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# Markov chain Monte Carlo test of toric homogeneous Markov chains

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## Abstract

Markov chain models are used in various fields, such behavioral sciences or econometrics. Although the goodness of fit of the model is usually assessed by large sample approximation, it is desirable to use conditional tests if the sample size is not large. We study Markov bases for performing conditional tests of the toric homogeneous Markov chain model, which is the envelope exponential family for the usual homogeneous Markov chain model. We give a complete description of a Markov basis for the following cases: i) two-state, arbitrary length, ii) arbitrary finite state space and length of three. The general case remains to be a conjecture. We also present numerical examples of conditional tests based on our Markov basis.

## 1 Introduction

Consider a Markov chain  $X_t$ ,  $t = 1, \dots, T$  ( $\geq 3$ ), over a finite state space  $\mathcal{S} = \{1, \dots, S\}$  ( $S \geq 2$ ). Let  $\pi_i$ ,  $i \in \mathcal{S}$ , denote the initial distribution of  $X_1$  and let  $p_{ij}^{(t)} = P(X_{t+1} = j \mid X_t = i)$  denote the transition probability from time  $t$  to  $t + 1$ . We want to test the null hypothesis of homogeneity

$$H_0 : p_{ij}^{(t)} = p_{ij}, \quad t = 1, \dots, T - 1. \quad (1)$$

This model is used as a standard model in many fields. See Haccou and Meelis [9] for behavioral sciences and Fühwirth-Schnatter [8] for econometrics. Usually the goodness of fit of the model is assessed by large sample approximation (Anderson and Goodman [3], Billingsley [5]). However when the sample size is not large, it is desirable to use conditional tests. The Markov basis methodology (Diaconis and Sturmfels [6]) is attractive for performing them.

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In this paper we study Markov bases for performing conditional tests of the null hypothesis of homogeneity. However the homogeneous Markov chain model (1) is a curved exponential family due to the constraints  $\sum_{j \in \mathcal{S}} p_{ij} = 1, \forall i \in \mathcal{S}$ , and we cannot directly apply conditional tests to  $H_0$  in (1). Instead, by the Markov basis methodology we can test a larger null hypothesis  $\bar{H}_0$  that  $X_t, t = 1, \dots, T$ , are observations from a *toric* homogeneous Markov chain (cf. Section 1.4 of Pachter and Sturmfels [13]), which is the envelope exponential family (cf. Küchler and Sørensen [11] and Küchler and Sørensen [12], Chapter 7) of the homogeneous Markov chain model (1). In Section 2.1 we discuss interpretations of the toric homogeneous Markov chain model and its difference from the usual homogeneous Markov chain model.

In the following for notational simplicity we write THMC for “toric homogeneous Markov chain”. Note that in Section 1.4 of Pachter and Sturmfels [13] they consider a model without parameters for the initial distribution, whereas our THMC model contains parameters for the initial distribution. As an alternative hypothesis to THMC model we can take non-homogeneous Markov chain model, which is an (affine or full) exponential family model which includes THMC model as a submodel.

In this paper we derive complete description of Markov bases for THMC model for the case of  $S = 2$  (arbitrary  $T$ ) and the case of  $T = 3$  (arbitrary  $S$ ). For other combinations of  $(S, T)$  with small  $S$  and  $T$ , we can use a computer algebra package 4ti2 ([1]). Complete description of Markov bases for general  $S$  and  $T$  seems to be a difficult problem at present.

The organization of this paper is as follows. In Section 2 we first set up our model and then give some preliminary results. We derive a Markov basis for the case of  $S = 2$  in Section 3 and for  $T = 3$  in Section 4. In Section 5 we present applications of our Markov bases to some data sets. In Section 6 we give some discussions on Markov bases for general  $S$  and  $T$ .

## 2 Toric homogeneous Markov chain model

### 2.1 THMC model and its interpretation

Let  $\omega = (s_1, \dots, s_T) \in \mathcal{S}^T$  denote an observed path of a Markov chain. Each path is considered as one frequency of a  $|\mathcal{S}|^T$  contingency table. The usual homogeneous Markov chain model (1) specifies the probability of the path  $\omega$  as

$$H_0 : p(\omega) = \pi_{s_1} p_{s_1 s_2} \cdots p_{s_{T-1} s_T}, \quad (2)$$

where the normalization is  $\sum_{i \in \mathcal{S}} \pi_i = 1$  and  $\sum_{j \in \mathcal{S}} p_{ij} = 1, \forall i \in \mathcal{S}$ . In THMC model, the normalization is only assumed for the total probability. In order to avoid confusion, let  $\gamma_i, i \in \mathcal{S}$ , and  $\beta_{ij}, i, j \in \mathcal{S}$ , be free nonnegative parameters. We specify THMC model by

$$\bar{H}_0 : p(\omega) = c \gamma_{s_1} \beta_{s_1 s_2} \cdots \beta_{s_{T-1} s_T}, \quad (3)$$

where  $c$  is the overall normalizing constant. THMC model (3) is the envelope exponential family of the homogeneous Markov chain model (2), i.e., the linear hull of logarithms of

the probabilities in (2) coincides with the set of logarithms of probabilities in (3). This simply follows from the fact that the linear hull of elementwise logarithms of probability vector

$$\{(\log p_1, \dots, \log p_S) \mid p_i > 0, i \in \mathcal{S}, \sum_{i \in \mathcal{S}} p_i = 1\}$$

is the whole  $\mathbb{R}^S$ . The THMC model  $\bar{H}_0$  contains the usual homogeneous Markov chain model  $H_0$  and the difference in degrees of freedom is  $S - 1$ .

As discussed in Küchler and Sørensen [11] an envelope exponential family is often difficult to interpret. For THMC model we give the following interpretation. Write

$$\beta_{ij} = \alpha_i p_{ij}, \quad \sum_{j \in \mathcal{S}} p_{ij} = 1.$$

Then (3) is written as

$$p(\omega) = c \gamma_{s_1} \alpha_{s_1} p_{s_1 s_2} \dots \alpha_{s_{T-1}} p_{s_{T-1} T} = c \gamma_{s_1} p_{s_1 s_2} \dots p_{s_{T-1} T} \times (\alpha_{s_1} \dots \alpha_{s_{T-1}}).$$

Compared to (2),  $\alpha_i$  specifies a magnifying ratio of probability of a path visiting the state  $i$ . We can interpret  $\alpha_i$  as an internal growth rate or “birth rate” of state  $i$ , which is not affected by immigration or emigration.

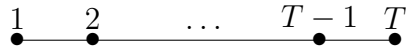
As an alternative hypothesis we can take the non-homogeneous Markov chain model

$$H_1 : p(\omega) = \pi_{s_1} p_{s_1 s_2}^{(1)} \dots p_{s_{T-1} s_T}^{(T-1)}. \quad (4)$$

By reparametrization this model can be simply written as the linearly ordered conditional independence model:

$$p(\omega) = c \beta_{s_1 s_2}^{(1)} \beta_{s_2 s_3}^{(2)} \dots \beta_{s_{T-1} s_T}^{(T-1)}.$$

This is a decomposable model of a  $T$ -way contingency table, with its independence graph given by the following linear tree:



This model is a full exponential family model containing THMC model.

In this paper we consider testing  $\bar{H}_0$  against  $H_1$  via Markov basis approach. Although by this procedure we are not directly testing  $H_0$ , it should be noted that we can reject  $H_0$  if  $\bar{H}_0$  is rejected. When  $\bar{H}_0$  is accepted, we further need to test  $H_0$  against  $\bar{H}_0$ . However at present there is no general procedure for finite sample exact tests of curved exponential family.

