Markov Bases for Two-way Subtable Sum Problems

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Abstract

It has been well-known that for two-way contingency tables with fixed row sums and column sums the set of square-free moves of degree two forms a Markov basis. However when we impose an additional constraint that the sum of a subtable is also fixed, then these moves do not necessarily form a Markov basis. Thus, in this paper, we show a necessary and sufficient condition on a subtable so that the set of square-free moves of degree two forms a Markov basis.

1 Introduction

Since Sturmfels [1996] and Diaconis and Sturmfels [1998] showed that a set of binomial generators of a toric ideal for a statistical model of discrete exponential families is equivalent to a Markov basis and initiated Markov chain Monte Carlo approach based on a Gröbner basis computation for testing statistical fitting of the given model, many researchers have extensively studied the structure of Markov bases for models in computational algebraic statistics (e.g. Hoşten and Sullivant [2002], Dobra [2003], Dobra and Sullivant [2004], Geiger et al. [2006]).

In this article we consider Markov bases for two-way contingency tables with fixed row sums, column sums and an additional constraint that the sum of a subtable is also fixed. We call this problem a *two-way subtable sum problem*. From statistical viewpoint this problem is motivated by a block interaction model or a two-way change-point model proposed by Hirotsu [1997], which has been studied from both theoretical and practical viewpoint(Ninomiya [2004]) and has important applications to dose-response clinical trials with ordered categorical responses.

Our model also relates to the quasi-independence model for incomplete two-way contingency tables which contain some structural zeros (Aoki and Takemura [2005], Rapallo [2006]). Essentially the same problem has been studied in detail from algebraic viewpoint in a series of papers by Ohsugi and Hibi (Ohsugi and Hibi [1999a], Ohsugi and Hibi [1999b], Ohsugi and Hibi [2005]).

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Example 1. *Suppose we have a 3×3 table with the following cell counts.*

7	5	1
5	10	6
2	6	8

If we fix the row sums $(13, 21, 16)$ *and column sums* $(14, 21, 15)$*, and also if we fix the sum of two cells at* $(1, 1)$ *and* $(2, 1)(7 + 5 = 12$ *in this example), a Markov basis consists of square-free moves of degree two. However, if we fix the sum of two cells at* $(1, 1)$ *and* $(2, 2)(7 + 10 = 17$ *in this example), then a Markov basis contains non-square-free moves such as*

1	1	−2
−1	−1	2
0	0	0

In this paper we show a necessary and sufficient condition on a subtable so that a corresponding Markov basis consists of square-free moves of degree two. The results here may give some insights into Markov bases for statistical models for general multi-way tables with various patterns of statistical interaction effects.

Because of the equivalence between a Markov basis and a set of binomial generators of a toric ideal, a theory of this paper can be entirely translated and developed in an algebraic framework. However, in this paper we make extensive use of pictorial representations of tables and moves. Therefore we prefer to develop our theory using tables and moves. See Aoki et al. [2005] for a discussion of this equivalence.

This paper is organized as follows: In section 2, we describe our problem and summarize some preliminary facts. Section 3 gives a necessary and sufficient condition that a Markov basis consists of square-free moves of degree two. We end this paper with some concluding remarks in Section 4.

2 Preliminaries

2.1 Subtable sum problem and its Markov bases

Let $\mathbb{N} = \{0, 1, 2, \ldots\}$ and let $X = \{x_{ij}\}$, $x_{ij} \in \mathbb{N}$, $i = 1, \ldots, R$, $j = 1, \ldots, C$, be an $R \times C$ table with nonnegative integer entries. Let $\mathcal{I} = \{(i, j) \mid 1 \le i \le R, 1 \le j \le C\}$. Using statistical terminology, we call X a *contingency table* and $\mathcal{I}$ the set of *cells*.

Denote the row sums and column sums of X by

$$x_{i+} = \sum_{j=1}^{C} x_{ij}, \quad i = 1, \ldots, R, \qquad x_{+j} = \sum_{i=1}^{R} x_{ij}, \quad j = 1, \ldots, C.$$

Let S be a subset of $\mathcal{I}$. Define the subtable sum $x(S)$ by

$$x(S) = \sum_{(i,j)\in S} x_{ij}.$$

Denote the set of row sums, column sums and $x(S)$ by

$$\boldsymbol{b} = \{x_{1+}, \ldots, x_{R+}, x_{+1}, \ldots, x_{+C}, x(S)\}.$$

For $S = \emptyset$ or $S = \mathcal{I}$, we have $x(\emptyset) \equiv 0$ or $x(\mathcal{I}) = \deg X := \sum_{(i,j)\in\mathcal{I}} x_{ij} = \sum_i x_{i+}$. In these cases $x(S)$ is redundant and our problem reduces to a problem concerning tables with fixed row sums and column sums. Therefore in the rest of this paper, we consider S which is a non-empty proper subset of $\mathcal{I}$. Also note that $x(S^c) = \deg X - x(S)$, where S^c is the complement of S. Therefore fixing $x(S)$ is equivalent to fixing $x(S^c)$.

We consider $\boldsymbol{b}$ as a column vector with dimension $R + C + 1$. We also order the elements of X with respect to a lexicographic order and regard X as a column vector with dimension $|\mathcal{I}|$. Then the relation between X and $\boldsymbol{b}$ is written by

$$A_S X = \boldsymbol{b}. \tag{1}$$

Here A_S is an $(R + C + 1) \times |\mathcal{I}|$ matrix consisting of 0's and 1's. The set of columns of A_S is a configuration defining a toric ideal I_{A_S}. In this paper we simply call A_S the *configuration* for S. The set of tables $X \in \mathbb{N}^{\mathcal{I}}$ satisfying (1) is called the *fiber* for $\boldsymbol{b}$ and is denoted by $\mathcal{F}(\boldsymbol{b})$.

An $R \times C$ integer array $B = \{b_{ij}\}_{(i,j)\in\mathcal{I}}$ satisfying

$$A_S B = \boldsymbol{0} \tag{2}$$

is called a *move* for the configuration A_S. Let

$$\mathcal{M}_S = \{B \mid A_S B = \boldsymbol{0}\}$$

denote the set of moves for A_S. Let $\mathcal{B} \subset \mathcal{M}_S$ be a subset of $\mathcal{M}_S$. Note that if B is a move then $-B$ is a move. We call $\mathcal{B}$ sign-invariant if $B \in \mathcal{B} \Rightarrow -B \in \mathcal{B}$. According to Diaconis and Sturmfels [1998], a Markov basis for A_S is equivalent to a set of binomial generators of the corresponding toric ideal for I_{A_S} and defined as follows.

Definition 1. *A Markov basis for A_S is a sign-invariant finite set of moves $\mathcal{B} = \{B_1, \dots, B_L\} \subset \mathcal{M}_S$ such that, for any $\boldsymbol{b}$ and X, $Y \in \mathcal{F}(\boldsymbol{b})$, there exist $\alpha > 0$, $B_{t_1}, \dots, B_{t_\alpha} \in \mathcal{B}$ such that*

$$Y = X + \sum_{s=1}^{\alpha} B_{t_s} \quad \text{and} \quad Y = X + \sum_{s=1}^{a} B_{t_s} \in \mathcal{F}(\boldsymbol{b}) \quad \text{for } 1 \le a \le \alpha.$$

In this paper, for simplifying notation and without loss of generality, we only consider sign-invariant sets of moves as Markov bases.

For $i \neq i'$ and $j \neq j'$, consider the square-free move of degree two with $+1$ at cells (i,j), (i',j') and -1 at cells (i,j') and (i',j) :

$$\begin{array}{ccc} & j & j' \\ i & 1 & -1 \\ i' & -1 & 1 \end{array}$$

For simplicity we call this a *basic move* and and denote it by

$$B(i,i';j,j') = (i,j)(i',j') - (i,j')(i',j).$$

It is well-known that the set of all basic moves

$$\mathcal{B}_0 = \{B(i,i';j,j') \mid (i,j) \in \mathcal{I}, (i',j') \in \mathcal{I}, i \neq i', j \neq j'\}$$

forms a unique minimal Markov basis for $A_\emptyset$, i.e. the problem concerning tables with fixed rows sums and column sums. If $B(i,i';j,j') \in \mathcal{M}_S$, we call it a basic move for S. Define

$$\mathcal{B}_0(S) = \mathcal{B}_0 \cap \mathcal{M}_S$$

which is the set of all basic moves for S. Note that $\mathcal{B}_0(S)$ coincides with the set of square-free moves of degree two for A_S, since the row sums and columns sums are fixed.

