Markov bases and subbases for bounded contingency tables

Fabio Rapallo   Ruriko Yoshida

Abstract

In this paper we study the computation of Markov bases for contingency tables whose cell entries have an upper bound. In general a Markov basis for unbounded contingency table under a certain model differs from a Markov basis for bounded tables. Rapallo and Rogantin (2007) applied Lawrence lifting to compute a Markov basis for contingency tables whose cell entries are bounded. However, in the process, one has to compute the universal Gröbner basis of the ideal associated with the design matrix for a model which is, in general, larger than any reduced Gröbner basis. Thus, this is also infeasible in small- and medium-sized problems. In this paper we focus on bounded two-way contingency tables under independence model and show that if these bounds on cells are positive, i.e., they are not structural zeros, the set of basic moves of all 2×2 minors connects all tables with given margins. We end this paper with an open problem that if we know the given margins are positive, we want to find the necessary and sufficient condition on the set of structural zeros so that the set of basic moves of all 2×2 minors connects all incomplete contingency tables with given margins.

keywords: Structural zeros Markov basis Universal Gröbner basis

1 Introduction

The study of statistical models to detect complex structures in contingency tables has received great attention in the last decades. (See Agresti (2002) for an overview of such models). Among the main research themes in this field, here we consider incomplete contingency tables (or equivalently, tables with structural zeros) and models to go beyond independence in two-way tables, such as quasi-independence models.

Contingency tables with upper bounds on the cell counts have recently been considered in, e.g., Cryan *et al.* (2005). Bounded contingency tables can come, for instance, in the analysis of designed experiments with multinomial response, as in Aoki and Takemura (2006), and in logistic regression models, as in e.g. Chen *et al.* (2005). We will use some examples from these applications later in the paper.

In recent years, the use of algebraic and geometric techniques in statistics has produced at least two relevant advances. One is a better understanding of statistical models in terms of varieties and polynomial equations, through the notion of toric models, as described in Chapter 6 of Pistone *et al.* (2001). Moreover, algebraic statistics has introduced a non-asymptotic method for goodness-of-fit tests following a Markov Chain Monte Carlo approach (see Diaconis and Sturmfels (1998)). Such an algorithm is based on the notion of Markov basis. In the last years the computation of Markov bases for special statistical models has involved both statisticians and algebraists.

In this paper we consider the computation of Markov bases for bounded contingency tables. A general algorithm to compute Markov bases for this case was described in Rapallo and Rogantin (2007), using the notions of Lawrence lifting and Universal Gröbner basis of a polynomial ideal. When a Markov basis is computed through a Universal Gröbner basis, we say that it is *Universal Markov basis*. The Markov bases for these kind of tables are in general very large, and we will show some explicit computations later in the paper. Therefore the computation of smaller Markov bases or subbases for special tables is a problem of major interest.

In practice, computing the Markov basis for the bounded contingency tables is infeasible because the number of elements in the Markov basis is very large. However, for some cases, if we know that the given margins are positive then the number of moves connecting all tables is smaller than the number of elements in a Markov basis for tables under the model. Such connecting sets were formalized in Chen *et al.* (2006) with the terminology *Markov subbases*. In this paper we consider bounded $I \times J$ tables under independence model. These tables are equivalent to $I \times J \times 2$ tables under the models of no-2-way interaction. Using this fact and the result from Chen *et al.* (2009), in this paper, we show that if we know the bounds of cells are all positive, that is, there are no structural zeros, then the set of basic moves of all 2×2 minors connects all bounded two-way contingency tables with given margins.

The organization of this paper is as follows. In Section 2 we recall the basic facts about Markov bases and bounded contingency tables. In Section 3 we present a characterization of Universal Markov bases for incomplete tables, showing that there is a simple connection between the Universal Markov basis for an incomplete table and the corresponding complete table. We present some explicit examples, focusing in particular on quasi-independence models for two-way tables. In Section 4 we show how to compute Markov bases when the bounds involve only a subset of cell counts. In Section 5 we show our main theorem, that is, we consider bounded two-way contingency tables under independence model. If we know all bounds are positive (equivalently there are no structural zeros), then the set of basic moves of all 2×2 minors connects all bounded two-way contingency tables with given margins. We end this paper with an open problem for incomplete contingency tables with positive margins.

2 Bounded contingency tables and Markov bases

Let $\mathbf{n}$ be a contingency table with k cells. In order to simplify the notation, we denote by $\mathcal{X} = \{1, \ldots, k\}$ the sample space of the contingency table. In the special case of two-way tables with I rows and J columns, we will also denote the sample space with

$\mathcal{X} = \{1, \ldots, I\} \times \{1, \ldots, J\}$.

Let $\mathbb{N}$ be the set of nonnegative integers, i.e., $\mathbb{N} = \{0, 1, 2, \ldots\}$ and let $\mathbb{Z}$ be the set of all integers, i.e., $\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2, \ldots\}$. Without loss of generality, in this paper, we represent a table by a vector of counts $\mathbf{n} = (n_1, \ldots, n_k)$. Under this point of view, a contingency table $\mathbf{n}$ can be regarded as a function $\mathbf{n} : \mathcal{X} \longrightarrow \mathbb{N}$, but it can also be viewed as a vector $\mathbf{n} \in \mathbb{N}^k$.

The fiber of an observed table $\mathbf{n}_{\mathrm{obs}}$ with respect to a function $T : \mathbb{N}^k \longrightarrow \mathbb{N}^s$ is the set

$$\mathcal{F}_T(\mathbf{n}_{\mathrm{obs}}) = \left\{ \mathbf{n} \mid \mathbf{n} \in \mathbb{N}^k \ , \ T(\mathbf{n}) = T(\mathbf{n}_{\mathrm{obs}}) \right\} . \tag{1}$$

When the dependence on the specific observed table is irrelevant, we will write simply $\mathcal{F}_T$ instead of $\mathcal{F}_T(\mathbf{n}_{\mathrm{obs}})$.

In mathematical statistics framework, the function T is usually the minimal sufficient statistic of some statistical model and the usefulness of enumeration of the fiber $\mathcal{F}_T(\mathbf{n}_{\mathrm{obs}})$ follows from classical theorems such as the Rao-Blackwell theorem, see e.g. Shao (1998).

When the function T is linear, it can be extended in a natural way to an homomorphism from $\mathbb{R}^n$ in $\mathbb{R}^s$, T is represented by a $s \times k$-matrix A_T, and its generic element $A_T(\ell, h)$ is

$$A_T(\ell, h) = T_\ell(h), \tag{2}$$

where T_ℓ is the ℓ-th component of the function T. In terms of the matrix A_T, the fiber $\mathcal{F}_T$ can be easily rewritten in the form:

$$\mathcal{F}_T = \left\{ \mathbf{n} \mid \mathbf{n} \in \mathbb{N}^k \ , \ A_T(\mathbf{n}) = A_T(\mathbf{n}_{\mathrm{obs}}) \right\} . \tag{3}$$

To navigate inside the fiber $\mathcal{F}_T$, i.e., to connect any two tables of the fiber $\mathcal{F}_T$ with a path of nonnegative tables, algebraic statistics suggests an approach based on the notion of Markov moves and Markov bases. A Markov move is any table $\mathbf{m}$ with integer entries that preserves the linear function T, i.e. $T(\mathbf{n} \pm \mathbf{m}) = T(\mathbf{n})$ for all $\mathbf{n} \in \mathcal{F}_T$.