## 2.2 Sufficient statistic and moves for THMC model

Suppose that we observe  $N$  paths  $\omega_1, \dots, \omega_N$  from a homogeneous Markov chain (1). We write  $W = \{\omega_1, \dots, \omega_N\}$ . Here multiple paths are allowed in  $W$  and hence  $W$  is a multiset.

Let  $x(\omega)$  denote the frequency of the path  $\omega$  in  $W$ . Then the data set is summarized in a  $T$ -way contingency table  $\mathbf{x} = \{x(\omega), \omega \in \mathcal{S}^T\}$ .

Let  $x_{ij}^t$  denote the number of transitions from  $s_t = i$  to  $s_{t+1} = j$  in  $W$  and let  $x_i^t$  denote the frequency of the state  $s_t = i$  in  $W$ . In particular  $x_i^1$  is the frequency of the initial state  $s_1 = i$ . Let

$$x_{ij}^+ = \sum_{t=1}^{T-1} x_{ij}^t$$

denote the total number of transitions from  $i$  to  $j$  in  $W$ . Under  $H_0$  the joint probability of  $\mathbf{x}$  is written as

$$\begin{aligned} p(\mathbf{x}) &= \frac{N!}{\prod_{\omega \in \mathcal{S}^T} x(\omega)!} \prod_{\omega \in \mathcal{S}^T} (\pi_{s_1} p_{s_1 s_2} \cdots p_{s_{T-1} s_T})^{x(\omega)} \\ &= \frac{N!}{\prod_{\omega \in \mathcal{S}^T} x(\omega)!} \prod_{s \in \mathcal{S}} \pi_s^{x_s^1} \prod_{i, j \in \mathcal{S}} p_{ij}^{x_{ij}^+}. \end{aligned}$$

Therefore the sufficient statistic for  $H_0$  is given by the initial frequencies and the frequencies of transitions

$$\mathbf{b} = \mathbf{b}(\mathbf{x}) = \{x_i^1, i \in \mathcal{S}\} \cup \{x_{ij}^+, i, j \in \mathcal{S}\}. \quad (5)$$

In fact this sufficient statistic for  $H_0$  is minimal sufficient and it is also the sufficient statistic for THMC model. This simply reflects the fact that THMC model is the envelope exponential family of the homogeneous Markov chain model. Since THMC model (3) is an exponential family with integral sufficient statistic, we can perform the conditional test of  $\bar{H}_0$  by the Markov basis methodology. Therefore our goal in this paper is to obtain Markov bases for  $\bar{H}_0$  with various  $S$  and  $T$ .

If we order paths of  $\mathcal{S}^T$  appropriately and write  $\mathbf{x}$  as a column vector according to the order,  $\mathbf{b} = \mathbf{b}(\mathbf{x})$  in (5) is written in a matrix form

$$\mathbf{b} = A\mathbf{x},$$

where  $A$  is an  $S(S+1) \times S^T$  matrix consisting of non-negative integers. The set of all contingency tables sharing  $\mathbf{b}$  is called a *fiber* and denoted by  $\mathcal{F}_{\mathbf{b}} = \{\mathbf{x} \in \mathbb{Z}_{\geq 0}^{S^T} \mid A\mathbf{x} = \mathbf{b}\}$ , where  $\mathbb{Z}_{\geq 0} = \{0, 1, \dots\}$ . A move  $\mathbf{z}$  for THMC model is an integer array satisfying  $A\mathbf{z} = 0$ . Then  $\mathbf{z}$  is expressed by a difference of two contingency tables  $\mathbf{x}$  and  $\mathbf{y}$  in the same fiber:

$$\mathbf{z} = \mathbf{x} - \mathbf{y}, \quad z(\omega) = x(\omega) - y(\omega), \quad \omega \in \mathcal{S}^T.$$

We write  $z_i^t = x_i^t - y_i^t$  and  $z_{ij}^t = x_{ij}^t - y_{ij}^t$ . Note that  $\sum_{i \in \mathcal{S}} z_i^t = 0$  for all  $t$ , because  $N = \sum_{i \in \mathcal{S}} x_i^t = \sum_{i \in \mathcal{S}} y_i^t$  is the number of paths. Also since  $\mathbf{x}$  and  $\mathbf{y}$  is in the same fiber  $\sum_{t=1}^{T-1} z_{ij}^t = 0$  for all  $i, j \in \mathcal{S}$ .

**Example 1.** For illustration we consider the case of  $S = 2$  and  $T = 4$ . The configuration

$A$  is written as

$$\begin{array}{rcccccccccccccccc}
 & 1111 & 1112 & 1121 & 1122 & 1211 & 1212 & 1221 & 1222 & 2111 & 2112 & 2121 & 2122 & 2211 & 2212 & 2221 & 2222 \\
 A = & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 \text{"11"} & 3 & 2 & 1 & 1 & 1 & 0 & 0 & 0 & 2 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
 \text{"12"} & 0 & 1 & 1 & 1 & 1 & 2 & 1 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 0 \\
 \text{"21"} & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 2 & 1 & 1 & 1 & 1 & 0 \\
 \text{"22"} & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 2 & 0 & 0 & 0 & 1 & 1 & 1 & 2 & 3
 \end{array} \tag{6}$$

The first two rows of  $A$  correspond to  $x_1^+$  and  $x_2^+$ . The other rows correspond to  $x_{11}^+$ ,  $x_{12}^+$ ,  $x_{21}^+$ ,  $x_{22}^+$  respectively. The columns of  $A$  are indexed by the paths  $\omega \in \{1, 2\}^4$  in the lexicographic order. Note that compared to a similar configuration in Section 1.4.1 of [13],  $A$  in (6) has additional two rows corresponding to initial frequencies.

An interesting feature of the above  $A$  is that it contains identical columns. The columns 1121 and 1211 are identical. This means that the difference of the two paths  $\mathbf{z} = \{z(\omega) \mid \omega \in \mathcal{S}^T\}$

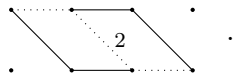
$$z(\omega) = \begin{cases} 1, & \text{if } \omega = 1121, \\ -1, & \text{if } \omega = 1211, \\ 0, & \text{otherwise} \end{cases}$$

forms a degree one move. We depict the degree one move as



where a solid line from  $(i, t)$  to  $(j, t + 1)$  represents  $z_{ij}^t = 1$  and a dotted line from  $(i, t)$  to  $(j, t + 1)$  represents  $z_{ij}^t = -1$ . We note that the columns 2122 and 2212 are also identical. We could remove redundant columns from  $A$  and only leave a representative column from the set of identical columns. However it seems better to leave identical columns in view of the symmetry in  $A$  and we will work with the above form of  $A$ .

In the following we often use the graph representation of moves as (7). We call such a graph a move graph. A node of a move graph is a pair  $(i, t)$  of state  $i$  and time  $t$  and an edge from  $(i, t)$  to  $(j, t + 1)$  represents the value of  $z_{ij}^t$ . If  $|z_{ij}^t| = 0$ , there is no corresponding edge in the graph. If  $|z_{ij}^t| \geq 2$ , we write the value of  $|z_{ij}^t|$  beside the edge. For example, the move for  $S = 2$  and  $T = 4$  such that  $z_{11}^1 = z_{22}^3 = -1$ ,  $z_{12}^2 = -2$  and  $z_{12}^1 = z_{22}^2 = z_{11}^2 = z_{12}^3 = 1$  is represented by

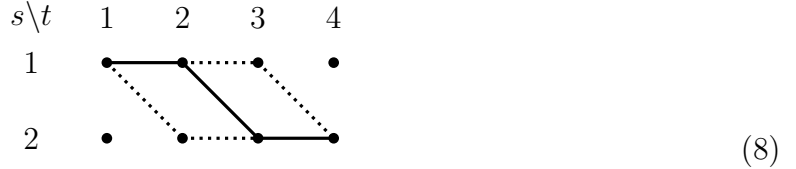


We note that a move graph does not have a one-to-one correspondence to a move and more than one move have the same move graph in general.

