Algebraic Algorithm for Direct Sampling from Toric Models and Hypergeometric Functions

By

SHUHEI MANO and NOBUKI TAKAYAMA
(The Institute of Statistical Mathematics and Kobe University, Japan)

Abstract. We show that Pfaffians or contiguity relations of hypergeometric functions of several variables give a direct sampling algorithm from toric models in statistics, which is a Markov chain on a lattice generated by a matrix $A$. A correspondence among graphical models and $A$-hypergeometric system is discussed and we give a sum formula of special values of $A$-hypergeometric polynomials. Some hypergeometric series which are interesting in view of statistics are presented.

Key Words and Phrases. $A$-hypergeometric system, discrete exponential family, GKZ-hypergeometric system, graphical model, Markov chain Monte Carlo

2020 Mathematics Subject Classification Numbers. 33C65, 33C90, 33F99, 62H17, 62R01, 65C05

1 Introduction

Consider a discrete sample with state space $[m] := \{1, 2, \ldots, m\}$ for $m \in \mathbb{N}$, where $\mathbb{N}$ is the set of positive integers. In this paper, we will discuss the discrete exponential families in statistics, which are also called log-affine models or toric models.

Definition 1. Let $A = (a_{ij}) \in \mathbb{Z}^{d \times m}$ be a matrix of integers such that $(1, \ldots, 1) \in \text{rowspan}(A)$ and let $y \in \mathbb{R}^m_{>0}$. The toric model associated with $A$ is the set of probability distributions

$$\{p \in \text{int}(\Delta_{m-1}) : \log p \in \log y + \text{rowspan}(A)\},$$

where $\Delta_{m-1}$ is the standard $d$-dimensional simplex. If $y = 1$, the model is called a log-linear model.

Suppose we have parameters $\phi \in \mathbb{R}^d_{>0}$. For the matrix $A = (a_{ij}) \in \mathbb{Z}^{d \times m}$ with $(1, \ldots, 1) \in \text{rowspan}(A)$, the vector $p$ in Definition 1 may be parameterized as

$$p_j = \frac{y_j}{Z(\phi, y)} \prod_{i \in [d]} \phi^{a_{ij}}, \quad j \in [m] \tag{1}$$
with the normalization constant $Z(\phi, y)$ such that $\sum_{j \in [m]} p_j = 1$. The set determined by the linear transformation

$$F_b(A) := \{ u : Au = b, u \in \mathbb{N}_0^m \}, \quad \mathbb{N}_0 := \{0\} \cup \mathbb{N}$$

is called the $b$-fiber associated to configuration matrix $A$ with the minimal sufficient statistics $b \in \mathbb{N}_0 A := \sum_{j \in [m]} \mathbb{N}_0 a_j$ for $\phi$, where $a_j$ denotes the $j$-th column vector of $A$. We will use the notation $u := \sum_{j \in [m]} u_j$, where the centered dot $(\cdot)$ in the position of the index $j$ means that the index $j$ is summed up. A sample consisting of observations in which counts of the $j$-th state is $u_j$, $j \in [m]$ taken from the multinomial distribution specified by the probability mass function (1) follows the probability law

$$P(U = u, AU = b) = \frac{u!}{\{Z(\phi, y)\}_u} \prod_{i \in [d]} \phi_i^b \prod_{j \in [m]} y_j^{u_j} u_j!.$$  

The conditional distribution given the minimal sufficient statistics $b$ is

$$P(U = u | AU = b) = \frac{1}{Z_A(b; y)} y_u^u, \quad y_u := \prod_{j \in [m]} y_j^{u_j}, \quad u! := \prod_{j \in [m]} u_j!.$$  

Here, the normalization constant

$$Z_A(b; y) := \sum_{u \in F_b(A)} y_u^u u!$$

is called the $A$-hypergeometric polynomial, or the GKZ-hypergeometric polynomial, defined by Gel’fand, Kapranov, and Zelevinsky in the end of the 1980’s [9]. We adopt the convention $Z_A(b; y) = 0$ if $b \notin \mathbb{N}_0 A$. It is straightforward to see that a sample consisting of the Poisson random variables whose means are given by the probability mass function (1) also follows the conditional distribution (3). Takayama et al. [27] called the probability distribution (3) the $A$-hypergeometric distribution.

**Definition 2** ([27]). For a matrix $A = (a_{ij}) \in \mathbb{Z}^{d \times m}$ such that $(1, \ldots, 1) \in \text{rowspan}(A)$ and $b \in \mathbb{N}_0 A$, the probability distribution of the vector $u \in \mathbb{N}_0^m$ given by the probability mass function

$$p(u; y) = \frac{1}{Z_A(b; y)} y_u^u u!,$$

with parameters $y \in \mathbb{R}^m_0$ is called the $A$-hypergeometric distribution. The support is the $b$-fiber $F_b(A)$ defined in (2).
A typical use of sampling from toric models in statistics is a hypothesis testing. Testing the hypothesis $y = 1$ is specifically called Fisher’s exact test. Consider a two-by-two contingency table. Under the independence of rows and columns, the conditional distribution given marginal sums is called the hypergeometric distribution, which is an $A$-hypergeometric distribution with $y = 1$. It is known that sampling from the hypergeometric distribution is achieved by an urn model (see Subsection 3.1 for the details). The conditional distribution with $y \neq 1$, where $y$ is the odds ratio of the interaction between rows and columns, is called the generalized hypergeometric distribution. To the best of the authors knowledge, in contrast to the hypergeometric distribution, sampling from the generalized hypergeometric distribution had not been known. Moreover, if a toric model is not graphical, or graphical but not chordal (see Subsection 3.2 for the definitions), sampling from such models had not been known even with $y = 1$. It had been considered that sampling from such models is difficult. The difficulty motivates the use of the Metropolis chain, which is one of the most common tools in the Markov chain Monte Carlo methods, see, e.g., [10, 14]. In the Metropolis chain, the unique stationary distribution of an ergodic Markov chain is designed to be the distribution which we need. Diaconis and Sturmfels [3] proposed the use of Gröbner bases of the toric ideal of a configuration matrix $A$ to construct a basis of moves in the Metropolis chain. They called such a basis, or a generating set for the toric ideal, a Markov Basis. The state space of the chain is the $b$-fiber, and in an implementation of the chain the ratio of two monomials, which correspond to the current state and the proposed next state, should be computed in each step of the chain. A comprehensive treatment of Markov bases is [2].

Recently, Mano [15] showed that direct sampling from the conditional distribution of any toric models given the minimal sufficient statistics, or the $A$-hypergeometric distribution, is possible with utilizing a holonomic ideal, called the $A$-hypergeometric ideal. Extensive discussion on the algorithm is available in the monograph [16]. Throughout this paper, we call a sampling from a distribution exactly a direct sampling to distinguish it from approximate samplings resorting the use of a Metropolis chain. In the context of graphical models, it might be surprising that direct sampling is possible even when the Markov property represented by the interaction graph does not hold, because the Markov property is the key for direct sampling from chordal graphical models ever known, see, e.g., Section 4.4 of [13]. In fact, the proposed algorithm in [15] utilizes another kind of Markov property which any toric model possesses. The purpose of this paper is two fold. The first purpose is to present an efficient implementation of the algorithm when the transition probability of the Markov chain run by the algorithm is not avail-
able, by introducing a notion of the Markov lattice defined in Section 2. The Markov lattice represents the Markov property mentioned above. The second purpose is to present concrete examples to show how the algorithm works with aids of Pfaffians or contiguity relations of hypergeometric functions of several variables for well-known toric models including graphical models, because the paper [13] focused on toric models associated with configuration matrices of two rows.

To give an important remark on our terminology concerning the hierarchical log-linear model, here we define it. A simplicial complex with ground set $V$ is a set $\Gamma \subseteq 2^V$ such that if $F \in \Gamma$ and $F' \subseteq F$, then $F' \in \Gamma$. An element of $\Gamma$ will be called the faces of $\Gamma$, and the inclusion maximal faces are the facets of $\Gamma$. A simplicial complex is specified by listing its facets. For instance, $\Gamma = [12][13][23]$ is the bracket notation of the simplicial complex

$$\Gamma = \{\emptyset, \{1\}, \{2\}, \{3\}, \{1, 2\}, \{1, 3\}, \{2, 3\}\}.$$  

The brackets are also used to represent sets of integers, but the distinction will be obvious from the context. Consider the ground set $V = \{1, \ldots, |V|\} = [[|V|]]$ and discrete random variables, $X_1, \ldots, X_{|V|}$, where $X_i \in [r_i]$ for some level $r_i \in \mathbb{N}$, $i \in V$. If $r_1 = \cdots = r_{|V|} = 2$, the model is called binary. The joint state space of a random vector $X = (X_1, \ldots, X_{|V|})$ is $\mathcal{I}_V = \prod_{i \in V} [r_i]$. For example, when $\Gamma = [1][2] \subset 2^{(1,2)}$ and the levels are $r_1 = 2$ and $r_2 = 3$, $\mathcal{I}_V = \{(1,1), (1,2), (1,3), (2,1), (2,2), (2,3)\}$. For a state $i_V = (i_1, \ldots, i_{|V|}) \in \mathcal{I}_V$ and a subset $F = \{f_1, f_2, \ldots\} \subset V$, we write $i_F = (\cdots, i_{f_1}, \cdots, i_{f_2}, \cdots, \cdots)$, where the centered dots (·) are used to keep the places of $V \setminus F$. In other words, $i_j$ of $i_F$ takes a value in $[r_j]$ if $j \in F$ and $i_j = \cdot$ if $j \notin F$. For example, for the binary simplicial complex $\Gamma = [12][14] \subset 2^{(1,2,3,4)}$, the set $\mathcal{I}_F$ with $F = \{1, 2\}$ is $\{(1,1,\cdot,\cdot), (1,2,\cdot,\cdot), (2,1,\cdot,\cdot), (2,2,\cdot,\cdot)\}$. Commas in states will be omitted hereafter, if it causes no confusion. The random vector $X_F = (X_f)_{f \in F}$ has the state space $\mathcal{I}_F = \prod_{f \in F} [r_f]$.

**Definition 3.** Let $\Gamma \subseteq 2^V$ be a simplicial complex. For each facet $F \in \Gamma$, we introduce a set of $|\mathcal{I}_F|$ positive parameters $\phi_{i_F}$. In addition, for each face $F' \in \text{face}(V) \setminus \Gamma$, we introduce a set of positive parameters $\psi_{i_{F'}}$. The hierarchical log-linear model associated with $\Gamma$ is the set of all probability distributions

$$\mathcal{M}_\Gamma = \left\{ p \in \text{int}(\Delta_{|\mathcal{I}_V|-1}) : p_{i_V} = \frac{1}{Z(\phi, \psi)} \prod_{F \in \text{facet}(\Gamma)} \phi_{i_F} \prod_{F' \in \text{face}(V) \setminus \Gamma} \psi_{i_{F'}}, \ i_V \in \mathcal{I}_V \right\},$$  

where $Z(\phi, \psi)$ is the normalizing constant.
Since the parameterization (6) is a form of the parameterization (1), the conditional distribution of the hierarchical log-linear model given minimal sufficient statistics for \( \phi \) is the \( A \)-hypergeometric distribution. The configuration matrix \( A \) is a binary matrix with \( m = |I_V| \) columns and \( d = \sum_{F \in \Gamma} |I_F| \) rows, and determines the \( b \)-fiber (2). Let \( F, F' \subseteq V \). If states of subsets \( i_F \in I_F \) and \( i_{F'} \in I_{F'} \) have no contradiction, that is, if all the elements are not different between \( i_F \) and \( i_{F'} \) by regarding \( \cdot \) as a wildcard and the number of \( \cdot \) in \( i_F \) is smaller than that of \( i_{F'} \), we write \( i_F \subset i_{F'} \). For example, \((11 \cdot 1) \subset (\cdot 1 \cdot 1) \) but \((11 \cdot 1) \not\subset (\cdot 2 \cdot 1) \). This is a consistent notation if we regard the \( i \)-th \( \cdot \) as the set \([r_i]\). Let \( u(i_V) \in \mathbb{N}_0^{r |V|} \) be an \( r_1 \times \cdots \times r_{|V|} \) contingency table, which is also denoted by \( u_{i_V} \) for saving space. For any subset \( F = \{f_1, f_2, \ldots \} \subseteq V \), let \( u(i_F) \) be the \( r_{f_1} \times r_{f_2} \times \cdots \) marginal table such that \( u(i_F) = \sum_{j \in I_V \setminus F} u(i_F, j) \). In other words, the symbol \( u(i_F) \) is the sum of the count \( u(i_V) \) of the state \( i_V \in I_V \) such that \( i_V \subset i_F \). For example, \( u_{1 \cdot 2} = u(1 \cdot 2) = \sum_{i_1 \in [r_1]} \sum_{i_2 \in [r_2]} u(i_1 i_2 2) \). Hence, for a simplicial complex \( \Gamma = [F_1][F_2] \cdots \), the configuration matrix \( A \) determines the linear transformation \( u(i_V) \mapsto (u(i_{F_1}), u(i_{F_2}), \ldots) \), or minimal sufficient statistics for \( \phi \).

**Remark 1.1.** The standard definition of the hierarchical log-linear model is the probability distributions (6) with parameters \( \psi = 1 \) [13, 24]. In fact, tests in hierarchical log-linear models are frequently performed between larger and smaller models in terms of inclusion of the associated simplicial complexes with \( \psi = 1 \) (see Subsection 4.3.2 of [13]). In this paper, we define the hierarchical log-linear model in a broader sense. The definition has a statistical meaning. If a hierarchical log-linear model with \( \psi = 1 \) is used as the null model for Fisher’s exact test, the model with \( \psi \neq 1 \) but associated with the same simplicial complex as the model with \( \psi = 1 \) provides an alternative model.

