice and $i = 3$ slice, all the patterns are either of

- Case 1-1: $z_{313} < 0, z_{314} \geq 0, z_{323} \leq 0, z_{324} > 0$, or
- Case 1-2: $z_{313} \geq 0, z_{314} < 0, z_{323} > 0, z_{324} \leq 0$.

Case 1-1: $z_{313} < 0, z_{314} \geq 0, z_{323} \leq 0, z_{324} > 0$

$$\begin{array}{|cccc|}\hline + & - & \ast & 0+ \\ - & + & 0- & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & + & 0- \\ + & 0+ & 0+ & - \\ \ast & \ast & - & + \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0+ & + & - & 0+ \\ 0- & - & 0- & + \\ \ast & \ast & \ast & \ast \\ \hline\end{array}$$

Since $z_{3\cdot 3} = z_{3\cdot 4} = 0$, it follows that $z_{333} > 0$ and $z_{334} < 0$.

$$\begin{array}{|cccc|}\hline + & - & \ast & 0+ \\ - & + & 0- & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & + & 0- \\ + & 0+ & 0+ & - \\ \ast & \ast & - & + \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0+ & + & - & 0+ \\ 0- & - & 0- & + \\ \ast & \ast & + & - \\ \hline\end{array}$$

But we can add $\boldsymbol{M}_8(132, 123, 2134)$ to $\boldsymbol{X}$ (or $\boldsymbol{M}_8(123, 123, 1234)$ to $\boldsymbol{Y}$) wcne and make $|\boldsymbol{Z}|$ smaller. This implies that Case 1-1 contradicts the assumption.

Case 1-2: $z_{313} \geq 0, z_{314} < 0, z_{323} > 0, z_{324} \leq 0$

$$\begin{array}{|cccc|}\hline + & - & \ast & 0+ \\ - & + & 0- & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & + & 0- \\ + & 0+ & 0+ & - \\ \ast & \ast & - & + \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0+ & + & 0+ & - \\ 0- & - & + & 0- \\ \ast & \ast & \ast & \ast \\ \hline\end{array}$$

But we can add $\boldsymbol{M}_6^J(132, 21, 123)$ to $\boldsymbol{X}$ wcne and $\boldsymbol{M}_6^J(132, 12, 124)$ to $\boldsymbol{Y}$ wcne and make $|\boldsymbol{Z}|$ smaller, which contradicts the assumption.

Case 2: Since there exists no rectangle in the 3×4 i-slices or j-slices of $\boldsymbol{Z}$, it follows that $z_{122}, z_{212} \leq 0$. We write $z_{222} \geq 0$ because otherwise we can add $\boldsymbol{M}_4(12, 12, 12)$ to $\boldsymbol{Y}$ wcne and make $|\boldsymbol{Z}|$ smaller.

$$\begin{array}{|cccc|}\hline + & - & \ast & \ast \\ - & 0- & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & \ast & \ast \\ + & 0+ & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline \ast & \ast & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array}$$

Since z_{112} has to be a member of a rectangle in $k = 2$ slice, $z_{132} > 0, z_{312} > 0$ and $z_{332} < 0$ are derived.

$$\begin{array}{|cccc|}\hline + & - & \ast & \ast \\ - & 0- & \ast & \ast \\ \ast & + & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & \ast & \ast \\ + & 0+ & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline \ast & + & \ast & \ast \\ \ast & \ast & \ast & \ast \\ \ast & - & \ast & \ast \\ \hline\end{array}$$

It is seen that

- if $z_{131} < 0$, there appears a rectangle in $i = 1$ slice, and
- if $z_{311} < 0$, there appears a rectangle in $j = 1$ slice,

which return to Case 1. Then it follows $z_{131}, z_{311} \geq 0$. Here we write $z_{123} > 0$ wlog, since $z_{12\cdot} = 0$.

$$\begin{array}{|cccc|}\hline + & - & * & * \\ - & 0- & + & * \\ 0+ & + & * & * \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & * & * \\ + & 0+ & * & * \\ * & * & * & * \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0+ & + & * & * \\ * & * & * & * \\ * & - & * & * \\ \hline\end{array}$$

