

A Finiteness Theorem for Markov Bases of Hierarchical Models

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Abstract

We show that the complexity of the Markov bases of multidimensional tables stabilizes eventually if a single table dimension is allowed to vary. In particular, if this table dimension is greater than a computable bound, the Markov bases consist of elements from Markov bases of smaller tables. We give an explicit formula for this bound in terms of Graver bases. We also compute these Markov and Graver complexities for all $K \times 2 \times 2 \times 2$ tables.

1 Introduction

Let d_1, \dots, d_n be positive integers where $d_i \geq 2$. A multidimensional contingency table is an $d_1 \times \dots \times d_n$ array of nonnegative integers. Such a table represents the results of a census of individuals for which n discrete random variables X_1, \dots, X_n are observed (where we assume the random variable X_i takes values in $[d_i] := \{1, \dots, d_i\}$). Inferences about the collected data are made based on a statistical model or collection of models. This paper is concerned with the family of *hierarchical log-linear models* for which one assumes a set of interaction factors between the random variables [8]. Performing the exact test of conditional inference requires knowledge of the Markov basis of a given hierarchical model, which we describe below.

When we assume that the sampling distribution of a table of observations is Poisson or multinomial, the sufficient statistics of any hierarchical model are given by certain marginal totals. The particular marginal totals that are sufficient statistics depend on the hierarchical model. For instance, for a $d_1 \times d_2 \times d_3$ contingency table, the *no three-way interaction model* has sufficient statistics that are the three 2-way margins of the table:

$$u_{+jk} = \sum_{i=1}^{d_1} u_{ijk}, \quad u_{i+k} = \sum_{j=1}^{d_2} u_{ijk}, \quad u_{ij+} = \sum_{k=1}^{d_3} u_{ijk},$$

where u_{ijk} are the entries of the table.

In general, a hierarchical model (and hence the marginal totals) is described by the list of the maximal faces F_1, \dots, F_r of a simplicial complex Δ on n vertices. Computing marginal totals corresponds to a linear map from the space of tables to the space of marginals:

$$\pi_{\Delta} : \mathbb{N}^D \longrightarrow \bigoplus_{k=1}^r \mathbb{N}^{D_k}$$

where $D = \prod_{i=1}^n d_i$ and $D_k = \prod_{j \in F_k} d_j$. This map is defined by

$$(u_{i_1, \dots, i_n} : i_j \in [d_j]) \longrightarrow \bigoplus_{k=1}^r \sum_{(i_j : j \notin F_k)} u_{i_1, \dots, i_n}.$$

Two tables \mathbf{t} and \mathbf{u} are said to be in the same *fiber* of π_{Δ} if $\pi_{\Delta}(\mathbf{t}) = \pi_{\Delta}(\mathbf{u})$. In other words, two tables are in the same fiber if they have the same margins with respect to Δ . We say that \mathbf{t} and \mathbf{u} are connected by the sequence of *moves* $\mathbf{v}_1, \dots, \mathbf{v}_s$ if each move \mathbf{v}_i is in $\ker_{\mathbb{Z}}(\pi_{\Delta})$ (that is, \mathbf{v}_i has zero margins), $\mathbf{t} + \sum_{i=1}^p \mathbf{v}_i$ is a table with nonnegative entries for each $1 \leq p \leq s$, and $\mathbf{u} = \mathbf{t} + \sum_{i=1}^s \mathbf{v}_i$.

By a theorem of Diaconis and Sturmfels [4, Theorem 3.1], for each hierarchical model given by Δ and $d = (d_1, \dots, d_n)$, there exists a finite set of moves called a *Markov basis* such that any two tables that are in the same fiber of π_{Δ} are connected by the moves in the Markov basis. Computing Markov bases via *Gröbner bases* for the use in MCMC methods was initiated in [4], and since this first work computing Markov bases efficiently and describing Markov bases succinctly have been the major focuses of research. Recently substantial progress has been made. Simple Markov bases (consisting of moves with four nonzero entries) for *decomposable models* have been determined [5], and similar Markov bases are known for *reducible models* [6, 9]. The case of *binary graph models* (where $d_1 = \dots = d_n = 2$ and Δ is a graph on n vertices) is worked out up to $n = 5$ [3].

The contribution of this paper is the most general form of a result first obtained in [1] for the no three-way interaction model for $K \times 3 \times 3$ tables. Our main theorem and its proof rely on ideas from [10] which treats the case of $K \times d_2 \times \dots \times d_n$ tables where $\{2, 3, \dots, n\}$ is a maximal face of Δ —the so-called *logit models*.