A finite set of moves $\mathcal{M} = \{\mathbf{m}_1, \ldots, \mathbf{m}_r\}$ is called a *Markov basis* if it is possible to connect any two tables of $\mathcal{F}_T$ with moves in $\mathcal{M}$. More formally, for all $\mathbf{n}_1$ and $\mathbf{n}_2$ in $\mathcal{F}_T$, there exist a sequence of moves $\{\mathbf{m}_{i_1}, \ldots, \mathbf{m}_{i_A}\}$ and a sequence of signs $\{\epsilon_{i_1}, \ldots, \epsilon_{i_A}\}$ such that

$$\mathbf{n}_2 = \mathbf{n}_1 + \sum_{a=1}^{A} \epsilon_{i_a} \mathbf{m}_{i_a} \tag{4}$$

and

$$\mathbf{n}_1 + \sum_{j=1}^{a} \epsilon_{i_j} \mathbf{m}_{i_j} \geq 0 \quad \text{ for all } \ a = 1, \ldots, A \, . \tag{5}$$

See Diaconis and Sturmfels (1998) for further details on Markov bases. Given a Markov basis, the Diaconis-Sturmfels algorithm for sampling from a distribution σ on $\mathcal{F}_T$ starts from a table $\mathbf{n} \in \mathcal{F}_T$ and proceeds at each step as follows:

- Choose a move $\mathbf{m} \in \mathcal{M}$ and a sign $\epsilon = \pm 1$ with probability 1/2 each independently on $\mathbf{m}$;

- Generate a random number u from the uniform distribution $\mathcal{U}[0,1]$;
- If $\mathbf{n} + \epsilon\mathbf{m} \in \mathcal{F}_T$ and $\min\{\sigma(\mathbf{n} + \epsilon\mathbf{m})/\sigma(\mathbf{n}), 1\} > u$, then the Markov chain moves from the current table $\mathbf{n}$ to $\mathbf{n} + \epsilon\mathbf{m}$; otherwise, it stays at $\mathbf{n}$.

To actually compute Markov bases, we associate to the problem two distinct polynomial rings. First, we define $\mathbb{R}[\mathbf{x}] = \mathbb{R}[x_1, \ldots, x_k]$, i.e., we associate an indeterminate x_h to any cell of the table; then, we define $\mathbb{R}[\mathbf{y}] = \mathbb{R}[y_1, \ldots, y_s]$, with an indeterminate y_ℓ for any component of the linear function T. In the following we will use some facts from commutative algebra, to be found in, e.g., Cox *et al.* (1992).

The simplest method to compute Markov bases uses the elimination algorithm:

- For each column of the matrix A_T, define the polynomial

$$f_h = x_h - \prod_{\ell=1}^{s} y_\ell^{A_T(\ell,h)} \quad \text{for} \quad h = 1, \ldots, k\,; \tag{6}$$

  Then, consider the ideal generated by the polynomials $f_1, \ldots, f_k$:

$$\mathcal{I} = \langle f_1, \ldots, f_k \rangle \tag{7}$$

  in the polynomial ring $\mathbb{R}[\mathbf{x}, \mathbf{y}]$;

- Eliminate the $\mathbf{y}$'s indeterminates, and obtain the ideal

$$\mathcal{I}_{A_T} = \mathrm{Elim}(\mathbf{y}, \mathcal{I}) \tag{8}$$

  in the polynomial ring $\mathbb{R}[\mathbf{x}]$. The ideal $\mathcal{I}_{A_T}$ in Equation (8) is by definition the toric ideal associated to A_T;

- A Gröbner basis of $\mathcal{I}_{A_T}$ is formed by binomials. Each binomial defines a move of a Markov basis taking the exponents. Namely, the correspondence between the binomials and the moves is given by the log-transformation

$$\log(\mathbf{x}^a - \mathbf{x}^b) = a - b \in \mathbb{R}^k\,.$$

Although faster algorithms have been implemented to compute toric ideals, the elimination-based algorithm is the simplest one and we will use this technique in some of the proofs. For details on computational methods for toric ideals, see Bigatti *et al.* (1999) and the implementation in `4ti2` (4ti2 team, 2008).

As noted in e.g. Rapallo and Rogantin (2007) and Chen *et al.* (2005), when the entries of table have an upper bound, the classical notion of Markov basis is not sufficient to connect all the tables in a fiber. In fact, the fiber in the bounded case:

$$\mathcal{F}_T^{\mathbf{b}} = \left\{\mathbf{n} \mid \mathbf{n} \in \mathbb{N}^k\ ,\ T(\mathbf{n}) = T(\mathbf{n}_{\mathrm{obs}})\ ,\ \mathbf{n} \le \mathbf{b}\right\} \tag{9}$$

is in general smaller than the unrestricted one.

As shown in Sections 3 and 4 as well as Rapallo and Rogantin (2007), the constraint $\mathbf{n} \leq \mathbf{b}$ translates into a linear system by introducing dummy counts $\overline{n}_1, \ldots, \overline{n}_k$ with $n_h + \overline{n}_h = b_h$ for all $h = 1, \ldots, k$. Therefore, in the presence of upper bounds of the cell counts, the Markov basis must be computed through a Universal Gröbner basis of the ideal $\mathcal{I}_{A_T}$.

The procedure to compute a Universal Gröbner basis of the ideal $\mathcal{I}_{A_T}$ is fully described in Chapter 7 of Sturmfels (1996). Here we summarize the main steps of the algorithm. Given the matrix A_T, its Lawrence lifting is a matrix $\Lambda(A_T)$ with dimensions $(s+k)\times(2k)$ and with block representation

$$\Lambda(A_T) = \begin{pmatrix} A_T & 0 \\ I_k & I_k \end{pmatrix} , \tag{10}$$

where 0 is a null matrix with dimensions $s \times k$ and I_k is the identity matrix with dimension $k \times k$.

The Universal Gröbner basis of A_T is then computed with the algorithm below:

- Define k new indeterminates $\overline{x}_1, \ldots, \overline{x}_k$;
- Compute a Gröbner basis of the toric ideal $\mathcal{I}_{\Lambda(A_T)}$ in the polynomial ring $\mathbb{R}[\mathbf{x}, \overline{\mathbf{x}}]$, the toric ideal associated to the Lawrence lifting $\Lambda(A_T)$ of A_T;
- Substitute $\overline{x}_h = 1$ for all $h = 1, \ldots, k$.

The interested reader can find all details and the proof of the correctness of this algorithm in Sturmfels (1996), Chapter 7. In terms of Markov bases, we state the following definition.

Definition 1. *A Markov basis computed through a Universal Gröbner basis is a* Universal Markov basis*.*

The following section is devoted to the computation of Universal Markov bases in special settings, such as incomplete tables, bounds acting on a subset of the full sample space, or strictly positive bounds.

3 Universal Markov bases and incomplete tables

The computation of Universal Markov bases is not easy in practice, especially for two distinct circumstances:

- The computation of a Universal Markov basis is based on twice the number of indeterminates than the standard Markov basis;
- The number of moves of a Universal Markov basis increases quickly with the dimension of the contingency table.

Example 1. *Let us consider $I \times J$ contingency tables under independence model. With fixed marginal totals, and without upper bounds, a Gröbner basis is formed by all 2×2 minors (see Diaconis and Sturmfels (1998)). This fact can be proved theoretically and does not need symbolic computations.*

In this special case we are also able to characterize the Universal Gröbner basis. Combining Algorithm 7.2 and Corollary 14.12 in Sturmfels (1996), the Universal Gröbner basis is formed by all the binomials:

$$x_{i_1 j_1} x_{i_2 j_2} \ldots x_{i_s j_s} - x_{i_2 j_1} x_{i_3 j_2} \ldots x_{i_1 j_s} \, , \tag{11}$$

where $(i_1, j_1), (j_1, i_2), \ldots, (j_s, i_1)$ is a circuit in the complete bipartite graph with I and J vertices.

This implies that the number of moves needed for the Universal Markov basis increases much faster with respect to the Markov basis for the unbounded problem. Just to give the idea of such increase, we present in the following table the number of moves of the Gröbner bases for square $I \times I$ tables for the first I's.

	2	3	4	5	6	7
Standard Markov basis	1	9	36	100	225	441
Universal Markov basis	1	15	204	3,940	113,865	4,027,161

To overcome this difficulty it is of major interest to have some results for the theoretical computation of Universal Markov bases. The first result in this direction that we present in this section is related to tables with structural zeros (or incomplete tables).