As clarified in Section 3, $\mathcal{B}_0(S)$ does not always form a Markov basis for A_S. In Section 3, we derive a necessary and sufficient condition on S that $\mathcal{B}_0(S)$ is a Markov basis.

2.2 Reduction of L_1-norm of a move and Markov bases

In proving that $\mathcal{B}_0(S)$ is a Markov basis for a given S, we employ the norm-reduction argument of Takemura and Aoki [2005] and Aoki and Takemura [2003]. Suppose that we have two tables X and Y in the same fiber $\mathcal{F}$. Denote

$$X - Y = \{x_{ij} - y_{ij}\}_{(i,j)\in\mathcal{I}}$$

and define the L_1-norm of $X - Y$ by $\|X - Y\|_1 = \sum_{(i,j)\in\mathcal{I}} |x_{ij} - y_{ij}|$. We define that $\|X - Y\|_1$ can be reduced (in several steps) by $\mathcal{B}_0(S)$ as follows.

Definition 2. *For $X \neq Y$ in the same fiber $\mathcal{F}$, we say that $\|X-Y\|_1$ can be reduced by $\mathcal{B}_0(S)$ if there exist $\tau^+ \geq 0, \tau^- \geq 0$, $\tau^+ + \tau^- > 0$, and sequences of moves $B_t^+ \in \mathcal{B}_0(S)$, $t = 1, \ldots, \tau^+$, and $B_t^- \in \mathcal{B}_0(S)$, $t = 1, \ldots, \tau^-$, satisfying*

$$\begin{cases} \|X - Y + \sum_{t=1}^{\tau^+} B_t^+ + \sum_{t=1}^{\tau^-} B_t^- \|_1 < \|X-Y\|_1, \\ X + \sum_{t=1}^{\tau'} B_t^+ \in \mathcal{F}, \quad \textit{for} \quad \tau' = 1, \ldots, \tau^+, \\ Y - \sum_{t=1}^{\tau'} B_t^- \in \mathcal{F}, \quad \textit{for} \quad \tau' = 1, \ldots, \tau^-. \end{cases} \tag{3}$$

In Takemura and Aoki [2005] we have mainly considered the case that $\|X-Y\|_1$ can be reduced in one step: $\tau^+ + \tau^- = 1$. However as discussed in Section 4.2 of Takemura and Aoki [2005], it is clear that $\mathcal{B}_0(S)$ is a Markov basis for A_S if for every fiber $\mathcal{F}(\boldsymbol{b})$ and for every $X \neq Y$ in $\mathcal{F}(\boldsymbol{b})$, $\|X-Y\|_1$ can always be reduced by $\mathcal{B}_0(S)$. Here the number of steps $\tau^+ + \tau^-$ needed to reduce $\|X-Y\|_1$ can depend on X and Y. Therefore we consider a condition that $\|X-Y\|_1$ can be reduced by $\mathcal{B}_0(S)$.

As in Aoki and Takemura [2003], we look at the patterns of the signs of $X-Y$. Suppose that $X-Y$ has the pattern of signs as in Figure 1-(i). This means

$$x_{i'j} < y_{i'j}, \quad x_{ij'} < y_{ij'}$$

and the signs of $x_{ij} - y_{ij}$ and $x_{i'j'} - y_{i'j'}$ are arbitrary. Henceforth let $*$ represent that the sign of the cell is arbitrary as in Figure 1. Because $x_{i'j} \geq 0$, $x_{ij'} \geq 0$, we have

$$y_{i'j} > 0, \quad y_{ij'} > 0.$$

Therefore for $B^- = (i,j)(i',j') - (i,j')(i',j) \in \mathcal{B}_0(S)$, we have $Y - B^- \in \mathcal{F}$ and we note that $\|X - Y + B^-\|_1 \leq \|X-Y\|_1$ regardless of the signs of $x_{ij} - y_{ij}$ and $x_{i'j'} - y_{i'j'}$. If $x_{ij} \leq y_{ij}$ and $x_{i'j'} \leq y_{i'j'}$,

$$\|X - Y + B^-\|_1 = \|X-Y\|_1.$$

On the other hand, if $x_{ij} > y_{ij}$ or $x_{i'j'} > y_{i'j'}$, i.e. $X-Y$ has the pattern of signs as in Figure 2-(i) or (ii), we have

$$\|X - Y + B^-\|_1 < \|X-Y\|_1. \tag{4}$$

In this case $\tau^+ = 0$, $\tau^- = 1$ and $B_1^- = B^-$ satisfy (3). By interchanging the role of X and Y, we can see that the patterns in (i) and (ii) in Figure 1 are interchangeable. Hence similar argument can be done for the patterns (ii) in Figure 1 and (iii), (iv) in Figure 2.

Denote $Z = Z_0 = X - Y$. For a sequence of basic moves $B_t \in \mathcal{B}_0(S)$, $t = 1, \ldots, \tau$ denote $Z_t = X - Y + B_1 + \cdots + B_t$, $t = 1, \ldots, \tau$. Based on the above arguments, we obtain the following lemma. The proof is easy and omitted.

Lemma 1. *$\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$ if there exist $\tau > 0$ and a sequence of basic moves $B_t \in \mathcal{B}_0(S)$, $t = 1, \ldots, \tau$ such that Z_t, $t = 0 \ldots, \tau - 1$, have either of the sign patterns in Figure 1 and Z_τ has either of the patterns in Figure 2.*

This lemma will be repeatedly used from Section 3.3 on.

$$\begin{array}{ccc} & j & j' \\ i & * & - \\ i' & - & * \end{array} \qquad \begin{array}{ccc} & j & j' \\ i & * & + \\ i' & + & * \end{array}$$

(i) (ii)

Figure 1: Patterns of signs in a 2×2 subtable

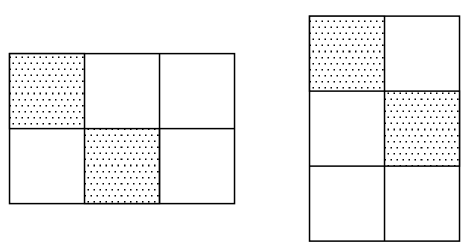
$$\begin{array}{ccc} & j & j' \\ i & + & - \\ i' & - & * \end{array} \qquad \begin{array}{ccc} & j & j' \\ i & * & - \\ i' & - & + \end{array} \qquad \begin{array}{ccc} & j & j' \\ i & - & + \\ i' & + & * \end{array} \qquad \begin{array}{ccc} & j & j' \\ i & * & + \\ i' & + & - \end{array}$$

(i) (ii) (iii) (iv)

Figure 2: Patterns of signs in a 2×2 subtable

3 A necessary and sufficient condition

In this section we give a necessary and sufficient condition on the subtable sum problem so that a Markov basis consists of basic moves, i.e. $\mathcal{B}_0(S)$ forms a Markov basis for A_S. Figure 3 shows patterns of 2×3 and 3×2 tables. A shaded area shows a cell belonging to S. Henceforth let a shaded area represent a cell belonging to S or rectangular blocks of cell belonging to S. We call these two patterns in Figure 3 the pattern $\mathcal{P}$ and $\mathcal{P}^t$, respectively. Then a necessary and sufficient condition is expressed as follows.



$\mathcal{P}$ $\mathcal{P}^t$

Figure 3: The pattern $\mathcal{P}$ and $\mathcal{P}^t$

Theorem 1. *$\mathcal{B}_0(S)$ is a Markov basis for A_S if and only if there exist no patterns of the form $\mathcal{P}$ or $\mathcal{P}^t$ in any 2×3 and 3×2 subtable of S or S^c after any interchange of rows and columns.*

We give a proof of Theorem 1 in the following subsections. Note that if $\mathcal{B}_0(S)$ is a Markov basis for A_S, then it is the *unique minimal Markov basis*, because the basic moves in $\mathcal{B}_0(S)$ are all indispensable.

The outline of this section is as follows. Section 3.1 gives a proof of the necessary condition. In Section 3.2 we introduce two patterns of S, 2×2 block diagonal set and triangular set, and show that S or S^c contain patterns of the form $\mathcal{P}$ or $\mathcal{P}^t$ if and only if S is equivalent to either of the two patterns. Then the sufficiency can be rewritten that $\mathcal{B}_0(S)$ forms a Markov basis for S equivalent to a 2×2 block diagonal set or a triangular set. In Section 3.3 we prepare some ingredients to prove the sufficiency. In Section 3.4 and Section 3.5 we show proofs of the sufficient condition for 2×2 block diagonal set and triangular set, respectively.

3.1 A proof of the necessary condition

The necessary condition of Theorem 1 is easy to prove.