It is seen that

- if $z_{113} < 0$, there appears a rectangle in $i = 1$ slice, and
- if $z_{223} < 0$, there appears a rectangle in $j = 2$ slice,

which return to Case 1. Then it follows $z_{113}, z_{223} \geq 0$.

$$\begin{array}{|cccc|}\hline + & - & 0+ & * \\ - & 0- & + & * \\ 0+ & + & * & * \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & * & * \\ + & 0+ & 0+ & * \\ * & * & * & * \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0+ & + & * & * \\ * & * & * & * \\ * & - & * & * \\ \hline\end{array}$$

Since z_{123} has to be a member of a rectangle in $k = 3$ slice, $z_{133} < 0, z_{323} < 0$ and $z_{333} > 0$ are derived.

$$\begin{array}{|cccc|}\hline + & - & 0+ & * \\ - & 0- & + & * \\ 0+ & + & - & * \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline - & 0- & * & * \\ + & 0+ & 0+ & * \\ * & * & * & * \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0+ & + & * & * \\ * & * & - & * \\ * & - & + & * \\ \hline\end{array}$$

But there appears a rectangle $(z_{132}, z_{133}, z_{333}, z_{332})$ in $j = 3$ slice, which implies that Case 2 itself returns to Case 1. Note that $k = 4$ slice is irrelevant for Case 2. This implies that Case 2 returns to Case 1 for any value of $K \geq 4$.

From these considerations, a set of the basic moves, the moves of degree 6 and degree 8 is shown to be a Markov basis for $3 \times 3 \times 4$ case. The minimality is obvious as in the proof of Theorem 1. Q.E.D.

3.4 Proof of Theorem 3.

Theorem 2 implies that a (minimal) Markov basis for $3 \times 3 \times 5$ case has to include a set of basic moves, moves of degree 6 and degree 8. In addition, if the pattern of $\boldsymbol{Z} = \boldsymbol{X} - \boldsymbol{Y}$ is expressed as

$$\begin{array}{|ccccc|}\hline + & - & 0 & 0 & 0 \\ - & + & 0 & - & + \\ 0 & 0 & 0 & + & - \\ \hline\end{array} \qquad \begin{array}{|ccccc|}\hline - & 0 & + & 0 & 0 \\ + & 0 & 0 & 0 & - \\ 0 & 0 & - & 0 & + \\ \hline\end{array} \qquad \begin{array}{|ccccc|}\hline 0 & + & - & 0 & 0 \\ 0 & - & 0 & + & 0 \\ 0 & 0 & + & - & 0 \\ \hline\end{array},$$

it is observed that we cannot add any basic move, move of degree 6 and degree 8 to $\boldsymbol{X}$ or $\boldsymbol{Y}$ wcne. This implies that a set of basic moves, moves of degree 6 and degree 8 is not a Markov basis for $3 \times 3 \times 5$ case. Accordingly, to prove Theorem 3, all we have to show is that the pattern of $\boldsymbol{Z}$ must be of all zero entries after minimizing $|\boldsymbol{Z}|$ by adding the basic moves, the moves of degree 6, degree 8 or degree 10, wcne on the way.

Suppose $\boldsymbol{Z}$ has nonzero entries. As we have already seen, Case 2 in the proof of Theorem 2 returns to Case 1 regardless of the value of $K \geq 4$. This implies that for $3 \times 3 \times K$ case, there exists at least one rectangle in the $3 \times K$ slice of $\boldsymbol{Z}$ and all we have to consider is the pattern of Case 1 in the proof of Theorem 2. For the similar reason leading to (7) in the proof of Theorem 2, we can restrict the patterns to

$$\begin{array}{|ccccc|}\hline + & - & * & 0+ & * \\ - & + & 0- & * & * \\ * & * & * & * & * \\ \hline\end{array} \qquad \begin{array}{|ccccc|}\hline - & 0- & + & 0- & * \\ + & 0+ & 0+ & - & * \\ * & * & - & + & * \\ \hline\end{array} \qquad \begin{array}{|ccccc|}\hline 0+ & + & * & * & * \\ 0- & - & * & * & * \\ * & * & * & * & * \\ \hline\end{array}$$

wlog. Since $z_{31\cdot} = z_{32\cdot} = 0$, at least one of $z_{313}, z_{314}, z_{315}$ has to be negative and at least one of $z_{323}, z_{324}, z_{325}$ has to be positive. But we have already seen that