Let $\mathcal{X}_0 \subset \mathcal{X}$ be the set of structural zeros of the table, let T' be the function T restricted to $\mathcal{X}' = \mathcal{X} \setminus \mathcal{X}_0$ and let $\mathcal{I}'_{A_T}$ be the toric ideal associated with $A_{T'}$

Theorem 1. *Let $\mathbf{n}$ be a contingency table and let $\mathcal{F}_T^{\mathbf{b}}$ be its bounded fiber under the bound $\mathbf{n} \leq \mathbf{b}$. Let $\mathcal{X}_0$ be the set of structural zeros. Then a Universal Gröbner basis for the ideal $\mathcal{I}'_{A(T)}$ is obtained from the Universal Gröbner basis of $\mathcal{I}_{A(T)}$ by removing the binomials involving indeterminates in $\mathcal{X}_0$.*

Proof. Using Theorem 7.1 in Sturmfels (1996), the Universal Gröbner basis has the following two properties: (a) it is unique; (b) it is a Gröbner basis with respect to all term orderings on $\mathbb{R}[\mathbf{x}]$.

Without loss of generality, let us suppose that the structural zeros are the first cells, i.e., $\mathcal{X}_0 = \{1, \ldots, k'\}$. The unique Universal Gröbner basis is, from property (b) above, a basis with respect to the elimination term ordering for the first k' indeterminates. Then, we apply Theorem 4 in Rapallo (2006) and the elimination algorithm.

Following the scheme in Equations (6) through (7) with the matrix $\Lambda(A_T)$, we define the polynomials

$$f_h = x_h - \overline{y}_h \prod_{\ell=1}^{s} y_\ell^{A_T(\ell,h)} \quad \text{for} \quad h = 1, \ldots, k$$

and

$$f_{k+h} = \overline{x}_h - \overline{y}_h \quad \text{for} \quad h = 1, \ldots, k \, .$$

The ideal in Equation (7) becomes

$$\mathcal{I} = \langle f_1, \ldots, f_k, f_{k+1}, \ldots, f_{2k} \rangle$$

in the polynomial ring $\mathbb{R}[\mathbf{x}, \overline{\mathbf{x}}, \mathbf{y}, \overline{\mathbf{y}}]$. Therefore, the toric ideal $\mathcal{I}_{\Lambda(A_T)}$ as in Equation (8) is

$$\mathcal{I}_{\Lambda(A_T)} = \mathrm{Elim}(\{\mathbf{y}, \overline{\mathbf{y}}\}, \mathcal{I}) \,. \tag{12}$$

When $x_1, \ldots, x_{k'}$ are indeterminates associated to structural zeros, the relevant ideal is

$$\mathcal{I}' = \mathrm{Elim}(\{x_1, \ldots, x_{k'}\}, \mathcal{I})$$

and the Universal Gröbner basis of $\mathcal{I}'_{A_T}$ is computed through

$$\mathrm{Elim}(\{\mathbf{y}, \overline{\mathbf{y}}\}, \mathcal{I}') = \mathrm{Elim}(\{\mathbf{y}, \overline{\mathbf{y}}\}, \mathrm{Elim}(\{x_1, \ldots, x_{k'}\}, \mathcal{I})) =$$

$$= \mathrm{Elim}(\{x_1, \ldots, x_{k'}\}, \mathrm{Elim}(\{\mathbf{y}, \overline{\mathbf{y}}\}, \mathcal{I})) = \mathrm{Elim}(\{x_1, \ldots, x_{k'}\}, \mathcal{I}_{\Lambda(A_T)})$$

and then substituting $\overline{x}_h = 1$ for all h. As the Universal Gröbner basis is in particular a basis with respect to the elimination term ordering for the indeterminates $x_1, \ldots, x_{k'}$, this proves that to remove the binomials involving $x_1, \ldots, x_{k'}$ from $\mathcal{I}_{\Lambda(A_T)}$ is equivalent to compute the Universal Gröbner basis for the incomplete table. □

If one has the Universal Markov basis for the complete configuration, Theorem 1 applies easily. In fact, using the correspondence between moves and binomials, the theorem above is clearly equivalent to the following:

Corollary 1. *Let* $\mathbf{n}$ *be a contingency table and let* $\mathcal{F}_T^{\mathbf{b}}$ *be its bounded fiber under the bound* $\mathbf{n} \leq \mathbf{b}$. *Let* $\mathcal{X}_0$ *be the set of structural zeros. Then a Universal Markov basis for* $\mathcal{F}_{T'}^{b}$ *is obtained from a Universal Markov basis for* $\mathcal{F}_T^{b}$ *by removing the moves involving the cells in* $\mathcal{X}_0$.

Example 2. *Let us consider* 4×4 *contingency tables with fixed marginal totals, as in Example 1. Without structural zeros, the Universal Markov basis is formed by* 204 *binomials:* 36 *moves involving* 4 *cells:* 96 *moves involving* 6 *cells: and* 72 *moves involving* 8 *cells.*

Suppose that the cell $(1,1)$ *is a structural zero. This kind of table is depicted below, where* 0 *means a structural zero, while the symbol* $\bullet$ *denotes a non-zero cell.*

$$\begin{pmatrix} 0 & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \end{pmatrix}$$

From the complete Universal Markov basis we can remove all moves involving the structural zero. Applying Corollary 1, we remove: 9 *moves involving* 4 *cells:* 36 *moves involving* 6 *cells: and* 36 *moves involving* 8 *cells. The Universal Markov basis in this case has* 123 *moves.*

Suppose now that the whole main diagonal contains structural zeros, as in the figure below.

$$\begin{pmatrix} 0 & \bullet & \bullet & \bullet \\ \bullet & 0 & \bullet & \bullet \\ \bullet & \bullet & 0 & \bullet \\ \bullet & \bullet & \bullet & 0 \end{pmatrix}$$

In this situation we remove: 30 *moves involving* 4 *cells:* 80 *moves involving* 6 *cells: and* 66 *moves involving* 8 *cells. Finally, the Universal Markov basis has only* 28 *moves.*

The last example is a prototype for the quasi-independence models. Now consider $I \times J$ contingency tables with structural zeros under quasi-independence model. Aoki and Takemura (2005) computed a unique minimum Markov basis for $I \times J$ contingency tables with structural zeros under quasi-independence model.

Definition 2 (Aoki and Takemura (2005))**.** *Let $\mathcal{X} = \{(i,j) \mid 1 \le i \le I, 1 \le j \le J\}$ be the sample space and let $\mathcal{X}' = \mathcal{X} \setminus \mathcal{X}_0$ be the set of cells that are not structural zeros. Also let*

$$F_0(S) = \left\{ \mathbf{m} \,\middle|\, \sum_{j=1}^{J} m_{ij} = \sum_{i=1}^{I} m_{ij} = 0, \text{ and } m_{ij} = 0 \text{ for } (i,j) \notin S \right\}.$$

A loop (or loop move) of degree r on $\mathcal{X}'$ is an $I \times J$ integer array $M_r(i_1, \ldots, i_r; j_1, ..., j_r) \in F_0(S)$, for $1 \le i_1, \ldots, i_r \le I$, $1 \le j_1, \ldots, j_r \le J$, where $M_r(i_1, \ldots, i_r; j_1, \ldots, j_r)$ has the elements

$$m_{i_1 j_1} = m_{i_2 j_2} = \ldots = m_{i_{r-1} j_{r-1}} = m_{i_r j_r} = 1,$$
$$m_{i_1 j_2} = m_{i_2 j_3} = \ldots = m_{i_{r-1} j_r} = m_{i_r j_1} = -1,$$

and all other elements are zero. Also the level indices $i_1, i_2, \ldots,$ and $j_1, j_2, \ldots$ are all distinct, i.e.

$$i_m \ne i_n \text{ and } j_m \ne j_n \text{ for all } m \ne n\,.$$

Specifically, a degree 2 loop $M_2(i_1, i_2; j_1, j_2)$ is called a basic move.

The support of a loop $M_r(i_1, \ldots, i_r; j_1, ..., j_r)$ is the set of its non-zero cells. A loop $M_r(i_1, \ldots, i_r; j_1, ..., j_r)$ is called df 1 if $R(i_1, \ldots, i_r; j_1, \ldots, j_r)$ does not contain support of any loop on S of degree $2, \ldots, r-1$, where $R(i_1, \ldots, i_r; j_1, \ldots, j_r) = \{(i,j) | i \in \{i_1, \ldots, i_r\}, j \in \{j_1, \ldots, j_r\}\}$.