This paper is organized as follows. In Section 2 after reviewing the direct sampling algorithm proposed in [15], or Algorithm 2.1, the Markov lattice, which is a bounded integer lattice generated by the configuration matrix \( A \), is introduced. A single run of Algorithm 2.1 produces a sample path of the Markov chain on the Markov lattice, where the transition probability is given by the \( A \)-hypergeometric polynomials. If a closed form of an \( A \)-hypergeometric polynomial is known for a special value, we will call it an \( A \)-hypergeometric sum formula. For such a case, the implementation is straightforward. Otherwise, how to compute the transition probability in each step of the algorithm is the key for an efficient implementation. It is shown that the computation can be done along with each sample path on the Markov lattice, if Pfaffians for the \( A \)-hypergeometric system is given. The
method is summarized as Algorithm 2.2. In Section 3, the cases that the $A$-
hypergeometric sum formula is known are discussed. The celebrated formula
of the normalization constants of chordal graphical models given by Sundberg
[25] is revisited as an $A$-hypergeometric sum formula. In Section 4 some con-
crete examples are discussed. Algorithms 2.1 and 2.2 are implemented for the
univariate Poisson regression model and two-way contingency tables, and the
performances are evaluated and compared with those of approximate sam-
plings by Metropolis chains. The non $l$ ($\geq 3$)-way interaction model, which is
an important class of non-graphical toric models, is also discussed. Inspired
by the case that levels are larger than two, we define a generalization of the
Aomoto–Gel’fand hypergeometric series.

There is a remarkable analogy between the direct sampling discussed in
this paper and the Metropolis chain. In the Metropolis chain, transitions
are along with the Markov basis with probabilities given by the ratio of two
monomials within the $b$-fiber, or $\{y^b : b \in \mathcal{F}_b(A)\}$, while in the direct sam-
pling discussed in this paper transitions are along with the Markov lattice
whose maximum is $b$ with probabilities given by the polynomials whose sup-
port is $\mathcal{F}_v(A)$, $v \prec b$. Generally speaking, the Metropolis chain is useful in
the situation that the normalization constants of the distribution which we
need are not available. The direct sampling algorithm discussed in this paper
is useful if the normalization constants can be evaluated recursively.

This paper describes an interplay between the direct sampling algorithm
and the theory of hypergeometric functions of several variables. The direct
sampling algorithm proposes interesting classes of hypergeometric functions
and also the graphical toric model gives an interesting new formula of hyper-
geometric polynomials. On the opposite side, studies of contiguity relations
of hypergeometric functions will give an efficient direct sampler. There are
general algorithms to derive the relations, but they are not efficient. New
algorithms and theories for hypergeometric functions are expected.

2 The direct sampling on the Markov lattice

In this section we introduce the Markov lattice, which is a bounded integer
lattice generated by the configuration matrix. The notion of the Markov
lattice aids to construct the direct sampling algorithms. The computational
complexity of the algorithms are evaluated.

Recall that the $A$-hypergeometric polynomial (4) is a solution of the $A$-
hypergeometric system.

Definition 4. For a matrix $A = (a_{ij}) \in \mathbb{Z}^{d \times m}$ and a vector $b \in \mathbb{C}^d$, the
$A$-hypergeometric system is the following system of linear partial differential
equations for an indeterminate function $f = f(y)$:

\[
(\sum_{j \in [m]} a_{ij}\theta_j - b_i) \cdot f = 0, \quad i \in [d], \quad \theta_j := y_j\partial_j, \quad \partial_j := \frac{\partial}{\partial y_j}, \quad \text{and} \quad (7)
\]

\[
(\partial^{z^+} - \partial^{z^-}) \cdot f = 0, \quad z \in \text{Ker} A \cap \mathbb{Z}^m, \quad \partial^{z} := \prod_{j \in [m]} \partial^{z_j}, \quad (8)
\]

where $z^+_j = \max\{z_j, 0\}$ and $z^-_j = -\min\{z_j, 0\}$. The second group of operators in (8) generates the toric ideal $I_A$ of $A$.

Let $H_A(b)$ denotes the left ideal of the Weyl algebra generated by (7) and (8). We call $H_A(b)$ the $A$-hypergeometric ideal with parameters $b$. In the following discussion, we will work with the ring of differential operators $R = C(y_1, \ldots, y_m)\langle \partial_1, \ldots, \partial_m \rangle$ with the commutation rule

\[
\partial_j \cdot h(y) = h(y) \cdot \partial_j + \partial_j h(y), \quad h(y) \in C(y_1, \ldots, y_m).
\]

If $(1, \ldots, 1) \in \text{rowspan}(A)$, the condition (7) demands homogeneity of the $A$-hypergeometric polynomial $Z_A(b; y)$:

\[
(\sum_{j \in [m]} \theta_j - \text{deg}(b)) \cdot Z_A(b; y) = 0,
\]

where $\text{deg}(b) := \text{deg}(Z_A(b; y))$. It is known that $A$-hypergeometric polynomials satisfy the contiguity relation (9):

\[
\partial_j Z_A(b; y) = Z_A(b - a_j; y), \quad j \in [m],
\]

which leads to

\[
\sum_{j \in [m]} e_{A}(b, b - a_j; y) \frac{\text{deg}(b)}{\text{deg}(b)} = 1, \quad e_{A}(b, b - a_j; y) := \frac{Z_A(b - a_j; y)}{Z_A(b; y)} y_j.
\]

Here, $e_{A}(b, b - a_j; y)$ is the marginal expectation of $u_j$ when the random vector $(u_1, \ldots, u_m)$ follows the $A$-hypergeometric distribution (5) with parameters $y$. Let us consider a Markov chain of a vector in $\mathbb{N}_0 A$ runs over an integer lattice embedded in $\mathbb{N}_0 A$ with the transition probability

\[
\mathbf{P}(b - a_j | b) = \frac{e_{A}(b, b - a_j; y)}{\text{deg}(b)} =: M(b, b - a_j), \quad b - a_j \in \mathbb{N}_0 A, \quad j \in [m],
\]

and $\mathbf{P}(b - a_j | b) = 0$ if $b - a_j \notin \mathbb{N}_0 A$. Since the contiguity relation (9) implies that $\text{deg}(b - a_j) = \text{deg}(b) - 1$, the unique absorbing state of the Markov
chain is the zero vector. A sample path of the Markov chain is specified by a sequence \( (j_1, \ldots, j_{\deg(b)}) \in [m]^{\deg(b)} \), and the probability is

\[
P\{ (j_1, \ldots, j_{\deg(b)}) \} = M(b, b-a_{j_1}) M(b-a_{j_1}, b-a_{j_1}-a_{j_2}) \]

\[
\cdots M(b-a_{j_1} - \cdots - a_{j_{\deg(b)-1}}, b-a_{j_1} - \cdots - a_{j_{\deg(b)}} = 0) \]

\[
e^{(b, b-a_{j_1}; y)} e^{(b-a_{j_1}, b-a_{j_1}-a_{j_2}; y)} \frac{\deg(b)}{\deg(b)-1} \cdots \frac{e^{(b-a_{j_1} - \cdots - a_{j_{\deg(b)-1}}, 0; y)}}{1} = \frac{1}{\deg(b)!} y^u Z_A(b; y),
\]

where \( u_j := |\{ t : j_t = j, t \in [\deg(b)]\}|, j \in [m] \). Accounting the order of appearance of \([m]\) in the multiset \( \{j_1, \ldots, j_{\deg(b)}\} \), the \( A \)-hypergeometric distribution appears:

\[
P(U = u) = \frac{u!}{u_1! \cdots u_m!} P\{ (j_1, \ldots, j_{\deg(b)}) \} = \frac{1}{Z_A(b; y)} y^u u!.
\]

This argument is summarized as the following algorithm.

**Algorithm 2.1 ([13]).**

*Input:* A matrix \( A \in \mathbb{Z}^{d \times m} \), a vector \( b \in \mathbb{N}_0 A \), parameters \( y \in \mathbb{R}_{>0}^m \), and the \( A \)-hypergeometric polynomials \( Z_A(b; y) \) defined in (4).

*Output:* The vector \( (u_1, \ldots, u_m) \) following the \( A \)-hypergeometric distribution associated with \( A \) and \( b \).

*Step 1:* Let \( t = 1 \) and \( n = \deg(b) \).

*Step 2:* Compute \( \tilde{e}(b, b-a_j; y) = Z_A(b-a_j; y_j), \forall j \in [m] \).

*Step 3:* Divide the interval \([0, 1]\) with the ratio

\[e(b, b-a_j; y) : e(b-a_j, b-a_{j+1}; y) : \cdots : e(b-a_1, b-a_m; y),\]

where the \( j \)-th interval is zero if \( b-a_j \notin \mathcal{L}_A(b) \). (see below for \( \mathcal{L}_A(b) \).)

*Step 4:* Get a random number of the uniform distribution on \([0, 1]\). If the number falls in the interval of \( \tilde{e}(b, b-a_j; y) \), then put \( j_t = j \).

*Step 5:* If \( \deg(b-a_{j_t}) = 0 \), go to Step 6. Else, set \( t \leftarrow t+1, b \leftarrow b-a_{j_t} \), and go to Step 2.

*Step 6:* Output the vector \( (u_1, \ldots, u_m) \), \( u_j := |\{ t : j_t = j, t \in [n]\}| \).
If the transition probability, or \( \tilde{e}(b, b - a_j; y) \), is known, the computational complexity of Algorithm 2.1 is \( O(md\nu) \), whose dominant contribution comes from updating \( b \in \mathbb{N}_0^d \) for each \( j \in [m] \) in Step 2. If a closed form of the \( A \)-hypergeometric polynomial, or the \( A \)-hypergeometric sum formula, is available, it is straightforward to compute \( \tilde{e}(b, b - a_j; y) \). Even otherwise, in principle, we can compute the \( A \)-hypergeometric polynomial for any matrix \( A \). To introduce Algorithm 2.2, we reproduce how to compute the \( A \)-hypergeometric polynomial.

Consider a coset of \( R \) modulo the \( A \)-hypergeometric ideal \( H_A(b) \), or \( R/H_A(b) \). A monomial \( u \notin \mathcal{I}(H_A(b)) \) with respect to a monomial term order \( \prec \) is called a standard monomial with respect to the initial ideal \( \mathcal{I}(H_A(b)) \). The set of standard monomials \( \{ \partial^{\mu(0)} = 1, \partial^{\mu(1)}, \ldots, \partial^{\mu(r-1)} \} \) forms a basis of the vector space \( R/H_A(b) \), where the dimension \( r \) is called the holonomic rank of \( H_A(b) \). It is known that \( r = \text{vol}(A) \), where \( \text{vol}(A) \) is the volume of the convex hull of \( \{0, a_1, \ldots, a_m\} \) with the unit being the volume of the unit simplex \( \{0, e_1, \ldots, e_d\} \) and \( e_i \) is a unit vector in \( \mathbb{N}^d \) whose \( i \)-th component is 1 and the other components are zero (Theorem 3 of [19]). The hypergeometric system \( H_A(b) \) can be transformed into the Pfaffian system

\[
\theta_j \cdot q(b; y) = P_j(b; y)q(b; y), \quad j \in [m]
\]

with

\[
q(b; y) := (\theta^{u(k)} Z_A(b; y) : k \in 0 \cup [r - 1])^\top, \quad (10)
\]

where the elements of the \( r \times r \) matrix \( P_j(b; y) \) are rational functions of \( y \), and the vector \( q(b; y) \) will be called the Gauss–Manin vector of \( Z_A(b; y) \). They are obtained via a Gröbner basis normal form with respect to a Gröbner basis of the hypergeometric ideal generated by \( H_A(b) \) (Theorem 1.4.22 of [23]). By using the contiguity relation (9), we have a recursion for the vector \( q \),

\[
y_j q(b - a_j; y) = \tilde{P}_j(b; y) q(b; y), \quad j \in [m], \quad q(0; y) = (1, 0, \ldots, 0)^\top,
\]

where

\[
\tilde{P}_j(b; x) = (E_r + S_j) P_j(b; x), \quad S_j = \begin{pmatrix}
0 & 0 & \cdots & 0 \\
-y_j^{-1}\theta^{u(1)}(y_j) & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
-y_j^{-1}\theta^{u(r-1)}(y_j) & 0 & \cdots & 0
\end{pmatrix}
\]

and \( E_r \) is the \( r \times r \) identity matrix. Ohara and Takayama [20] showed that \( q_0(b; y) = Z_A(b; y) \) is obtained by the matrix multiplications:

\[
q(b; y) = y_{j_1} \cdots y_{j_{\deg(b)}}
\times \tilde{P}_{j_1}^{-1}(b; y) \tilde{P}_{j_2}^{-1}(b - a_{j_1}; y) \cdots \tilde{P}_{j_{\deg(b)-1}}^{-1}(b - a_{j_1} - \cdots - a_{j_{\deg(b)-1}}; y)
\times q(0; y), \quad (11)
\]
for a sequence of vectors $b, b - a_j, \ldots, 0$, and called this method to obtain the Gauss–Manin vector the difference holonomic gradient method. Hence, in principle, we can obtain $\tilde{c}(b, b - a_j) = Z_A(b - a_j; y)_j$, since the set of standard monomials forms a basis of the vector space $R/H_A(b)$. In practice, computation of a Gröbner basis is expensive, but such computation can be avoided if the matrices $P_j, j \in [m]$ are computed by another way with using specific properties of each $A$-hypergeometric system. See Section 4 for some examples.