- if $(z_{313}, z_{324}) = (-, +)$, there appears a same pattern as Case 1-1 in the proof of Theorem 2 and
- if $z_{314} < 0$ or $z_{323} > 0$, there appears a same pattern as Case 1-2 in the proof of Theorem 2.

In addition, if $(z_{315}, z_{325}) = (-, +)$, it follows that $z_{115} \leq 0$ and $z_{125} \geq 0$, (otherwise we can add $\boldsymbol{M}_4(13, 12, 25)$ to $\boldsymbol{X}$ wcne and $\boldsymbol{M}_4(13, 12, 52)$ to $\boldsymbol{Y}$ wcne and make $|\boldsymbol{Z}|$ smaller) and $(z_{215}, z_{225}) = (+, -)$ since $z_{\cdot 15} = z_{\cdot 25} = 0$. But we can add $\boldsymbol{M}_6^J(132, 21, 125)$ to $\boldsymbol{X}$ wcne and $\boldsymbol{M}_6^J(132, 12, 125)$ to $\boldsymbol{Y}$ wcne and make $|\boldsymbol{Z}|$ smaller. All of these contradict the assumption. The remaining patterns are $(z_{313}, z_{325}) = (-, +)$ or $(z_{315}, z_{324}) = (-, +)$. Considering the symmetry, we write $(z_{313}, z_{325}) = (-, +)$ wlog. Then the patterns are wlog summarized as

$$\begin{array}{|ccccc|}\hline + & - & * & 0+ & * \\ - & + & 0- & * & * \\ * & * & * & * & * \\ \hline\end{array} \qquad \begin{array}{|ccccc|}\hline - & 0- & + & 0- & * \\ + & 0+ & 0+ & - & * \\ * & * & - & + & * \\ \hline\end{array} \qquad \begin{array}{|ccccc|}\hline 0+ & + & - & 0+ & 0+ \\ 0- & - & 0- & 0- & + \\ * & * & * & * & * \\ \hline\end{array} \; .$$

Since $z_{\cdot 24} = z_{1\cdot 4} = z_{3\cdot 3} = z_{3\cdot 5} = 0$, it follows that $z_{124} > 0, z_{134} < 0, z_{333} > 0, z_{335} < 0$.

$$\begin{array}{|ccccc|}\hline + & - & * & 0+ & * \\ - & + & 0- & + & * \\ * & * & * & - & * \\ \hline\end{array} \qquad \begin{array}{|ccccc|}\hline - & 0- & + & 0- & * \\ + & 0+ & 0+ & - & * \\ * & * & - & + & * \\ \hline\end{array} \qquad \begin{array}{|ccccc|}\hline 0+ & + & - & 0+ & 0+ \\ 0- & - & 0- & 0- & + \\ * & * & + & * & - \\ \hline\end{array}$$

Since z_{325}, z_{335} have to be members of a rectangle in the $k = 5$ slice, (z_{125}, z_{135}) and/or (z_{225}, z_{235}) has to be $(-, +)$. But

- if $(z_{225}, z_{235}) = (-, +)$, then we can add $\boldsymbol{M}_8(123, 213, 1253)$ to $\boldsymbol{X}$ (or $\boldsymbol{M}_8(123, 123, 1235)$ to $\boldsymbol{Y}$) wcne and make $|\boldsymbol{Z}|$ smaller and
- if $(z_{125}, z_{135}) = (-, +)$, then we can add $\boldsymbol{M}_{10}(123, 321, 45321)$ to $\boldsymbol{X}$ (or $\boldsymbol{M}_{10}(123, 123, 12354)$ to $\boldsymbol{Y}$) wcne and make $|\boldsymbol{Z}|$ smaller,

which contradict the assumption.