Proposition 1. *If S or S^c contains the pattern $\mathcal{P}$ or $\mathcal{P}^t$, $\mathcal{B}_0(S)$ is not a Markov basis for A_S.*

Proof. Assume that S has the pattern $\mathcal{P}$. Without loss of generality we can assume that $\mathcal{P}$ belongs to $\{(i,j) \mid i = 1,2,\ j = 1,2,3\}$. Consider a fiber such that

- $x_{1+} = x_{2+} = 2$, $x_{+1} = x_{+2} = 1$, $x_{+3} = 2$;
- $x_{i+} = 0$ and $x_{+j} = 0$ for all $(i,j) \notin \{(i,j) \mid i = 1,2,\ j = 1,2,3\}$;
- $\sum_{(i,j) \in S} x_{ij} = 1$;

Then it is easy to check that this fiber has only two elements shown in Figure 4. Hence the difference of these two tables

$$B = \begin{array}{|r|r|r|} \hline 1 & 1 & -2 \\ \hline -1 & -1 & 2 \\ \hline \end{array} \qquad (5)$$

is an indispensable move. Therefore if S has the pattern $\mathcal{P}$, there does not exist a Markov basis consisting of basic moves. When S has the pattern $\mathcal{P}^t$, a proof is similar.

□

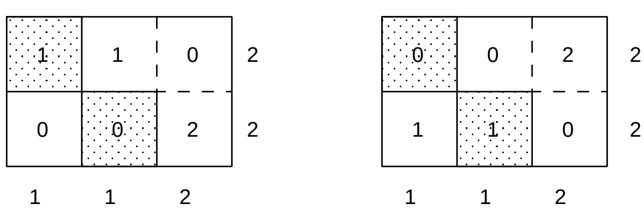


Figure 4: Two elements of the fiber

It is of interest to note that the toric ideal for the 2×3 table with the pattern $\mathcal{P}$ of S is a principal ideal generated by a single binomial corresponding to (5) whose both monomials are non-square-free.

3.2 Block diagonal sets and triangular sets

After an appropriate interchange of rows and columns, if S satisfies that

$$S = \{(i, j) \mid i \le r, j \le c\} \cup \{(i, j) \mid i > r, j > c\}$$

for some $r < R$ and $c < C$, we say that S is equivalent to a 2×2 block diagonal set. Figure 5 shows a 2×2 block diagonal set. A 2×2 block diagonal set is decomposed into four blocks consisting of one or more cells. We index each of the four blocks as in Figure 5. Note that S is a 2×2 block diagonal set if and only if S^c is a 2×2 block diagonal set.

For a row index i, let $\mathcal{J}(i) = \{j | (i, j) \in S\}$ denote a slice of S at row i. If for every pair i and i', either $\mathcal{J}(i)$ is a subset of $\mathcal{J}(i')$ or $\mathcal{J}(i)$ is a superset of $\mathcal{J}(i')$, we say that S is equivalent to a *triangular set*. A triangular set is expressed as in Figure 6 after an appropriate interchange of rows and columns. In general, if we allow transposition of tables, triangular sets can be decomposed into $n \times (n + 1)$ or $n \times n$ blocks as in Figure 6. Figure 6 shows examples of $n \times (n + 1)$ and $n \times n$ triangular sets with $n = 4$. We index each block as in Figure 6. Let $\mathcal{F}^T$ be a fiber of an $n \times (n + 1)$ triangular set. Define $\mathcal{J}_{n+1} = \{j \mid (i, j) \in \mathcal{I}_{k,n+1}\}$. Then we note that if $\mathcal{F}^T$ satisfies $\sum_{i=1}^{R} x_{ij} = 0$ for all $j \in \mathcal{J}_{n+1}$, the fiber is equivalent to a fiber for an $n \times n$ triangular set. Hence an $n \times n$ triangular set is interpreted as a special case of an $n \times (n + 1)$ triangular set. Hereafter we consider only $n \times (n + 1)$ triangular sets and let a triangular set mean $n \times (n + 1)$ triangular set. Note also that S is a triangular set if and only if S^c is a triangular set. In other words, a triangular set is symmetric with respect to 180° rotation of the table.

Proposition 2. *There exist no patterns of the form $\mathcal{P}$ or $\mathcal{P}^t$ in any 2×3 and 3×2 subtable of S after any interchange of rows and columns if and only if S is equivalent to a 2×2 block diagonal set or a triangular set.*

Proof. Assume that S does not contain $\mathcal{P}$ and $\mathcal{P}^t$ and that S contains a (cell-wise) 2×2 crossing sub-pattern presented in Figure 7. Without loss of generality the crossing pattern belongs to $\{(i, j) \mid i = 1, 2, j = 1, 2\}$. Since S does not contain $\mathcal{P}$ and $\mathcal{P}^t$, $\{(i, j) \mid i = 1, 2\}$ and $\{(i, j) \mid j = 1, 2\}$ have to have the pattern as in Figure 8 after an appropriate

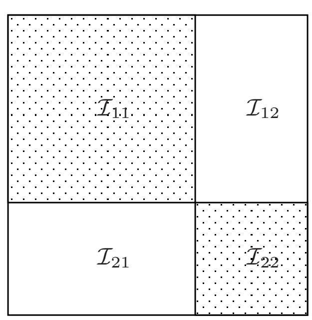


Figure 5: 2×2 block diagonal set

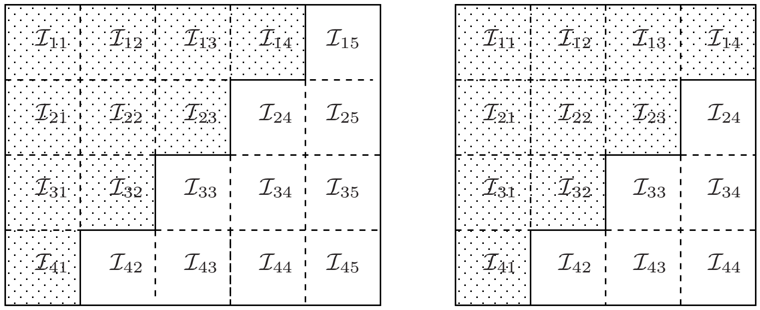


Figure 6: (block-wise) 4×5 and 4×4 triangular sets

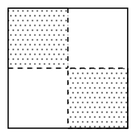


Figure 7: 2×2 (cell-wise) crossing pattern

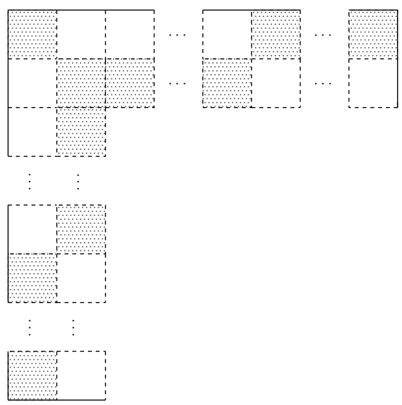


Figure 8: The pattern of $\{(i, j) \mid i = 1, 2\}$ and $\{(i, j) \mid j = 1, 2\}$

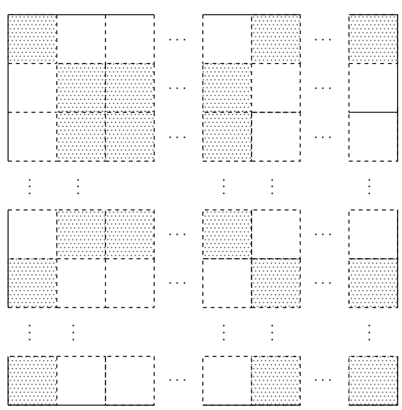


Figure 9: The pattern of S which has a (cell-wise) 2×2 crossing pattern

interchange of rows and columns. In the same way the rest of the table $\{(i,j) \mid i \geq 3, j \geq 3\}$ has to have the pattern as in Figure 9. It is clear that the pattern in Figure 9 is equivalent to a 2×2 block diagonal pattern after interchanging rows and columns.

From the definition of triangular set, S is not equivalent to a triangular set if and only if there exists i, i', $i \neq i'$, and j, j', $j \neq j'$, such that $j \in \mathcal{J}(i)$, $j \notin \mathcal{J}(i')$, $j' \in \mathcal{J}(i')$ and $j' \notin \mathcal{J}(i)$. But this is equivalent to the existence of a 2×2 crossing pattern. □

3.3 Signs of blocks

Based on Proposition 2, for the sufficient condition of Theorem 1 we only need to show that $\mathcal{B}_0(S)$ forms a Markov basis for S equivalent to a 2×2 block diagonal set or a triangular set. As mentioned above, a 2×2 block diagonal set and a triangular set can be decomposed into some rectangular blocks. In general each block consists of more than one cell. For the rest of this section, we use the following lemma.