Corollary 2 (Aoki and Takemura (2005))**.** *The set of df* 1 *loops of degree* $2, \ldots, \min\{I, J\}$ *constitutes a unique minimal Markov basis for $I \times J$ contingency tables with structural zeros under quasi-independence model.*

The examples above show that in many cases the computation of Universal Markov bases for incomplete tables inherits benefit from complete tables. In terms of computations, an incomplete table has less cells than the corresponding complete table and therefore an incomplete table implies the use of a smaller number of indeterminates. Nevertheless, in a complete table with symmetric constraints the Markov bases can be characterized theoretically (e.g., independence model presented here), and in many cases the symmetry of the combinatorial problem can lead to substantial simplifications in the symbolic computation (see in particular (Aoki and Takemura, 2008)). Moreover, following Theorem 1, in the computation of Universal Markov bases through elimination we do not introduce new polynomials and, therefore, we do not increase the degree of the moves, as usual in the unbounded problems (see Rapallo (2006)).

Example 3. *As a different example, where Markov bases are much simpler, we present a computation for a 2^{3-1} fraction of a factorial design. The use of Markov bases for fractions are useful for experiments with Poisson-distributed response variable and the upper bounds are needed when the response variable is Binomial (see Aoki and Takemura (2006)). Here we consider the lattice $\{-1,1\}^3$ for an experiment with 3 factors A, B, and C. The fraction defined by the aliasing equation $AB = 1$ consists of 4 cells:*

$$(-1,-1,-1), \quad (-1,-1,1), \quad (1,1,-1), \quad (1,1,1). \tag{13}$$

These 4 points can be viewed as an incomplete three-way table. Computing with `CoCoA` *(CoCoATeam, 2007), the standard Markov basis for this incomplete table under the complete independence model (i.e., with the one-way marginal totals fixed), we obtain only one move, represented by the binomial:*

$$x_{-1-1-1}x_{111} - x_{-1-11}x_{11-1}. \tag{14}$$

From this computation we note that:

- *In this example the standard Markov basis has only one polynomial and therefore it is by definition a Universal Markov basis;*
- *The standard Markov basis for the corresponding complete table with 8 cells is formed by 9 quadratic square-free binomials, and the corresponding Universal Markov basis for the bounded problem has 20 binomials:*

```
-x[-1,1,-1]x[1,-1,1] + x[-1,-1,-1]x[1,1,1],
-x[-1,1,1]x[1,-1,-1] + x[-1,-1,-1]x[1,1,1],
-x[-1,1,-1]x[1,-1,-1] + x[-1,-1,-1]x[1,1,-1],
x[-1,1,1]x[1,1,-1] - x[-1,1,-1]x[1,1,1],
-x[-1,-1,1]x[-1,1,-1] + x[-1,-1,-1]x[-1,1,1],
-x[-1,1,1]x[1,-1,-1] + x[-1,-1,1]x[1,1,-1],
x[-1,1,1]x[1,-1,-1] - x[-1,1,-1]x[1,-1,1],
x[-1,-1,1]x[1,-1,-1] - x[-1,-1,-1]x[1,-1,1],
-x[1,-1,1]x[1,1,-1] + x[1,-1,-1]x[1,1,1],
-x[-1,1,1]x[1,-1,1] + x[-1,-1,1]x[1,1,1],
-x[-1,1,-1]x[1,-1,1] + x[-1,-1,1]x[1,1,-1],
-x[-1,-1,1]x[1,1,-1] + x[-1,-1,-1]x[1,1,1],
-x[-1,1,1]x[1,-1,1]x[1,1,-1] + x[-1,-1,-1]x[1,1,1]^2,
-x[-1,-1,1]x[-1,1,-1]x[1,-1,-1] + x[-1,-1,-1]^2x[1,1,1],
```

```
x[-1,-1,1]x[1,1,-1]^2 - x[-1,1,-1]x[1,-1,-1]x[1,1,1],
x[-1,1,1]x[1,-1,-1]^2 - x[-1,-1,-1]x[1,-1,1]x[1,1,-1],
-x[-1,-1,-1]x[-1,1,1]x[1,-1,1] + x[-1,-1,1]^2x[1,1,-1],
x[-1,1,1]^2x[1,-1,-1] - x[-1,-1,1]x[-1,1,-1]x[1,1,1],
-x[-1,1,-1]^2x[1,-1,1] + x[-1,-1,-1]x[-1,1,1]x[1,1,-1],
-x[-1,1,-1]x[1,-1,1]^2 + x[-1,-1,1]x[1,-1,-1]x[1,1,1]
```

Notice that in a Metropolis-Hastings algorithm one can also make use of the complete Markov basis and then discard the chosen move at a given step if it modifies a cell with a structural zero. But the computations for this example show that the use of such a strategy leads to a slower convergence of the Markov chain to the stationary distribution. The use of the Markov basis with the unique applicable move is essential for a correct use of the Metropolis-Hastings algorithm.

4 Markov bases for partially bounded tables

While the problem in the previous section has a positive answer, in this section we present a problem without a theoretical solution. Nevertheless, we show how to write the relevant symbolic computations and we describe explicitly some special examples.

When working with bounded contingency tables, it is a common situation to have some cell counts bounded and other counts unbounded. Moreover, some bounds can be treated as unessential. In this section, we consider two-way contingency tables under independence model.

It is well known that under the marginal totals each cell count n_{ij} can not exceed $\min\{n_{i+}, n_{+j}\}$, where n_{i+} is the i-th row total and n_{+j} is the j-th column total. Thus, any bound exceeding such value can be ignored. Now, we know that:

- With no upper bounds, we need a Markov basis formed by the basic moves of the form $\begin{pmatrix} +1 & -1 \\ -1 & +1 \end{pmatrix}$ for all 2×2 minors of the table;
- With an upper bound for each cell count, we need the Universal Markov basis formed by all the closed circuits in the complete bipartite graph with I and J vertices, as discussed in the previous section.

Example 1 shows that the differences between such two situations are noticeable in terms of number of moves. We can conjecture that with some cells bounded and other cells without bounds we will fall into an intermediate situation, with a Gröbner basis formed by all the degree two by two minors and some other square-free binomials.

As pointed out in the previous section, the bounds on the cell counts are represented as linear constraints through the two identity matrices I_k in the Lawrence lifting $\Lambda(A_T)$, see Equation (10). Thus, for the computation of Markov bases for partially bounded table, we have to remove from the block $[I_k, I_k]$ of $\Lambda(A_T)$ the rows corresponding to cells without upper bound.

To show the behavior of Universal Markov bases with partial bounds, we present here some numerical examples of Markov bases computed with `CoCoA`.

Example 4. *Consider a* 3×3 *contingency table under independence model. With a bound on all the cells, the Universal Markov basis has* 15 *moves:* 9 *moves of the form* $\begin{pmatrix} +1 & -1 \\ -1 & +1 \end{pmatrix}$ *for all* 2×2 *minors of the table plus the* 6 *moves of degree* 3 *below:*

$$\mathbf{m}_1 = \begin{pmatrix} 0 & -1 & +1 \\ -1 & +1 & 0 \\ +1 & 0 & -1 \end{pmatrix} ,$$

$$\mathbf{m}_2 = \begin{pmatrix} 0 & -1 & +1 \\ +1 & 0 & -1 \\ -1 & +1 & 0 \end{pmatrix} ,$$

$$\mathbf{m}_3 = \begin{pmatrix} -1 & 0 & +1 \\ +1 & -1 & 0 \\ 0 & +1 & -1 \end{pmatrix} ,$$

$$\mathbf{m}_4 = \begin{pmatrix} -1 & 0 & +1 \\ 0 & +1 & -1 \\ +1 & -1 & 0 \end{pmatrix} ,$$

$$\mathbf{m}_5 = \begin{pmatrix} -1 & +1 & 0 \\ 0 & -1 & +1 \\ +1 & 0 & -1 \end{pmatrix} ,$$

$$\mathbf{m}_6 = \begin{pmatrix} -1 & +1 & 0 \\ +1 & 0 & -1 \\ 0 & -1 & +1 \end{pmatrix} .$$

Now we have computed the Universal Markov basis in three different situations, with different types of bounds:

- *with a bound only on the cell* $(1,1)$*, the Universal Markov basis has* 10 *moves: the* 9 *basic moves and* $\mathbf{m}_2$*;*
- *with a bound on the three cells on the main diagonal, the Universal Markov basis has* 13 *moves: the* 9 *basic moves, plus* $\mathbf{m}_1$*,* $\mathbf{m}_2$*,* $\mathbf{m}_4$ *and* $\mathbf{m}_6$*;*
- *with a bound on the five block-diagonal cells:* $(1,1)$*,* $(2,2)$*,* $(2,3)$*,* $(3,2)$ *and* $(3,3)$*, the Universal Markov basis has* 12 *moves: the* 9 *basic moves, plus* $\mathbf{m}_1$*,* $\mathbf{m}_2$ *and* $\mathbf{m}_4$*;*
- *with a bound on all cells but the* $(1,1)$*, the Universal Markov basis has* 13 *moves: the* 9 *basic moves, plus* $\mathbf{m}_3$*,* $\mathbf{m}_4$*,* $\mathbf{m}_5$ *and* $\mathbf{m}_6$*.*

Example 5 (Aoki and Takemura (2005)). *Consider* 6×6 *contingency tables of the following form:*

$$\begin{pmatrix} 0 & \bullet & \bullet & 0 & 0 & \bullet \\ \bullet & 0 & \bullet & \bullet & 0 & 0 \\ \bullet & \bullet & 0 & 0 & \bullet & 0 \\ 0 & 0 & \bullet & 0 & \bullet & \bullet \\ \bullet & 0 & 0 & \bullet & 0 & \bullet \\ 0 & \bullet & 0 & \bullet & \bullet & 0 \end{pmatrix}.$$

The reduced Gröbner basis with the degree reverse lexicographical ordering consists of three basic moves, 20 degree 3 loops, 10 degree 4 loops, and 3 degree 5 loops. Note that the loops of degree 4 and 5 are not df 1. On the other hand, all the 20 loops of degree 3 are df 1. Hence by Corollary 2, the above three basic moves and 20 degree 3 loops constitute the unique minimal Markov basis.

5 Markov subbases for bounded and incomplete two-way contingency tables

Despite the computational advances presented in the previous sections, there are applied problems where one may never be able to compute a Markov basis. Models of no-3-way interaction and constraint matrices of Lawrence type seem to be arbitrarily difficult, namely if we vary I and J for $(I, J, K)-$tables, the degree and support of elements in a minimal Markov bases can be arbitrarily large (De Loera and Onn, 2005). In general, the number of elements in a minimal Markov basis for a model can be exponentially many. Thus, it is important to compute a reduced number of moves which connect all tables instead of computing a Markov basis. Chen *et al.* (2009) discussed that in some cases, such as logistic regression, positive margins are shown to allow a set of Markov connecting moves that are much simpler than the full Markov basis. One such example is shown in Hara *et al.* (2008) where a Markov basis for a multiple logistic regression is computed by the Lawrence lifting of this basis. In the case of bivariate logistic regression, Hara *et al.* (2008) showed a simple subset of the Markov basis which connects all fibers with a positive sample size for each combination of levels of covariates. Such connecting sets were formalized in Chen *et al.* (2006) with the terminology *Markov subbasis*.

In this section we use a sample space indexed as $\{1, \ldots, k\}$ instead of $\{1, \ldots, I\} \times \{1, \ldots J\}$ whenever possible, in order to make the formulae easier to read.

Definition 3 (Chen *et al.* (2006)). *A Markov subbasis* $M_{A_T,\mathbf{n}_{obs}}$ *for* $\mathbf{n}_{obs} \in \mathbb{N}^k$ *and integer matrix* A_T *is a finite subset of* $\ker(A_T) \cap \mathbb{Z}^k$ *such that, for each pair of vectors* $\mathbf{u}$, $\mathbf{v} \in \mathcal{F}_T$, *there is a sequence of vectors* $\mathbf{m}_i \in M_{A_T,\mathbf{n}_{obs}}$, $i = 1, \ldots, l$, *such that*

$$\mathbf{u} = \mathbf{v} + \sum_{i=1}^{l} \mathbf{m}_i,$$

$$0 \leq \mathbf{v} + \sum_{i=1}^{j} \mathbf{m}_i,\ j = 1, \ldots, l.$$

The connectivity through nonnegative lattice points only is required to hold for this specific $\mathbf{n}_{obs}$.

Note that $M_{A_T,\mathbf{n}_{\text{obs}}}$ for every $\mathbf{n}_{\text{obs}} \in \mathbb{N}^k$ and for a given A_T is a Markov basis $\mathcal{M}$ for A_T.

In this section we first study Markov subbases $M_{A_T,\mathbf{n}_{\text{obs}}}$ for any bounded two-way contingency tables $\mathbf{n}_{\text{obs}} \in \mathbb{N}^k$ with positive bounds, i.e., no structural zeros, under independence model. Then we study Markov subbases $M_{A_T,\mathbf{n}_{\text{obs}}}$ for any incomplete $I \times J$ contingency tables $\mathbf{n}_{\text{obs}} \in \mathbb{N}^k$ with positive margins, i.e., $A_T(\mathbf{n}_{\text{obs}}) > 0$, under independence model.

To analyze these cases we recall some definitions from commutative algebra:

- An ideal $\mathcal{I} \subset \mathbb{R}[\mathbf{x}]$ is *radical* if

$$\{f \in \mathbb{R}[\mathbf{x}] \mid f^n \in \mathcal{I} \text{ for some } n\} = \mathcal{I}\,;$$

- Let $\mathcal{I},\ \mathcal{J} \subset \mathbb{R}[\mathbf{x}]$ be ideals. The quotient ideal $(\mathcal{I} : \mathcal{J})$ is defined by:

$$(\mathcal{I} : \mathcal{J}) = \{f \in \mathbb{R}[\mathbf{x}] \mid f \cdot \mathcal{J} \subset \mathcal{I}\}\ ;$$

- Let $\mathcal{I},\ \mathcal{J} \subset \mathbb{R}[\mathbf{x}]$ be ideals. The saturation of $\mathcal{I}$ with respect to $\mathcal{J}$ is the ideal defined by:

$$(\mathcal{I} : \mathcal{J}^\infty) = \{f \in \mathbb{R}[\mathbf{x}] \mid g^m \cdot f \in \mathcal{I},\ g \in \mathcal{J},\ \text{for some } m > 0\}\,;$$

- Let $Z = \{z_1, \ldots, z_s\} \subset \mathbb{R}^k$. A lattice L generated by Z is defined:

$$L = \mathbb{Z}Z.$$

  $M \subset \mathbb{R}^k$ is called a lattice basis of L if each element in L can be written as a linear integer combination of elements in M. Now a lattice basis for $\ker(A_T)$ has the property that any two tables can be connected by its vector increments if one is allowed to swing negative in the connecting path (see Chapter 12 of Sturmfels (1996) for definitions and properties of a lattice basis).

The reader can find in Cox *et al.* (1992) more details on the definitions above.

Theorem 2 (Chen *et al.* (2009))**.** *Suppose* $\mathcal{I}_M$ *is a radical ideal, and suppose* M *is a lattice basis. Let* $p = x_1 \cdots x_k$. *For each index* ℓ *with* $(A_T)_\ell > 0$, *let* $\mathcal{I}_\ell = \langle x_h \rangle_{(A_T)_{\ell,h}>0}$ *be the monomial ideal generated by indeterminates for cells that contribute to margin* ℓ. *Let* $\mathcal{L}$ *be the collection of indices* ℓ *with* $(A_T\mathbf{n})_\ell > 0$. *Define*

$$\mathcal{I}_{\mathcal{L}} = \left(\mathcal{I}_M : \prod_{\ell \in \mathcal{L}} \mathcal{I}_\ell\right).$$

If
$$(\mathcal{I}_{\mathcal{L}} : (\mathcal{I}_{\mathcal{L}} : p)) = \langle 1 \rangle \tag{15}$$
then the moves in M connect all the tables in $\mathcal{F}_T$.

For computing the following examples we have used the software `Singular` (Greuel *et al.*, 2009).