For notational simplicity we denote the edge from  $(i, t)$  to  $(j, t)$  as  $t : ij$ . Given a contingency table  $\mathbf{x}$ ,  $x_i^t$  is the number of paths passing through the node  $(i, t)$  and  $x_{ij}^t$  is the number of paths passing through the edge  $t : ij$ . Consider a partial path  $(s_t, s_{t+1}, \dots, s_{t'})$  starting at time  $t$  and ending at time  $t' > t$ . We write this partial path as  $t : s_t s_{t+1} \dots s_{t'}$ .  $x_{s_t s_{t+1} \dots s_{t'}}^t$  denotes the frequency of the partial path  $t : s_t s_{t+1} \dots s_{t'}$  in  $W$ . For a particular path  $\omega \in \mathcal{S}^T$  we say that  $\omega$  passes through  $t : s_t s_{t+1} \dots s_{t'}$  if  $\omega$  is of the form  $(*, \dots, *, s_t, s_{t+1}, \dots, s_{t'}, *, \dots, *)$  where  $*$  is arbitrary.

Let  $\mathbf{z} = \mathbf{x} - \mathbf{y}$ . If  $z_i^t > 0$  we say that  $\mathbf{x}$  dominates  $\mathbf{y}$  at the node  $(i, t)$ . Similarly if  $z_{ij}^t > 0$  we say that  $\mathbf{x}$  dominates  $\mathbf{y}$  in the edge  $t : ij$ . Consider a partial path  $t : s_t \dots s_{t'}$ . If all of  $z_{s_t, s_{t+1}}^t, z_{s_{t+1}, s_{t+2}}^{t+1}, \dots, z_{s_{t'-1}, s_{t'}}^{t'-1}$  are positive, we say that  $\mathbf{x}$  dominates  $\mathbf{y}$  in the partial path  $t : s_t \dots s_{t'}$ .

Given the signs of some  $z_{ij}^t$ 's, we depict the pattern of signs as an undirected graph with thick edges. Positive edges are depicted by thick solid lines and negative edges by thick dotted line. In the case of  $S = 2$  and  $T = 4$ , when  $z_{11}^1, z_{12}^2$  and  $z_{22}^3$  are positive and  $z_{12}^1, z_{11}^2, z_{22}^2$  and  $z_{12}^3$  are negative, the corresponding graph is depicted by



regardless of the signs of  $z_{22}^1, z_{21}^1, z_{21}^2, z_{21}^3$  and  $z_{11}^3$  where no edge is depicted. We call such graphs edge-sign pattern graphs. We note that edges of an edge-sign pattern graph have only the information on the signs of  $z_{ij}^t$  and do not have the information on the value of  $z_{ij}^t$  like a move graph.

For considering our Markov basis it is important to note that THMC model possesses the symmetry with respect to time reversal. The following fact is well known, as discussed in Section 2 of Billingsley [5].

**Lemma 1.** *For all  $\mathbf{x}$  in the same fiber  $\mathcal{F}_{\mathbf{b}}$  of THMC model, the terminal frequencies  $x_j^T$ ,  $j \in \mathcal{S}$ , are common.*

In terms of moves, the above lemma implies that  $z_i^T = 0$  for all  $i \in \mathcal{S}$ . Since  $z_i^1 = 0$ , we have

$$\sum_{t=2}^{T-1} z_i^t = 0. \quad (9)$$

Lemma 1 shows that given  $\mathbf{b}$ , the paths of the original homogeneous Markov chain and the paths of the time-reversed homogeneous Markov chain has the same conditional distribution. This symmetry with respect to time reversal is important in considering a Markov basis for the present problem.

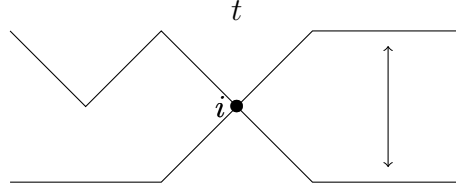


## 2.3 Linearly ordered conditional independence model and crossing path swapping

Let  $\mathbf{x}$  and  $\mathbf{y}$  in the same fiber be given. We call  $\mathbf{x}$  and  $\mathbf{y}$  *edge-wise equivalent* if  $z_{ij}^t = 0$  for all  $t$  and for all  $i, j$ . Edge-wise equivalence does not mean that  $\mathbf{x}$  and  $\mathbf{y}$  are identical as a multiset of  $N$  paths. However consider a non-homogeneous Markov chain  $H_1$  in (4), which is a linearly ordered conditional independence model of  $T$ -way contingency tables. Then  $x_{ij}^t$ ,  $1 \leq t \leq T - 1$  and  $i, j \in \mathcal{S}$ , constitute the sufficient statistic for the model. Therefore moves for  $H_1$  is expressed by the difference of two edge-wise equivalent paths and their move graphs have no edges.

We note that  $H_1$  is a decomposable model for contingency tables. By Dobra [7] there exists a Markov basis for this model consisting of square-free degree two moves. These square-free degree two moves are related to the idea of swapping of two paths meeting (or crossing) at a node. Let  $\bar{\omega} = (s_1, \dots, s_T)$  and  $\bar{\omega}' = (s'_1, \dots, s'_T)$  be two paths. We say that these two paths meet (or cross) at the node  $(i, t)$  if  $i = s_t = s'_t$ . If  $\omega$  and  $\omega'$  cross at the node  $(i, t)$ , consider the swapping of these two paths like

$$\begin{aligned} \{\omega, \omega'\} &= \{ (s_1, \dots, s_{t-1}, i, s_{t+1}, \dots, s_T), (s'_1, \dots, s'_{t-1}, i, s'_{t+1}, \dots, s'_T) \} \\ &\leftrightarrow \{ (s_1, \dots, s_{t-1}, i, s'_{t+1}, \dots, s'_T), (s'_1, \dots, s'_{t-1}, i, s_{t+1}, \dots, s_T) \} := \{\tilde{\omega}, \tilde{\omega}'\} \end{aligned} \quad (10)$$



Then the difference  $\mathbf{z}$  of  $(\omega, \omega')$  and  $(\tilde{\omega}, \tilde{\omega}')$

$$z(\omega) = \begin{cases} 1 & \text{if } \omega = \bar{\omega} \text{ or } \bar{\omega}' \\ -1 & \text{if } \omega = \tilde{\omega} \text{ or } \tilde{\omega}' \\ 0 & \text{otherwise} \end{cases}$$

forms a move for  $H_1$ . We call this move a “crossing path swapping”. By Dobra [7] we have the following proposition.

**Proposition 1.** *The set of crossing path swappings in (10) constitutes a Markov basis for the linearly ordered conditional independence model.*

Therefore once  $\mathbf{x}$  and  $\mathbf{y}$  of the same fiber are brought to be edge-wise equivalent, they can be further brought to be identical as multisets by crossing path swappings. Therefore for constructing a Markov basis for THMC model, we need to find an additional finite set of moves, which can make two elements of the same fiber edge-wise equivalent.

Crossing path swapping has the following implication. Suppose that  $\mathbf{x}$  dominates  $\mathbf{y}$  in the partial path  $t: s_t \dots s_{t'}$ . Then clearly there exists a path  $\omega$  in  $\mathbf{x}$  passing through the edge  $t: s_t s_{t+1}$ . Similarly there exists a path  $\omega'$  in  $\mathbf{x}$  passing through the edge  $t+1: s_{t+1} s_{t+2}$ .