The Markov chain of a vector in $\mathbb{N}_0^d$ discussed above runs over an integer lattice embedded in $\mathbb{N}_0 A$. A drawback of Algorithm 2.1 is that if the number of elements of the lattice is huge, it is practically impossible to compute the $A$-hypergeometric polynomials for all the elements in advance. An efficient procedure to compute the transition probability, or $\tilde{c}(b, b - a_j; y)$, is needed. Algorithm 2.2 is based on such a procedure. To describe the procedure, let us introduce the notion of the Markov lattice. The Hasse diagram of an example of the Markov lattice is shown as Figure 1.

**Definition 5.** Consider a matrix $A = (a_{ij}) \in \mathbb{Z}^{d \times m}$ and a vector $b \in \mathbb{N}_0 A = \sum_{j \in [m]} \mathbb{N}_0 a_j \subset \mathbb{N}_0^d$. The Markov lattice $\mathcal{L}_A(b)$ is the bounded integer lattice
embeded in \( \mathbb{N}_0A \) equipped with the partial order

\[ v \in \mathbb{N}_0A \text{ and } v - a_j \in \mathbb{N}_0A \Rightarrow v - a_j \prec v, \]

and the maximum and the minimum are \( b \) and 0, respectively.

A lattice consists of a partially ordered set in which any two elements have a unique supremum and a unique infimum. In fact, the Markov lattice is a lattice, because the unique supremum and infimum of two elements \( v = \sum_{j \in [m]} v_j a_j \) and \( w = \sum_{j \in [m]} w_j a_j \) are \( \sum_{j \in [m]} \max\{v_j, w_j\} a_j \) and \( \sum_{j \in [m]} \min\{v_j, w_j\} a_j \), respectively.

The state space of the Markov chain run by Algorithm 2.2 is the Markov lattice \( \mathcal{L}_A(b) \), where the states are the elements of \( \mathcal{L}_A(b) \). An element \( v \) of the Markov lattice specifies the \( v \)-fiber \( \mathcal{F}_v(A) \), or the \( A \)-hypergeometric polynomial \( Z_A(v; y) \). The transitions with positive probabilities occur between neighbors, or from an element \( v \) to an element \( u \) satisfying \( u \prec v \).

Define a vector

\[ \tilde{q}(v; y) := (\theta_1, \ldots, \theta_m)^\top \cdot Z_A(v; y), \quad v \in \mathcal{L}_A(b). \]

Since the set of standard monomials forms a basis of the vector space \( R/H_A(b) \), there exists an \( m \times r \) matrix \( T(v, y) \) whose elements are rational functions of \( y \) satisfying

\[ \tilde{q}(v; y) = T(v; y)q(v; y), \]

where \( q(v; y) \) is the Gauss–Manin vector defined in (10). The transition probabilities can be obtained along with a sample path \((j_1, j_2, \ldots)\) as follows. For the first step, we compute

\[ \tilde{e}(b, b - a_j; y) = \tilde{q}_j(b; y) = \sum_{k \in 0 \cup [r-1]} t_{jk}(b; y)q_k(b; y), \quad j \in [m]. \]

If \( j = j_1 \) is chosen, we update the Gauss–Manin vector

\[ q_k(b - a_{j_1}; y) = y_{j_1}^{-1}\{\tilde{P}_{j_1}(b; y)q(b; y)\}_k \]
\[ = y_{j_1}^{-1}\sum_{l \in 0 \cup [r-1]} \{\tilde{P}_{j_1}(b; y)\}_klq_k(b; y), \quad k \in 0 \cup [r-1], \]

which gives

\[ \tilde{e}(b - a_{j_1}; b - a_{j_1} - a_j; y) = \sum_{k \in 0 \cup [r-1]} t_{jk}(b - a_{j_1}; y)q_k(b - a_{j_1}; y), \quad j \in [m]. \]

Then, if \( j = j_2 \) is chosen, we update the Gauss–Manin vector

\[ q_k(b-a_{j_1}-a_{j_2}; y) = y_{j_2}^{-1}\sum_{l \in 0 \cup [r-1]} \{\tilde{P}_{j_2}(b-a_{j_1}; y)\}_klq_l(b-a_{j_1}; y), \quad k \in 0 \cup [r-1], \]
which gives
\[
\hat{e}(b - a_{j_1} - a_{j_2}; b - a_{j_1} - a_{j_2} - a_j) = \sum_{k \in 0, j[r-1]} t_{jk}(b - a_{j_1} - a_{j_2}; y) q_k(b - a_{j_1} - a_{j_2}; y), \quad j \in [m].
\]

Note that only the sequence \( q_k(b; y), q_k(b - a_{j_1}; y), q_k(b - a_{j_1} - a_{j_2}; y), \ldots \) is computed. In other words, we do not have to exhaust the Gauss–Manin vectors \( \{q_k(v) : v < b\} \) for all \( v \in \mathcal{L}_A(b) \). The procedure leads to a version of Algorithm 2.1.

**Algorithm 2.2.**

*Input:* A matrix \( A \in \mathbb{Z}^{d \times m} \), a vector \( b \in \mathbb{N}_0 A \), and parameters \( y \in \mathbb{R}_d^d > 0 \).

*Output:* The vector \((u_1, \ldots, u_m)\) following the \( A \)-hypergeometric distribution associated with \( A \) and \( b \).

**Step 1:** Initialize the Gauss–Manin vector \( q(b; y) \) defined in (10), which can be computed by using the matrix multiplication (11).

**Step 2:** Let \( t = 1 \) and \( n = \deg(b) \).

**Step 3:** Compute \( \hat{e}(b, b - a_j; y) = \{T(b; y)q(b; y)\}_{j}, \forall j \in [m] \).

**Step 4:** Divide the interval \([0, 1]\) with the ratio
\[
\hat{e}(b, b - a_j; y) : \hat{e}(b, b - a_2; y) : \cdots : \hat{e}(b, b - a_m; y),
\]
where the \( j \)-th interval is zero if \( b - a_j \notin \mathcal{L}_A(b) \).

**Step 5:** Get a random number of the uniform distribution on \([0, 1]\). If the number falls in the interval of \( \hat{e}(b, b - a_j; y) \), then put \( j_t = j \).

**Step 6:** If \( \deg(b - a_{j_1}) = 0 \), go to Step 7. Else, compute
\[
q_k(b - a_{j_1}; y) = y_{j_2}^{-1} \{\tilde{P}_{j_1}(b; y)q(b; y)\}_k, \quad k \in 0 \cup [r - 1],
\]
set \( t \leftarrow t + 1, \ b \leftarrow b - a_{j_t}, \) and go to Step 3.

**Step 7:** Output the vector \((u_1, \ldots, u_m)\), \( u_j := |\{t : j_t = j, t \in [n]\}| \).
Let us see the computational complexity of Algorithm 2.2. We ignore the cost demanded by the initialization, or Step 1, because we do not have to repeat the computation. Since Step 3 demands $O(mr)$, Step 4 demands $O(r^2)$, and the other steps demand smaller costs, we have the following estimate, which was announced as Theorem 2 in [28].

**Theorem 2.3.** The computational complexity of the direct sampling of a random vector following the $A$-hypergeometric distribution associated with a configuration matrix $A \in \mathbb{Z}^{d \times m}$ and a vector $b \in \mathbb{N}^A$ by Algorithm 2.2 is $O(\max\{m, r\}rn)$, where $n = \deg(Z_A(b; y))$ and $r = \text{vol}(A)$, with assuming costs of rational arithmetic to be $O(1)$.

**Remark 2.4.** The computational complexity of the direct sampling of a random vector by Algorithm 2.2 is $O(\max\{m, r\}rn)$. On the other hand, the computational complexity of simulating a Metropolis chain of random vectors of length $N$ is $O(\max\{|\mathcal{B}|, U\}N)$, where $|\mathcal{B}|$ is the size of a Markov basis $\mathcal{B}$ and $U$ is the number of elements to be updated at each step of the chain. The cost of $O(|\mathcal{B}|)$ comes from the choice of an element from $|\mathcal{B}|$ elements. The algorithms 2.1 and 2.2 can be performed in parallel if random numbers of the uniform distribution used in Step 4 for Algorithm 2.1 or Step 5 for Algorithm 2.2 are independent among the parallel processes.

### 3 Cases that sum formulae are known

In this section we discuss Algorithm 2.1 for the case that the $A$-hypergeometric sum formula is known. After warming up by considering independence model of two-way contingency tables, the celebrated formula of the normalization constant of chordal graphical models given by Sundberg [25] is revisited as the $A$-hypergeometric sum formula.

For $\alpha, \beta, \gamma \in \mathbb{C}$, if $\text{Re}(\gamma) > \text{Re}(\beta) > 0$, the Gauss hypergeometric series

$$2F_1(\alpha, \beta; \gamma; z) := \sum_{u \geq 0} \frac{(\alpha)_u(\beta)_u z^u}{(\gamma)_u u!}, \quad z \in \mathbb{C}, \quad (12)$$

where $(\alpha)_u$ is the Pochhammer symbol: $(\alpha)_u := \alpha(\alpha + 1) \cdots (\alpha + u - 1)$, has Euler’s integral

$$2F_1(\alpha, \beta; \gamma; z) = \frac{\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\gamma - \beta)} \int_0^1 t^{\beta - 1}(1 - t)^{\gamma - 1}(1 - tz)^{-\alpha} dt.$$ 

If $z = 1$ the right hand side becomes a beta-integral and we have the identity (Theorem 2.2.2 of [11])

$$2F_1(\alpha, \beta; \gamma; 1) = \frac{\Gamma(\gamma)\Gamma(\gamma - \alpha - \beta)}{\Gamma(\gamma - \alpha)\Gamma(\gamma - \beta)}, \quad \text{Re}(\gamma) > \text{Re}(\alpha + \beta), \quad -\gamma \notin \mathbb{N}_0.$$
This closed formula of the Gauss hypergeometric series is called the Gauss
hypergeometric theorem. For the classical univariate hypergeometric series
\[ k \mathbf{F}^k_{k-1}(c_1, \ldots, c_k; d_2, \ldots, d_k; z) := \sum_{u \geq 0} \frac{(c_1)_u \cdots (c_k)_u z^u}{(d_2)_u \cdots (d_k)_u u!}, \quad k \in \mathbb{N} \setminus \{1\}, \quad (13) \]
several identities at \( z = 1 \) are known, see, e.g. Sections 4.4 and 4.5 of [2],
Chapters 2 and 3 of [1]. If the \( A \)-hypergeometric sum formula is available
at a specific value, say \( y_0 \), the computation of the transition probability of
the Markov chain run by Algorithm 2.1 with \( y_0 \) is straightforward. The
independence model of two-way contingency tables is such an example.

3.1 Independence model of two-way tables
The two-way contingency table \((u_{ij} : i \in [r_1], j \in [r_2])\) given marginal sums
is the hierarchical log-linear model associated with the simplicial complex
\( \Gamma = [1][2] \) and the random variables \( i \in [r_1] \) and \( j \in [r_2] \). The conditional
distribution given marginal sums \( \mathbf{b} \) is the \( A \)-hypergeometric distribution asso-
ciated with matrix \( A \) and vector \( \mathbf{b} \) satisfying
\[ A = \begin{pmatrix} E_{r_1} \otimes 1_{r_2} \\ 1_{r_1} \otimes E_{r_2} \end{pmatrix}, \quad \mathbf{b} = (u_{11}, \ldots, u_{1r_1}, u_{21}, \ldots, u_{2r_2}, \ldots, u_{r_11}, \ldots, u_{r_1r_2})^\top, \quad 1_r := (1, \ldots, 1), \quad (14) \]
for the state vector
\[(u_{11}, \ldots, u_{1r_2}, u_{21}, \ldots, u_{2r_2}, \ldots, u_{r_11}, \ldots, u_{r_1r_2})^\top, \]
where \( u_{ik} = \sum_{j \in [r_2]} \mathbf{u}_{ij} \) and \( \otimes \) denotes the Kronecker product of matrices.
By using the parameters
\[ z_{ij} = \frac{y_{ij} y_{r_1 r_2}}{y_{r_1} y_{r_2}}, \quad z_{i r_i} = z_{j r_2} = z_{r_1 r_2} = 1, \quad i \in [r_1 - 1], \quad j \in [r_2 - 1], \]
the conditional distribution given marginal sums is the \( A \)-hypergeometric
distribution with the matrix \( A \) and the vector \( \mathbf{b} \) given in (14). Here,
\[ (u_{r_1} + u_{r_2} - n)! \prod_{i \in [r_1 - 1]} u_i! \prod_{j \in [r_2 - 1]} u_{j}! Z_A(b; y) \]
is a hypergeometric polynomial of type \((r_1, r_1 + r_2)\), or an Aomoto–Gel’fand
hypergeometric polynomial associated with the matrix \( A \) and the vector \( \mathbf{b} \) in
The hypergeometric polynomial of type \((r_1, r_1 + r_2)\) is defined as

\[
F(\alpha, \beta, \gamma; z) = \sum_{u \in \mathcal{F}_A} \frac{\prod_{i \in [r_1-1]} (\alpha_i) u_i - u_{r_2} \prod_{j \in [r_2-1]} (\beta_j) u_{-j} - u_{r_1}}{(\gamma) \prod_{i \in [r_1-1]} \prod_{j \in [r_2-1]} u_{ij}} \prod_{i \in [r_1-1]} \prod_{j \in [r_2-1]} \frac{z_{ij}^{u_{ij}}}{u_{ij}!},
\]

where \(\alpha = (-u_1, \ldots, -u_{r_1-1})\), \(\beta = (-u_1, \ldots, -u_{r_2-1})\), and \(\gamma = u_{r_1} + u_{r_2} - u. + 1\). A hypergeometric function of type \((r_1, r_1 + r_2)\) can be said to be a hypergeometric function on a Grassmannian, and various hypergeometric series appear as special cases. See Section 3 of [3] for the background.