Example 6 (Continue from Example 4)**.** *Consider again 3×3 tables with fixed row and column sums, which are the constraints from fixing sufficient statistics in independence model, and with all bounded cells. This is equivalent with $3 \times 3 \times 2$ tables with constraints $[A, C]$, $[B, C]$, $[A, B]$ for factors A, B, C, which would arise for example in case-control data with two factors A and B at three levels each.*

The constraint matrix that fixes row and column sums in a 3×3 table gives a toric ideal with a $\binom{3}{2} \times \binom{3}{2}$ element Gröbner basis. Each of these moves can be paired with its signed opposite to get 9 moves of $3 \times 3 \times 2$ tables that preserve sufficient statistics. This is equivalent to 9 moves of the form $\begin{pmatrix} +1 & -1 \\ -1 & +1 \end{pmatrix}$ for all 2×2 minors of the table for 3×3 tables under independence model (see Example 4). These elements make an ideal with a Gröbner basis that is square-free in the initial terms, and hence the ideal is radical (Proposition 5.3 of Sturmfels (2002)). Then applying Theorem 2 with nine margins of case-control counts, i.e., this is equivalent to having the positive constraints on bounds, namely we have non-zero bounds for all cells, shows that these 9 moves do connect tables with positive case-control sums. The full Markov basis has 15 moves. Therefore, the Markov subbasis for this table is the standard Markov basis for a 3×3 table under independence model.

Example 7 (Chen *et al.* (2009))**.** *Consider now 4×4 tables with fixed row and column sums as in Example 6, and with all bounded cells. Again, this is equivalent with $4 \times 4 \times 2$ tables with constraints $[A, C]$, $[B, C]$, $[A, B]$ for factors A, B and C, with factors A and B at four levels each.*

The constraint matrix that fixes row and column sums in a 4×4 table gives a toric ideal with a $\binom{4}{2} \times \binom{4}{2}$ element Gröbner basis. Each of these moves can be paired with its signed opposite to get 36 moves of $4 \times 4 \times 2$ tables that preserve sufficient statistics:
$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ + & 0 & - & 0 \\ 0 & 0 & 0 & 0 \\ - & 0 & + & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 0 & 0 \\ - & 0 & + & 0 \\ 0 & 0 & 0 & 0 \\ + & 0 & - & 0 \end{pmatrix}.$$
These elements make an ideal with a Gröbner basis that is square-free in the initial terms, and hence the ideal is radical (Proposition 5.3 of Sturmfels (2002)). Then applying Theorem 2 with sixteen margins of case-control counts, i.e., this is equivalent to having the positive conditions on bounds, namely we have non-zero bounds for all cells, shows that these 36 moves do connect tables with positive case-control sums. The full Markov basis has 204 moves. Therefore, the Markov subbasis for this table is the standard Markov basis for a 4×4 table with fixed row and column sums fixed without bounds.

In practice, the algorithm in Theorem 2 is not feasible for a large number of cells in a table.

From Examples 6 and 7 it seems that for bounded two-way tables with row and column sums fixed we only need a standard Markov basis for two-way tables with row and column sums fixed if these bounds are positive. In fact, by the following theorem, additional elements in a Universal Markov basis are needed for incomplete tables, i.e., structural zeros.

Theorem 3. *Consider $I \times J$ tables with row and column sums fixed and with all cells bounded. If these bounds are positive, then a Markov subbasis for the tables is the standard Markov basis for $I \times J$ tables with row and column sums fixed without bounds, i.e., the set of basic moves of all 2×2 minors.*

In order to prove Theorem 3 we need the following proposition.

Proposition 1. *Let $\mathcal{I}_h = \langle x_h,\ \overline{x}_h\rangle$ for $h = 1, \ldots, k = IJ$. Then we have:*

$$\prod_{h=1}^{k} \mathcal{I}_h = \langle z_1 \cdots z_k \mid z_j = x_j \text{ or } \overline{x}_j \text{ for } j = 1, \ldots, k\rangle .$$

Proof. One can prove this proposition by induction on k. For $k = 2$, one can verify that using `Singular` (Greuel *et al.*, 2009). Assume $\prod_{h=1}^{k} \mathcal{I}_h = \langle z_1 \cdots z_k \mid z_j = x_j$ or $\overline{x}_j$ for $j = 1, \ldots, k\rangle$ holds. We want to prove that $\prod_{h=1}^{k+1} \mathcal{I}_h = \langle z_1 \cdots z_{k+1} \mid z_j = x_j$ or $\overline{x}_j$ for $j = 1, \ldots, k+1\rangle$. We have:

$$\begin{aligned}\prod_{h=1}^{k+1} \mathcal{I}_h &= \left(\prod_{h=1}^{k} \mathcal{I}_h\right) \cdot \langle x_{k+1}, \overline{x}_{k+1}\rangle \\ &= \langle z_1 \cdots z_k \mid z_j = x_j \text{ or } \overline{x}_j \text{ for } j = 1, \ldots, k\rangle \cdot \langle x_{k+1}, \overline{x}_{k+1}\rangle \\ &= \langle z_1 \cdots z_{k+1} \mid z_j = x_j \text{ or } \overline{x}_j \text{ for } j = 1, \ldots, k+1\rangle .\end{aligned}$$

□

Let M be the set of vectors such that

$$M = \{\pm (e_{i_1 j_1} + e_{i_2 j_2} - e_{i_1 j_2} - e_{i_2 j_1})\},$$

where $e_{ij} = e_{ijk}$ is defined as an integral array with 1 at the cell $(i, j, 1)$ and -1 at the cell $(i, j, 2)$ and 0 every other cells. Also let

$$\mathcal{I}_M = \langle x_{i_1 j_1} x_{i_2 j_2} \overline{x}_{i_1 j_2} \overline{x}_{i_2 j_1} - x_{i_1 j_2} x_{i_2 j_1} \overline{x}_{i_1 j_1} \overline{x}_{i_2 j_2} \mid i_1 \neq i_2,\ j_1 \neq j_2\rangle. \tag{16}$$

Proposition 2.

$$\cap_{(z_{ij} = x_{ij} \text{ or } \overline{x}_{ij} \text{ for } i=1,\ldots,I, j=1,\ldots,J)} (\mathcal{I}_M : z_{11} \ldots z_{IJ}) = (\mathcal{I}_M : x_{11} \ldots x_{IJ}) .$$

Proof. Clearly $\cap_{(z_{ij}=x_{ij} \text{ or } \overline{x}_{ij} \text{ for } i=1,\dots,I, j=1,\dots,J)} (\mathcal{I}_M : z_{11} \dots z_{IJ}) \subset (\mathcal{I}_M : x_{11} \dots x_{IJ})$. So we have to show $(\mathcal{I}_M : x_{11} \cdots x_{IJ}) \subset \cap_{(z_{ij}=x_{ij} \text{ or } \overline{x}_{ij} \text{ for } i=1,\dots,I, j=1,\dots,J)} (\mathcal{I}_M : z_{11} \cdots z_{IJ})$. By symmetry on $I \times J \times 2$ tables we have to show

$$(\mathcal{I}_M : x_{11} \cdots x_{IJ}) \subset (\mathcal{I}_M : x_{11} \cdots x_{IJ-1}\overline{x}_{IJ}) ,$$

i.e., $\forall f \in (\mathcal{I}_M : x_{11} \cdots x_{IJ})$, $f \cdot x_{11} \cdots x_{IJ-1}\overline{x}_{IJ} \in \mathcal{I}_M$. Since $f \in (\mathcal{I}_M : x_{11} \cdots x_{IJ})$, $f \cdot x_{11} \cdots x_{IJ} \in \mathcal{I}_M$. Let $f \cdot x_{11} \cdots x_{IJ} = \sum_{i_1,i_2,j_1,j_2} \alpha_{i_1,i_2,j_1,j_2} \cdot (x_{i_1j_1}x_{i_2j_2}\overline{x}_{i_1j_2}\overline{x}_{i_2j_1} - x_{i_1j_2}x_{i_2j_1}\overline{x}_{i_1j_1}\overline{x}_{i_2j_2}) \in \mathcal{I}_M$. But notice that all generators for $\mathcal{I}_M$ are symmetric on x_{ij} and $\overline{x}_{ij}$. Thus we permute x_{IJ} and $\overline{x}_{IJ}$ on the coefficients α_{i_1,i_2,j_1,j_2} if α_{i_1,i_2,j_1,j_2} contains the variables x_{IJ} or $\overline{x}_{IJ}$. Thus $f \cdot x_{11} \cdots x_{II}\overline{x}_{IJ} \in \mathcal{I}_M$. □