Lemma 2. *Assume that S is equivalent to a 2×2 block diagonal set or a triangular set. Suppose that $Z = \{z_{ij}\}_{(i,j)\in\mathcal{I}}$ contains a block $\mathcal{I}_{kl}$ such that $(i,j) \in \mathcal{I}_{kl}$, $(i',j') \in \mathcal{I}_{kl}$, $z_{ij} > 0$ and $z_{i'j'} < 0$. Then $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$.*

Proof. Suppose that $j = j'$ and $i \neq i'$. Since any row sum of Z is zero, there exists j'' such that $z_{ij''} < 0$ as presented in Figure 10. Hence Z contains the sign pattern of Figure 1-(i) and $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$. When $i = i'$ and $j \neq j'$, we can show that $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$ in the similar way.

Next we consider the case where $i \neq i'$ and $j \neq j'$. If $z_{i'j} \neq 0$ or $z_{ij'} \neq 0$, we can reduce $\|Z\|_1$ by using the above argument regardless of the signs of them. So we suppose $z_{i'j} = 0$ and $z_{ij'} = 0$. There exists j'' such that $z_{ij''} < 0$ as presented in Figure 11-(i). If $(i,j'') \in \mathcal{I}_{kl}$, we can reduce $\|Z\|_1$ by using the above argument. If $(i,j'') \notin \mathcal{I}_{kl}$, let $B = (i,j'')(i',j') - (i,j')(i',j'') \in \mathcal{B}_0(S)$ and let $Z' = \{z'_{ij}\} = Z + B$. Since $z_{ij''} < 0$ and $z_{i'j'} < 0$, we have $\|Z'\|_1 \leq \|Z\|_1$. We also have $z'_{ij} > 0$ and $z'_{ij'} < 0$. Since $(i,j), (i,j') \in \mathcal{I}_{kl}$, $\|Z'\|_1$ can be reduced by $\mathcal{B}_0(S)$. Therefore Z satisfies the condition of Lemma 1 and $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$. □

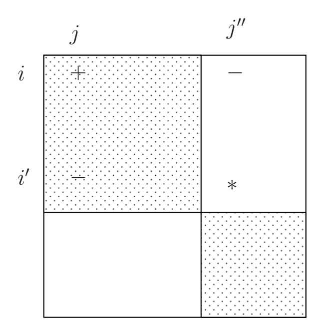


Figure 10: Z when $j = j'$

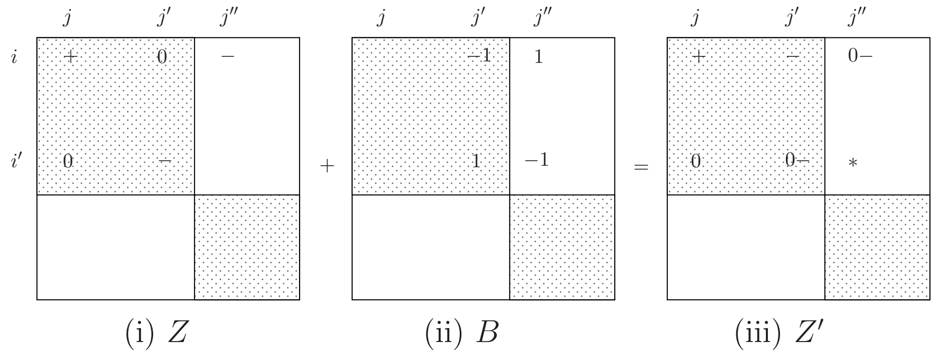


Figure 11: Z and Z'; when $j \neq j'$
("0−" represents the cell which is nonpositive)

Let "0+" and "0−" represent the cell which is nonnegative and nonpositive, respectively, as in Figure 11.

From Lemma 2 in order to prove the sufficient condition of Theorem 1, we only need to consider the case where Z does not have a block with both positive and negative cells. If all cells in $\mathcal{I}_{kl}$ are zeros, we denote it by $\mathcal{I}_{kl} = 0$. If $\mathcal{I}_{kl} \neq 0$ and all nonzero cells in $\mathcal{I}_{kl}$ are positive, we denote it by $\mathcal{I}_{kl} > 0$ and we say $\mathcal{I}_{kl}$ is positive. We define $\mathcal{I}_{kl} < 0$, $\mathcal{I}_{kl} \geq 0$ and $\mathcal{I}_{kl} \leq 0$ in the similar way. Then we say $\mathcal{I}_{kl}$ is negative, nonnegative and nonpositive, respectively. Then we obtain the following lemma.

Lemma 3. *Assume that S is equivalent to a triangular set. Suppose that Z has four blocks $\mathcal{I}_{kl}$, $\mathcal{I}_{k'l}$, $\mathcal{I}_{kl'}$ and $\mathcal{I}_{k'l'}$ which have either of the patterns of signs as follows,*

$$\begin{array}{ccc} & l & l' \\ k & + & - \\ k' & - & * \end{array} \qquad \begin{array}{ccc} & l & l' \\ k & * & - \\ k' & - & + \end{array} \qquad \begin{array}{ccc} & l & l' \\ k & - & + \\ k' & + & * \end{array} \qquad \begin{array}{ccc} & l & l' \\ k & * & + \\ k' & + & - \end{array}$$

(i) (ii) (iii) (iv)

where $*$ represents that the sign of the block is arbitrary. If there exist i, i', j, j' such that $(i,j) \in \mathcal{I}_{kl}$, $(i',j) \in \mathcal{I}_{k'l}$, $(i,j') \in \mathcal{I}_{kl'}$ $(i',j') \in \mathcal{I}_{k'l'}$, and $B(i,i';j,j') = (i,j)(i',j') - (i,j')(i',j) \in \mathcal{B}_0(S)$, then $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$.

Proof. Assume that the four blocks have the pattern of signs (i) and that

$$z_{i_b j_b} < 0, \quad (i_b, j_b) \in \mathcal{I}_{k'l}, \quad z_{i_c j_c} < 0, \quad (i_c, j_c) \in \mathcal{I}_{kl'}.$$

We note that $(i_c, j_b) \in \mathcal{I}_{kl}$. If $z_{i_c j_b} > 0$ or $z_{i_b j_c} > 0$, $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$. Suppose $z_{i_c j_b} = z_{i_b j_c} = 0$. Let $B = (i_b, j_b)(i_c, j_c) - (i_b, j_c)(i_c, j_b)$. Denote $Z' = \{z'_{ij}\}_{(i,j)\in\mathcal{I}} = Z + B$. Then we have $z'_{i_c j_b} < 0$. Since there exists $(i_a, j_a) \in \mathcal{I}_{kl}$ such that $z'_{i_a j_a} > 0$, Z' has both positive and negative cells in $\mathcal{I}_{kl}$. Hence $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$ from Lemma 1. Proofs for the other patterns are the same by symmetry. □

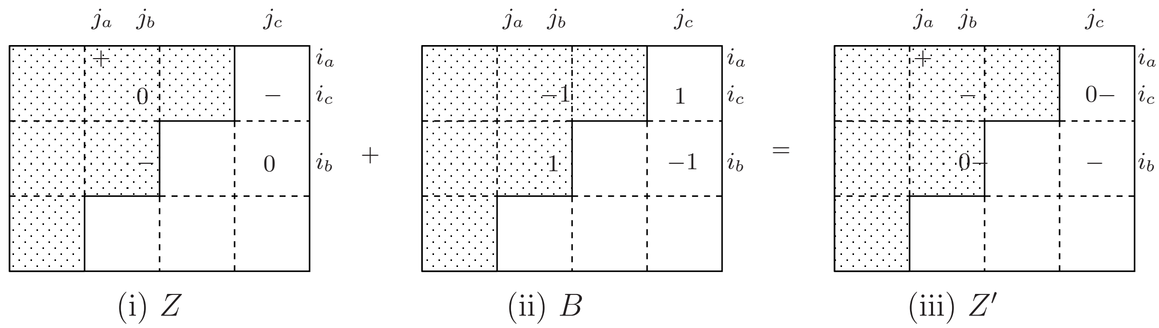


Figure 12: Z and Z' when $z_{i_c j_b} = z_{i_b j_c} = 0$

3.4 The sufficient condition for 2×2 block diagonal sets

In this subsection we give a proof of the sufficient condition of Theorem 1 when S is equivalent to a 2×2 block diagonal set.