From these considerations, a set of the basic moves, the moves of degree 6, degree 8 and degree 10 is shown to be a Markov basis for $3 \times 3 \times 5$ case. The minimality is obvious as in the proof of Theorem 1. Q.E.D.

3.5 Proof of Theorem 4.

Again we can begin with the following pattern.

+	−	∗	0+	∗	∗
−	+	0−	∗	∗	∗
∗	∗	∗	∗	∗	∗

−	0−	+	0−	∗	∗
+	0+	0+	−	∗	∗
∗	∗	−	+	∗	∗

0+	+	∗	∗	∗	∗
0−	−	∗	∗	∗	∗
∗	∗	∗	∗	∗	∗

As we have seen in the proof of Theorem 3, z_{313} and z_{314} have to be nonnegative and z_{323} and z_{324} have to be nonpositive, since $(z_{313}, z_{326}) = (-,+)$ or $(z_{316}, z_{324}) = (-,+)$ also contradict the assumption. The case of $(z_{316}, z_{326}) = (-,+)$ also contradicts the assumption for the similar reason that $(z_{315}, z_{325}) = (-,+)$ does. Hence the remaining pattern is $(z_{315}, z_{326}) = (-,+)$ or $(z_{316}, z_{325}) = (-,+)$. We write $(z_{315}, z_{326}) = (-,+)$ wlog.

+	−	∗	0+	∗	∗
−	+	0−	∗	∗	∗
∗	∗	∗	∗	∗	∗

−	0−	+	0−	∗	∗
+	0+	0+	−	∗	∗
∗	∗	−	+	∗	∗

0+	+	0+	0+	−	∗
0−	−	0−	0−	∗	+
∗	∗	∗	∗	∗	∗

Considering the symmetry in interchanging the roles of $\{+,-\}$, the roles of $\{z_{2jk}, z_{3jk}\}$ and the roles of $\{(z_{ij3}, z_{ij4}), (z_{ij5}, z_{ij6})\}$, we can restrict the patterns to

+	−	∗	0+	∗	0−
−	+	0−	∗	0+	∗
∗	∗	∗	∗	∗	∗

−	0−	+	0−	0−	0−
+	0+	0+	−	0+	0+
∗	∗	−	+	∗	∗

0+	+	0+	0+	−	0+
0−	−	0−	0−	0−	+
∗	∗	∗	∗	+	−

for the similar reason to Case 1-1 of the proof of Theorem 2. Since $z_{\cdot 13} = z_{\cdot 15} = z_{\cdot 24} = z_{\cdot 26} = 0$, it follows that $z_{113} < 0, z_{115} > 0, z_{124} > 0$ and $z_{126} < 0$. $z_{1\cdot 3} = z_{1\cdot 4} = z_{1\cdot 5} = z_{1\cdot 6} = 0$ also forces $z_{133} > 0, z_{134} < 0, z_{135} < 0$ and $z_{136} > 0$.

+	−	−	0+	+	0−
−	+	0−	+	0+	−
∗	∗	+	−	−	+

−	0−	+	0−	0−	0−
+	0+	0+	−	0+	0+
∗	∗	−	+	∗	∗

0+	+	0+	0+	−	0+
0−	−	0−	0−	0−	+
∗	∗	∗	∗	+	−

But this pattern includes moves of degree 6. We can add $\boldsymbol{M}_6^I(21, 132, 134)$ to $\boldsymbol{X}$, $\boldsymbol{M}_6^I(12, 132, 134)$ to $\boldsymbol{Y}$, $\boldsymbol{M}_6^I(13, 132, 256)$ to $\boldsymbol{X}$ or $\boldsymbol{M}_6^I(31, 132, 256)$ to $\boldsymbol{Y}$ wcne and make $|\boldsymbol{Z}|$ smaller, which contradicts the assumption.