If rows and columns are independent, or \(y = 1\), the \(A\)-hypergeometric distribution reduces to the multivariate hypergeometric distribution. The normalization gives a generalization of the Gauss hypergeometric theorem:

\[
Z_A(b; 1) = \sum_{u \in \mathcal{F}_A} \frac{1}{u!} = \frac{n!}{\prod_{i \in [r_1]} u_i! \prod_{j \in [r_2]} u_{-j}!},
\]

which can be confirmed with Euler’s integral associated with the hypergeometric polynomial of type \((r_1, r_1 + r_2)\) (Theorem 3.3 of [3]). Let \(a_{(i,j)}\) denotes the column vector of the matrix \(A\) which specifies the \((i,j)\)-entry of the contingency table. The transition probability of the Markov chain run by Algorithm 2.1 becomes

\[
e(b, b - a_{(i,j)}; 1) = Z_A(b - a_{(i,j)}; 1) \frac{1}{u.} = \frac{u_i u_{-j}}{u_. u.}.
\]

Then, Algorithm 2.1 reduces to sampling from the multivariate hypergeometric distribution, because a sample path giving the array \((u_{ij} : i \in [r_1], j \in [r_2])\) has the probability

\[
\frac{\prod_{i \in [r_1]} u_i! \prod_{j \in [r_2]} u_{-j}!}{(u_.!)^2},
\]

and multiplying the multinomial coefficient \(u_.! / u!\) gives the multivariate hypergeometric distribution.

Remark 3.1. It is known that a direct sampling from the multivariate hypergeometric distribution is achieved by an urn scheme. Consider \(n\) balls with colors indexed by \([r_2]\) are in the urn, where the number of balls of color \(j\) is \(u_j\). If we put the balls into the boxes indexed by \([r_1]\) randomly such that the number of balls in the box \(i\) is \(u_i\), the table \((u_{ij} : i \in [r_1], j \in [r_2])\), where \(u_{ij}\) is the number of balls of color \(j\) in box \(i\), follows the multivariate hypergeometric distribution. In a sense, running Algorithm 2.1 with the transition
probability (17) is a reversed urn scheme. Consider the set of all tables $u$ satisfying $Au = b$. In the right hand side of (17), the first factor can be interpreted as the proportion of the balls in the box $i$, and the second factor as the proportion of the balls of color $j$. Pick a ball of color $j$ from the box $i$ with the probability given by the product of these two factors, which means the independence of rows and columns. Then, the resulting set of tables is the set of tables $u'$ satisfying $Au' = b - a_{(ij)}$. Running Algorithm 2.1 with the transition probability (17) is equivalent to repeating this procedure. In this sense, Algorithm 2.1 provides a generalization of the reversed urn scheme.

3.2 Chordal graphical models with parameters $\psi = 1$

Let us recall some basic concepts around graphical models. See Subsections 2.1 and 4.4 of [13] for the details. Note that our discussion is restricted to discrete random variables.

With a hierarchical log-linear model $\mathcal{M}_\Gamma$ associated with the simplicial complex $\Gamma$, we associate the undirected graph $\mathcal{G}(\Gamma) = (V, E)$ with edges satisfying

$$a \sim b \iff \{a, b\} \subseteq F \text{ for some } F \in \Gamma.$$ 

This graph is called the interaction graph of the hierarchical log-linear model. Different hierarchical log-linear models may have the same interaction graph. For instance, both simplicial complexes [123] and [12][13][23] have the complete three-graph as their interaction graph. A hierarchical log-linear model is graphical if the associated simplicial complex $\Gamma$ exactly consists of the cliques (maximal complete subgraph) of its interaction graph, namely, the facets of $\Gamma$ are the cliques of $\mathcal{G}(\Gamma)$. Thus [123] is graphical whereas [12][13][23] is not.

A subset $S$ of the vertex set $V$ is said to be $(f, f')$-separator if all paths from a vertex $f$ to $f'$ intersect $S$. The subset $S$ is said to separate $F$ from $F'$ if it is an $(f, f')$-separator for every $f \in F$, $f' \in F'$. A triple $(F, F', S)$ of disjoint subsets of the vertex set $V$ of an undirected graph $\mathcal{G}$ is said to form a decomposition of $\mathcal{G}$ if $V = F \cup F' \cup S$, where the separator $S$ is a complete subset of $V$ and separates $F$ from $F'$. We allow some of the sets in $(F, F', S)$ to be empty. If the set of $F$ and $F'$ are both non-empty, the decomposition is called proper. An undirected graph is said to be decomposable if it is complete, or if there exists a proper decomposition $(F, F', S)$ into decomposable subgraphs $\mathcal{G}_{F \cup S}$ and $\mathcal{G}_{F' \cup S}$. A graphical model is called decomposable if the interaction graph is decomposable. It is known that an undirected graph is decomposable if and only if it is chordal, namely, every cycle of length larger than three possesses a chord (Proposition 2.5 of [13]).
Let $B_1, \ldots, B_k$ be a sequence of the vertex set $V$ of an undirected graph $G$. Let

$$H_j = B_1 \cup \cdots \cup B_j, \quad S_{j+1} = H_j \cap B_{j+1}, \quad j \in [k-1].$$

The sequence $B_1, \ldots, B_k$ is said to be perfect if the following conditions are satisfied.

(i) for all $i > 1$ there exists a $j < i$ such that $S_i \subseteq B_j$;

(ii) the sets (separators) $S_i$ are complete for all $i$.

A separator $S$ may occur several times in a perfect sequence. The number of occurrence $\nu(S)$ is called multiplicity. In addition, a separator can be the empty set.

The boundary $\text{bd}(A)$ of a subset $A$ of vertices is the set of vertices in $V \setminus A$ that are neighbours to vertices in $A$, and the closure of a subset $A$ is $\text{cl}(A) = A \cup \text{bd}(A)$. A perfect numbering of the vertices $V$ of $G$ is a numbering $\alpha_1, \alpha_2, \ldots, \alpha_{|V|}$ such that

$$B_l = \text{cl}(\alpha_l) \cap \{\alpha_1, \ldots, \alpha_l\}, \quad l \in [|V|]$$

is a perfect sequence of sets. A characterization of chordal graphs is as follows (Proposition 2.17 of [13]).

**Proposition 3.2.** The following conditions are equivalent for an undirected graph $G$.

(i) the graph $G$ is chordal.

(ii) the vertices of $G$ admit a perfect numbering.

(ii) the cliques of $G$ can be numbered to form a perfect sequence.

If the boundary of a vertex is complete, then the vertex is called simplicial. A vertex without neighbor is also called simplicial. Since a clique consists of separators and simplicial vertices, removing all the simplicial vertices from a chordal graph induces backward elimination of cliques from a perfect sequence.

**Example 1.** Consider the simplicial complex $\Gamma = [123][124][135][246][247]$. The interaction graph $G(\Gamma)$ is shown in the left of Figure 2. The model is graphical since $\Gamma$ exactly consists of the cliques of $G(\Gamma)$. Moreover, $G(\Gamma)$ is chordal. The vertices of $G(\Gamma)$ are in a perfect numbering. A perfect sequence of cliques is $C_1 = \{1, 2, 3\}$, $C_2 = \{1, 2, 4\}$, $C_3 = \{1, 3, 5\}$, $C_4 = \{1, 4, 5\}$, $C_5 = \{2, 3, 4\}$, $C_6 = \{2, 3, 5\}$, $C_7 = \{2, 4, 5\}$, $C_8 = \{3, 4, 5\}$.
Figure 2: The process of removing simplicial vertices from the simplicial complex \([123][124][135][246][247]\).

\(\{2, 4, 6\}\), and \(C_5 = \{2, 4, 7\}\). The separator for this perfect sequence is \(S_2 = \{1, 2\}, S_3 = \{1, 3\}, S_4 = S_5 = \{2, 4\}\), where the separator \(\{2, 4\}\) has the multiplicity of two. The vertices 7, 6, and 5 are simplicial. Removing these simplicial vertices eliminates cliques \(C_5\), \(C_4\), and \(C_3\), respectively. Then, we have the simplicial complex \([123][124]\) with the simplicial vertices 4 and 3. Removing these simplicial vertices eliminates cliques \(C_2\) and \(C_1\), respectively. The process of removing simplicial vertices from \(\Gamma\) is shown in Figure 2.

As we have seen in Section 1, the configuration matrix \(A\) of a simplicial complex \(\Gamma = [F_1][F_2] \cdots\) determines the linear transformation \(u(i_V) \mapsto (u(i_{F_1}), u(i_{F_2}), \ldots), i_V \in I_V, i_{F_1} \in I_{F_1}, i_{F_2} \in I_{F_2}, \ldots\) Therefore, the rows of \(A\) consist of the states of the subsets in \(I_{F_1}, I_{F_2}, \ldots\), and the columns of \(A\) consists of the states in \(I_V\). The order of \(i_F\) in the rows will be denoted by \(\text{Pos}(i_F)\) and that of \(i_V\) in the columns will be denoted by \(\text{Pos}(i_V)\). For example, for the simplicial complex \(\Gamma = [123][124]\), \(\text{Pos}(1111) = 1, \text{Pos}(1112) = 2, \ldots,\) and \(\text{Pos}(111\cdot) = 1, \text{Pos}(112\cdot) = 2, \ldots,\) for the facet \(F = [123]\). An expression of \(A\) is given by the following proposition. We can read off the correspondence between the indices of the hierarchical log-linear model and those of the configuration matrix. The derivation uses neither graphical nor chordal. For a graphical model, the rows are states of the cliques.

**Proposition 3.3.** Consider a hierarchical log-linear model \(\mathcal{M}_\Gamma\) associated with the simplicial complex \(\Gamma = [F_1][F_2] \cdots\). Let the rows and the columns of the configuration matrix \(A\) are states of the minimal sufficient statistics and the joint states, respectively, and they are ordered in the lexicographic order
with $1 > 2 > \cdots$. For a facet $F \subset [m]$, define
\[
\begin{align*}
  s_i & := \min\{j : j \in F, j > s_{i-1}, j - 1 \notin F\}, \\
  t_i & := \min\{j : j \notin F, j > t_{i-1}, j - 1 \in F\},
\end{align*}
\]
for $1 \leq i \leq \{j : t_j = m \text{ or } m + 1\}$ with $s_0 = t_0 = 0$. Let
\[
A_F = 1_{r_1 \times \cdots \times r_{s_1-1}} \otimes E_{r_1 \times \cdots \times r_{t_1-1}} \otimes 1_{r_1 \times \cdots \times r_{s_2-1}} \otimes E_{r_2 \times \cdots \times r_{t_2-1}} \otimes \cdots,
\]
if $s_1 > 2$ and
\[
A_F = E_{r_1 \times \cdots \times r_{t_1-1}} \otimes 1_{r_1 \times \cdots \times r_{s_2-1}} \otimes E_{r_2 \times \cdots \times r_{t_2-1}} \otimes 1_{r_2 \times \cdots \times r_{s_3-1}} \otimes \cdots,
\]
if $s_1 = 1$. In other words, put $1$ for the maximal contiguous vertices which do not appear in $F$, and put $E$ for the maximal contiguous vertices in $F$. Then, the matrix $A$ has the form
\[
A_F = \begin{pmatrix} A_{F_1} \\ A_{F_2} \\ \vdots \end{pmatrix},
\]
where the column vector of the matrix $A_F$ is indexed by the elements of $\mathcal{I}_V$. Let $a_{ij}$ be the $(i, j)$-entry of the matrix $A_F$. For $\text{Pos}(i_F) = i$ and $\text{Pos}(i_V) = j$, $a_{ij} = 1$ if $i_F \subset i_V$ and $a_{ij} = 0$ otherwise.

Proof. To avoid messy expressions, the case of the facet $F = [13]$ is shown. Similar proof works for any facet. If the $i$-th row of $A_F$ determines the minimal sufficient statistic $\mu_{p_1, \ldots, p_3}$, which is an element of $u(i_{[13]})$, $i = p_1 r_3 + p_3$. For the $i$-th row, the $(i, j)$-entry of $A_F$ is one if $j = p_1 (r_2 r_3) + q_2 r_3 + p_2$, $q_2 \in 0 \cup [r_2 - 1]$, and zero otherwise, that is,
\[
(a_{[13]})_{ij} = \sum_{q_2=0}^{r_2-1} \delta_{p_1 (r_2 r_3) + q_2 r_3 + p_2, j}.
\]
But the right hand side is equivalent to the $(i, j)$-entry of $E_{r_1} \otimes 1_{r_2} \otimes E_{r_3}$. □

Graphical models are used to study conditional independence in the situation where we have a collection of random variables. A probability measure of $X = (X_1, \ldots, X_{|V|})$ taking values in the joint state space $\mathcal{I}_V = \prod_{i=1}^{|V|} [r_i]$ is said to be obeying the \textit{global Markov property} relative to an undirected graph $\mathcal{G}$, if for any triple $(F, F', S)$ of disjoint subsets of $V$ such that $S$ separates $F$ from $F'$ in $\mathcal{G}$, $X_F$ and $X_{F'}$ are conditionally independent given $X_S$, which will be written as
\[
X_F \independent X_{F'} | X_S.
\]
(19)
Note that the global Markov property represented by the interaction graph $G(\Gamma)$ of the hierarchical log-linear model $\mathcal{M}_\Gamma$ holds if and only if $\psi = 1$ in the probability function (6), because $\psi \neq 1$ means that there exist interactions which are not represented by $G(\Gamma)$. If $\psi = 1$, the conditional distribution given minimal sufficient statistics is the A-hypergeometric distribution with parameters $y = 1$.

