

## 分割表の列挙とグレブナー基底

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### Abstract

In this paper, we propose a Markov chain for sampling  $(m+1)$ -dimensional contingency tables indexed by  $\{1, 2\}^m \times \{1, 2, \dots, n\}$ . Stationary distribution of our chain is the uniform distribution. The mixing time of our chain is bounded by  $(1/2)n(n-1) \ln(dn/\varepsilon)$  where  $d$  is the average of the values in cells and  $\varepsilon$  is a given error bound. We use the path coupling method for estimating the mixing time of our chain and showed that our chain is rapidly mixing. Lastly, we introduce some results using Gröbner bases for enumerating all contingency tables.

## 1 Introduction

We propose a Markov chain for sampling  $(m+1)$ -dimensional contingency tables indexed by  $\{1, 2\}^m \times \{1, 2, \dots, n\}$ . Our chain has the uniform distribution as a unique stationary distribution. The mixing time of our chain is bounded by  $(1/2)n(n-1) \ln(dn/\varepsilon)$  where  $d$  is the average of the values in cells and  $\varepsilon$  is a given error bound. We use the path coupling method [5, 6] for estimating the mixing time of our chain.

Contingency tables are used in statistics to store data from sample surveys. Consider a scenario where  $N$  subjects are categorized into a table according to some attributes. Data is often analyzed under assumption that the attributes are independent; that is, the joint distribution is uniquely determined by the marginal probabilities. We often assume that each table was generated from the uniform distribution over the set of all the contingency tables (see [1, 2, 8, 15] for example). One of the commonly used measure of independence is the  $\chi^2$  statistics [23]. A typical test of the independence asks what fraction (the sum of probabilities) of tables have  $\chi^2$  value smaller than a parameter  $t$ , as  $t$  varies. When the marginal totals are sufficiently large, we can apply the Pearson chi-square test [23]. In case that marginal totals includes a small number, we need an exact inference for contingency tables [15]. For the analysis of  $2 \times 2$  contingency tables, an alternative to maximum likelihood estimation and  $\chi^2$  goodness-of fit tests is the use of Fisher's exact test for independence [16].

Exact test can be done by systematic enumeration of all the tables. When the number of tables is huge, exact enumeration is impractical. Mehta and Patel [22] proposed a network algorithm for exact counting (not for enumeration) of contingency tables. However, the computational efforts and memory requirement of their algorithm is bounded by the table sum and so impractical when the table sum is large. For estimating the moments of  $\chi^2$  statistics efficiently, a standard technique is the ordinary Monte Carlo method if we have a method for sampling from the set of contingency tables. By using a rapidly

mixing Markov chain with the desired stationary distribution, we can sample a contingency table after enough number of transitions of the Markov chain from arbitrary initial state.

It is known that the problem for generating 3-dimensional contingency tables is intractable. More precisely, when we deal with 3-dimensional tables, the problem for checking the existence of at least one table satisfying the given marginal totals is NP-complete [18]. Moreover Diaconis and Strumfels [11] proposed algebraic algorithms for finding Markov bases for higher dimensional contingency tables. Recently, Aoki and Takemura discussed Markov bases for some classes of 3-dimensional contingency tables [4, 27]. In this paper, we deal with a special class of  $(m + 1)$ -dimensional contingency tables such that the cells are indexed by  $\{1, 2\}^m \times \{1, 2, \dots, n\}$ . For this class, a natural Markov basis exists, which is a direct extension of 2-dimensional case. This class of contingency tables arises in many practical situations [14, 25]. There also exist some theoretical results on testing the independency of attributes of  $2 \times 2 \times K$  tables (see Agresti's survey paper [1] for example).

The problem of almost uniform sampling of contingency tables can be solved by using a Markov chain that converges to the uniform distribution. Diaconis and Saloff-Coste [10] discussed the rate of convergence of a natural Markov chain for 2-dimensional contingency tables. They have shown that the ordinary chain mixes polynomial time in the table sum when the numbers of rows and columns are fixed. Dyer, Kannan and Mount [13] proposed a different Markov chain for counting the number of 2-dimensional contingency tables. In case of sufficiently large marginal totals, their chain mixes polynomial time in the number of rows and columns. For 2-dimensional contingency tables with two rows, Hernek [17] showed that the mixing time of the ordinary Markov chain is bounded by a polynomial of table sum and number of columns. Hernek bounded the mixing time of the chain by using coupling lemma shown by Aldous [3]. Dyer and Greenhill [12] proposed a rapidly mixing Markov chain for two rowed contingency tables. Their chain mixes polynomial time in the logarithm of table sum and the number of columns. They analyzed the mixing rate of their chain by using path coupling technique proposed by Bubley and Dyer [5, 6]. Kannan, Tetali and Vempala [21] gave a Markov chain with polynomial-time convergence for the 0-1 case with nearly equal marginal totals. In contrast, Chung, Graham and Yau [7] proposed a Markov chain for contingency tables with large enough marginal sums and showed that their chain converges in pseudo polynomial time.