From these considerations, it is shown that a set of the basic moves, the moves of degree 6, degree 8 and degree 10 is also a Markov basis for $3 \times 3 \times K$ $(K \geq 5)$ case. The minimality is again obvious. Note that although we have displayed 3x3x6 tables, the above argument does not involve k-slices for $k \geq 7$. Therefore we obtain the same contradiction for $3 \times 3 \times K$ $(K \geq 7)$ tables. Q.E.D.

4 Computational examples

Using the Markov basis obtained above, we can perform various tests by Monte Carlo method. In this section, we show simple examples of testing the hypothesis of no three-factor interaction. We consider the null distribution of the classical goodness-of-fit chi-squared statistic. It is known that, under the hypothesis of no three-factor interaction, the conditional probability of cell counts is the hypergeometric distribution. Our concern is to compute the finite sample null distribution of the goodness-of-fit chi-squared statistic, not using the large sample theory.

The settings of the examples are as follows. The size of the contingency table is $3 \times 3 \times 8$ and the total frequency $x_{\cdots}$ is taken to be 72 and 216. The marginal totals are assumed to be completely uniform, i.e., $x_{i \cdot k} = x_{\cdot jk} = 3$ or 9, $x_{ij\cdot} = 8$ or 24 for all i, j, k. For this case, as we have seen, a set of $2 \times 2 \times 2$ basic moves, $2 \times 3 \times 3, 3 \times 2 \times 3, 3 \times 3 \times 2$ moves of degree 6, $3 \times 3 \times 4$ moves of degree 8 and $3 \times 3 \times 5$ moves of degree 10 forms a Markov basis. For constructing a Markov chain which has the hypergeometric distribution as a stationary distribution, we use the Metropolis procedure described in Lemma 2.2 of Diaconis and Sturmfels (1998). To compare the obtained sample to the asymptotic distribution, we make a Q-Q plot of the permutation distribution of the chi-square statistic versus the limiting chi-square distribution with 28 degrees of freedom. Figure 7 and 8 show the cases of $x_{\cdots} = 72$ and 216, respectively. It is seen that the approximation is not good especially for the cases of $x_{\cdots} = 72$.

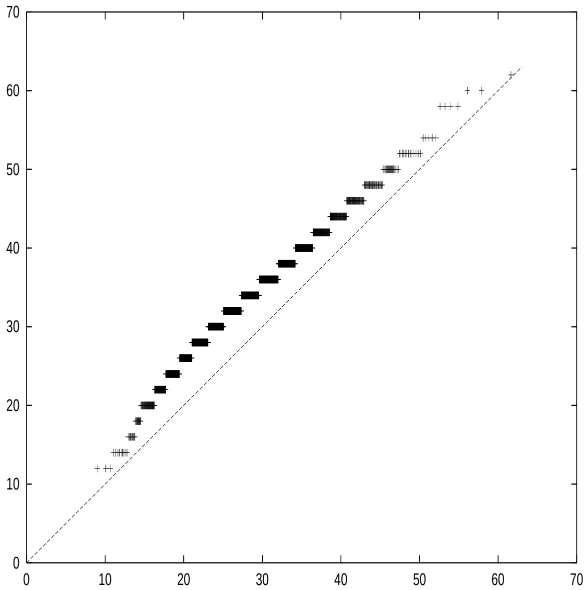

Figure 7: Q-Q plot of the permutation distribution of chi-square statistic versus asymptotic distribution ($x_{\cdots} = 72$).