We can then make the crossing path swapping of these two paths and make  $\omega$  go through the partial path  $t: s_t s_{t+1} s_{t+2}$ . Repeating this procedure, by a sequence of crossing path swappings of paths of  $\mathbf{x}$ , we can assume that  $\mathbf{x}$  contains a path  $\omega$  which goes through the partial path  $t: s_t \dots s_{t'}$ . We state this as a lemma.

**Lemma 2.** *Let  $\mathbf{x}$  and  $\mathbf{y}$  be two elements of the same fiber. If  $\mathbf{x}$  dominates  $\mathbf{y}$  in the partial path  $t: s_t \dots s_{t'}$ , then by crossing path swappings of paths in  $\mathbf{x}$ , we can transform  $\mathbf{x}$  to  $\tilde{\mathbf{x}}$ , such that there exists a path in  $\tilde{\mathbf{x}}$  going through the partial path  $t: s_t \dots s_{t'}$ .*

Note that during the sequence of crossing path swappings, the values of  $\{z_{ij}^t\}$  stay the same. By Lemma 2, we can identify all  $\mathbf{x}$ 's with the same edge frequencies, whenever we are concerned about decreasing  $\sum_{t,i,j} |z_{ij}^t|$  for our distance reduction argument in Sections 3 and 4.

## 2.4 Some properties of moves for THMC model

In this subsection we present an important class of moves for THMC model. Consider two different states  $i_1 \neq i_2$  at time  $t$  and two different states  $j_1 \neq j_2$  at time  $t+1$ . Let  $t: i_1 j_1$  and  $t: i_2 j_2$  be two edges joining these states. Now consider  $t': i_1 j_2$  and  $t': i_2 j_1$ , which swaps the transitions  $i_1 j_1, i_2 j_2$  of time  $t$ . Suppose that all of  $x_{i_1 j_1}^t, x_{i_2 j_2}^t, x_{i_1 j_2}^{t'}, x_{i_2 j_1}^{t'}$  are positive. Choose (not necessarily distinct) four paths  $\omega_1, \omega_2, \omega_3, \omega_4$  from  $\mathbf{x}$  passing through  $t: i_1 j_1, t: i_2 j_2, t': i_1 j_2, t': i_2 j_1$ , respectively:

$$\begin{aligned} \omega_1 &= (s_{11} \dots, s_{1,t-1}, i_1, j_1, s_{1,t+2}, \dots, s_{1T}), \quad \omega_2 = (s_{21} \dots, s_{2,t-1}, i_2, j_2, s_{2,t+2}, \dots, s_{2T}) \\ \omega_3 &= (s_{31} \dots, s_{3,t'-1}, i_1, j_2, s_{3,t'+2}, \dots, s_{3T}), \quad \omega_4 = (s_{41} \dots, s_{4,t'-1}, i_2, j_1, s_{4,t'+2}, \dots, s_{4T}). \end{aligned}$$

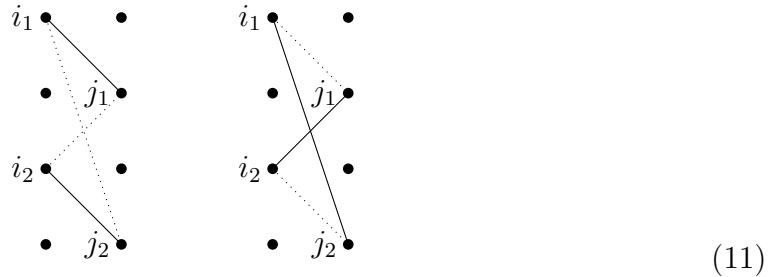
Then we consider swapping the transitions in  $\{t: i_1 j_1, t: i_2 j_2\}$  and those in  $\{t': i_1 j_2, t': i_2 j_1\}$  in  $\mathbf{x}$  as  $\{\omega_1, \omega_2, \omega_3, \omega_4\} \leftrightarrow \{\tilde{\omega}_1, \tilde{\omega}_2, \tilde{\omega}_3, \tilde{\omega}_4\}$ , where

$$\begin{aligned} \tilde{\omega}_1 &= (s_{11} \dots, s_{1,t-1}, i_1, j_2, s_{1,t+2}, \dots, s_{1T}), \quad \tilde{\omega}_2 = (s_{21} \dots, s_{2,t-1}, i_2, j_1, s_{2,t+2}, \dots, s_{2T}), \\ \tilde{\omega}_3 &= (s_{31} \dots, s_{3,t'-1}, i_1, j_1, s_{3,t'+2}, \dots, s_{3T}), \quad \tilde{\omega}_4 = (s_{41} \dots, s_{4,t'-1}, i_2, j_2, s_{4,t'+2}, \dots, s_{4T}). \end{aligned}$$

The resulting move  $\mathbf{z} = \{z(\omega) \mid \omega \in \mathcal{S}^T\}$  is written as

$$z(\omega) = \begin{cases} 1 & \text{if } \omega = \omega_1, \dots, \omega_4, \\ -1 & \text{if } \omega = \tilde{\omega}_1, \dots, \tilde{\omega}_4, \\ 0 & \text{otherwise.} \end{cases}$$

We call this move a “2 by 2 swap”. The corresponding move graph is depicted as follows,



We denote the set of 2 by 2 swaps sharing the move graph (11) by

$$\{t:i_1j_1, t:i_2j_2\} \leftrightarrow \{t':i_1j_2, t':i_2j_1\}. \quad (12)$$

As noted above,  $\omega_1, \omega_2, \omega_3$  and  $\omega_4$  are not necessarily distinct. It may be the case that  $\omega_1 = \omega_3$ ,  $\omega_1 = \omega_4$ ,  $\omega_2 = \omega_3$  or  $\omega_2 = \omega_4$ . In the 2 by 2 swap in (12) and (11), the paths are only partially specified. Therefore it corresponds to a set of moves in term of fully specified paths. In particular, depending on which paths are the same, a 2 by 2 swap may be of degree 2,3, or 4 in terms of the fully specified paths.

The above 2 by 2 swap can be extended in various ways. First it can be extended to a permutation of more states

$$\{t:i_1j_1, \dots, t:i_mj_m\} \leftrightarrow \{t':i_1j_{\sigma(1)}, \dots, t':i_mj_{\sigma(m)}\}, \quad (13)$$

where  $\sigma$  is an element of the symmetric group  $S_m$ . We call this move an “ $m$  by  $m$  permutation”. The degree of this move is at most  $2m$  in terms of paths. The degree is smaller if  $\sigma(l) = l$  for some  $l$ , because swapping  $t:i_lj_l$  and  $t':i_lj_l = t':i_lj_{\sigma(l)}$  does not change anything.

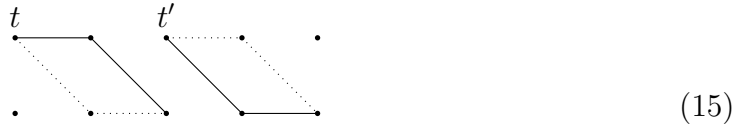
Second, it can be extended to swapping of two partial paths

$$\underbrace{t:i * \dots * j}_k \leftrightarrow \underbrace{t':i * \dots * j}_k, \quad (t \neq t'),$$

where ‘\*’ is arbitrary. For example we can swap  $t:112$  and  $t':122$ , ( $t \neq t'$ ):

$$\begin{aligned} & \{s_1 \dots s_{t-1} 112 s_{t+3} \dots s_T, s'_1 \dots s'_{t'-1} 122 s'_{t'+3} \dots s'_T\} \\ & \leftrightarrow \{s_1 \dots s_{t-1} 122 s_{t+3} \dots s_T, s'_1 \dots s'_{t'-1} 112 s'_{t'+3} \dots s'_T\}, \end{aligned} \quad (14)$$

which can be depicted as



### 3 Markov basis for two state space case

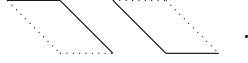
In this section we give an explicit form of a Markov basis for the case of  $S = 2$ . The length  $T$  of the Markov chain is arbitrary.