In Section 2, we introduce some notations and summarize the path coupling method. In Section 3, we describe our first chain whose stationary distribution is uniform. Section 4, we introduce some results using Gröbner bases for enumerating all contingency tables.

## 2 Notations and Definitions

We denote the set of integers (non-negative integers, positive integers) by  $Z$  ( $Z_+$ ,  $Z_{++}$ ), respectively. In this paper, we consider a set of  $(m + 1)$ -dimensional contingency tables indexed by  $B^m \times J$  where  $B = \{1, 2\}$  and  $J = \{1, 2, \dots, n\}$ . Any index in  $J$  is called a *column index*. For any vector  $x \in Z^{B^m \times J}$ , both  $x(i; j)$  and  $x(i_1, i_2, \dots, i_m; j)$  denote the element of  $x$  indexed by  $i = (i_1, i_2, \dots, i_m) \in B^m$  and  $j \in J$ . For any column index  $j \in J$ ,  $x(j) \in Z^{B^m}$  denotes the subvector of  $x \in Z^{B^m \times J}$  consists of elements defined by indices in  $B^m \times \{j\}$ . Given a vector of indices  $i \in B^m$  and an index  $l \in \{1, 2, \dots, m\}$ ,  $i_{\bar{l}}$  denotes the vector of indices  $(i_1, \dots, i_{l-1}, i_{l+1}, \dots, i_m) \in B^{m-1}$  and we also denote the vector  $i$  by  $(i_{\bar{l}}, i_l)$  by changing the order of elements. For any vector  $x \in Z^{B^m \times J}$  and  $l \in \{1, 2, \dots, m\}$ ,  $x(i_{\bar{l}}, i_l; j)$  denotes

$x(1,1;1)$	$x(1,1;2)$	$x(1,1;3)$	$x(1,1;4)$	$x(1,1;5)$	$x(1,1;6)$
$x(1,2;1)$	$x(1,2;2)$	$x(1,2;3)$	$x(1,2;4)$	$x(1,2;5)$	$x(1,2;6)$
$x(2,1;1)$	$x(2,1;2)$	$x(2,1;3)$	$x(2,1;4)$	$x(2,1;5)$	$x(2,1;6)$
$x(2,2;1)$	$x(2,2;2)$	$x(2,2;3)$	$x(2,2;4)$	$x(2,2;5)$	$x(2,2;6)$

2	5	1	4	5	9
6	3	6	3	2	0
5	2	7	1	0	3
6	4	4	3	8	8

$r^2(1;1)$	$r^2(1;2)$	$r^2(1;3)$	$r^2(1;4)$	$r^2(1;5)$	$r^2(1;6)$

8	8	7	7	7	9

$r^2(2;1)$	$r^2(2;2)$	$r^2(2;3)$	$r^2(2;4)$	$r^2(2;5)$	$r^2(2;6)$

11	6	11	4	8	11

$r^1(1;1)$	$r^1(1;2)$	$r^1(1;3)$	$r^1(1;4)$	$r^1(1;5)$	$r^1(1;6)$
$r^1(2;1)$	$r^1(2;2)$	$r^1(2;3)$	$r^1(2;4)$	$r^1(2;5)$	$r^1(2;6)$

7	7	8	5	5	12
12	7	10	6	10	8

$c(1,1)$					
$c(1,2)$					

26					
20					

$c(2,1)$					
$c(2,2)$					

18					
33					

Figure 1: An example of  $B \times B \times J$  ( $|J| = 6$ ) table (denoted by  $\mathbf{x}^*$ ).

the element  $x(i; j)$ .