Proposition 3. *If S is equivalent to a 2×2 block diagonal set, $\mathcal{B}_0(S)$ is a Markov basis for A_S.*

Proof. Suppose that $Z \neq 0$. If Z contains a block $\mathcal{I}_{kl}$ which has both positive and negative cells, $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$ from Lemma 1.

Next we suppose that all four blocks are nonnegative or nonpositive. Without loss of generality we can assume that $\mathcal{I}_{11} \geq 0$. Since all row sums and column sums of Z are zeros, we have $\mathcal{I}_{12} \leq 0$, $\mathcal{I}_{21} \leq 0$ and $\mathcal{I}_{22} \geq 0$. On the other hand, since $\sum_{(i,j)\in S} z_{ij} = 0$, we have $\mathcal{I}_{22} \leq 0$. However this implies $Z = 0$ and contradicts the assumption. $\square$

3.5 The sufficient condition for triangular sets

In this subsection we give a proof of the sufficient condition of Theorem 1 when S is equivalent to an $n \times (n+1)$ triangular set in Figure 6. We only need to consider this case if we allow transposition of the tables and because of the fact that an $n \times n$ triangular set can be considered as a special case of an $n \times (n+1)$ triangular set as discussed in Section 3.2.

In general, as mentioned, each block consists of more than one cell. However for simplicity we first consider the case where every block consists of one cell. As seen at the end of this section, actually it is easy to prove the sufficient condition of Theorem 1 for general triangular set, once it is proved for the triangular sets with each block consisting of one cell. Therefore the main result of this section is the following proposition.

Proposition 4. *Suppose that S is equivalent to an $n \times (n+1)$ triangular set in Figure 6 and every block consists of one cell. Then $\mathcal{B}_0(S)$ is a Markov basis for A_S.*

We prove this proposition based on a series of lemmas. In all lemmas we assume that S is equivalent to an $n \times (n+1)$ triangular set. If $n = 1$, each fiber has only one element. Hence we assume that $n \geq 2$.

Lemma 4. *If Z contains a row i_a such that the signs of z_{i_a1} and $z_{i_a,n+1}$ are different, then $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$.*

Proof. Without loss of generality we can assume that $z_{i_a1} > 0$ and $z_{i_a,n+1} < 0$. Since $\sum_{i=1}^{n} z_{i,n+1} = 0$, there exists i_b such that $z_{i_b,n+1} > 0$ as presented in Figure 13. Hence if we set $B = (i_a, n+1)(i_b, 1) - (i_a, 1)(i_b, n+1)$, $B \in \mathcal{B}_0(S)$ and $\|Z + B\|_1 < \|B\|_1$. □

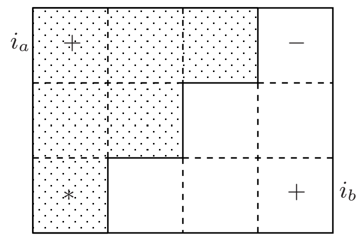


Figure 13: The case of $n = 3$, $i_a = 1$ and $i_b = 3$

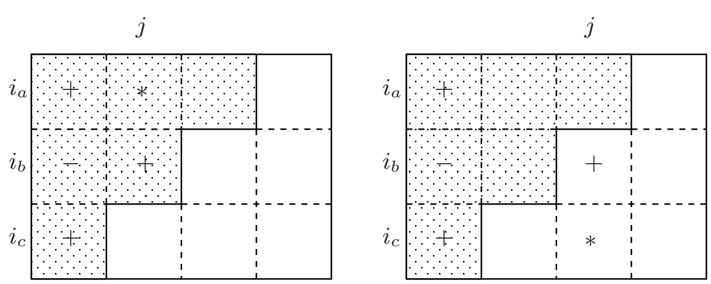
Lemma 5. *Suppose that Z has three rows $i_a < i_b < i_c$ satisfying either of the following conditions,*

(i) $z_{i_a1} > 0$, $z_{i_b1} < 0$ *and* $z_{i_c1} > 0$*;*

(ii) $z_{i_a1} < 0$, $z_{i_b1} > 0$ *and* $z_{i_c1} < 0$*;*

Then $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$.

Proof. It suffices to prove the case of (i). Since $z_{i_b1} < 0$, there exists j such that $2 \leq j \leq n+1$ and $z_{i_bj} > 0$. If $(i_b, j) \in S$ as presented in Figure 14-(i), $B = (i_a, j)(i_b, 1) - (i_a, 1)(i_b, j) \in \mathcal{B}_0(S)$ and $\|Z + B\|_1 < \|Z\|_1$. If $(i_b, j) \notin S$ as presented in Figure 14-(ii), $B' = (i_c, j)(i_b, 1) - (i_c, 1)(i_b, j) \in \mathcal{B}_0(S)$ and $\|Z + B'\|_1 < \|Z\|_1$. □



(i) $(i_b, j) \in S$ (ii) $(i_b, j) \notin S$

Figure 14: The case of $n = 3$, $i_a = 1$, $i_b = 2$ and $i_c = 3$

Lemma 6. *Suppose that Z contains four rows i_a, i_b, i_c and i_d satisfying*

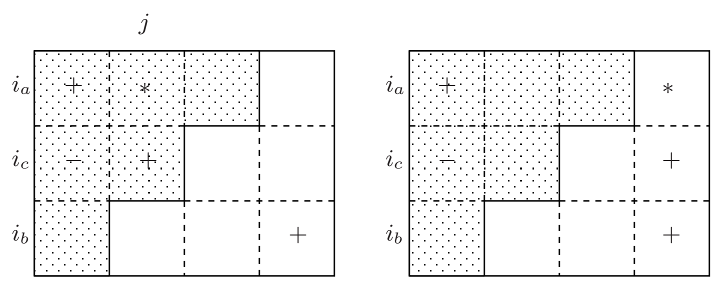
$$z_{i_a 1} > 0, \quad z_{i_b,n+1} > 0, \quad z_{i_c 1} < 0 \quad \text{and} \quad z_{i_d,n+1} < 0$$

and satisfying either of the following conditions,

$$\text{(i) } i_a < i_c < i_b, \quad \text{(i}'\text{) } i_a < i_d < i_b, \quad \text{(ii) } i_b < i_c < i_a, \quad \text{(ii}'\text{) } i_b < i_d < i_a \ .$$

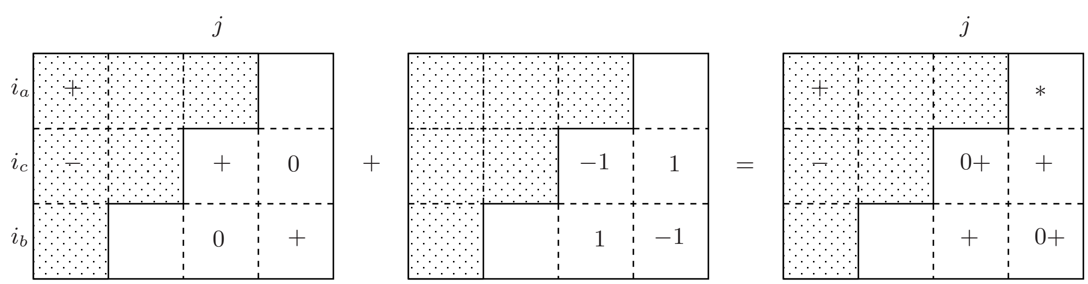
Then $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$.

Proof. Suppose (i) $i_a < i_c < i_b$. Since any row sum is zero, there exists j such that $z_{i_c j} > 0$ and $j \geq 2$. If $(i_c, j) \in S$ or $j = n+1$, $B = (i_a, j)(i_c, 1) - (i_a, 1)(i_c, j) \in \mathcal{B}_0(S)$ and $\|Z + B\|_1 < \|Z\|_1$ (Figure 15 shows an example for this case). Suppose that $(i_c, j) \in S^c$ and $j \neq n+1$. If $z_{i_c,n+1} < 0$, $B = (i_b, j)(i_c, n+1) - (i_b, n+1)(i_c, j) \in \mathcal{B}_0(S)$ and $\|Z + B\|_1 < \|Z\|_1$. If $z_{i_c,n+1} = 0$, $\|Z'\|_1 = \|Z + B\|_1 \leq \|Z\|_1$ and $z'_{i_c,n+1} > 0$. Since $z'_{i_a,1} > 0$ and $z'_{i_c,1} < 0$, $\|Z_1\|$ can be reduced by $\mathcal{B}_0(S)$. Hence $\|Z\|_1$ can be also reduced by $\mathcal{B}_0(S)$ (Figure 16 shows an example for this case).