**Theorem 1.** *A Markov basis for  $S = 2$ ,  $T \geq 4$ , consists of the following moves:*

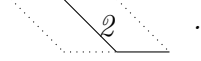
1. *Crossing path swappings.*
2. *Degree one moves.*

3. *2 by 2 swaps of the following form:* 

4. Moves of the following form:



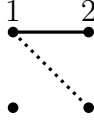
This includes the case of a double transitions in the middle:



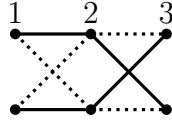
For  $T = 3$  a Markov basis consists of the first three types of moves.

*Proof.* We use an induction on the length  $T$  of the Markov chain combined with the distance reduction argument in [15] for the distance  $|\mathbf{z}| := \sum_{t,i,j} |z_{ij}^t|$ .

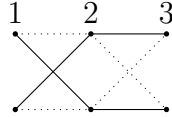
If  $z_{ij}^1 = 0, \forall i, j$ , then we can ignore the transitions  $1:ij, i, j \in \mathcal{S}$ , in both  $\mathbf{x}$  and  $\mathbf{y}$  and regard the chain as starting from  $t = 2$ . Similarly if  $z_{ij}^{T-1} = 0, \forall i, j$ , then we can regard the chain as ending at time  $t = T - 1$ . Therefore we can assume that  $z_{ij}^1 \neq 0$  for some  $i, j$  and  $z_{ij}^{T-1} \neq 0$  for some  $i, j$ . In view of the symmetry of the model and the fact that  $z_1^1 = z_2^1 = 0$ , we can assume without loss of generality that  $z_{11}^1 > 0$  and  $z_{12}^1 < 0$ :



As the initial step of the induction we assume  $T = 3$ . Then by (9)  $z_i^2 = 0, i = 1, 2$ . This necessarily implies that the edge-sign pattern of  $\mathbf{z}$  is of the following form:



By Lemma 2, we can assume that  $\mathbf{x}$  contains the path 112 and 221. Therefore by adding the 2 by 2 swap



to  $\mathbf{x}$ , we can reduce  $|\mathbf{z}|$  by eight. This takes care of the case of  $T = 3$ .

Now consider the case of  $T \geq 4$ . First we explain our strategy. We claim that by moves in Theorem 1 we can always achieve one of the following two things:

- 1)  $|\mathbf{z}|$  is reduced without increasing  $\sum_{i,j} |z_{ij}^1| + \sum_{i,j} |z_{ij}^{T-1}|$ ;
- 2)  $\sum_{i,j} |z_{ij}^1| + \sum_{i,j} |z_{ij}^{T-1}|$  is reduced.

Then either  $|\mathbf{z}|$  can be reduced to zero and we are done, or if we can not further decrease  $|\mathbf{z}|$  then, we can now reduce  $\sum_{i,j} |z_{ij}^1| + \sum_{i,j} |z_{ij}^{T-1}|$ , noting that  $\sum_{i,j} |z_{ij}^1| + \sum_{i,j} |z_{ij}^{T-1}|$  has not increased. By this strategy we can either make  $|\mathbf{z}| = 0$  or employ induction on  $T$ . Therefore Theorem 1 is implied by the above claim.

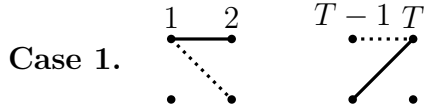
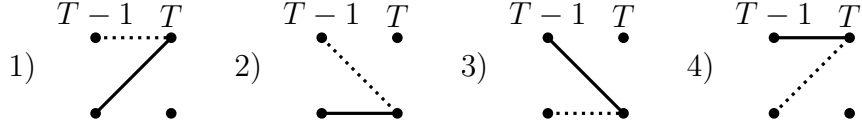
As a preliminary step consider a path of  $\mathbf{x}$  passing through  $s = 1, t = 2$ . If this path ever moves to  $s = 2$  and then comes back to  $s = 1$  before  $T - 1$ , i.e., if this path contains

$t:12$  and  $t':21$ ,  $t < t' < T - 1$ , then we can apply a degree 1 move of the following form

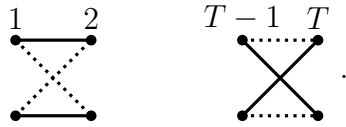


and reduce  $\sum_{i,j} |z_{ij}^1|$  without affecting  $\sum_{i,j} |z_{ij}^{T-1}|$ . Therefore in the following we only need to consider the case that every path of  $\mathbf{x}$  passing through  $s = 1, t = 2$  either always stays at  $s = 1$  until  $T - 1$  or moves once to  $s = 2$  and then stays at  $s = 2$  thereafter until  $T - 1$ .

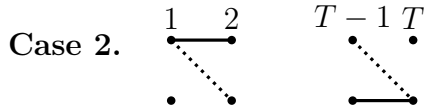
We now check four possible sign patterns of  $\{z_{ij}^{T-1}\}$ .



As shown above, a path in  $\mathbf{x}$  passing through the node  $s = 1, t = 1, 2$  has to either stay at  $s = 1$  until  $T - 1$  or has to transit once to  $s = 2$  and stay  $s = 2$  thereafter until  $T - 1$ . Consider the latter case. If a transition from  $s = 1$  to  $s = 2$  occurs before  $T - 1$ , then in view of  $z_{21}^{T-1} > 0$ , we can assume that the path also contains  $T - 1 : 21$  by Lemma 2. Then we can apply a degree one move to  $\mathbf{x}$  and then  $\sum_{i,j} |z_{ij}^1| + \sum_{i,j} |z_{ij}^{T-1}|$  is reduced. Therefore we only need to consider the case where every path in  $\mathbf{x}$  passing through the node  $s = 1, t = 1, 2$  move to  $s = 2$  at  $T - 1$ . By Lemma 2, we can assume that there is no transition  $t:12$ ,  $t = 2, \dots, T - 1$  in  $\mathbf{x}$  and therefore  $z_{12}^t \leq 0$ , for  $t = 2, \dots, T - 1$ . Then  $z_{12}^{T-1} > 0$  in view of  $z_{12}^1 < 0$ . Interchanging the roles of  $\mathbf{x}$  and  $\mathbf{y}$  and reversing the time direction we similarly have  $z_{21}^1 < 0$ . From the fact that  $z_2^1 = z_2^T = 0$ , we have  $z_{22}^1 > 0$  and  $z_{22}^{T-1} < 0$ , i.e.  $\mathbf{z}$  has a sign pattern

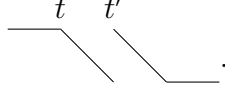


Therefore  $|\mathbf{z}|$  is reduced by eight by a 2 by 2 swap.