Sundberg [25] established the following A-hypergeometric sum formula of parameter $y = 1$ for chordal graphical models by using factorization of the probability measure of $X$ (see Subsection 4.4.1 of [13]). We will see an alternative derivation by using the A-hypergeometric integral.

**Theorem 3.4.** Consider a chordal graphical model associated with the simplicial complex $\Gamma$. The A-hypergeometric polynomial with parameters $y = 1$ associated with the matrix $A\Gamma$ in (18) and the vector $b\Gamma = u(i_C : i_C \in I_C, C \in C)$ has an expression

$$Z_{A\Gamma}(b\Gamma; 1) = \sum_{\{v(i'): \sum_{i' : i' \in V} v(i') = u(i_C), \forall C \in C\} \ i_V \in I_V} \prod_{i_V \in I_V} \frac{1}{v(i_V)!}$$

$$= \prod_{S \in S} \{\prod_{i_S \in I_S} u(i_S)!\}^{\nu(S)} \prod_{C \in C} \prod_{i_C \in I_C} u(i_C)!,$$

(20)

where $C$ is the set of cliques of the interaction graph $G(\Gamma) = (V, E)$, $S$ is the set of separators with multiplicities $\nu$ in any perfect sequence, and $v(i_V)$ are variables, which takes values in $\mathbb{N}_0$, indexed by the elements of $I_V$.

The transition probability of the Markov chain run by Algorithm 2.1 immediately follows by Theorem 3.4.

**Corollary 3.5.** Consider a chordal graphical model associated with the simplicial complex $\Gamma$. The transition probability of the Markov chain run by Algorithm 2.1 for the A-hypergeometric distribution with parameters $y = 1$ associated with the matrix $A\Gamma$ in (18) and the vector $b\Gamma = u(i_C : i_C \in I_C, C \in C)$ is given by

$$e(b\Gamma, b\Gamma - a\Gamma_j; 1) = \frac{\prod_{C \in C} \prod_{\{i_C : i_C \in I_C, i_C \supset j\}} u(i_C)}{\prod_{S \in S} \{\prod_{i_S \in I_S} u(i_S)!\}^{\nu(S)}} \forall j \in [m],$$

(21)

where $a\Gamma_j$ is the $j$-th column vector of $A\Gamma$ and $\text{Pos}(i_j) = j$, $i_j \in I_V$.

**Example 2.** Consider a binary chordal graphical model with the simplicial complex $\Gamma = [123][124]$. The matrix $A\Gamma = \begin{pmatrix} E_8 \otimes 1_2 \\ E_4 \otimes 1_2 \otimes E_2 \end{pmatrix}$ and the vector
\begin{align*}
  b_\Gamma &= \begin{pmatrix}
    1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
    1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\
  \end{pmatrix}
\end{align*}

where the columns of $A_\Gamma$ specify the joint states in $\mathcal{I}_V = \{1111, 1112, 1121, 1122, 1211, \ldots, 2222\}$.

The separator is $\{1, 2\}$. Consider sampling from the model with parameters $\psi = 1$ by Algorithm 2.1. When $j = 1$, $(11 \cdot \cdot \cdot), (11 \cdot 1), (11 \cdot \cdot), (11 \cdot 11) \supset (1111) = i_1$, and the transition probability of the Markov chain run by Algorithm 2.1 given by (21) becomes

\[
  e(b_\Gamma, b_\Gamma - a_{\Gamma_1}; 1) = \frac{u_{111,111,1}}{u_{111,111,1}}.
\]

Remark 3.6. Since the chordal graphical model in Example 2 with parameters $\psi = 1$ has the global Markov property (19) $X_3 \Perp \Perp X_4 | X_{(1,2)}$, we have

\[
  P(X = (1, 1, 1, 1)) = P(X_3 = 1 | X_1 = X_2 = 1)P(X_4 = 1 | X_1 = X_2 = 1)
  \times P(X_1 = X_2 = 1) = \frac{u_{111,111,111,111}}{u_{111,111,111,111}}.
\]

Algorithm 2.1 provides a sampling utilizes this conditional independence, and generalizes the reversed urn scheme for the independence model of two-way contingency tables discussed in Remark 3.1.
It is known that the $A$-hypergeometric integral
\[
\int_{\gamma} \left( \prod_{j \in [m]} \prod_{i \in [d]} y_j t_i^{a_{ij}} \right)^n \prod_{i \in [d-1]} t_i^{-b_i-1} dt_i, \quad t_d = 1,
\]
for a $(d-1)$-cycle $\gamma$ in $C^{*d}$ (Theorem 5.4.2 of [23]), where $C^* := C \setminus \{0\}$ and $n = \deg(Z_A(b; y))$, is annihilated by the $A$-hypergeometric ideal $H_A(b)$. The integration at $y = 1$ yields Theorem 3.4.

We prepare the following proposition. Note that $t$ should be indeterminants, because in the proof of Theorem 3.4 we use $t$ as variables for the integration along with $\gamma \in C^{*d}$.

**Proposition 3.7.** If a polynomial $f(t) \in \mathbb{Q}[t_1, \ldots, t_d]$ is zero for all $t = T \in \mathbb{N}^d$, then we have $f(t) = 0$ as a polynomial.

**Proof.** We use an induction in $d$. When $d = 1$, if the univariate polynomial $f(t)$ is not the zero polynomial, the number of zeros of $f(t)$ is up to the degree of $f(t)$. It contradicts the assumption, and $f(t)$ should be the zero polynomial. When $d = n > 1$, the expansion in $t_n$ for some $m$:
\[
f(t) = \sum_{k=0}^{m} f_k(t') t_n^k, \quad t' = (t_1, \ldots, t_{n-1})
\]
determines polynomials $f_k(t') \in \mathbb{Q}[t_1, \ldots, t_{n-1}]$. If we fix $T' \in \mathbb{N}^{n-1}$, $f(t)$ reduces to a univariate polynomial, and the argument for $d = 1$ gives $f_k(T') = 0$. By the assumption of the induction for $d = n - 1$, $f_k(t') = 0$ as a polynomial. Hence $f(t)$ is the zero polynomial.

The following lemma for a factorization is the key for the proof of Theorem 3.4.

**Lemma 3.8.** Consider a chordal graphical model associated with the simplicial complex $\Gamma$. We fix the state of all the separators $S$ to be $i_S$. For the set of indeterminants $t(i_V), i_V \in \mathcal{I}_V$, we have
\[
\sum_{i_V \subset i_S} \prod_{C \in \mathcal{C}} t(i_C) 1\{i_V \subset i_C\} = \prod_{C \in \mathcal{C}} \sum_{i_C \subset i_S} t(i_C)
\]
as a polynomial equality, where $\mathcal{C}$ is the set of cliques of the interaction graph $G(\Gamma) = (V, E)$, $t(i_F) = \sum_{j \in \mathcal{I}_V \setminus F} t(i_F, j)$ for any subset $F \subset V$, and $1\{\cdot\}$ is the indicator function, i.e. $1\{\cdot\} = 1$ if $\cdot$ is true and zero otherwise.
Proof. Consider a probability measure of $X$ taking values in the joint state space $I_V$. We fix the state of all the separators $S$ to be $i_S$ with satisfying $P(X_S = i_S) > 0$. We may write

$$P(X = i_V | X_S = i_S) = \frac{t(i_V)}{t(i_S)}, \quad \forall i_V \subseteq i_S.$$ 

On the other hand, for each clique $C$ we may write

$$P(X = i_V | X_S = i_S) = \frac{t(i_C)}{\sum_{i'_C \subseteq i_S} t(i'_C)}, \quad \forall i_V \subseteq i_S.$$ 

Since the global Markov property (19) implies

$$P(X = i_V | X_S = i_S) = \prod_{C \in \mathcal{C}} P(X = i_C | X_S = i_S),$$

we have

$$\frac{t(i_V)}{t(i_S)} = \prod_{C \in \mathcal{C}} \frac{t(i_C)}{\sum_{i'_C \subseteq i_S} t(i'_C)}, \quad \forall i_V \subseteq i_S,$$

where $i_V \subseteq i_C \subseteq i_S$, $\forall C \in \mathcal{C}$. Since the denominator of the right hand side does not depend on $i_V \setminus S$ and $\sum_{i_V \subseteq i_S} t(i_V) = t(i_S)$, we have

$$\sum_{i_V \subseteq i_S} \prod_{C \in \mathcal{C}} t(i_C) 1\{i_V \subseteq i_C\} = \prod_{C \in \mathcal{C}} \sum_{i_C \subseteq i_S} t(i_C).$$

Since this argument holds for any probability measure of $X$, Proposition 3.7 guarantees that (23) holds even if $t(i_V), i_V \in I_V$ are indeterminants.

Proof of Theorem 3.4. Let the interaction graph $G(\Gamma)$ be a chordal graph with at least four vertices. We use a backward inductive argument with respect to the number of vertices. Figure 2 shows the process of integration for the simplicial complex [123][124][135][246][247]. The set of simplicial vertices is denoted by $V \setminus S =: V_*$. Then, $G(\Gamma)$ has at least two simplicial vertices (Lemma 2.9 of [13]). If states of all separators are fixed to be $i_S$,

$$\sum_{\{j : j \in [m], i_j \subseteq i_S\}} \prod_{i \in [d]} t_i^{a_{ij}} = \sum_{\{j : j \in [m], i_j \subseteq i_S\}} \prod_{C \in \mathcal{C}} t_{i_C} 1\{i_j \subseteq i_C\} = \prod_{C \in \mathcal{C}} \sum_{i_C \subseteq i_S} t_{i_C}, \quad (24)$$

where the factorization of the second equality follows by the formula (23) of
Lemma 3.8 and Proposition 3.7. The multinomial expansion yields
\[
\left( \sum_{j \in [m]} \prod_{i \in [d]} t_{ij}^{a_{ij}} \right)^n = \sum_{\{v(is): \sum_{is} v(is) = n\}} \frac{n!}{\prod_{is} v(is)!} \prod_{C \in \mathcal{C}} \left( \sum_{t_{ic}} \right)^{v(is)}
\]
\[
= \sum_{\{v(is): \sum_{is} v(is) = n\}} \frac{n!}{\prod_{is} v(is)!} \prod_{C \in \mathcal{C}} \prod_{is} \left( \sum_{t_{ic}} \right)^{v(is)}.
\]

Here \( v(is) \) is a variable which takes a value in \( \mathbb{N}_0 \) indexed by the elements of \( \mathcal{I}_S \). If a clique does not contain simplicial vertices, the indices of the clique are completely specified by the condition \( i_C \subset i_S \) and we have
\[
\prod_{is} \left( \sum_{t_{ic}} \right)^{v(is)} = \prod_{i_C} t_{i_C}^{v(i_C)},
\]
Otherwise,
\[
\prod_{is} \left( \sum_{t_{ic}} \right)^{v(is)} = \prod_{i_C \subset i_S} \left( \sum_{t_{ic}} \right)^{v(i_C \setminus V_s)}
\]
\[
= \prod_{i_C \setminus V_s} \left( \sum_{\{v(i_C): \sum_{i_C \subset C \in \mathcal{C}_s \setminus V_s} v(i_C) = v(i_C \setminus V_s)\}} \frac{v(i_C \setminus V_s)!}{\prod_{i_C \subset i_C \setminus V_s} v(i_C)!} \prod_{i_C \subset i_C \setminus V_s} t_{i_C}^{v(i_C)} \right).
\]

Note that \( C \setminus V_s \subset S \) and the inclusion can be strict. Finally,
\[
\prod_{i \in [d-1]} t_i^{-b_i-1} dt_i = \prod_{C \in \mathcal{C}} \prod_{i_C} t_{i_C}^{-u(i_C)-1} dt_{i_C}.
\]