(i) $(i_c, j) \in S$ (ii) $j = n+1$

Figure 15: The case of $n = 3$ and $i_a < i_c < i_b$

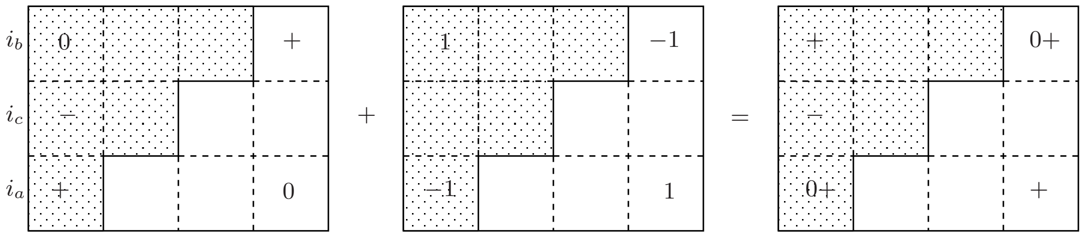


(i) Z (ii) B (iii) Z'

Figure 16: The case of $n = 3$ and $i_a < i_c < i_b$

In the case (i') $i_a < i_d < i_b$, we can prove the lemma in the same way by the symmetry of $n \times (n+1)$ triangular pattern.

Suppose that (ii) $i_b < i_c < i_a$ or (ii') $i_b < i_d < i_a$. If $z_{i_a,n+1} < 0$ or $z_{i_b,1} < 0$, the lemma holds from Lemma 4. So we suppose that $z_{i_a,n+1} \geq 0$ and $z_{i_b,1} \geq 0$. Let



(i) Z (ii) B (iii) Z'

Figure 17: The case of $n = 3$ and $i_b < i_c < i_a$

$B = (i_a, n+1)(i_b, 1) - (i_a, 1)(i_b, n+1)$. Then we have $\|Z'\| = \|Z + B\|_1 \le \|Z\|_1$ and $z'_{i_a,n+1} > 0$, $z'_{i_b,1} > 0$. Since $z'_{i_c,1} = z_{i_c,1} < 0$ and $z'_{i_d,n+1} = z_{i_d,n+1} < 0$, we can prove the lemma by applying the above argument (Figure 17 shows an example for this case). $\square$

From the definition of L_1-norm, $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$, if and only if $\|-Z\|_1$ can be reduced by $\mathcal{B}_0(S)$. Thus without loss of generality we can assume that $z_{11} \ge 0$. From Lemma 4, 5 and 6, it suffices to show that $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$ if Z satisfies

$$\begin{cases} \exists i_0 \ge 1 \quad \text{s.t.} \\ z_{i1} \ge 0 \quad \text{and} \quad z_{i,n+1} \ge 0 \quad \text{for} \quad i \le i_0, \\ z_{i1} \le 0 \quad \text{and} \quad z_{i,n+1} \le 0 \quad \text{for} \quad i > i_0, \end{cases} \tag{6}$$

as shown in Figure 18.

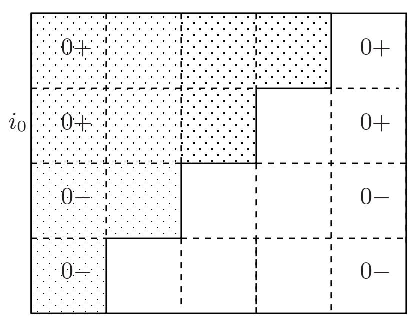


Figure 18: The case of $n = 4$ and $i_0 = 2$

We look at rows of Figure 18 from the bottom and find the last row i_1 such that at least one of $z_{i_1 1}$ or $z_{i_1,n+1}$ is negative, i.e., define i_1 by the following conditions.

$$\begin{array}{ll} \text{(i)} & z_{i_1 1} \le 0 \text{ and } z_{i_1,n+1} \le 0; \\ \text{(ii)} & z_{i_1 1} < 0 \text{ or } z_{i_1,n+1} < 0; \\ \text{(iii)} & z_{i1} = 0 \text{ and } z_{i,n+1} = 0 \text{ for } i > i_1; \end{array} \tag{7}$$

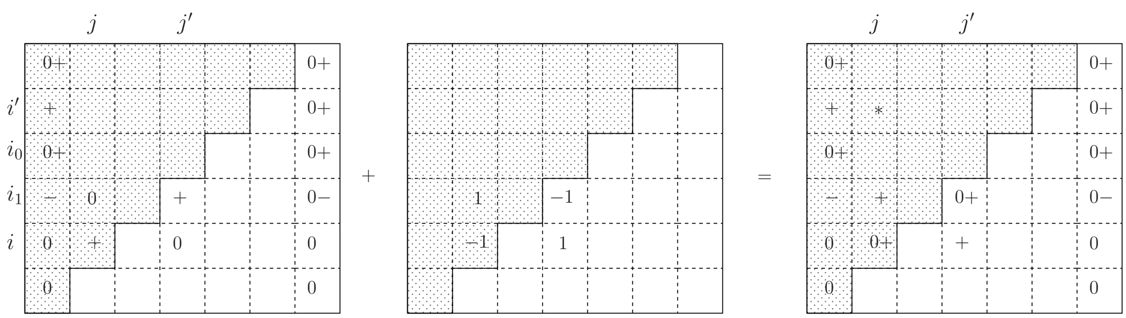
Note that if there exists no i_1 satisfying these conditions, then the first column and the last column of the table consists of only zeros and we can use the induction on n. Therefore for Lemmas 7–9 below, we assume that there exists i_1 satisfying (7). We also note that $i_1 > i_0$ when i_1 exists.

Lemma 7. *Suppose Z satisfies (6) and define i_1 by (7) assuming that i_1 exists. $\|Z\|_1$ can be reduced if there exists $z_{ij} > 0$ for some $(i, j) \in S$ and $i \geq i_1$.*

Proof. Consider the case $z_{i_1 1} < 0$. We note that there has to exist $i' < i_0$ such that $z_{i'1} > 0$ from the condition (6). Suppose that $i = i_1$. Let B be $B = (i_1, 1)(i', j) - (i_1, j)(i', 1)$. Then $\|Z + B\|_1 < \|Z\|_1$. Suppose that $i > i_1$ and $z_{i_1 j} \leq 0$ for $(i_1, j) \in S$. There has to exist j' such that $z_{i_1 j'} > 0$. Let $B = (i_1, j)(i, j') - (i_1, j')(i, j)$. If $z_{i_1 j} < 0$ or $z_{ij'} < 0$, $\|Z'\|_1 = \|Z + B\|_1 < \|Z\|_1$. If $z_{i_1 j} = 0$ or $z_{ij'} = 0$, $\|Z'\|_1 = \|Z + B\|_1 \leq \|Z\|_1$. As shown in Figure 19, since $z'_{i'1} > 0$, $z'_{i_0 1} < 0$ and $z'_{i_0 j} > 0$, $\|Z'\|$ can be reduced by $\mathcal{B}_0(S)$. Hence $\|Z\|_1$ can also be reduced by $\mathcal{B}_0(S)$.

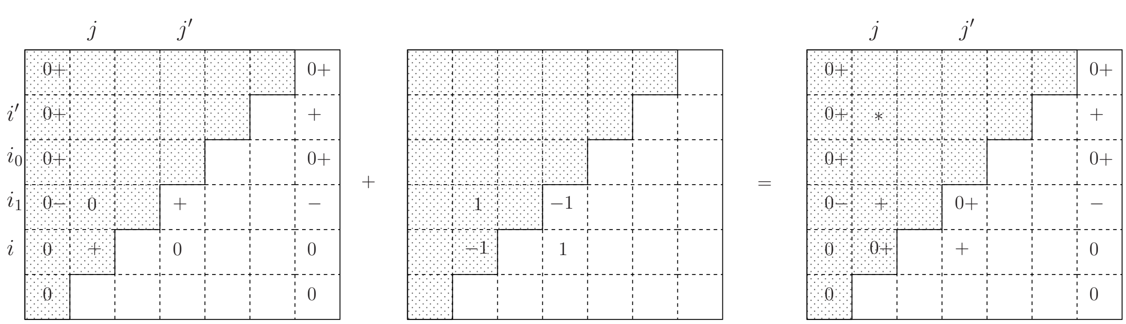
Next we consider the case $z_{i_1, n+1} < 0$. Then there has to exist $i' < i_0$ such that $z_{i', n+1} > 0$ from the condition (6). When $i = i_1$, let $B = (i_1, n+1)(i', j) - (i_1, j)(i', n+1)$. Then $\|Z + B\|_1 < \|Z\|_1$. When $i > i_1$ and $z_{i_1 j} \leq 0$ for $(i_1, j) \in S$, a similar proof to the case $z_{i_1 1} < 0$ can be given as shown in Figure 20