Let  $(\mathbf{r}^1, \mathbf{r}^2, \dots, \mathbf{r}^m; \mathbf{c})$  be a sequence of non-negative integer vectors where  $\mathbf{r}^l \in \mathbb{Z}_+^{B^{m-1} \times J}$  for each  $l \in \{1, 2, \dots, m\}$  and  $\mathbf{c} \in \mathbb{Z}_+^{B^m}$ . The element of  $\mathbf{r}^l$  indexed by  $(i'; j) \in B^{m-1} \times J$  is denoted by  $r^l(i'; j)$ . The set of contingency tables corresponding to  $(\mathbf{r}^1, \mathbf{r}^2, \dots, \mathbf{r}^m; \mathbf{c})$  is defined by

$$\mathcal{T} \stackrel{\text{def.}}{=} \left\{ \mathbf{x} \in \mathbb{Z}_+^{B^m \times J} \mid \begin{array}{l} x(i_{\bar{l}}, 1; j) + x(i_{\bar{l}}, 2; j) = r^l(i_{\bar{l}}; j) \quad (\forall l \in \{1, 2, \dots, m\}, \forall i_{\bar{l}} \in B^{m-1}, \forall j \in J), \\ \sum_{j \in J} x(i; j) = c(i) \quad (\forall i \in B^m) \end{array} \right\}.$$

Each element in  $\mathcal{T}$  is called a *table* for simplicity. In the following,  $\sum_{i \in B^m} c(i)$  is denoted by  $N$ . Clearly, for any table  $\mathbf{x} \in \mathcal{T}$ , the sum total of elements of  $\mathbf{x}$  is equal to  $N$ .

In the rest of this section, we briefly review the path coupling technique proposed by Bubley and Dyer [5]. We use the technique in later sections to estimate the mixing time of our Markov chain. Here we deal with a Markov chain  $\mathcal{M}$  with state space  $\mathcal{T}$ . Assume that  $\mathcal{M}$  has a unique stationary distribution  $\pi : \mathcal{T} \rightarrow [0, 1]$ . For any probability distribution function  $\pi'$  on  $\mathcal{T}$ , define the *total variation distance* between  $\pi$  and  $\pi'$  to be

$$D_{\text{TV}}(\pi, \pi') \stackrel{\text{def.}}{=} \max_{\mathcal{T}' \subseteq \mathcal{T}} \left| \sum_{\mathbf{x} \in \mathcal{T}'} \pi(\mathbf{x}) - \sum_{\mathbf{x} \in \mathcal{T}'} \pi'(\mathbf{x}) \right| = (1/2) \sum_{\mathbf{x} \in \mathcal{T}} |\pi(\mathbf{x}) - \pi'(\mathbf{x})|.$$

If the initial state of the chain  $\mathcal{M}$  is  $\mathbf{x}$ , we denote the distribution of the chain at time  $t$  by  $P_{\mathbf{x}}^t : \mathcal{T} \rightarrow [0, 1]$ , i.e.,

$$P_{\mathbf{x}}^t(\mathbf{y}) \stackrel{\text{def.}}{=} \Pr[X_t = \mathbf{y} \mid X_0 = \mathbf{x}] \quad (\forall \mathbf{y} \in \mathcal{T}).$$

The rate of convergence to stationary from the initial state  $\mathbf{x}$  may be measured by

$$\tau_{\mathbf{x}}(\varepsilon) \stackrel{\text{def.}}{=} \min\{t \mid D_{\text{TV}}(\pi, P_{\mathbf{x}}^t) \leq \varepsilon \text{ for all } t' \geq t\}$$

where the error bound  $\varepsilon$  is a given positive constant. The *mixing time*  $\tau(\varepsilon)$  of  $\mathcal{M}$  is defined by

$$\tau(\varepsilon) \stackrel{\text{def.}}{=} \max_{\mathbf{x} \in \mathcal{T}} \tau_{\mathbf{x}}(\varepsilon),$$

which is independent of the initial state.

Next, we define a special Markov process with respect to  $\mathcal{M}$  called joint process. A *joint process* of  $\mathcal{M}$  is a Markov chain  $(X_t, Y_t)$  defined on  $\mathcal{T} \times \mathcal{T}$  satisfying that each of  $(X_t), (Y_t)$ , considered marginally, is a faithful copy of the original Markov chain  $\mathcal{M}$ . More precisely, we require that

$$\begin{aligned}\Pr[X_{t+1} = \mathbf{x}' | (X_t, Y_t) = (\mathbf{x}, \mathbf{y})] &= P_{\mathcal{M}}(\mathbf{x}, \mathbf{x}'), \\ \Pr[Y_{t+1} = \mathbf{y}' | (X_t, Y_t) = (\mathbf{x}, \mathbf{y})] &= P_{\mathcal{M}}(\mathbf{y}, \mathbf{y}'),\end{aligned}$$

for all  $\mathbf{x}, \mathbf{y}, \mathbf{x}', \mathbf{y}' \in \mathcal{T}$  where  $P_{\mathcal{M}}(\mathbf{x}, \mathbf{x}')$  and  $P_{\mathcal{M}}(\mathbf{y}, \mathbf{y}')$  denotes the transition probability from  $\mathbf{x}$  to  $\mathbf{x}'$  and from  $\mathbf{y}$  to  $\mathbf{y}'$  of the original Markov chain  $\mathcal{M}$ , respectively.