Theorem 1.1. *Let Δ and $d = (d_1, \dots, d_n)$ define a hierarchical model. Then there exists a constant $m := m(\Delta; d_2, \dots, d_n)$ such that for all $d_1 \geq m$ the universal Markov basis $\mathcal{M}_{\Delta, d}$ consists of tables of the format $r \times d_2 \times \dots \times d_n$ where $r \leq m$.*

In other words, if we fix a hierarchical model together with the $n - 1$ dimensions d_2, \dots, d_n while varying the single dimension d_1 , then for large enough d_1 the universal Markov basis $\mathcal{M}_{\Delta, d}$ will be obtained from Markov bases of small fixed-size tables; see Definition 3.1. In particular, as a function of d_1 , the complexity of computing and storing a Markov basis is bounded.

We give the details of the proof of Theorem 1.1 in Sections 2 and 3, where we give an explicit computable upper bound for $m(\Delta; d_2, \dots, d_n)$. We also present, in Section 3, a lower bound for $m(\Delta; d_2, \dots, d_n)$ which only applies in some cases. In the fourth section, we consider strengthenings and generalizations of the main result when more than one level is allowed to vary. In the final section we explicitly compute the complexity bound $m(\Delta; 2, 2, 2)$ for all tables of the form $K \times 2 \times 2 \times 2$.

2 From Models to Matrices

In this section we describe how to obtain a matrix A_Δ corresponding to the linear transformation π_Δ where the simplicial complex Δ describes a hierarchical model. We describe a decomposition for A_Δ that is fundamental to the proof of Theorem 1.1.

Given the vector $d = (d_1, \dots, d_n)$, and a subset $F = \{j_1 < \dots < j_s\} \subseteq [n]$ we let $d_F = (d_{j_1}, d_{j_2}, \dots, d_{j_s})$. The columns of A_Δ are in bijection with the D entries of a $d_1 \times \dots \times d_n$ table, and we label each such column with the vector indexing the table entry $(i_1, \dots, i_n) \in [d_1] \times \dots \times [d_n]$. Moreover, we order these columns lexicographically:

$$(1, 1, \dots, 1, 1) \prec (1, 1, \dots, 1, 2) \prec \dots \prec (1, 1, \dots, 1, d_n) \prec$$

$$(1, 1, \dots, 2, 1) \prec (1, 1, \dots, 2, 2) \prec \dots \prec (1, 1, \dots, 2, d_n) \prec \dots$$

$$(d_1, d_2, \dots, d_{n-1}, 1) \prec (d_1, d_2, \dots, d_{n-1}, 2) \prec \dots \prec (d_1, d_2, \dots, d_{n-1}, d_n).$$

Each row is labeled by a pair (F, e) where $F = \{j_1, j_2, \dots, j_s\}$ is a facet of Δ and $e = (e_{j_1}, e_{j_2}, \dots, e_{j_s}) \in [d_{j_1}] \times [d_{j_2}] \times \dots \times [d_{j_s}]$ indexing the marginal corresponding to F . We first list the rows (F, e) where $1 \in F$. We impose a linear order on the facets where $1 \in F$ and set $(F, e) \prec (G, f)$ if $e_1 < f_1$, or if $e_1 = f_1$ and $F \prec G$, and in the case when $e_1 = f_1$ and $F = G$ we use an arbitrary but fixed order of the indices. The rest of the rows will be listed again by some arbitrary but fixed order which will not play a role for the rest of the article. The entry of A_Δ in the column indexed by (i_1, \dots, i_n) and the row $(F = \{j_1, \dots, j_s\}, (e_{j_1}, \dots, e_{j_s}))$ will be equal to one if $i_{j_1} = e_{j_1}$, $i_{j_2} = e_{j_2}, \dots$, and $i_{j_s} = e_{j_s}$; and it will be zero otherwise.

Example 2.1. Let $\Delta = \{\{1, 2\}, \{1, 4\}, \{2, 3\}, \{3, 4\}\}$ and $d_1 = d_2 = d_3 = d_4 = 2$. This is the binary 4-cycle model.

$$A_\Delta = \begin{array}{c} \left[\begin{array}{cccccccc|cccccccc} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ \hline 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{array} \right] \end{array}$$

Here the 16 columns are indexed as $(1, 1, 1, 1) \prec (1, 1, 1, 2) \prec (1, 1, 2, 1) \prec (1, 1, 2, 2) \prec \dots \prec (2, 2, 2, 1) \prec (2, 2, 2, 2)$. The first four rows are indexed by $(F_1, (1, 1)), (F_1, (1, 2)), (F_2, (1, 1)),$ and $(F_2, (1, 2))$ where $F_1 = \{1, 2\}$ and $F_2 = \{1, 4\}$. The second block of four rows are indexed by $(F_1, (2, 1)), (F_1, (2, 2)), (F_2, (2, 1)),$ and $(F_2, (2, 2))$. For the rest of the rows we have chosen the order $(F, (i, j)) \prec (G, (s, t))$ if $F = \{2, 3\}$ and $G = \{3, 4\}$, or if $F = G$ and $(i, j) \prec (s, t)$ lexicographically.