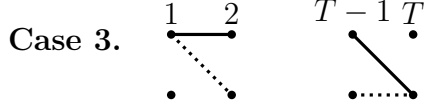


Since  $z_{12}^1 < 0, z_{12}^{T-1} < 0$ , either there exists  $2 \leq t \leq T - 1$  such that  $z_{ij}^t \geq 2$  or there exist  $2 \leq t < t' \leq T - 1$  such that  $z_{12}^t, z_{12}^{t'} > 0$ . In the former case write  $t' = t$ . By the symmetry with respect to time reversal of THMC model, we can assume that a path in  $\mathbf{x}$  passing through the node  $s = 2, t = T, T - 1$  stays at  $s = 2$  until  $t = 2$  or transits once

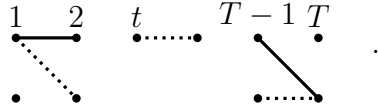
to  $s = 1$  and stays  $s = 1$  until  $t = 2$ . By Lemma 2, we can assume that there exist two paths passing through  $t - 1 : 112$  and  $t' : 122$ , respectively:



Then by subtracting a move of type 4, we can widen the difference  $t' - t$ . By iterating this procedure until either  $t = 1$  or  $t' = T - 1$ , we can reduce  $\sum_{i,j} |z_{ij}^1| + \sum_{i,j} |z_{ij}^{T-1}|$ .



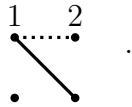
We can assume  $z_{11}^{T-1} \geq 0$  because we have already covered Case 1. Then there has to be  $2 \leq t \leq T - 1$  such that  $z_{11}^t < 0$ :



Also it can be easily seen that  $z_{21}^1 < 0$  (hence  $z_{22}^1 > 0$ ) is reduced to Case 1 by a symmetry consideration. Therefore we can assume  $z_{21}^1 \geq 0$ . Then

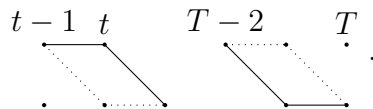
$$z_1^2 = z_{11}^1 + z_{21}^1 > 0,$$

i.e.,  $\mathbf{x}$  dominates  $\mathbf{y}$  at the node  $s = 1, t = 2$ . Then  $z_2^2 < 0$  because  $z_1^2 + z_2^2 = 0$ . Similar consideration shows that  $z_1^{T-1} > 0$  and  $z_2^{T-1} < 0$ . Suppose that a path of  $\mathbf{y}$  passing  $1 : 12$  arrives at  $s = 1$  at time  $t$ . By Lemma 2 we can assume that the path stays at  $s = 1$  at time  $t + 1$ . Denote the path by  $w = (12s_3 \cdots s_{t-1}1s_{t+2} \cdots s_T)$ . Let  $w' = (112s_3 \cdots s_{t-1}1s_{t+2} \cdots s_T)$ . Then the difference of  $w$  and  $w'$  forms a degree one move with a sign pattern

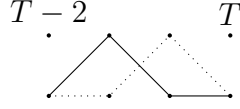


By adding it to  $\mathbf{x}$ , we can reduce  $\sum_{i,j} |z_{ij}^1|$  by two without affecting  $\sum_{i,j} |z_{ij}^{T-1}|$ . Therefore we only need to consider the case where there is no path of  $\mathbf{y}$  passing the node  $s = 2, t = 2$  and arriving at  $s = 1$  at time  $t$ .

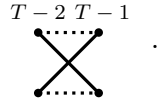
Since  $z_1^2 > 0$ , there has to be some  $t' \leq t$  such that  $z_{12}^{t'} > 0$ . Now assume that  $t' < T - 2$  and choose the minimum  $t'$  with  $z_{12}^{t'} > 0$ . Then a path in  $\mathbf{x}$  passing through  $(s, t) = (1, 2)$  and  $t' : 12$  has to stay at  $s = 2$  from  $t' + 1$  to  $T - 1$ . Recall  $0 < z_1^{T-1} = z_{11}^{T-2} + z_{21}^{T-2}$  and suppose that  $z_{11}^{T-2} > 0$ . Then we can assume that there exists a path passing through  $T - 2 : 112$ . Therefore we can apply type 4 move



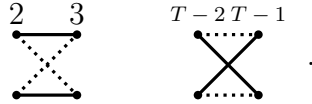
and we can reduce  $\sum_{i,j} |z_{ij}^{T-1}|$  without affecting  $\sum_{i,j} |z_{ij}^1|$ . Suppose that  $z_{21}^{T-2} > 0$ . Then we can assume that there exists a path passing through  $T - 3 : 2212$  and hence we can apply a degree one move



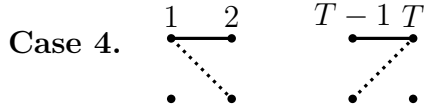
to reduce  $\sum_{i,j} |z_{ij}^{T-1}|$  without affecting  $\sum_{i,j} |z_{ij}^1|$ . Therefore we only need to consider the case of  $t' = t = T - 2$ . Since  $z_1^{T-1} > 0$  and  $z_{11}^{T-2} < 0$ , we have  $z_{21}^{T-2} > 0$ . In the same way we also have  $z_{12}^{T-2} < 0$ . Hence  $\mathbf{z}$  has a sign pattern



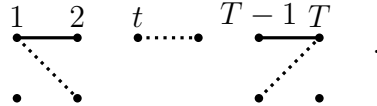
By symmetry we can easily see that  $\mathbf{z}$  has a sign pattern



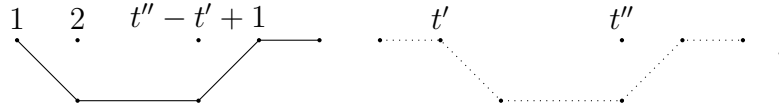
Then we can decrease  $|\mathbf{z}|$  by a 2 by 2 swap.



By a consideration as in the previous case there exists  $t$  such that  $z_{11}^t < 0$ :



As in the previous case there should exist (the minimum)  $t' \leq t$  with  $z_{12}^{t'} > 0$ . By symmetry there also exists (the maximum)  $t'' \geq t + 1$  with  $z_{21}^{t''} > 0$ . Then we can apply a degree 1 move



to decrease  $\sum_{i,j} |z_{ij}^1|$ . This completes the proof of Theorem 1.  $\square$

## 4 Markov basis for the case of length of three

In this section we give an explicit form of a Markov basis for the case of  $T = 3$ . The number of states  $S = |\mathcal{S}|$  is arbitrary.

Let  $i_1, \dots, i_m$ ,  $m \leq S$ , be distinct elements of  $\mathcal{S}$ . Similarly let  $j_1, \dots, j_m$ ,  $m \leq S$ , be distinct elements of  $\mathcal{S}$ . In the  $m$  by  $m$  permutation of (13) let  $t = 1, t' = 2$  and

$$\sigma(1) = m, \sigma(2) = 1, \dots, \sigma(k) = m - 1.$$

Then the resulting set of  $m$  by  $m$  permutation is denoted by

$$\mathcal{Z}(i_1, \dots, i_m; j_1, \dots, j_m) : \{1:i_1j_1, 1:i_2j_2, \dots, 1:i_mj_m\} \leftrightarrow \{2:i_1j_m, 2:i_2j_1, \dots, 2:i_mj_{m-1}\}. \quad (16)$$

A move graph of a permutation for  $S = 6$  with  $m = 4$ ,  $(i_1, i_2, i_3, i_4) = (1, 2, 4, 5)$ ,  $(j_1, j_2, j_3, j_4) = (1, 3, 5, 6)$  is depicted in Figure 1. Now we state the following theorem on

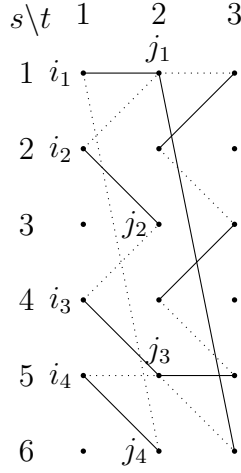


Figure 1: A typical permutation

a Markov basis for the case of  $T = 3$ .