**Path coupling lemma** [Bubley and Dyer [5]]

Let  $G$  be a directed graph with vertex set  $\mathcal{T}$  and arc set  $A \subseteq \mathcal{T} \times \mathcal{T}$ . Let  $\ell : A \rightarrow \mathbb{Z}_{++}$  be a positive length defined on the arc set. We assume that  $G$  is strongly connected. For any ordered pair of vertices  $(\mathbf{x}, \mathbf{x}')$  of  $G$ , the distance from  $\mathbf{x}$  to  $\mathbf{x}'$ , denoted by  $\ell(\mathbf{x}, \mathbf{x}')$ , is the length of the shortest path from  $\mathbf{x}$  to  $\mathbf{x}'$ , where the length of a path is the sum of the lengths of arcs in the path. Suppose that there exists a joint process  $(X, Y) \mapsto (X', Y')$  with respect to  $\mathcal{M}$  satisfying that

$$1 > \exists \beta > 0, \forall (X, Y) \in A, \mathbb{E}[\ell(X', Y')] \leq \beta \ell(X, Y).$$

Then the mixing time  $\tau(\varepsilon)$  of the original Markov chain  $\mathcal{M}$  satisfies  $\tau(\varepsilon) \leq (1 - \beta)^{-1} \ln(D/\varepsilon)$  where  $D$  denotes the diameter of  $G$ , i.e., the distance of a farthest (ordered) pair of vertices.

### 3 Markov Chain for Uniform Distribution

First, we show a lemma which implies an irreducible Markov chain defined on the set of tables  $\mathcal{T}$ . We define the *parity function*  $p : \mathbb{Z} \rightarrow \{1, -1\}$  by

$$p(x) = \begin{cases} 1 & (x \text{ is an even integer}), \\ -1 & (x \text{ is an odd integer}). \end{cases}$$

For any index  $\mathbf{i} \in \mathbb{B}^m$ , we denote  $p(i_1 + i_2 + \dots + i_m)$  by  $p(\mathbf{i})$ . The vector  $\Delta \in \{1, -1\}^{\mathbb{B}^m}$  is defined by  $\Delta(\mathbf{i}) \stackrel{\text{def.}}{=} p(\mathbf{i})$  for each index  $\mathbf{i} \in \mathbb{B}^m$ . Given an ordered pair of distinct column indices  $(j', j'')$ , we define the vector  $\Delta[j', j''] \in \mathbb{Z}^{\mathbb{B}^m \times J}$  by

$$\Delta[j', j''](j) \stackrel{\text{def.}}{=} \begin{cases} 0 & (j \in J \setminus \{j', j''\}), \\ \Delta & (j = j'), \\ -\Delta & (j = j''). \end{cases}$$

For any table  $\mathbf{x} \in \mathcal{T}$ , we introduce the set of neighboring tables;

$$\mathcal{N}^0(\mathbf{x}) \stackrel{\text{def.}}{=} \{\mathbf{x}' \in \mathcal{T} \mid \exists (j', j'') \in J \times J, j' \neq j'', \mathbf{x}' = \mathbf{x} + \Delta[j', j'']\}.$$

It is easy to see that if  $\mathbf{x}' = \mathbf{x} + \Delta[j', j'']$ , then  $\mathbf{x} = \mathbf{x}' - \Delta[j', j''] = \mathbf{x}' + \Delta[j'', j']$ , and so  $\mathbf{x}' \in \mathcal{N}^0(\mathbf{x})$  implies  $\mathbf{x} \in \mathcal{N}^0(\mathbf{x}')$ . For any pair of vectors  $\mathbf{x}, \mathbf{x}' \in \mathbb{Z}^{\mathbb{B}^m \times J}$ ,  $\|\mathbf{x} - \mathbf{x}'\|_1$  denotes the distance

$$\sum_{(\mathbf{i}; j) \in \mathbb{B}^m \times J} |\mathbf{x}(\mathbf{i}; j) - \mathbf{x}'(\mathbf{i}; j)| \text{ between } \mathbf{x} \text{ and } \mathbf{x}'.$$