The integrand is holomorphic on \( \mathbb{C}^{*d-1} \). By using Cauchy’s integral theorem, the integral \( \int_{\gamma} \) with taking the \((d-1)\)-cycle \( \gamma \) as the \((d-1)\)-complex torus \( T^{d-1} = \mathbb{C}^{*d-1} \) around the origin is evaluated as
\[
Z_{\lambda_{T^*}}(b_T; 1) \propto \sum_{\{v(is): \sum_{is} v(is) = n\}} \frac{\prod_{C \in \mathcal{C}_0} \prod_{i_C} 1(v(i_C) = u(i_C))}{\prod_{is} v(is)!} \]
\[
\times \prod_{i_C \subset i_C \setminus V_s} \left( \sum_{\{v(i_C): \sum_{i_C \subset C \in \mathcal{C}_s \setminus V_s} v(i_C) = v(i_C \setminus V_s)\}} \frac{v(i_C \setminus V_s)!}{\prod_{i_C \subset i_C \setminus V_s} v(i_C)!} 1(v(i_C) = u(i_C)) \right)
\]
\[
= \sum_{\{v(is): \sum_{is} v(is) = n\}} \frac{\prod_{C \in \mathcal{C}_0} \prod_{i_C} 1(v(i_C) = u(i_C))}{\prod_{is} v(is)!} \prod_{C \in \mathcal{C}_0} \prod_{i_C \setminus V_s} \frac{1(v(i_C) = u(i_C))}{\prod_{i_C \subset i_C \setminus V_s} u(i_C)!}.
\]
where \( C_0 \) is the set of cliques containing no simplicial vertices. The summation appears in the last expression is the \( A \)-hypergeometric polynomial associated with the graph \( \mathcal{G}(\Gamma) \) with removing \( V_* \), say \( Z_{A\mathcal{G}_0}(b_{\Gamma_0}; 1) \). A chordal graph whose simplicial vertices are removed is again a chordal graph. By the assumption of the induction, we should have

\[
Z_{A\mathcal{G}_0}(b_{\Gamma_0}; 1) = \frac{\prod_{S \in \mathcal{S}} \{ \prod_{i \in \mathcal{I}_S} b(i_S) \}^{\nu_0(S)}}{\prod_{C \in C_0} \prod_{i_c \in \mathcal{I}_C} b(i_C)!},
\]

where \( \nu_0(S) \) is the multiplicity of separator \( S \) in a perfect sequence of the cliques in the set \( C_0 \). This observation proves the assertion for \( Z_A(b; 1) \), because when we remove \( V_* \) from \( \mathcal{G}(\Gamma) \) the set \( C \setminus V_* \), \( C \in C \setminus C_0 \) becomes a separator. Therefore, we have

\[
\prod_{C \subseteq C \setminus C_0} \prod_{i \in \mathcal{I}_{C \setminus V_*}} b(i_{C \setminus V_*})! = \prod_{S \in \mathcal{S}} \{ \prod_{i \in \mathcal{I}_S} b(i_S)! \}^{\nu(S) - \nu_0(S)}.
\]

By the backward induction, our task reduces to confirm the assertion for a set of disconnected simplices. If the set consists of a single simplex, the computation is trivial, because \( A = E_m \) and \( Z_A(b; 1) = m^n/n! \). Otherwise, an \( A \)-hypergeometric integral is involved. We discuss the case with two vertices, but other cases can be discussed in similar ways. The graph coincides that of the independence model of two-way contingency tables discussed in Section 3.1. For simplicity, we display explicit expressions for the binary case. Taking the 3-cycle \( \gamma \) as the 3-complex torus \( T^3 \) around the origin, the integral becomes

\[
\int_{T^3} (t_1 + t_2)^n (1 + t_1)^n t_1^{-u_1 - 1} t_2^{-u_2 - 1} dt_1 dt_2 dt_1
\]

\[
= \int_{T^3} \sum_{v_1 = 0}^n \sum_{v_1 = 0}^n \binom{n}{v_1} \binom{n}{v_1} t_1^{v_1 - u_1 - 1} t_2^{v_1 - u_1 - 1} dt_1 dt_2 dt_1
\]

\[
= \int_{T} \sum_{v_1 = 0}^n \binom{n}{v_1} t_1^{v_1 - u_1 - 1} dt_1 \int_{T} \sum_{v_1 = 0}^n \binom{n}{v_1} t_1^{v_1 - u_1 - 1} dt_1 dt_2 dt_1
\]

\[
= 2\pi \sqrt{-1} \binom{n}{u_1} \int_{T} \left\{ \sum_{v_1 = 0}^n \binom{n}{v_1} t_1^{v_1 - u_1 - 1} \right\} dt_2
\]

\[
= (2\pi \sqrt{-1})^2 \binom{n}{u_1} \int_{T} \sum_{v_1 = 0}^n \binom{n}{v_1} t_1^{v_1 - u_1 - 1} dt_1 = \frac{(2\pi \sqrt{-1})^3 n!^2}{u_1! u_2! u_1! u_2!},
\]

where the last three equalities follow by Cauchy’s integral theorem. The proportional constant can be fixed by the case that \( b \) is the zero vector, and we obtain the expression \( [16] \) for the \( A \)-hypergeometric polynomial.

\( \square \)
Example 3. Consider a binary chordal graphical model with parameters $\psi = 1$ associated with the simplicial complex $\Gamma = [123][124][135][246]$. The simplicial vertices are 5 and 6. A perfect sequence of cliques is $C_1 = \{1, 2, 3\}$, $C_2 = \{1, 2, 4\}$, $C_3 = \{1, 3, 5\}$ and $C_4 = \{2, 4, 6\}$, and the separators are $S_2 = \{1, 2\}$, $S_3 = \{1, 3\}$, and $S_4 = \{2, 4\}$. The summation \[24\] in the proof of Theorem 3.4 consists of terms with fixing possible set of indices of $S = \{1, 2, 3, 4\}$ becomes

$$
\sum_{j \in [2^n]} \prod_{i \in [8 \times 4]} t_i^{a_{ij}} = t_{111\ldots t_{11.1}} \cdot (t_{1.1.1} \cdot t_{1.1.2} + t_{1.1.1} \cdot t_{1.1.1} + t_{1.1.2} \cdot t_{1.1.2})
$$

$$
\quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad + \ldots
$$

$$
\quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad = t_{111\ldots t_{11.1}} \cdot (t_{1.1.1} + t_{1.1.2}) \cdot (t_{1.1.1} + t_{1.1.2}) + \text{(other 15 terms)},
$$

where the first term of the right hand side appears for $i_S = (1111 \cdots)$. The second equality comes from the factorization formula \[23\] in Lemma 3.8 with the global Markov property $X_5 \perp X_6 | X_{\{1,2,3,4\}}$, where the states of the cliques $C_1$ and $C_2$ are uniquely determined by $i_S$. The multinomial expansion of the $n$-th power of this expression is

$$
\sum_{v_{1111}, \ldots, v_{2222}} \frac{n!}{v_{1111}! \cdots v_{2222}!} (t_{111\ldots t_{11.1}} \cdot (t_{1.1.1} + t_{1.1.2}) \cdot (t_{1.1.1} + t_{1.1.2}))^{v_{1111} \ldots v_{2222}}
$$

$$
= \sum_{v_{1111}, \ldots, v_{2222}} \frac{n!}{v_{1111}! \cdots v_{2222}!} (t_{111\ldots t_{11.1}} \cdot (t_{1.1.1} + t_{1.1.2})^{v_{1111} \ldots v_{2222}})
$$

$$
= \sum_{v_{1111}, \ldots, v_{2222}} \frac{n!}{v_{1111}! \cdots v_{2222}!} (v_{1111}! \cdot v_{11.2}! \cdot v_{1.1.1}! \cdot v_{1.1.2}! \cdot v_{22.1}! \cdot v_{2.2.1}! \cdot v_{2.1.2}! \cdot v_{1.2.2}! \cdot v_{1.1.2}! \cdot v_{1.1.1}! \cdot v_{22.1}! \cdot v_{2.2.1}! \cdot v_{2.1.2}! \cdot v_{1.2.2}!)
$$

The $A$-hypergeometric integral leads to

$$
\frac{u_{1.1.1}! \cdot u_{1.1.2}! \cdot u_{1.2.1}! \cdot u_{1.2.2}! \cdot u_{2.1.1}! \cdot u_{2.2.1}! \cdot u_{2.2.2}!}{u_{1.1.1}! \cdot u_{1.1.2}! \cdot u_{1.2.1}! \cdot u_{1.2.2}! \cdot u_{2.1.1}! \cdot u_{2.2.1}! \cdot u_{2.2.2}!}
$$

$$
\times \sum_{\{v_{1111}, \ldots, v_{2222}\} : v_{1111} = u_{1111}, \ldots, v_{2222} = u_{2222}} \frac{1}{v_{1111}! \cdots v_{2222}!}
$$

up to a constant. Here, the summation is the $A$-hypergeometric polynomial associated with the simplicial complex $[123][124]$, which was already obtained in Example 2. The expression

$$
\frac{u_{111!} \cdots u_{222!}}{u_{111!} \cdots u_{222!}},
$$

confirms the formula \[20\].
4 Examples

For non-chordal graphical models and non-graphical toric models, the $A$-hypergeometric sums formulae are generally not available. Even for a chordal graphical model, the $A$-hypergeometric sum formula is not available if a parameter is not unity. This section is devoted to demonstrate direct samplings by using Algorithms 2.1 and 2.2 from toric models including such models. For the univariate Poisson regression model and two-way contingency tables, these algorithms were implemented and the performances were examined. The non $l(\geq 3)$-way interaction model, which is an important class of non-graphical toric models, is also discussed.

Direct samplings by Algorithms 2.1 and 2.2 and approximate samplings with the Metropolis chain were implemented on a computer algebra system Risa/Asir version 20190328 [18]. The following timing results were taken on a CPU (Intel Core i5-4308U CPU, 2.80GHz) of a machine with 8GB memory. A single core was used unless otherwise noted. Since we are interested in evaluation of performance of algorithms without numerical errors, the following computations were conducted in the rational number arithmetic. If we compromise on accuracy, e.g., by using floating-point arithmetics, computations could be done in shorter times. A comparison of performance between a direct sampling and an approximate sampling resorting the use of a Metropolis chain is nontrivial, because steps of a Metropolis chain are not independent. To account for the autocorrelation among steps of a chain, we employed the notion of the effective sample size [10]. The effective sample size of $N$ steps is defined as $N/(1 + 2\sum_{t=1}^{\infty} \rho_t)$, where $\rho_t$ is the autocorrelation of chi-squares at lag $t$. The estimate was based on the sample autocorrelation, and the sum was cut at the lag such that the sample autocorrelation was larger than some small positive value, where 0.05 was chosen.

4.1 Univariate Poisson regressions

Consider the univariate Poisson regression model, that is, random variables $X_j$, $j \in [m]$ independently follow the Poisson distribution with mean $\alpha + \beta j$, where $\alpha$ and $\beta$ are the nuisance parameters. The conditional distribution given the sufficient statistics $b_1 = \sum_{j=1}^{m} j x_j$ and $b_2 = \sum_{j=1}^{m} x_j$ is the $A$-hypergeometric distribution with matrix

\[
A = \begin{pmatrix}
1 & 2 & \cdots & m \\
1 & 1 & \cdots & 1
\end{pmatrix}
\]

and parameters $\psi = 1$. The $A$-hypergeometric distributions of various parameters associated with a configuration matrix of two rows appear also as
distributions of random Young diagrams of weight $b_1$ and length $b_2$, see [16]. An explicit expression of the Pfaffian system was obtained by using a recurrence relation of the partial Bell polynomials [15]. Since $\text{vol}(A) = m - 1$ and $\text{deg}(Z_A(b; y)) = b_2$, if the $A$-hypergeometric sum formulae are known, the computational complexity of the direct sampling by Algorithm 2.1 is $O(2mb_2)$. Otherwise, that by Algorithm 2.2 is $O(m^2b_2)$. A minimal Markov basis is

$$\mathcal{B} = \{e_i + e_j - e_{i+1} - e_{j-1} : 1 \leq i < j \leq m, i + 2 \leq j\},$$

where $|\mathcal{B}| = O(m^4)$. Surprisingly, according to Theorem 2.3, the computational complexity of the direct sampling by Algorithms 2.1 and 2.2 can be smaller than that of a single step of the Metropolis chain, if $m$ is sufficiently larger than $\sqrt{b_1}$.

If $m \geq b_1 - b_2 + 1$, the $A$-hypergeometric polynomial has the closed form $(b_1 - 1)!/[\{(b_2 - 1)!(b_1 - b_2)!b_2\}$, or the $A$-hypergeometric sum formula, which is the signless Lah number with divided by $b_1!$. Otherwise, no closed formula is available. Nevertheless, the $A$-hypergeometric polynomials on all the elements of the Markov lattice can be computed efficiently by using the recurrence relation for the partial Bell polynomials mentioned above. In fact, there exists bijection between the partial Bell polynomials $B_{b_1b_2}(\cdot!)$ and the elements $(b_1, b_2)^\top$ of the Markov lattice, and computing the partial Bell polynomials $B_{b_1b_2}(\cdot!)$ from the partial Bell polynomials $B_{b_1b_2} = \delta_{b_1b_2}$ by using the recurrence relation is equivalent to computing the hypergeometric polynomials of all elements of the Markov lattice with the maximum $(b_1, b_2)^\top$ from the minimum 0. Hence, direct sampling of tables following the conditional distribution of the univariate Poisson regression model by Algorithm 2.1 was implemented. The Metropolis chain was also implemented. As a benchmark problem, we considered the case of $m = 5$, $b = (288, 120)^\top$, whose approximate sampling by the Metropolis chain was discussed by Diaconis et al. [4]. Following [4], metropolis chains of 9,000 steps with 1,000 burn-in steps were generated. The average computation time and the average effective sample size for a chain based on 100 trials were 10.72 seconds and 1,977.3, respectively. Computation of the $A$-hypergeometric polynomials for all the elements of the Markov lattice was 8.92 seconds. Then, we conducted 100 trials of generation of 1,977 tables by using Algorithm 2.1. The average computation time was 5.50 seconds. We may say that the direct sampling by Algorithm 2.1 is more efficient than the Metropolis chain. We have little reason to use the Metropolis chain.
4.2 Two-way contingency tables