**Theorem 2.** *A Markov basis for THMC model with  $T = 3$  is given by the set of crossing path swappings in (10) and the set of  $m \times m$  permutations  $\mathcal{Z}(i_1, \dots, i_m; j_1, \dots, j_m)$  in (16), where  $m = 2, \dots, S$ ,  $i_1, \dots, i_m$  are distinct, and  $j_1, \dots, j_m$  are distinct.*

For proving Theorem 2 we need more detailed consideration of these moves.

Let

$$\mathcal{I} = \{i_1, \dots, i_m\}, \quad \mathcal{J} = \{j_1, \dots, j_m\}.$$

For each  $j \in \mathcal{I} \cap \mathcal{J}$ , there exist unique indices  $i(j), i'(j) \in \mathcal{I}$ ,  $k(j), k'(j) \in \mathcal{J}$ , such that

$$\begin{aligned} 1:i(j)j &\in \{1:i_1j_1, 1:i_2j_2, \dots, 1:i_mj_m\}, \\ 2:jk'(j) &\in \{2:i_1j_1, 2:i_2j_2, \dots, 2:i_mj_m\}, \\ 1:i'(j)j &\in \{1:i_1j_m, 1:i_2j_1, \dots, 1:i_mj_{m-1}\}, \\ 2:jk(j) &\in \{2:i_1j_m, 2:i_2j_1, \dots, 2:i_mj_{m-1}\}. \end{aligned}$$



For example consider  $j = 1$  in Figure 1. Then  $i(1)1k(1) = 116$  is a solid path and  $i'(1)1k'(1) = 211$  is a dotted path. Next, for each  $j \in \mathcal{I} \setminus \mathcal{J}$ , there exist unique indices  $k(j), k'(j)$  such that

$$2:j k(j) \in \{2:i_1 j_m, 2:i_2 j_1, \dots, 2:i_m j_{m-1}\}, \quad 2:j k'(j) \in \{2:i_1 j_1, 2:i_2 j_2, \dots, 2:i_m j_m\}.$$

For  $j = 2$  in Figure 1,  $k(j) = 1, k'(j) = 3$ ,  $2:21$  is a solid edge and  $2:23$  is a dotted edge. Finally for each  $j \in \mathcal{J} \setminus \mathcal{I}$  there exist unique indices  $i(j), i'(j)$  such that

$$1:i(j)j \in \{1:i_1 j_1, 1:i_2 j_2, \dots, 1:i_m j_m\}, \quad 1:i'(j)j \in \{1:i_1 j_m, 1:i_2 j_1, \dots, 1:i_m j_{m-1}\}.$$

For  $j = 3$  in Figure 1,  $i(j) = 2, i'(j) = 4$ ,  $1:23$  is a solid edge and  $1:43$  is a dotted edge. Define the set of paths  $W_1$  and  $W_2$  as follows,

$$\begin{aligned} W_1 &= \{i(j)jk(j), j \in \mathcal{I} \cap \mathcal{J}\} \cup \{s_j j k(j), j \in \mathcal{I} \setminus \mathcal{J}\} \cup \{i(j)j \tilde{s}_j, j \in \mathcal{J} \setminus \mathcal{I}\} \\ W_2 &= \{i'(j)jk'(j), j \in \mathcal{I} \cap \mathcal{I}\} \cup \{s_j j k'(j), j \in \mathcal{I} \setminus \mathcal{J}\} \cup \{i'(j)j \tilde{s}_j, j \in \mathcal{J} \setminus \mathcal{I}\}, \end{aligned}$$

where  $s_j, j \in \mathcal{I} \setminus \mathcal{J}$  and  $\tilde{s}_j, j \in \mathcal{J} \setminus \mathcal{I}$  are arbitrary states. Then we consider a set of moves  $\bar{Z}(i_1, \dots, i_m; j_1, \dots, j_m) = \{\bar{z}(\omega \mid i_1, \dots, i_m; j_1, \dots, j_m) \mid \omega \in \mathcal{S}^T\}$ ,

$$\bar{z}(\omega \mid i_1, \dots, i_m; j_1, \dots, j_m) = \begin{cases} 1 & \text{if } \omega \in W_1 \\ -1 & \text{if } \omega \in W_2 \\ 0 & \text{otherwise} \end{cases} \quad (17)$$

$\bar{Z}(i_1, \dots, i_m; j_1, \dots, j_m)$  is easily shown to be an  $m$  by  $m$  permutation. Now we have the following proposition, which implies Theorem 2.

**Proposition 2.** *A Markov basis for THMC model for  $T = 3$  is given by the set of crossing path swappings in (10) and moves of  $\bar{Z}(i_1, \dots, i_m; j_1, \dots, j_m)$  of the form (17), where  $m = 2, \dots, S$ ,  $i_1, \dots, i_m$  are distinct, and  $j_1, \dots, j_m$  are distinct.*

*Proof.* For  $T = 3$ , (9) implies that node frequencies are common for two elements  $\mathbf{x}$  and  $\mathbf{y}$  of the same fiber. Therefore the edge-sign pattern graph  $G$  has the following property (P1):

$$\begin{aligned} \text{If } z_{ij}^1 > 0 \text{ } (< 0), \text{ there exists } i' \text{ such that } z_{i'j}^1 < 0 \text{ } (> 0). \\ \text{If } z_{ij}^2 > 0 \text{ } (< 0), \text{ there exists } j' \text{ such that } z_{ij'}^2 < 0 \text{ } (> 0). \end{aligned}$$

Clearly similar property holds for initial nodes at  $t = 1$  and terminal nodes at  $t = 3$ . Also for  $T = 3$  we have  $z_{ij}^1 + z_{ij}^2 = 0$  and therefore  $z_{ij}^1 > 0$  ( $< 0$ ) if and only if  $z_{ij}^2 < 0$  ( $> 0$ ). This means that  $G$  for  $t = 2, 3$  is a copy of  $G$  for  $t = 1, 2$  with signs of edges reversed.

Suppose that  $\mathbf{x}$  and  $\mathbf{y}$  are not edge-wise equivalent. Then by the above properties  $G$  has some positive edge  $1:i_1 j_1$ . We follow the edge from  $t = 1$  to  $t = 2$ . Then by (P1), we can follow a negative edge  $1:i_2 j_1$  back to  $t = 1$ . Then we can again follow a positive edge  $1:i_2 j_2$  to  $t = 2$ , etc. By continuing this, the same node is eventually visited twice and a loop is formed. By considering the shortest loop, it can be easily shown that there exists the following simple loop of  $G$  for  $t = 1, 2$ :

There are distinct indices  $i_1, \dots, i_m$  and distinct indices  $j_1, \dots, j_m$  such that  $1 : i_1 j_1, 1 : i_2 j_2, \dots, 1 : i_m j_m$  are positive edges of  $G$  and  $1 : i_1 j_m, 1 : i_2 j_1, \dots, 1 : i_m j_{m-1}$  are negative edges of  $G$ .

Now we employ the distance reduction argument of Takemura and Aoki [15]. As above let  $\mathcal{I} = \{i_1, \dots, i_m\}$  and  $\mathcal{J} = \{j_1, \dots, j_m\}$ . By Lemma 2 we can assume that  $x(i(j)jk(j)) > 0$  for  $j \in \mathcal{I} \cap \mathcal{J}$ . For  $j \in \mathcal{I} \setminus \mathcal{J}$  we can find a path  $\omega = s_j j k(j)$  with  $x(\omega) > 0$ . Similarly for  $j \in \mathcal{J} \setminus \mathcal{I}$  we can find a path  $\omega = i(j) j \tilde{s}_j$  such that  $x(\omega) > 0$ . Now we can subtract a move in (17) from  $\mathbf{x}$ . This reduces  $|z|$  by  $4m$ . This completes the proof of Proposition 2.  $\square$

## 5 Numerical examples

In this section we give two numerical examples for testing THMC model against the non-homogeneous Markov chain model using our Markov bases.