5 Discussion and higher tables

Our main contribution in this paper is twofold. First, an explicit form of a minimal Markov basis for $3 \times 3 \times K$ contingency tables is provided, by considering all the patterns that do not contradict the constraints. These enable us to construct a connected Markov chain over $3 \times 3 \times K$ contingency tables. Adjusting this chain to have a given stationary distribution by the Metropolis procedure, we can perform various tests by Monte Carlo method. A typical example of the applications is the Monte Carlo simulation of the finite sample distribution of

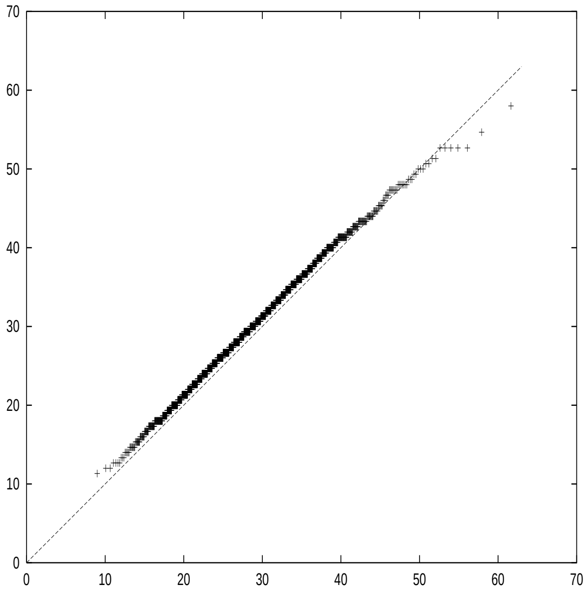

Figure 8: Q-Q plot of the permutation distribution of chi-square statistic versus asymptotic distribution ($x_{\cdots} = 216$).

the goodness-of-fit chi-square statistic under the hypothesis of no three-factor interaction in Section 4. Our approach is also applicable to the problem of data security, where very sparse contingency tables with fixed marginals are treated. See Irving and Jerrum (1994), for example. Second, a general method to obtain a Markov basis is provided. It is true that our method is laborious one as seen in Section 3. But Theorem 4 assures us that no other moves are needed to construct a connected Markov chain regardless of the value of K. This result is attractive since it may not be derived by performing algebraic algorithms.

On the other hand, our approach seems to be difficult to generalize to larger tables. For illustration, we here present a Markov basis for the $3 \times 4 \times 4$ — the next simplest — case. By the similar consideration to Section 3, it can be shown that a minimal Markov basis for the $3 \times 4 \times 4$ case is composed of basic moves, moves of degree 6 ($2 \times 3 \times 3, 3 \times 2 \times 3, 3 \times 3 \times 2$), moves of degree 8 ($3 \times 3 \times 4, 3 \times 4 \times 3$), moves of degree 8 ($2 \times 4 \times 4$) like

$$
\boxed{\begin{array}{cccc} +1 & -1 & 0 & 0 \\ 0 & +1 & -1 & 0 \\ 0 & 0 & +1 & -1 \\ -1 & 0 & 0 & +1 \end{array}}
\qquad
\boxed{\begin{array}{cccc} -1 & +1 & 0 & 0 \\ 0 & -1 & +1 & 0 \\ 0 & 0 & -1 & +1 \\ +1 & 0 & 0 & -1 \end{array}}
\qquad
\boxed{\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}}\ ,
$$

moves of degree 9 ($3 \times 4 \times 4$, Figure 9) like

$$
\boxed{\begin{array}{cccc} +1 & -1 & 0 & 0 \\ -1 & 0 & +1 & 0 \\ 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{array}}
\qquad
\boxed{\begin{array}{cccc} -1 & +1 & 0 & 0 \\ +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & +1 \end{array}}
\qquad
\boxed{\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 \\ 0 & -1 & +1 & 0 \\ 0 & +1 & 0 & -1 \end{array}}\ ,
$$

and moves of degree 10 ($3 \times 4 \times 4$, Figure 10) like

$$\boxed{\begin{matrix} +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ 0 & 0 & +1 & -1 \\ 0 & 0 & -1 & +1 \end{matrix}} \qquad \boxed{\begin{matrix} -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 \\ 0 & -1 & +1 & 0 \end{matrix}} \qquad \boxed{\begin{matrix} 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ -1 & 0 & 0 & +1 \\ 0 & +1 & 0 & -1 \end{matrix}} .$$

Among the newly obtained moves, the $3 \times 4 \times 4$ move of degree 10 is interpreted as the type 2 combination of a basic move and a move of degree 8, which is similar to the $3 \times 3 \times 5$ move of degree 10 shown in Section 2.4. However, the $3 \times 4 \times 4$ move of degree 9 is new in the sense that this is a type 2 combination of a basic move and a move of degree 7. In other words, this move is composed of three basic moves and two of these basic moves are type 1 combinations. Recall that the move of degree 7 itself is not needed to construct a connected Markov chain. The move of degree 9 suggests the difficulty in forming a conjecture on a minimal Markov basis for larger tables.