0	-1	0	1	0	0
0	1	0	-1	0	0

2	5	1	4	5	9
6	3	6	3	2	0

2	4	1	5	5	9
6	4	6	2	2	0

  

0	1	0	-1	0	0
0	-1	0	1	0	0

5	2	7	1	0	3
6	4	4	3	8	8

5	3	7	0	0	3
6	3	4	4	8	8

$\Delta[4, 2]$ 
 $\mathbf{x}^*$ 
 $\mathbf{x}^* + \Delta[4, 2]$

Figure 2: The vector  $\Delta[4, 2]$ .

**Lemma 1** Let  $G^0$  be an undirected graph with vertex set  $\mathcal{T}$  and for any pair of vertices  $\{\mathbf{x}, \mathbf{x}'\}$ , there exists an edge between  $\mathbf{x}$  and  $\mathbf{x}'$  if and only if  $\mathbf{x}' \in \mathcal{N}^0(\mathbf{x})$ . Then the graph  $G^0$  is connected, i.e., for any pair of vertices  $\{\mathbf{x}, \mathbf{x}'\}$  of  $G^0$ , there exists a path on  $G^0$  between  $\mathbf{x}$  and  $\mathbf{x}'$ . The diameter (the distance of farthest pair of vertices) is less than or equal to  $N/2^{m+1}$

**Proof.** Assume on the contrary that  $G^0$  is not connected. Let  $\{\mathbf{x}, \mathbf{x}'\}$  be a pair of vertices which minimizes  $\|\mathbf{x} - \mathbf{x}'\|_1$  subject to the condition that there does not exist any path between  $\mathbf{x}$  and  $\mathbf{x}'$ . Without loss of generality, we can assume that  $\exists j' \in J$ ,  $x(\mathbf{2}; j') < x'(\mathbf{2}; j')$ , where  $\mathbf{2}$  is the all-two vector in  $B^m$ . It directly implies the followings;

1.  $x(\mathbf{i}; j') < x'(\mathbf{i}; j')$  for any  $\mathbf{i} \in B^m$  satisfying  $p(\mathbf{i}) = p(\mathbf{2})$ ,
2.  $x(\mathbf{i}; j') > x'(\mathbf{i}; j')$  for any  $\mathbf{i} \in B^m$  satisfying  $p(\mathbf{i}) \neq p(\mathbf{2})$ ,
3.  $|x(\mathbf{i}; j') - x'(\mathbf{i}; j')| = |x(\mathbf{2}; j') - x'(\mathbf{2}; j')|$  for any  $\mathbf{i} \in B^m$ .

Since  $\sum_{j \in J} x(\mathbf{2}; j) = \sum_{j \in J} x'(\mathbf{2}; j)$ , there exists a column index  $j''$  satisfying  $x(\mathbf{2}; j'') > x'(\mathbf{2}; j'')$ . Then we have the following properties;

1.  $x(\mathbf{i}; j'') > x'(\mathbf{i}; j'')$  for any  $\mathbf{i} \in B^m$  satisfying  $p(\mathbf{i}) = p(\mathbf{2})$ ,
2.  $x(\mathbf{i}; j'') < x'(\mathbf{i}; j'')$  for any  $\mathbf{i} \in B^m$  satisfying  $p(\mathbf{i}) \neq p(\mathbf{2})$ ,
3.  $|x(\mathbf{i}; j'') - x'(\mathbf{i}; j'')| = |x(\mathbf{2}; j'') - x'(\mathbf{2}; j'')|$  for any  $\mathbf{i} \in B^m$ .

The vector  $\mathbf{x}'' = \mathbf{x} + \Delta[j', j'']$  is non-negative and so  $\mathbf{x}'' \in \mathcal{T}$ . Since  $\mathbf{x}'' \in \mathcal{N}^0(\mathbf{x})$ , there does not exist any path between  $\mathbf{x}''$  and  $\mathbf{x}'$ . The inequality  $\|\mathbf{x} - \mathbf{x}'\|_1 > \|\mathbf{x}'' - \mathbf{x}'\|_1$  contradicts with the minimality of  $\|\mathbf{x} - \mathbf{x}'\|_1$ . The definition of  $\mathbf{x}''$  implies that  $\|\mathbf{x} - \mathbf{x}''\|_1 = 2^{m+1}$ .