### 5.1 Respiratory illness example

Table 1: Results of breath test at four ages

|         |          | age = 11 |    |          |     |
|---------|----------|----------|----|----------|-----|
|         |          | 1        |    | 2        |     |
| age = 9 | age = 10 | age = 12 |    | age = 12 |     |
|         |          | 1        | 2  | 1        | 2   |
| 1       | 1        | 94       | 30 | 15       | 28  |
| 1       | 2        | 14       | 9  | 12       | 63  |
| 2       | 1        | 19       | 15 | 10       | 44  |
| 2       | 2        | 17       | 42 | 35       | 572 |

1: wheeze, 2: no wheeze

Table 5.1 refers to a longitudinal study of incidence of respiratory illness in children caused by effects of air pollution (e.g. [18, 2]). The children were examined annually at ages 9 through 12 and classified according to the process of the presence or absence of wheeze.

We examine the goodness-of-fit of homogeneity of Markov chain model  $H_0$  with  $(S, T) = (2, 4)$  by testing the goodness-of-fit of THMC model  $\bar{H}_0$ . We use Pearson's  $\chi^2$  statistic. For data in Table 5.1 we have  $\chi^2 = 129.59$ .

We computed the exact distribution of  $\chi^2$  via MCMC with a Markov basis derived in Theorem 1. We sampled 100,000 tables after 50,000 burn-in steps. The histogram of the sampling distribution of  $\chi^2$  is shown in Figure 5.1. The solid line in the figure represents the density function of the asymptotic  $\chi^2$  distribution with degrees of freedom 11. The asymptotic  $p$ -value and the exact  $p$ -value are almost zeros and THMC model is rejected. Since THMC model is rejected, the homogeneity of Markov chain model is also rejected.

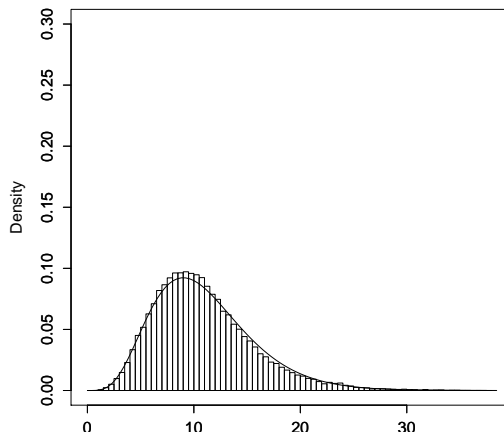


Figure 2: Sampling distribution of  $\chi^2$  via MCMC

## 5.2 Marijuana use example

Table 2: Marijuana use data

|      |          | 1978   |       |       |      |  |  |      |  |  |
|------|----------|--------|-------|-------|------|--|--|------|--|--|
|      |          | 1      |       |       | 2    |  |  | 3    |  |  |
| 1977 | 1979     | 1979   |       |       | 1979 |  |  | 1979 |  |  |
|      | 1 2 3    | 1 2 3  | 1 2 3 | 1 2 3 |      |  |  |      |  |  |
| 1    | 140 13 8 | 5 17 6 | 1 1 4 |       |      |  |  |      |  |  |
| 2    | 4 1 0    | 4 3 3  | 1 2 9 |       |      |  |  |      |  |  |
| 3    | 0 0 1    | 1 1 1  | 0 3 8 |       |      |  |  |      |  |  |

Table 5.2 refers to a longitudinal data from 1977 to 1979 on marijuana use of 237 respondents who were age 14 in 1977 (e.g [17]). The degrees of dependence are categorized into the following three levels, 1. never use; 2. no more than once a month; 3. more than once a month.

We examine the goodness-of-fit of  $H_0$  with  $(S, T) = (3, 3)$  by testing  $\bar{H}_0$ . We again use Pearson's  $\chi^2$ . We have  $\chi^2 = 39.791$ .

We computed the exact distribution of  $\chi^2$  via MCMC with a Markov basis derived in Theorem 2. We sampled 100,000 tables after 50,000 burn-in steps. Figure 5.2 represents the histogram of the sampling distribution of  $\chi^2$  and the solid line in the figure is the density function of the asymptotic  $\chi^2$  distribution with degrees of freedom 16. The asymptotic  $p$ -value and the exact  $p$ -value are  $8.352 \times 10^{-4}$  and 0.02078 and THMC model is rejected. Also for this example the homogeneity of Markov chain model is rejected, since THMC model is rejected. However, note that the approximation by  $\chi^2$  distribution is not very good for this data. This is probably due to small frequencies in the data set.

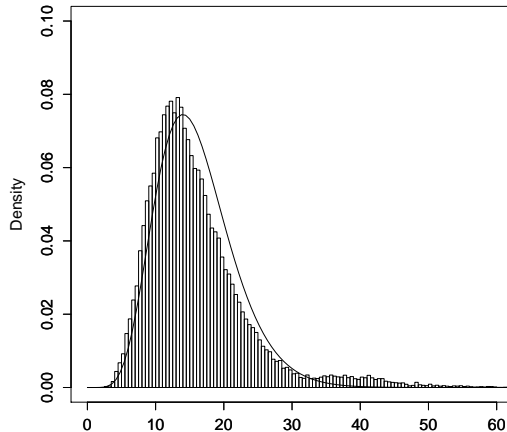


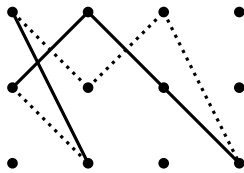
Figure 3: Sampling distribution of  $L$  via MCMC

## 6 Discussion and a conjecture for general case

From the viewpoint of application, it is clearly desirable to obtain Markov bases for general  $S$  and  $T$ . By 4ti2 we can obtain a Markov basis for  $S = 3$  and  $T = 5$ . However currently this case seems to be the largest case which can be handled by a software.

Even if obtaining a Markov basis is difficult, it is of theoretical interest to know some properties of Markov bases for general  $S$  and  $T$ . Note that the description of Markov basis for  $S = 2$  is common for all  $T \geq 4$ . This is very similar to the notion of Markov complexity ([10], [14], [4]) and we believe that there exists some bound of complexity of Markov basis in  $T$  for a given  $S$ .

We have done extensive investigation of edge-sign pattern graphs  $G$  for the case  $S = 3$  and  $T = 4$ . We will discuss these edge-sign pattern graphs in [16]. It seems that the following notion of *extended simple loop* of the edge-sign pattern graph  $G$  is important. Here we give only a rough definition of an extended simple loop. An extended simple loop is a loop, such that when we are moving towards the future we follow positive edges and when we are moving towards the past we follow negative edges of  $G$ . Also we require that each node is passed at most once. An important example of an extended simple loop for  $S = 3$  and  $T = 4$  is depicted as follows.



We have used the term “extended” to indicate that the lengths of partial paths may be greater than one. If all the edges are of length one (in this case the loop involves only two time points  $t$  and  $t + 1$ ), we call it a *simple loop*.

Note that for the case of  $S = 2$ , a Markov basis consists of moves, which are sum of at most two extended simple loops. For the case of  $S = 3$  and  $T = 4$  we checked that a Markov basis consists of moves, which are sums of at most three extended simple loops. Therefore our conjecture at this point is that for each  $S$ , there exists  $k_S$ , such that a Markov basis consists of moves which are sums of at most  $k_S$  extended simple loops. A stronger conjecture is  $k_S = S$ .

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