Two-way contingency tables were discussed in Subsection 3.1. In this subsection, we consider models with and without independence of rows and columns. For an $A$-hypergeometric system associated with two-way contingency tables, an explicit expression for the Pfaffian system was obtained via computation of intersection forms of the twisted cohomology groups in associated hypergeometric integral [11]. We have $m = r_1 r_2$,

$$r = \text{vol}(A) = \begin{pmatrix} r_1 + r_2 - 2 \\ r_1 - 1 \end{pmatrix}$$

(see Subsection 3.6 of [3]), and $n = \text{deg}(Z_A(b; y)) = n...$. Goto and Matsumoto [11] discussed evaluation of the Gauss–Manin vector using the matrix multiplication (11), and the procedure was summarized as Algorithm 7.8 in [11]. As for Algorithm 2.2, Step 3 is their Corollary 7.1, and the update of the Gauss–Manin vector in Step 6 is their Corollary 6.3. See Tachibana et al. [26] for explicit expressions for the binary two-way contingency table. Moreover, Tachibana et al. discussed an efficient implementation of the matrix multiplication (11) by the modular method in computational algebra. According to Theorem 2.3, the computational complexity of the direct sampling by Algorithm 2.2 is $O(\max\{r_1 r_2, r\} n)$. A formula in Corollary 7.2 of [11] implies that Step 2 is computed with a cost of $O(r_1^2 r_2^2)$, which leads to the complexity of $O(\max\{r_1^2 r_2^2, r^2\} n)$. In either case, $r^2 n$ dominates for large $r$, because $r$ grows rapidly than $r_1 r_2$. For example, $(r_1 r_2, r) = (4, 2), (9, 6), (16, 20), (25, 70)$ for $r_1 = r_2 = 2, 3, 4, 5$, respectively. The unique minimal Markov basis up to sign is $\mathcal{B} = (z_{ij} : i \in [r_1], j \in [r_2])$, where

$$z_{ij} = \begin{cases} +1 & (i, j) = (i_1, j_1), (i_2, j_2), \\ -1 & (i, j) = (i_1, j_2), (i_2, j_1), \\ 0 & (i, j) = \text{others}, \end{cases} \quad 1 \leq i_1 < i_2 \leq r_1, \ 1 \leq j_1 < j_2 \leq r_2,$$

(25)

and $|\mathcal{B}| = O(r_1^2 r_2^2)$. Roughly speaking, if $r_1$ and $r_2$ are fixed, the ratio of computational complexities of the direct sampling by Algorithm 2.2 to that of a single step of the Metropolis chain scales with $n$. Therefore, as a rule of thumb, the computational complexities of the direct sampling by Algorithm 2.2 and that of the Metropolis chain of length $n$ are comparative.

Direct samplings of two-way contingency tables by Algorithms 2.1 and 2.2 and by the Metropolis chain were implemented. The implementation of Algorithm 2.2 is published as the package $\texttt{gtt_ds}$ for Risa/Asir. As a benchmark problem, we considered sampling $3 \times 4$ tables whose marginal
For the independence model, 100 Metropolis chains of 10,000 steps with 1,000 burn-in steps were generated. The average computation time and the average effective sample size for a chain were 1.80 seconds and 425.1, respectively. Then, we conducted 100 trials of generation of 425 tables by using Algorithm 2.1. The average computation time was 0.21 seconds. We may say that the direct sampling by Algorithm 2.1 is nine times efficient than the Metropolis chain. As a model without independence, we considered parameters $(z_{ij}) = \begin{pmatrix} 1/2 & 1/11 & 1/13 & 1 \\ 1/7 & 1/3 & 1/5 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$.

We generated 100 Metropolis chains of 10,000 steps with 1,000 burn-in steps. The average computation time and the average effective sample size for a chain were 1.96 seconds and 280.9, respectively. In sharp contrast to the univariate Poisson regression model, computing the $A$-hypergeometric polynomials for all the elements of the Markov lattice is practically impossible, because the number of the elements is huge. Nevertheless, Algorithm 2.2 works because it does not exhaust computation of all the $A$-hypergeometric polynomials. We conducted 10 trials of generation of 281 tables by using Algorithm 2.2. The average computation time was 1645.6 seconds. The same computation was performed in 693.6 seconds by using four cores. Currently, our implementation of Algorithm 2.2 is far inefficient than the Metropolis chain. However, the fact that tables generated by Algorithm 2.2 follow independently to the exact distribution is a remarkable advantage, and the timing is practically reasonable if we use multiple cores of a CPU.

Remark 4.1. Propp and Wilson proposed the coupling from the past (CFTP) algorithm, which guarantees that a sample taken from an ergodic Markov chain is a sample taken from the unique stationary distribution [21]. The CFTP is another algorithm for taking samples exactly following the distribution which we need. The waiting time for taking the sample, called the coalescence, determines the performance. The mixing time of an ergodic Markov chain is defined as

$$t_{\text{mix}}(\epsilon) := \min\{t : \max_{x \in X} \|M^t(x, \cdot) - \pi\|_{\text{TV}} < \epsilon\}$$
for some $\epsilon > 0$, where $\| \cdot \|_{TV}$ is the total variation distance, $M$ is the transition matrix, and $\pi$ is the stationary distribution. For sampling two-row ($r_1 = 2$) contingency tables from the uniform distribution, not the conditional distribution given marginal sums, Dyer and Greenhill \[6\] showed that the upper bound of the mixing time of a Markov chain with moves of multiples of the Markov basis \[25\] at each step is $O(r_2^2 \log n)$.

By using the result, Kijima and Matsui \[12\] constructed a CFTP algorithm \[21\], whose expected waiting time of the coalescence is $O(r_3^2 \log n)$. For two-row contingency tables from the uniform distribution, their CFTP has smaller computational complexity than Algorithm \[2.2\]. However, note that the path coupling and the estimate of the waiting times rely on specific properties of two-row contingency tables and the uniform distribution.

4.3 Non $l(\geq 3)$-way interaction models and associated hypergeometric series

For an $l$-way contingency table $(u_{i_1 \cdots i_l} : i_1 \in [r_1], \ldots, i_l \in [r_l])$, the non $l$-way interaction model is the hierarchical log-linear model associated with the simplicial complex $[1 \cdots l] \setminus \{1, \ldots, l\}$. For example, $[12] \setminus \{1, 2\}$ is the simplicial complex $[12][23][31]$, which is the independence model of two-way contingency tables discussed in Subsection \[5.1\] and $[123] \setminus \{1, 2, 3\}$ is the simplicial complex $[12][23][31][32]$. If $l \geq 3$, the model is non-graphical. Note that if the parameters $\psi \neq 1$, there exists $l$-way interactions. The classical univariate hypergeometric polynomial \[13\] appears as the $A$-hypergeometric polynomial in the binary non $l$-way interaction model. For example, the hypergeometric polynomial $4F_3$ appears in the binary non 3-way interaction model of $2 \times 2 \times 2$ contingency tables, and the hypergeometric polynomial $8F_7$ appears in the binary non 4-way interaction model of $2 \times 2 \times 2 \times 2$ contingency tables.

Let us recall the following useful fact. The classical univariate hypergeometric series \[13\] can be represented as the $A$-hypergeometric series (Example 5.4.6 of \[23\]), while the classical univariate hypergeometric series satisfies the following ordinary differential equation, see, e.g., Section 4.2 of \[7\]:

$$\left\{ \prod_{i \in [k]} (\theta + d_i - 1) - z \prod_{i \in [k]} (\theta + c_i) \right\} \cdot kF_{k-1}(c_1, \ldots, c_k; d_2, \ldots, d_k; z) = 0,$$

where $d_1 = 1$ and $\theta = z\partial_z$. This ordinary differential equation yields the
following recurrence relation:

\[
\theta^k = \frac{\sum_{i \in [k]} d_i - k - z \sum_{i \in [k]} c_i}{z - 1} \theta^{k-1} \\
+ \sum_{2 \leq i < j \leq k} (d_i - 1)(d_j - 1) - z \sum_{1 \leq i < j \leq k} c_i c_j \theta^{k-2} \\
+ \cdots + \prod_{2 \leq i \leq k} (d_i - 1) - z \sum_{i \in [k]} \prod_{j \neq i} c_j \theta - \frac{z \prod_{i \in [k]} c_i}{z - 1}
\]

(26)
on \_F_{k \_1}(c; d; z), where \( z \neq 1 \). For \( z = 1 \), we have

\[
\theta^{k-1} = \frac{\sum_{2 \leq i < j \leq k} (d_i - 1)(d_j - 1) - \sum_{1 \leq i < j \leq k} c_i c_j \theta^{k-2} + \cdots}{k + \sum_{i \in [k]} (c_i - d_i)} \\
+ \frac{\prod_{2 \leq i \leq k} (d_i - 1) - \sum_{i \in [k]} \prod_{j \neq i} c_j}{k + \sum_{i \in [k]} (c_i - d_i)} \theta - \frac{\prod_{i \in [k]} c_i}{k + \sum_{i \in [k]} (c_i - d_i)},
\]
on \_F_{k \_1}(c; d; 1), where \( \sum_{i \in [k]} (d_i - c_i) \neq k \). These recurrence relations are useful to obtain Pfaffian systems for univariate \( A \)-hypergeometric polynomials. In addition, the initial Gauss–Manin vector of an univariate \( A \)-hypergeometric polynomial can be evaluated efficiently by the binary splitting algorithm, see, e.g., [17].

A joint state of a binary \( l \)-way contingency table is \( i_V = (i_1 \ldots i_l) \), \( i_1 \in [2], \ldots, i_l \in [2] \) with the joint state space \( \mathcal{I}_V = [2]^l \). A contingency table is the set of \( u(i_V) = u(i_1 \ldots i_l) = u_{i_1 \ldots i_l}, i_V \in [2]^l \).

**Proposition 4.2.** The normalization constant of the conditional distribution of the binary non \( l \) (\( \geq 2 \))-way interaction model is proportional to the classical univariate hypergeometric polynomial \((13)\) with \( k = 2^{l-1} \).

**Proof.** The joint state space \( \mathcal{I}_V = [2]^l \) can be identified with the hypercube and the sufficient statistics are the facets. For each state \( i_V \in [2]^l \), there exists a shortest path to the state \( (1 \cdots 1) \) whose length is the number of coordinates of \( i_V \) occupied by 2. Then, \( u(i_V) \) can be expressed by an alternating sum of sufficient statistics and \( u_{i_1 \ldots 1} \). For example, the state \( (1212) \) has a path \( (1212) \to (1112) \to (1111) \), which can expressed as

\[
u_{1212} = u_{112} - u_{1112} = u_{112} - u_{111} + u_{1111}.
\]

For such an expression, \( u(i_V)! \) can be represented by the Pochhammer symbol with subscript \( u_{i_1 \ldots 1} \), and \( y_i^k \) can be represented by power of \( y_i^{1 \ldots 1} \). For \( u_{1212}! \),

\[
u_{1212}! = (u_{112} - u_{111})(u_{112} - u_{111} + 1)u_{1111}
\]

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and \( y_{1212} \propto y_{1212}^{u} \). For the state \((1112)\), the unique shortest path to \((1111)\) gives
\[
u_{1112}! = (\nu_{111} - \nu_{1111})! = \frac{\nu_{111}!}{(-\nu_{111})!} (-1)^{\nu_{1111}}
\]
and \( y_{1222} \propto y_{1222}^{u} \). These observations lead to
\[
\frac{y^{u} u}{u!} \propto \prod_{\{i:j[2]^{l}, \text{number of 1 is odd}\}} (c_{i}) \nu_{1...1} \left( \prod_{\{i:j[2]^{l}, \text{number of 1 is even}\}} (d_{i}) \nu_{1...1} \right)^{u_{1...1}},
\]
which is the form of the summand of the classical univariate hypergeometric polynomial \([13]\) with \( k = 2^{l-1} \) and \( u = u_{1...1} \).

Let \( A^{(2)} \) denotes the configuration matrix. The above proof gives some insights of the toric ideal and the \( A \)-hypergeometric ideal generated by \( A^{(2)} \). The expression \((27)\) shows that the toric ideal is the principal ideal generated by the binomial
\[
\prod_{\{i:j[2]^{l}, \text{number of 1 is even}\}} \partial_{i} - \prod_{\{i:j[2]^{l}, \text{number of 1 is odd}\}} \partial_{i},
\]
which is the unique minimal Markov basis up to sign. The recurrence relation \((26)\) shows that the holonomic rank of \( A \)-hypergeometric ideal is \( 2^{l-1} \) and \( n = \deg(Z_{A^{(2)}}(b; y)) = u_{...} \). According to Theorem \(2.3\), computational complexity of the direct sampling by Algorithm \(2.2\) is \( O(2^{2l-1} n) \), while that of the Metropolis chain of length \( N \) is \( O(2^{l} N) \). By using the recurrence relation \((26)\), the explicit form of the Pfaffian system can be obtained immediately.

The case of \( l = 3 \) is as follows.