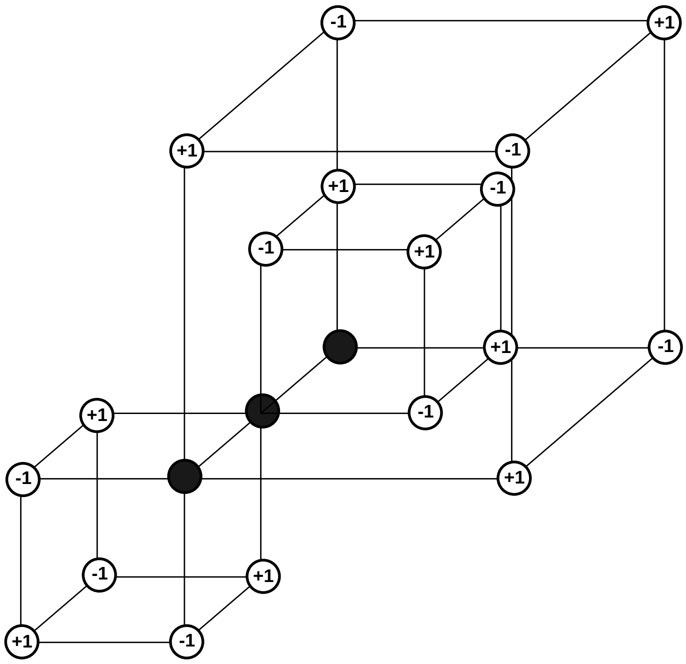

Figure 9: $3 \times 4 \times 4$ move of degree 9

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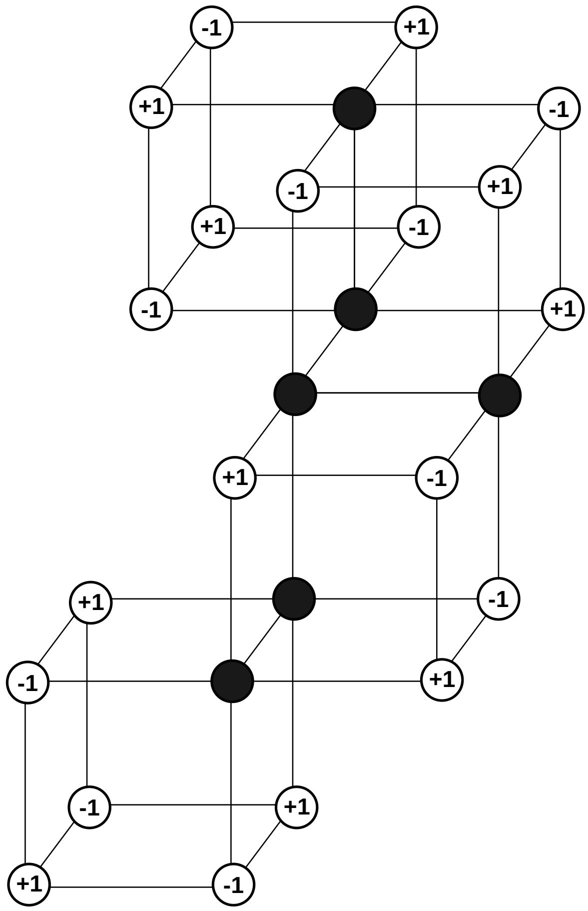

Figure 10: $3 \times 4 \times 4$ move of degree 10

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