The above procedure decreases the distance between a distinct pair of vertices and the decrement is  $2^{m+1}$ . If we apply the procedure  $\lfloor \|\mathbf{x} - \mathbf{x}'\|_1 / 2^{m+1} \rfloor$  times, the distance of two vertices is less than  $2^{m+1}$ . It implies that the obtained pair of vertices are identical. Thus the diameter of  $G^0$  is less than or equal to  $N/2^{m+1}$ .  $\square$

The above lemma indicates the existence of an irreducible Markov chain on  $\mathcal{T}$  such that the transition probability of an ordered pair of tables  $(\mathbf{x}, \mathbf{x}')$  is positive if and only if  $\mathbf{x}$  and  $\mathbf{x}'$  are adjacent on  $G^0$ . When  $m = 1$ , this chain is a special case of the Markov chain proposed by Diaconis and Saloff-Coste [10]. However, as discussed in Dyer and Greenhill [12], the mixing rate of Diaconis and Saloff-Coste's chain is low. In the following, we describe our chain, which is an extension of the chain discussed by Dyer and Greenhill [12] for contingency tables with two rows.

For any table  $\mathbf{x} \in \mathcal{T}$  and any pair of distinct column indices  $\{j', j''\}$ , we define the following set of tables;

$$\mathcal{N}(\mathbf{x}, \{j', j''\}) \stackrel{\text{def.}}{=} \left\{ (\mathbf{y}(j'), \mathbf{y}(j'')) \in \mathbb{Z}_+^{B^m \times \{j', j''\}} \mid \exists \theta \in \mathbb{Z}, (\mathbf{y}(j'), \mathbf{y}(j'')) = (\mathbf{x}(j'), \mathbf{x}(j'')) + \theta(\Delta, -\Delta) \geq \mathbf{0} \right\}.$$

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Figure 3: Vectors in  $\mathcal{N}(\mathbf{x}^*, \{1, 3\})$ .

### Markov Chain $\mathcal{M}$

We introduce our chain  $\mathcal{M}$  with state space  $\mathcal{T}$ . For any table  $\mathbf{x} \in \mathcal{T}$  and any pair of distinct column indices  $\{j', j''\}$ , we define the following set of tables;

$$\begin{aligned} \mathbb{N}^1(\mathbf{x}, \{j', j''\}) &\stackrel{\text{def.}}{=} \{ \mathbf{x}' \in \mathcal{T} \mid \mathbf{x}'(j) = \mathbf{x}(j) \ (\forall j \in J \setminus \{j', j''\}), (\mathbf{x}'(j'), \mathbf{x}'(j'')) \in \mathcal{N}(\mathbf{x}, \{j', j''\}) \} \\ &= \{ \mathbf{x}' \in \mathcal{T} \mid \exists \theta \in \mathbb{Z}, \mathbf{x}' = \mathbf{x} + \theta \Delta[j', j''] \geq \mathbf{0} \}. \end{aligned}$$

The Markov chain  $\mathcal{M}$  with the state space  $\mathcal{T}$  is defined by the following transition procedure. We denote the state of the chain  $\mathcal{M}$  at time  $t$  by  $X_t$  and the element of  $X_t$  indexed by  $(i; j)$  is denoted by  $X_t(i; j)$ . Then the state  $X_{t+1}$  at time  $t+1$  is determined as follows. First, choose a pair of distinct column indices  $\{j', j''\}$  randomly. Next, choose a table  $X_{t+1}$  from  $\mathbb{N}^1(X_t, \{j', j''\})$  at random.

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$\mathbf{x}^* + \Delta[1, 3]$	$\mathbf{x}^*$	$\mathbf{x}^* - \Delta[1, 3]$	$\mathbf{x}^* - 2\Delta[1, 3]$																																																

Figure 4: The set of neighbors  $\mathbb{N}^1(\mathbf{x}^*, \{1, 3\})$ .