Proof of Theorem 3. Consider the ideal $\mathcal{I}_M$ in Equation (16). Its Gröbner basis is square-free in the initial terms, and hence the ideal is radical (Proposition 5.3 of Sturmfels (2002)). Since $\mathcal{I}_M$ in Equation (16) is radical, we use Theorem 2. Let $\mathcal{I}_A$ be the toric ideal associate with the constraint matrix of the tables $I \times J \times 2$ with constraints $[A, C]$, $[B, C]$, $[A, B]$ for factors A, B, and C. We want to show

$$\left(\mathcal{I}_M : \prod_{i=1,\dots I,\ j=1\dots J} \mathcal{I}_{ij}\right) = \mathcal{I}_A ,$$

where $\mathcal{I}_{ij} = \langle x_{ij}, \overline{x}_{ij}\rangle$ for $i = 1, \dots, I,\ j = 1, \dots, J$. Clearly $\left(\mathcal{I}_M : \prod_{i=1,\dots I,\ j=1\dots J} \mathcal{I}_{ij}\right) \subset \mathcal{I}_A$. Thus we want to show $\mathcal{I}_A \subset \left(\mathcal{I}_M : \prod_{i=1,\dots I,\ j=1\dots J} \mathcal{I}_{ij}\right)$. By Propositions 1, 2, and Equation (5) on page 193 in (Cox *et al.*, 1992), we only have to show

$$\mathcal{I}_A \subset (\mathcal{I}_M : x_{11} \cdots x_{IJ}) .$$

Let $f \in \mathcal{I}_A$. Then by the definition of the quotient ideal, we only have to show

$$(x_{11} \cdots x_{IJ}) \cdot f \in \mathcal{I}_A .$$

Assume $I \le J$ without loss of generality. Also if $I < J$, we can reduce all moves to $I \times I \times 2$ tables and other columns are zeros. Thus we consider $I \times I \times 2$ tables. We will prove this by induction on I. For $I = 3$, one can verify that the statement holds using `Singular` (Greuel *et al.*, 2009). Assume that the statement holds for some $I - 1 \ge 3$. We want to show the statement holds for I. By the inductive assumption we can assume that $s = I$ in Equation (11). Let $f = x_{i_1j_1}x_{i_2j_2} \cdots x_{i_Ij_I}\overline{x}_{i_2j_1}\overline{x}_{i_3j_2} \cdots \overline{x}_{i_1j_I} - x_{i_2j_1}x_{i_3j_2} \cdots x_{i_1j_I}\overline{x}_{i_1j_1}\overline{x}_{i_2j_2} \cdots \overline{x}_{i_Ij_I}$. By the symmetry on the row and column operations on the table $I \times I \times 2$, without loss of generality we assume $f = x_{11}x_{22} \cdots x_{II}\overline{x}_{21}\overline{x}_{32} \cdots \overline{x}_{1I} -$

$x_{21}x_{32}\cdots x_{1I}\overline{x}_{11}\overline{x}_{22}\cdots\overline{x}_{II}$. This is a binomial representation of a move on $I\times I\times 2$ tables

$$\begin{pmatrix} 1 & 0 & \dots & 0 & 0 & -1 \\ -1 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & -1 & 1 & 0 \\ 0 & 0 & \dots & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & \dots & 0 & 0 & 1 \\ 1 & -1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & -1 & 0 \\ 0 & 0 & \dots & 0 & 1 & -1 \end{pmatrix} =$$

$$\begin{pmatrix} 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 1 & 0 \\ 0 & 0 & \dots & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & \dots & 0 & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 & 0 \\ 0 & 0 & \dots & 0 & 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & \dots & 0 & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 & 0 \\ 0 & 0 & \dots & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 1 & 0 \\ 0 & 0 & \dots & 0 & 0 & 1 \end{pmatrix},$$

where the first $I\times I$ table is the first level of the table and the second table is the second level. We claim that

$$(x_{11}\cdots x_{II})\cdot f = \sum_{(i,j)=(1,2)\dots,(I-1,I)} \mathbf{x}^{U(i,j)}\overline{\mathbf{x}}^{V(i,j)}\left(x_{1i}x_{jj}\overline{x}_{1j}\overline{x}_{ji} - x_{1j}x_{ji}\overline{x}_{1i}\overline{x}_{jj}\right), \qquad (17)$$

where

$$U(i,j) = \begin{cases} \begin{pmatrix} 2 & 1 & \dots & 1 \\ 1 & 2 & \dots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \dots & 2 \end{pmatrix} - \begin{pmatrix} 0 & \dots & 1 & 0 \\ 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & 1 \end{pmatrix} & \text{if } i = I-1, j = I \\ \Sigma_{(i',j')=(i+1,j+1),\dots,(I-1,I)} U(i',j') + (e_{1,j+1} + e_{j+1,i+1}) - (e_{1,i} + e_{j,j}) & \text{else} \end{cases}$$

and

$$V(i,j) = \begin{cases} \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & \dots & 0 & 1 \\ 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 1 & 0 \end{pmatrix} & \text{if } i = I-1, j = I \\ \Sigma_{(i',j')=(i+1,j+1),\dots,(I-1,I)} V(i',j') + (e_{1,i+1} + e_{j+1,j+1}) - (e_{1,j} + e_{j,i}) & \text{else} \end{cases},$$

where $e_{i,j}$ is the integral array with 1 at the cell (i,j) and otherwise all zeros. First we consider the right hand side in Equation (17). By the construction of each coefficient, each monomial in each term cancels out except the monomial with a negative sign in the first term of the sum and the monomial with a positive sign in the last term of the sum. Also simple calculations show that

$$u_1 := \begin{pmatrix} 0 & \dots & 1 & 0 \\ 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 0 & 1 \end{pmatrix} + U(I-1,I) = \begin{pmatrix} 2 & 1 & \dots & 1 \\ 1 & 2 & \dots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \dots & 2 \end{pmatrix}$$

and

$$v_1 := \begin{pmatrix} 0 & \dots & 0 & 1 \\ 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & 1 & 0 \end{pmatrix} + V(I-1, I) = \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{pmatrix}$$

and

$$u_2 := \begin{pmatrix} 0 & 1 & \dots & 0 & 0 \\ 1 & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 \end{pmatrix} + U(1,2) = \begin{pmatrix} 1 & 1 & \dots & 1 & 2 \\ 2 & 1 & \dots & 1 & 1 \\ 1 & 2 & \dots & 1 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \dots & 2 & 1 \end{pmatrix}$$

and

$$v_2 := \begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 \end{pmatrix} + V(1,2) = \begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix}.$$

Then we notice that

$$\begin{pmatrix} 1 & 1 & \dots & 1 & 1 & 1 \\ 1 & 1 & \dots & 1 & 1 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \dots & 1 & 1 & 1 \\ 1 & 1 & \dots & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 & 0 \end{pmatrix} \quad +$$

$$\begin{pmatrix} 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 1 & 0 \\ 0 & 0 & \dots & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & \dots & 0 & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 & 0 \\ 0 & 0 & \dots & 0 & 1 & 0 \end{pmatrix} \quad = (u_1)\,(v_1)$$

and

$$\begin{pmatrix} 1 & 1 & \dots & 1 & 1 & 1 \\ 1 & 1 & \dots & 1 & 1 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \dots & 1 & 1 & 1 \\ 1 & 1 & \dots & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 & 0 \end{pmatrix} +$$

$$\begin{pmatrix} 0 & 0 & \dots & 0 & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 & 0 \\ 0 & 0 & \dots & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 1 & 0 \\ 0 & 0 & \dots & 0 & 0 & 1 \end{pmatrix} = (u_2)\,(v_2)\,.$$

Thus, $\mathbf{x}^{u_1}\overline{\mathbf{x}}^{v_1} - \mathbf{x}^{u_2}\overline{\mathbf{x}}^{v_2}$ equals to the left hand side in Equation (17). □

Now we assume that the given margins are positive for bounded $I \times J$ tables, i.e., we assume that all row and column sums are positive. Without loss of generality, we can assume that all margins are positive because cell counts in rows and/or columns with zero marginals are necessary zeros and such rows and/or columns can be ignored in the conditional analysis.