□



(i) Z (ii) B (iii) Z'

Figure 19: The case of $n = 6$, $(i_0, i_1, i, i', j, j') = (3, 4, 5, 2, 2, 4)$ and $z_{i_1 1} < 0$



(i) Z (ii) B (iii) Z'

Figure 20: The case of $n = 6$, $(i_0, i_1, i, i', j, j') = (3, 4, 5, 2, 2, 4)$ and $z_{i_1, n+1} < 0$

We define some more sets. Let $\bar{S}^c$ and $\bar{S}^c_i$, $i = 2, \ldots, n$, be the sub-triangular set of S^c defined as

$$\bar{S}^c = \{(i', j') \in S^c \mid j' \neq n+1\}, \quad \bar{S}^c_i = \{(i', j') \in S^c \mid i' < i,\ j' \neq n+1\},$$

respectively. Figure 21 shows $\bar{S}^c$ and $\bar{S}^c_i$ for $n = 4$, $i = 4$. We note that

$$\sum_{(i,j)\in \bar{S}^c} z_{ij} = 0 \tag{8}$$

for all Z, because the last column sum is zero and $\sum_{(i,j)\in S^c} z_{ij} = 0$. We also define $\bar{S}^-_i$, $i = 2, \ldots, n$, by

$$\bar{S}^-_i = \{(i', j') \in \bar{S}^c_i \mid z_{i'j'} < 0\}.$$

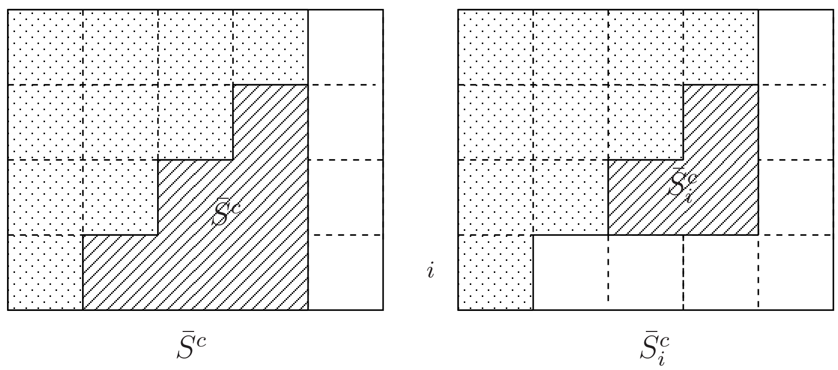


Figure 21: $\bar{S}^c$ and $\bar{S}^c_i$ for $n = 4$ and $i = 4$

From Lemma 7 it suffices to consider Z such that $z_{ij} \leq 0$ for all $(i, j) \in S$ and $i \geq i_1$. The following lemma states a property of such a Z.

Lemma 8. *Suppose that Z satisfies (6) and define i_1 by (7) assuming that i_1 exists. Furthermore assume that $z_{ij} \leq 0$ for all $(i, j) \in S$, $i \geq i_1$. Then*

$$|z_{i_1 1} + z_{i_1,n+1}| \leq \sum_{(i,j)\in \bar{S}^-_{i_1}} |z_{ij}|. \tag{9}$$

Proof. Assume that

$$|z_{i_1 1} + z_{i_1,n+1}| > \sum_{(i,j)\in \bar{S}^-_{i_1}} |z_{ij}|.$$

Since the roles of $z_{i_1 1}$ and $z_{i_1,n+1}$ are interchangeable, we assume that $|z_{i_1 1}| > 0$. Then there exist nonnegative integers w^1_{ij}, w^{n+1}_{ij} and the set of cells $S' \subseteq \bar{S}^-_{i_1}$ and $S'' \subseteq \bar{S}^-_{i_1}$ satisfying

$$w^1_{ij} + w^{n+1}_{ij} \leq |z_{ij}|, \quad \sum_{(i,j)\in S'} w^1_{ij} + \sum_{(i,j)\in S''} w^{n+1}_{ij} = \sum_{(i,j)\in \bar{S}^-_{i_1}} |z_{ij}|.$$

$$\sum_{(i,j)\in S'} w^1_{ij} < |z_{i_1 1}|, \qquad \sum_{(i,j)\in S''} w^{n+1}_{ij} \le |z_{i_1,n+1}|.$$

S' and S'' may have overlap if $|z_{ij}| \ge 2$ for some cell $(i,j) \in \bar{S}^-_{i_1}$. For $(i,j) \in \bar{S}^-_{i_1}$, let $B^1(i,j)$ and $B^{n+1}(i,j)$ be defined by

$$B^1(i,j) = (i,j)(i_1,1) - (i,1)(i_1,j), \quad B^{n+1}(i,j) = (i,j)(i_1,n+1) - (i,n+1)(i_1,j).$$

We note that $B^1(i,j) \in \mathcal{B}_0(S)$ and $B^{n+1}(i,j) \in \mathcal{B}_0(S)$ for any $(i,j) \in \bar{S}^-_{i_1}$. Denote

$$Z' = \{z'_{ij}\}_{(i,j)\in\mathcal{I}} = Z + \sum_{(i,j)\in S'} w^1_{ij} B^1(i,j) + \sum_{(i,j)\in S''} w^{n+1}_{ij} B^{n+1}(i,j). \tag{10}$$

Then we have $z'_{i_1 1} < 0$, $z'_{i_1,n+1} \le 0$, and $z'_{ij} \ge 0$ for all $(i,j) \in \bar{S}^c_{i_1}$. This implies that

$$\sum_{(i,j)\in\bar{S}^c\setminus\bar{S}^c_{i_1}} z'_{ij} \le 0. \tag{11}$$

On the other hand from the condition of Lemma 8

$$\sum_{(i,j)\in\bar{S}^c\setminus\bar{S}^c_{i_1}} z'_{ij} = \sum_{i=i_1}^{n}\sum_{j=1}^{n+1} z'_{ij} - \Big(\sum_{i\ge i_1,\,(i,j)\in S} z'_{ij} + \sum_{i=i_1}^{n} z'_{i,n+1}\Big) > 0,$$

which contradicts (11) (See Figure 22). □

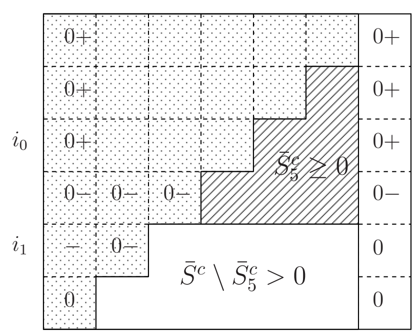


Figure 22: The case of $n = 6$ and $(i_0, i_1) = (3, 5)$

Lemma 9. *Suppose that Z satisfies (6) and the conditions of Lemma 8. Then*

(i) $i_1 \ge 3$;

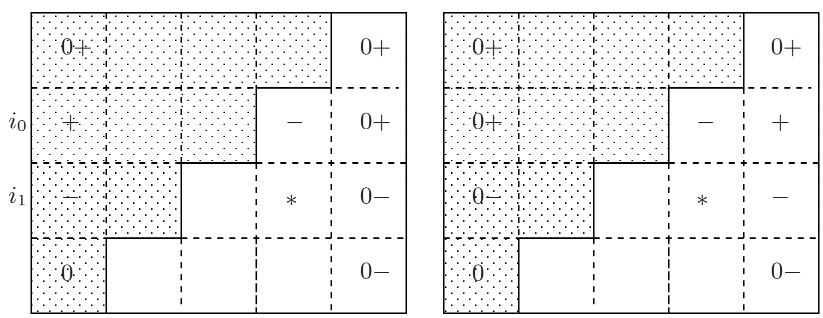
(ii) *If $i_1 = 3$, $\|Z\|_1$ can be reduced.*

Proof. (i) It is obvious that $i_1 \geq 2$. Suppose $i_1 = 2$. Since any row sum of Z is zero, we have

$$\sum_{(i,j)\in \bar{S}^c} z_{ij} > 0,$$

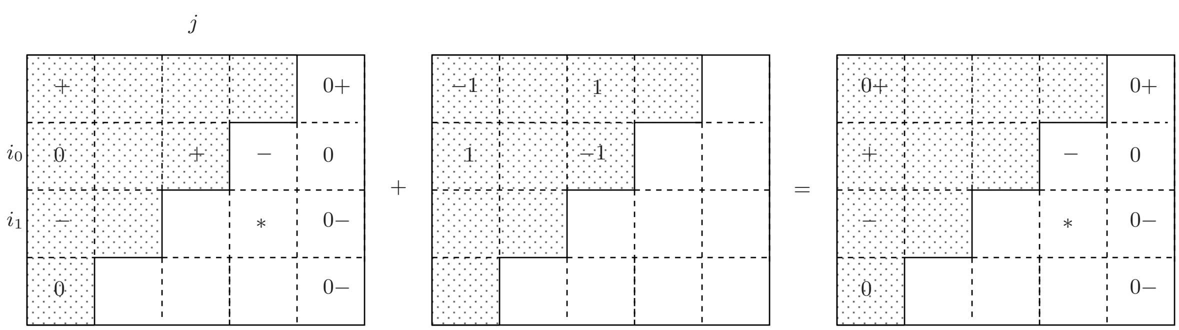
from (ii) and (iii) of (7). However this contradicts (8).