We estimate the mixing time of our chain  $\mathcal{M}$ . According to the definition, it is clear that  $\mathcal{M}$  is aperiodic and irreducible. The transition probability of  $\mathcal{M}$  from  $\mathbf{x}$  to  $\mathbf{y}$ , denoted by  $P_{\mathcal{M}}(\mathbf{x}, \mathbf{y})$  is

$$P_{\mathcal{M}}(\mathbf{x}, \mathbf{y}) = \begin{cases} \left( \binom{n}{2} |\mathcal{N}(\mathbf{x}, \{j', j''\})| \right)^{-1} & (\text{if } \mathbf{y} \in \mathbb{N}^1(\mathbf{x}, \{j', j''\})), \\ \sum_{j' < j''} \left( \binom{n}{2} |\mathcal{N}(\mathbf{x}, \{j', j''\})| \right)^{-1} & (\mathbf{x} = \mathbf{y}), \\ 0 & (\text{otherwise}). \end{cases}$$

Since  $P_{\mathcal{M}}(\mathbf{x}, \mathbf{y}) = P_{\mathcal{M}}(\mathbf{y}, \mathbf{x})$ , the stationary distribution of the chain is uniform.

First, we introduce a directed graph  $G$  with the vertex set  $\mathcal{T}$  and the arc set  $A = \{(\mathbf{x}, \mathbf{x}') \mid \mathbf{x}' \in N^0(\mathbf{x})\}$ . We define that the length  $\ell(a)$  of each arc  $a \in A$  is equal to 1. The distance of any ordered pair of vertices  $(\mathbf{x}, \mathbf{x}')$  on  $G$  is denoted by  $\ell(\mathbf{x}, \mathbf{x}')$ . Next, we define a joint process  $(X, Y) \mapsto (X', Y')$  with respect to  $\mathcal{M}$ . For any pair of tables  $(X, Y) \in A$ , we define the transition probability of our joint process from  $(X, Y)$  to  $(X', Y')$ . Without loss of generality, we can assume that  $X(1) \neq Y(1), X(2) \neq Y(2)$  and  $X(j) = Y(j)$  for all  $j \in J \setminus \{1, 2\}$ . In the joint process, we choose a pair of distinct column indices  $(j', j'')$ .

Case 1: When  $\{j', j''\} \subseteq \{3, \dots, n\}$ , it is clear that  $\mathcal{N}(X, \{j', j''\}) = \mathcal{N}(Y, \{j', j''\})$  and so we choose a pair  $(Z(j'), Z(j''))$  from  $\mathcal{N}(X, \{j', j''\})$  at random. We set  $X'$  and  $Y'$  to the contingency table obtained from  $X$  and  $Y$  by replacing  $(X(j'), X(j''))$  and  $(Y(j'), Y(j''))$  by  $(Z(j'), Z(j''))$ , respectively. Then, it is clear that  $(X', Y')$  is also in  $A$  and so  $\ell(X', Y') = 1$ .

Case 2: Next, consider the case that  $\{j', j''\} = \{1, 2\}$ . It is clear that  $\mathcal{N}(X, \{j', j''\}) = \mathcal{N}(Y, \{j', j''\})$ . We construct  $X'$  and  $Y'$  by using the same manner of Case 1. Then, we have  $X' = Y'$  and  $\ell(X', Y') = 0$ .

Case 3: Finally, we consider the case that  $j' = 1$  and  $j'' = 3$ . Other cases are treated in the same way as follows.

Case 3-1: Consider the case that  $|\mathcal{N}(X, \{j', j''\})| = |\mathcal{N}(Y, \{j', j''\})|$ .

We denote  $N^1(X, \{j', j''\}) = \{X^1, X^2, \dots, X^k\}$  and  $N^1(Y, \{j', j''\}) = \{Y^1, Y^2, \dots, Y^k\}$ . By arranging the order of the elements, we assume that  $X^1(1; 1) > X^2(1; 1) > \dots > X^k(1; 1)$  and  $Y^1(1; 1) > Y^2(1; 1) > \dots > Y^k(1; 1)$ . Then we choose  $(X', Y')$  randomly from  $\{(X^1, Y^1), (X^2, Y^2), \dots, (X^k, Y^k)\}$ . It is easy to see that  $(X', Y') \in A$  and so  $\ell(X', Y') = 1$ .