**Example 4.** Consider the binary non three-way interaction model associated with the simplicial complex \([12][13][23]\). Let
\[
A^{(2)} = \begin{pmatrix}
E_{2} \otimes 1_{2} \\
E_{2} \otimes 1_{2} \otimes E_{2} \\
1_{2} \otimes E_{2}^{2}
\end{pmatrix}, \quad b^{\top} = (u_{11}, u_{12}, u_{21}, u_{22}, u_{1,1}, \ldots, u_{2,2}, u_{1,1}, \ldots, u_{2,2}),
\]
where the columns of \( A^{(2)} \) specify the joint states in
\[
\mathcal{I}_{V} = \{111, 112, 121, 122, 211, \ldots, 222\}.
\]
The conditional distribution of \( u = u_{111} \) given marginal sums is
\[
P(U = u | A^{(2)} u = b) = \frac{1}{Z_{A^{(2)}}(b; y)} \frac{y^{u} u}{u!} = \frac{1}{4 F_{3}(c; d; z)} \frac{(c_{1})(c_{2})(c_{3})(c_{4}) z^{u}}{(d_{2})(d_{3})(d_{4}) u} u!,
\]
where \( Z_{A^{(2)}}(b; y) \) is the univariate hypergeometric polynomial.
where
\[ c = (-u_{11}, -u_{11}, -u_{11}, -u_{11}, u_{11}, u_{11}, u_{11}, u_{11}, -u_{11}) \]
\[ d = (1, u_{11}, -u_{11}, -u_{11} + 1, u_{11}, -u_{11} + 1, u_{11} - u_{11} - u_{11} + 1) \]
and
\[ z = \frac{y_{111}y_{121}y_{211}y_{221}}{y_{112}y_{121}y_{211}y_{222}}. \]

Therefore,
\[ Z_{A^{(23)}}(b; y) = c y^s F_3(c_1, c_2, c_3; d_2, d_3, d_4; z), \]
where
\[ c = \frac{1}{(-c_1)!(-c_2)!(-c_3)!(-c_4)!d_2!d_3!d_4!}, \quad y^s = \frac{d_2^{-1} d_3^{-1} d_4^{-1}}{y_{112}y_{121}y_{211}y_{222}}. \]

To avoid messy expressions with many subscripts, let
\[ (y_1, y_2, y_3, y_4, y_5, y_6, y_7, y_8) = (y_{111}, y_{112}, y_{122}, y_{121}, y_{212}, y_{211}, y_{221}, y_{222}). \]

The toric ideal of the matrix \( A^{(23)} \) is the principal ideal generated by the binomial \( \partial_1 \partial_2 \partial_3 \partial_4 - \partial_2 \partial_3 \partial_4 \partial_5 \), and the set of the standard monomials in reverse lexicographic term order with \( \partial_1 \succ \partial_2 \succ \cdots \) is \( \{1, \theta_8, \theta_8^2, \theta_8^3\} \), where \( \theta_1 = \theta_3 = \theta_5 = \theta_7 = \theta \) and \( \theta_2 = \theta_4 = \theta_6 = \theta_8 = -\theta \). The Gauss–Manin vector is \( (1, \theta_8, \theta_8^2, \theta_8^3)Z_{A^{(23)}}(b; y) \). The Pfaffian system is given by the following matrices (the fourth rows are not specified):

\[
\tilde{P}_8 = \begin{pmatrix}
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
\ast & \ast & \ast & \ast
\end{pmatrix},
\quad
\tilde{P}_1 = \begin{pmatrix}
-c_4 & -1 & 0 & 0 \\
0 & -c_4 & -1 & 0 \\
0 & 0 & -c_4 & -1 \\
\ast & \ast & \ast & \ast
\end{pmatrix},
\]

\[
\tilde{P}_2 = \begin{pmatrix}
c_4 - c_1 & 1 & 0 & 0 \\
0 & c_4 - c_1 & 1 & 0 \\
0 & 0 & c_4 - c_1 & 1 \\
\ast & \ast & \ast & \ast
\end{pmatrix},
\]

\[
\tilde{P}_4 = \begin{pmatrix}
c_4 - c_2 & 1 & 0 & 0 \\
0 & c_4 - c_2 & 1 & 0 \\
0 & 0 & c_4 - c_2 & 1 \\
\ast & \ast & \ast & \ast
\end{pmatrix},
\]

\[
\tilde{P}_6 = \begin{pmatrix}
c_4 - c_3 & 1 & 0 & 0 \\
0 & c_4 - c_3 & 1 & 0 \\
0 & 0 & c_4 - c_3 & 1 \\
\ast & \ast & \ast & \ast
\end{pmatrix},
\]

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Since the entries of the fourth rows of these matrices can be obtained as follows. With using the recurrence relation (26) denoted by \( \theta^4 = r_3(z)\theta^3 + r_2(z)\theta^2 + r_1(z)\theta + r_0(z) \), we can read off the fourth row of \( P \) and \( A \).

The entries of the fourth row of the other matrices can be obtained in a similar way.

If a level is larger than two, the associated \( A \)-hypergeometric polynomial becomes much more complicated. Consider the non-three-way interaction model with \( r_1 = r_2 = 3 \) and \( r_3 = 2 \). Let the matrix

\[
A^{(332)} = \begin{pmatrix}
E_{3^2} \otimes I_2 \\
E_3 \otimes I_3 \otimes E_2 \\
I_3 \otimes E_{3 \times 2}
\end{pmatrix}, \quad j^{(332)} = (u_{11}, \ldots, u_{33}, u_{3 \cdot 1}, \ldots, u_{3 \cdot 2}, u_{11}, \ldots, u_{32}),
\]

The entries of the fourth row of the other matrices can be obtained in a similar way.
where the columns of $A^{(332)}$ specify the joint states in

$$\mathcal{I}_V = \{111, 112, 121, 122, 131, 132, 211, \ldots, 332\}.$$  

The model can be represented by the following three tables:

| $u_{11}$ | $u_{121}$ | $u_{131}$ | $u_{11}$ | $u_{122}$ | $u_{132}$ | $u_{12}$ | $u_{12}$ | $u_{12}$ |
|----------|-----------|-----------|----------|-----------|-----------|----------|----------|----------|
| $u_{211}$ | $u_{221}$ | $u_{231}$ | $u_{21}$ | $u_{22}$ | $u_{23}$ | $u_{22}$ | $u_{22}$ | $u_{22}$ |
| $u_{311}$ | $u_{321}$ | $u_{331}$ | $u_{31}$ | $u_{32}$ | $u_{33}$ | $u_{32}$ | $u_{32}$ | $u_{32}$ |

Since the dimension of the kernel of $A^{(332)}$ is four, we take $(u_{111}, u_{121}, u_{211}, u_{221})$ as the independent variables. Then,

$$u_{112} = u_{11} - u_{111}, \quad u_{122} = u_{12} - u_{121}, \quad u_{212} = u_{21} - u_{211}, \quad u_{222} = u_{22} - u_{221},$$
$$u_{131} = u_{11} - u_{111} - u_{121}, \quad u_{231} = u_{21} - u_{211} - u_{221}, \quad u_{311} = u_{31} - u_{111} - u_{121},$$
$$u_{312} = u_{21} - u_{121} - u_{221}, \quad u_{321} = u_{31} - u_{111} - u_{121} + u_{211} + u_{211} + u_{221},$$
$$u_{132} = u_{13} - u_{11} + u_{12} + u_{121} + u_{211} + u_{211},$$
$$u_{322} = u_{23} - u_{21} - u_{211} + u_{221},$$
$$u_{332} = u_{33} - u_{31} + u_{11} + u_{21} - u_{111} - u_{121} - u_{211} - u_{221}.$$  

The expression

$$y^u \propto \left(\frac{y_{111}y_{131}y_{132}y_{312}}{y_{131}y_{131}y_{112}y_{332}}\right)^{u_{111}} \left(\frac{y_{121}y_{131}y_{132}y_{312}}{y_{131}y_{121}y_{332}}\right)^{u_{121}} \left(\frac{y_{211}y_{331}y_{32}y_{312}}{y_{231}y_{131}y_{312}}\right)^{u_{221}}$$

implies that a generator of the toric ideal of $A^{(332)}$ contains the following four binomials

$$\partial_{111}\partial_{331}\partial_{132}\partial_{312} - \partial_{131}\partial_{331}\partial_{112}\partial_{332}, \quad \partial_{121}\partial_{331}\partial_{132}\partial_{322} - \partial_{131}\partial_{321}\partial_{122}\partial_{332},$$
$$\partial_{211}\partial_{331}\partial_{232}\partial_{312} - \partial_{231}\partial_{331}\partial_{212}\partial_{332}, \quad \partial_{221}\partial_{331}\partial_{232}\partial_{322} - \partial_{231}\partial_{321}\partial_{222}\partial_{332},$$

where $\partial_{ijk} = \partial/\partial y_{ijk}$. Diaconis and Sturmfels called moves represented by quartic binomials basic $2 \times 2 \times 2$ moves. By the permutation of the indices of the above four binomials, we have nine basic $2 \times 2 \times 2$ moves. In addition, we have six moves of degree six, which appear in $y^u$ if we choose other sets of independent variables. In total, there are 15 moves up to sign and they form a minimal Markov basis. The normalized volume of $A^{(332)}$ was computed with the aid of the software polymake, and the result was 81. Thus, the
The holonomic rank of the $A$-hypergeometric ideal is 81. It is straightforward to see that

$$Z_A(332) (b(332); y) \propto \sum_{u \in \mathbb{F}_q(332)} (A(332)) \prod_{i \in [2], j \in [2]} \frac{-u_{ij} + u_{ij} \prod_{j \in [2]} (-u_{j1}) u_{j1} - u_{j1}}{\prod_{i \in [2]} (-u_i + u_i + u_i + u_i - u_i + u_i + u_i + u_i - u_i - u_i + u_i + u_i + u_i + u_i + 1) \sum_{j \in [2]} u_{ij1}} \times \prod_{j \in [2]} (-u_{j1} + u_{j1} + u_{j1} + u_{j1} - u_{j1} - u_{j1} + u_{j1} + u_{j1} + 1) \sum_{i \in [2], j \in [2]} u_{ij1} \times \frac{u_{111} u_{211} u_{221} u_{221} - u_{111} u_{121} u_{111} u_{221}}{u_{111} u_{211} u_{111} u_{221}!}!.$$ 

Proposition 4.2 implies that the normalization constant of the conditional distribution of the independence model of binary two-way contingency tables is proportional to the Gauss hypergeometric polynomial \((12)\). In Subsection 3.1, the hypergeometric polynomial of type \((r_1, r_1 + r_2)\) \((15)\) appeared as a generalization of the Gauss hypergeometric polynomial for two-way contingency tables with levels of larger than two. Hence, it is natural to define analogs of the hypergeometric series of type \((r_1, r_1 + r_2, \ldots, r_1 + \cdots + r_l)\) for non-\(l\)-way interaction models as a generalization of the classical univariate hypergeometric polynomial \(2^l - 1 F_{2^l - 1}(c; d; z)\). The hypergeometric series of type \((r_1, r_1 + r_2, \ldots, r_1 + \cdots + r_l)\) needs further investigation. The explicit expression for the case of \(l = 3\) is given below. The expressions for \(l \geq 4\) can be defined analogously.

**Definition 6.** The hypergeometric series of type \((r_1, r_1 + r_2, r_1 + r_2 + r_3)\) associated with the matrix and the vector

$$A = \begin{pmatrix} E_{r_1 r_2} \otimes 1_{r_1} & E_{r_1} \otimes 1_{r_2} \otimes E_{r_3} & 1_{r_1} \otimes E_{r_2 r_3} \end{pmatrix}, \quad b^T = (u_{11}, \ldots, u_{r_1 r_2}, u_{1,1}, \ldots, u_{r_1 r_3}, u_{1,1}, \ldots, u_{r_2 r_3}),$$

with \((u_{ijk}) \in \mathbb{N}_0^{r_1 \times r_2 \times r_3}\) and \((z_{ijk}) \in \mathbb{C}^{r_1 - 1, r_2 - 1, r_3 - 1}\) is

$$F(\gamma^{(1)}, \gamma^{(2)}, \gamma^{(3)}, \gamma^{(4)}, \delta^{(1)}, \delta^{(2)}, \delta^{(3)}, z) = \sum_{u \in \mathbb{F}_q(A)} \prod_{i \in [r_1 - 1], j \in [r_2 - 1]} (\gamma^{(1)}_{ij})_{u_{ij} - u_{ij} r_3} \prod_{i \in [r_1 - 1], k \in [r_3 - 1]} (\gamma^{(2)}_{ik})_{u_{ik} - u_{ik} r_2} \prod_{j \in [r_2 - 1], k \in [r_3 - 1]} (\delta^{(3)}_{jk})_{u_{jk} - u_{jk} r_3} \times \prod_{i \in [r_1 - 1], j \in [r_2 - 1], k \in [r_3 - 1]} (\delta^{(3)}_{ijk})_{u_{ijk} - u_{ijk} r_3}$$

$$\times \prod_{i \in [r_1 - 1], j \in [r_2 - 1], k \in [r_3 - 1]} \frac{z_{ijk} u_{ijk} u_{ijk}!}{u_{ijk}!}.$$
The normalization constant of the non three-way interaction model appears by taking

\[ \gamma_{ij}^{(1)} = -u_{ij}, \quad \gamma_{ik}^{(2)} = -u_{i+k}, \quad \gamma_{jk}^{(3)} = -u_{j+k}, \]

\[ \gamma^{(4)} = -u + u_{r1} + u_{r2} + u_{r3} - u_{r1r2} - u_{r1r3} - u_{r2r3}, \]

\[ \delta_i^{(1)} = -u_{i} + u_{ir2} + u_{ir3} + 1, \quad \delta_j^{(2)} = -u_{ij} + u_{r1j} + u_{jr3} + 1, \]

\[ \delta_k^{(3)} = -u_{.k} + u_{r1.k} + u_{r2k} + 1, \]

and if we take \( r_1 = r_2 = r_3 = 2 \) the classical univariate hypergeometric polynomial \( _4F_3(c; d; z) \) discussed in Example 4 recovers.

**Acknowledgements**

The first author was supported in part by JSPS KAKENHI Grants 18H00835 and 20K03742. The second author was supported in part by the JST, CREST Grant Number JP19209317.

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Shuhei Mano
The Institute of Statistical Mathematics, Tokyo 190-8562, Japan
E-mail: smano@ism.ac.jp

Nobuki Takayama
Department of Mathematics, Graduate School of Science, Kobe University,
Kobe 657-8501, Japan
E-mail: takayama@math.kobe-u.ac.jp