(ii) When $i_1 = 3$, $\bar{S}_3 = \{(2,n)\}$ and $z_{2n} < 0$ from Lemma 8. If $z_{21} > 0$, we have $z_{31} < 0$ from (iii) of (7). Therefore $B = (3,1)(2,n) - (2,1)(3,n)$ satisfies $\|Z+B\|_1 < \|Z\|_1$ (Figure 23-(i)). If $z_{2,n+1} > 0$, $z_{3,n+1} < 0$ from (iii) of (7). Hence $B = (2,n)(3,n+1) - (2,n+1)(3,n)$ satisfies $\|Z+B\|_1 < \|Z\|_1$(Figure 23-(ii)). Next we consider the case of $z_{21} = z_{2,n+1} = 0$. Then $z_{11} > 0$ or $z_{1,n+1} > 0$. Suppose that $z_{11} > 0$. This implies $z_{31} < 0$. Since $z_{2n} < 0$, there exists $2 \leq j \leq n-1$ such that $z_{2j} > 0$. Then if we set $B = (1,j)(2,1) - (1,1)(2,j)$, we have $\|Z'\|_1 = \|Z+B\|_1 \leq \|Z\|_1$ and $z'_{21} > 0$, $z'_{31} < 0$ and $z'_{2n} < 0$ (Figure 24). Then $\|Z'\|_1$ can be reduced by $\mathcal{B}_0(S)$. Therefore $\|Z\|_1$ can be also reduced by $\mathcal{B}_0(S)$. When $z_{1,n+1} > 0$, a proof is similar. □



(i) $z_{21} > 0$ (ii) $z_{25} > 0$

Figure 23: The case of $n = 4$ and $z_{21} > 0$ or $z_{25} > 0$



(i) Z (ii) B (iii) Z'

Figure 24: The case of $n = 4$, $z_{21} = 0$ and $z_{25} = 0$

By using Lemmas 4–9, we give a proof of Proposition 4.

Proof of Proposition 4. We prove this proposition by the induction on the number of rows n. Suppose that $n = 2$. Then

$$z_{1j} + z_{2j} = 0 \quad \text{for} \quad j = 1, 2, 3.$$

$$z_{11} + z_{12} + z_{21} = 0, \quad z_{22} + z_{13} + z_{23} = 0.$$

Hence $z_{12} = z_{22} = 0$. Therefore Z is equivalent to a move in the 2×2 pattern as in Figure 25 with fixed row sums and column sums. It is easy to see that that proposition holds for this pattern.

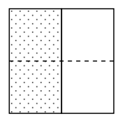


Figure 25: A 2×2 pattern

Suppose $n > 2$ and assume that this proposition holds for triangular sets smaller than $n \times (n + 1)$. From the results of Lemmas 4–9, it suffices to show that if Z satisfies (6) and the conditions of Lemma 8, $\|Z\|_1$ can be reduced by $\mathcal{B}_0(S)$. We prove this by the induction on i_1.

Suppose that $i_1^* > 3$ and assume that Z with $i_1 < i_1^*$ can be reduced by $\mathcal{B}_0(S)$. From Lemma 8, (9) holds. Thus there exist nonnegative integers w_{ij}^1, w_{ij}^{n+1} and the set of cells $S' \subseteq \bar{S}_{i_1}^-$ and $S'' \subseteq \bar{S}_{i_1}^-$ satisfying

$$w_{ij}^1 + w_{ij}^{n+1} \leq |z_{ij}|, \quad \sum_{(i,j) \in S'} w_{ij}^1 = |z_{i_1 1}|, \quad \sum_{(i,j) \in S''} w_{ij}^{n+1} = |z_{i_1, n+1}|.$$

Let Z' be defined as in (10). Then we have $\|Z'\|_1 \leq \|Z\|_1$. If $\|Z'\|_1 < \|Z\|_1$, this proposition holds. Suppose that $\|Z'\|_1 = \|Z\|_1$. Then Z' satisfies either of the following three conditions,

(i) $z'_{i1} = 0$ and $z'_{i,n+1} = 0$ for $i = 1, \ldots, n$;

(ii) there exists i such that $z'_{i1} \neq 0$ or $z'_{i,n+1} \neq 0$ and Z' does not satisfy (6).

(iii) there exists i such that $z'_{i1} \neq 0$ or $z'_{i,n+1} \neq 0$ and Z' satisfies (6).

In the case of (i), $\|Z'\|_1$ can be reduced by $\mathcal{B}_0(S)$ from the inductive assumption on n. In the case of (ii), $\|Z'\|_1$ can be reduced by by Lemma 6. In the case of (iii), noting that $z'_{i1} = 0$ and $z'_{i,n+1} = 0$ for $i \geq i_1$, $\|Z'\|_1$ can be reduced from the inductive assumption on i_1. □

So far we have given a proof when every block has only one cell. It remains to extend Proposition 4 to general triangular sets. Based on the results of Lemma 1 and 2, we see that Proposition 4 can be extended to the case where $n \geq 2$. Then it suffices to consider the case of $n = 1$ as in Figure 26.

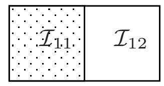


Figure 26: 1×2 triangular pattern

Lemma 10. *Suppose that S is equivalent to a 1×2 triangular set. Then $\mathcal{B}_0(S)$ is a Markov basis for A_S.*

Proof. Since Z satisfies $\sum_{(i,j)\in S} z_{ij} = 0$ and $\sum_{(i,j)\in S^c} z_{ij} = 0$, $Z \neq 0$ has to contain both positive and negative cells in at least one of $\mathcal{I}_{11}$ and $\mathcal{I}_{12}$. Hence $\|Z\|_1$ can be reduced from Lemma 1. □

Now we have completed a proof of the sufficient condition of Theorem 1 for general triangular set S.

4 Concluding remarks

In this paper we consider Markov bases consisting of square-free moves of degree two for two-way subtable sum problems. We gave a necessary and sufficient condition for the existence of a Markov basis consisting of square-free moves of degree two.

From our results, if S contains a pattern $\mathcal{P}$ or $\mathcal{P}^t$, a Markov basis has to include a move with degree higher than or equal to four. From theoretical viewpoint, it is interesting to study the structure of Markov bases for such cases. Our results may give insights into the problem. However it seems difficult at this point and left to our future research.

Consider a particular fiber with $x(S) = 0$ in the subtable sum problems. Then $x_{ij} = 0$ for all $(i, j) \in S$. This implies that this fiber is also a fiber for a problem where all cells of S are structural zeros. Therefore Markov bases for the subtable sum problems for S are also Markov bases for a problem where all cells of S are structural zeros. Various properties of Markov bases are known for structural zero problems. It is of interest to investigate which properties of Markov bases for structural zero problem for S can be generalized to subtable sum problem for S.

Ohsugi and Hibi have been investigating properties of Gröbner bases arising from finite graphs (Ohsugi and Hibi [1999a], Ohsugi and Hibi [1999b], Ohsugi and Hibi [2005]). With bipartite graphs, their problem is equivalent to two-way contingency tables with structural zeros. From the viewpoint of graphs of Ohsugi and Hibi, the subtable sum problem corresponds to a complete bipartite graph with two kinks of edges. It would be also very interesting to investigate subtable sum problem from the viewpoint of Gröbner bases.

We used the norm reduction argument to prove that $\mathcal{B}_0(S)$ is a Markov basis. It should be noted that $\mathcal{B}_0(S)$ for the subtable sum problem is not necessarily 1-norm reducing *in one step*, even when $\mathcal{B}_0(S)$ is the unique minimal Markov basis. Therefore the subtable sum problem is worth to be considered from the viewpoint of norm reduction by a Markov basis.

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