Let $\mathcal{X} = \{(i, j) \mid 1 \leq i \leq I, 1 \leq j \leq J\}$ and let $\mathcal{X}_0$ be a non-trivial subset of $\mathcal{X}$. Recall that $\mathcal{X}_0$ is the set of structural zeros of the table. For Examples 8 and 9, we used Theorem 2.

Example 8. *We consider* 3×3 *tables under independence model with all cells bounded. We assume row and column sums are positive. We have studied in which* $\mathcal{X}_0$ *the standard Markov basis for* 3×3 *tables, i.e., the set of the 9 moves of the form* $\begin{pmatrix} +1 & -1 \\ -1 & +1 \end{pmatrix}$ *for all* $2{\times}2$ *minors of the table, connects these bounded tables with positive conditions. If* $|\mathcal{X}_0| = 1$ *or* $|\mathcal{X}_0| = 2$ *then Equation in* (15) *holds. Thus, these 9 moves connect bounded tables. For* $|\mathcal{X}_0| = 3$*, if* $\mathcal{X}_0 = \{(1, 1), (2, 2), (3, 3)\}$ *after an appropriate interchange of rows and columns, i.e. there are 6 patterns of* $\mathcal{X}_0$*, then Equation in* (15) *does not hold. Otherwise for other patterns of* $\mathcal{X}_0$*, Equation in* (15) *holds. Thus, 9 moves connect bounded tables. For* $|\mathcal{X}_0| > 3$*, if* $\mathcal{X}_0$ *contains* $\{(1, 1), (2, 2), (3, 3)\}$ *after appropriate interchange of rows and columns, then Equation in* (15) *does not hold. Otherwise for other patterns of* S*, Equation in* (15) *holds. Thus, these 9 moves connect bounded tables. Even with the positive margin assumption, if* $\mathcal{X}_0 = \{(1, 1), (2, 2), (3, 3)\}$*, then the basic moves do not connect incomplete contingency tables, i.e., we need the Universal Markov basis.*

Example 9. *We also consider* 4×4 *tables under independence model with all cells bounded. We assume row and column sums are positive. After an appropriate interchange of rows and columns, if we have structural zero constraints on all diagonal cells (i.e., cells with indices in* $\mathcal{X}_0 = \{(i, j) : i = j \text{ for } i = 1, \dots, I\}$*), then Equation in* (15) *does not hold.*

Now we consider $I \times J$ contingency tables with only diagonal elements being structural zeros under assumption of positive conditions on row and column sums. Aoki and Takemura (2005) showed the following propositions.

Proposition 3. *Suppose we have $I \times J$ tables with fixed row and column sums. A set of basic moves is a Markov subbasis for $I \times J$ contingency tables, $I, \ J \geq 4$, with structural zeros in only diagonal elements under the assumption of positive marginals.*

From Examples 8, 9, and Proposition 3, we have the following open problem.

Problem 1. *Suppose we have $I \times J$ tables with fixed row and column sums. What is the necessary and sufficient condition on $\mathcal{X}_0$ so that a set of basic moves is a Markov subbasis for $I \times J$ contingency tables with structural zeros in $\mathcal{X}_0$ under the assumption of positive marginals.*

6 Discussions

In this paper we have studied Markov bases and Markov subbases for bounded contingency tables, showing many ways to compute them. While Theorem 1 applies to incomplete tables, Theorem 3 considers bounded tables with positive bounds. In particular, Theorem 3 shows that considering two-way tables under independence model for bounded tables with strictly positive bounds, then the set of basic moves, which is much smaller than the Universal Markov basis, connects the fibers with given margins. Thus, in practice we do not need to compute the Universal Markov basis.

In order to prove Problem 1 we may be able to apply Theorem 2 and mimic the proof for Theorem 3. If we can solve Problem 1 this would be very useful in practice because we know exactly when we only need the set of basic moves of all 2×2 minors for two-way incomplete contingency tables.

Acknowledgements

The authors thank Ian Dinwoodie (Duke University, Durham, NC) for computational help and Akimichi Takemura (University of Tokyo, Japan) for suggesting some of references. Also we would like to thank Seth Sullivant for useful comments to improve this paper.

References

4ti2 team (2008). 4ti2—a software package for algebraic, geometric and combinatorial problems on linear spaces. Available at www.4ti2.de.

Agresti, A. (2002). *Categorical Data Analysis*. John Wiley and Sons, 2nd ed.

Aoki, S. and Takemura, A. (2005). Markov chain Monte Carlo exact tests for incomplete two-way contingency table. *J. Stat. Comput. Simul.*, *75*(10), 787–812.

Aoki, S. and Takemura, A. (2006). Markov chain Monte Carlo tests for designed experiments. arXiv:math/0611463.

Aoki, S. and Takemura, A. (2008). The largest group of invariance for Markov bases and toric ideals. *J. Symb. Comput.*, *43*(5), 342–358.

Bigatti, A., La Scala, R., and Robbiano, L. (1999). Computing toric ideals. *J. Symb. Comput.*, *27*(4), 351–365.

Chen, Y., Dinwoodie, I., Dobra, A., and Huber, M. (2005). Lattice points, contingency tables, and sampling. In *Integer points in polyhedra—geometry, number theory, algebra, optimization*, Providence, RI: Amer. Math. Soc., vol. 374 of *Contemp. Math.*. 65–78.

Chen, Y., Dinwoodie, I. H., and Sullivant, S. (2006). Sequential importance sampling for multiway tables. *Ann. Statist.*, *34*(1), 523–545.

Chen, Y., Dinwoodie, I. H., and Yoshida, R. (2009). Markov chains, quotient ideals, and connectivity with positive margins. In P. Gibilisco, E. Riccomagno, and M. P. Rogantin (Eds.), *Algebraic and Geometric Methods in Statistics*, Cambridge University Press. 101 – 112.

CoCoATeam (2007). CoCoA: a system for doing Computations in Commutative Algebra. Available at `http://cocoa.dima.unige.it`.

Cox, D., Little, J., and O'Shea, D. (1992). *Ideals, Varieties, and Algorithms*. New York: Springer Verlag.

Cryan, M., Dyer, M., and Randall, D. (2005). Approximately counting integral flows and cell-bounded contingency tables. In *Proc. STOC'05*. Baltimore, Maryland, USA, 413–422.

De Loera, J. and Onn, S. (2005). Markov bases of three-way tables are arbitrarily complicated. *J. Symb. Comput.*, *41*(2), 173–181.

Diaconis, P. and Sturmfels, B. (1998). Algebraic algorithms for sampling from conditional distributions. *Ann. Statist.*, *26*(1), 363–397.

Greuel, G.-M., Pfister, G., and Schönemann, H. (2009). Singular 3.1.0 — A computer algebra system for polynomial computations. Http://www.singular.uni-kl.de.

Hara, H., Takemura, A., and Yoshida, R. (2008). On connectivity of fibers with positive marginals in multiple logistic regression. arXiv:0810.1793.

Pistone, G., Riccomagno, E., and Wynn, H. P. (2001). *Algebraic Statistics: Computational Commutative Algebra in Statistics*. Boca Raton: Chapman&Hall/CRC.

Rapallo, F. (2006). Markov bases and structural zeros. *J. Symb. Comput.*, *41*(2), 164–172.

Rapallo, F. and Rogantin, M. P. (2007). Markov chains on the reference set of contingency tables with upper bounds. *Metron*, *65*(1).

Shao, J. (1998). *Mathematical Statistics*. New York: Springer Verlag.

Sturmfels, B. (1996). *Gröbner bases and convex polytopes*, vol. 8 of *University lecture series (Providence, R.I.)*. American Mathematical Society.

Sturmfels, B. (2002). *Solving systems of polynomial equations*, vol. 97 of *CBMS Regional Conference Series in Mathematics*. Published for the Conference Board of the Mathematical Sciences, Washington, DC.