Case 3-2: We only need to consider the case that  $|\mathcal{N}(X, \{j', j''\})| > |\mathcal{N}(Y, \{j', j''\})|$  without loss of generality. Since  $(X, Y) \in A$ , it is easy to show that  $|\mathcal{N}(X, \{j', j''\})| = |\mathcal{N}(Y, \{j', j''\})| + 1$ . By arranging the order of elements in  $N^1(X, \{j', j''\}) = \{X^1, X^2, \dots, X^{k+1}\}$  and  $N^1(Y, \{j', j''\}) = \{Y^1, Y^2, \dots, Y^k\}$ , we can assume that  $X^1(1; 1) > X^2(1; 1) > \dots > X^{k+1}(1; 1)$  and  $Y^1(1; 1) > Y^2(1; 1) > \dots > Y^k(1; 1)$ . Then we choose  $(X', Y')$  as follows;

$$(X', Y') = \begin{cases} (X^i, Y^i) & \text{with probability } (k-i+1)/k(k+1) & \text{for } i \in \{1, 2, \dots, k\}, \\ (X^{i+1}, Y^i) & \text{with probability } i/k(k+1) & \text{for } i \in \{1, 2, \dots, k\}, \end{cases}$$

where the sum total of the probabilities is  $(1+2+\dots+k)/k(k+1) + (k+\dots+2+1)/k(k+1) = 1$ . Figure 5 shows an example. Clearly from the definition,  $(X^i, Y^i), (X^i, Y^{i+1}) \in A$  for each  $i \in \{1, 2, \dots, k\}$  and so  $\ell(X', Y') = 1$ .

From the above, we have

$$E[\ell(X', Y')] = \left(1 - \binom{n}{2}^{-1}\right).$$

It implies the following result.

**Theorem 1** *The Markov chain  $\mathcal{M}$  has the mixing time  $\tau(\varepsilon)$  satisfying that*

$$\tau(\varepsilon) \square (1/2)n(n-1) \ln(dn/(2\varepsilon)),$$

where  $d$  is the average of the values in cells, i.e.,  $d = N/(2^m n)$ .

3	5	0	4	5	9
5	3	7	3	2	0

$$X^1 = X + \Delta[1, 3]$$

$$= Y^1 + \Delta[1, 2]$$

2	5	1	4	5	9
6	3	6	3	2	0

$$X^2 = X$$

$$= Y^2 + \Delta[1, 2]$$

1	5	2	4	5	9
7	3	5	3	2	0

$$X^3 = X - \Delta[1, 3]$$

$$= Y^3 + \Delta[1, 2]$$

0	5	3	4	5	9
8	3	4	3	2	0

$$X^4 = X - 2\Delta[1, 3]$$

2	6	0	4	5	9
6	2	7	3	2	0

$$Y^1 = Y + \Delta[1, 3]$$

$$= X^2 + \Delta[2, 3]$$

1	6	1	4	5	9
7	2	6	3	2	0

$$Y^2 = Y = X + \Delta[2, 1]$$

$$= X^3 + \Delta[2, 3]$$

0	6	2	4	5	9
8	2	5	3	2	0

$$Y^3 = Y - \Delta[1, 3]$$

$$= X^4 + \Delta[2, 3]$$

$$\Pr[(X', Y') = (X^1, Y^1) | (j', j'') = (1, 3)] = 3/12, \quad \Pr[(X', Y') = (X^2, Y^1) | (j', j'') = (1, 3)] = 1/12,$$

$$\Pr[(X', Y') = (X^2, Y^2) | (j', j'') = (1, 3)] = 2/12, \quad \Pr[(X', Y') = (X^3, Y^2) | (j', j'') = (1, 3)] = 2/12,$$

$$\Pr[(X', Y') = (X^3, Y^3) | (j', j'') = (1, 3)] = 1/12, \quad \Pr[(X', Y') = (X^4, Y^3) | (j', j'') = (1, 3)] = 3/12.$$

Figure 5: An example of Case 3-2.

**Proof.** The diameter of the graph  $G$  is equal to that of  $G^0$  and so less than or equal to  $N/2^{m+1}$ . Path coupling lemma induces the desired result.  $\square$

Our chain is rapidly mixing. Moreover, our result indicates that the mixing time independent of the dimension  $m + 1$  of a contingency table in the case that the size is  $2 \times 2 \times \dots \times J$ .

## 4 Discussion

In this paper, we proposed the Markov chain for sampling  $2 \times 2 \times \dots \times J$  contingency tables. Though the author considered for constructing an efficient algorithm for finding all contingency tables, we couldn't propose it. With regard to enumeration algorithms for contingency tables, there are some results. Recently, to enumerate 2-dimensional contingency tables, Sturmfels proposed an algorithm using Gröbner bases which arise from algebraic geometry [26]. His enumeration algorithm is based on the reverse search technique. Sakata, Sawae and Kroumov have calculated Gröbner bases for months to enumerate  $4 \times 4 \times 4$  contingency tables [24]. Thus we need to consider about practical algorithms for enumerating contingency tables.

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