We observe that when the rows and columns are ordered as described, the matrix A_Δ exhibits a block structure. In the above example, the upper-left and lower-right blocks of the first eight rows are identical augmented with the two blocks of zeros. And the last eight rows are split into two identical matrices. We summarize this observation in the following lemma where we assume the ordering of the columns and rows of A_Δ that we introduced above.

Lemma 2.2. *Let $\Delta = \{F_1, \dots, F_r\}$ and $d = (d_1, \dots, d_n)$ define a hierarchical model. Then*

$$A_\Delta = \begin{bmatrix} A & 0 & 0 & \cdots & 0 \\ 0 & A & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & A \\ B & B & B & \cdots & B \end{bmatrix}$$

where A is a $\sum_{k=1}^s (D_k/d_1) \times (D/d_1)$ matrix with F_1, \dots, F_s being the facets containing the vertex 1, and where B is a $\sum_{k=s+1}^r D_k \times (D/d_1)$ matrix. Hence there are d_1 copies of A and B .

Remark. The matrices A and B are also matrices that come from hierarchical models. Note that the matrix A is the matrix A_Γ for the simplicial complex

$$\Gamma = \text{link}(\Delta) := \text{link}(\Delta, \{1\}) = \{F \setminus \{1\} \mid F \in \Delta \text{ and } 1 \in F\}$$

and the vector $d' = (2, 3, \dots, n)$. The matrix B is the matrix $A_{\Delta \setminus \{1\}}$ for the simplicial complex

$$\Delta \setminus \{1\} = \{F \mid F \in \Delta, 1 \notin F, \text{ and } F \text{ is a facet}\}.$$

3 Proof of the Finiteness Theorem

In this section, we proceed with the proof of Theorem 1.1. To do this, we will prove a finiteness theorem for the Markov bases of arbitrary matrices which come in a block form akin to the one demonstrated in Lemma 2.2.

Definition 3.1. Let $A \in \mathbb{N}^{d \times n}$ be an integer matrix with no zero columns. A finite set $\mathcal{M} \subset \ker_{\mathbb{Z}}(A)$ of integer vectors in the kernel of A is called a *Markov basis* of A if any two nonnegative integer vectors in the same fiber of A can be connected by a collection of the elements in \mathcal{M} . That is, for any $\mathbf{t}, \mathbf{u} \in \mathbb{N}^n$ with $A\mathbf{t} = A\mathbf{u}$, there exists a sequence of moves $\{\mathbf{v}_i\}_{i=1}^s \subset \mathcal{M}$ such that

$$\mathbf{t} + \sum_{i=1}^p \mathbf{v}_i \geq 0 \quad \text{for all } 1 \leq p \leq s \quad \text{and} \quad \mathbf{t} + \sum_{i=1}^s \mathbf{v}_i = \mathbf{u}.$$

A Markov basis \mathcal{M} of A is called *minimal* if no subset of \mathcal{M} is a Markov basis of A . The *universal Markov basis* $\mathcal{M}(A)$ of A is the union of all minimal Markov bases of A .

When $A = A_\Delta$ is the matrix associated to a hierarchical model, we use the shorthand $\mathcal{M}_{\Delta, d}$ to denote the universal Markov basis of A_Δ .

Definition 3.2. Let \mathbf{u}, \mathbf{v} , and \mathbf{v}' be nonzero vectors in $\ker_{\mathbb{Z}}(A)$. We say $\mathbf{u} = \mathbf{v} + \mathbf{v}'$ is a *conformal decomposition* of \mathbf{u} if $u_i \geq 0$ implies $0 \leq v_i, v'_i \leq u_i$, and $u_i \leq 0$ implies $u_i \leq v_i, v'_i \leq 0$ for all $1 \leq i \leq n$. The set $\mathcal{G}(A) \subset \ker_{\mathbb{Z}}(A)$ of integer vectors with no conformal decompositions is called the *Graver basis* of A .

One can show that $\mathcal{G}(A)$ is a finite set [11, Chapter 4] and any minimal Markov basis of A is a subset of $\mathcal{G}(A)$ [11, Chapter 5]. Thus, $\mathcal{M}(A)$ is a finite set.

Definition 3.3. Let A be a $d \times n$ matrix with columns a_1, \dots, a_n and B be a $p \times n$ matrix with columns b_1, \dots, b_n . The *r-th generalized Lawrence*

lifting of A with B is the $(rd + p) \times rn$ matrix $\Lambda(A, B, r)$, whose columns are the vectors

$$\Lambda(A, B, r) = \{a_i \otimes e_j \oplus b_i \mid 1 \leq i \leq n, 1 \leq j \leq r\}.$$

In particular, the matrices A_Δ are of the form $\Lambda(A, B, r)$ with $A = A_{\text{link}(\Delta)}$, $B = A_{\Delta \setminus \{1\}}$ and $r = d_1$. When B is the $n \times n$ identity matrix and $r = 2$, the matrix $\Lambda(A, B, r)$ is called the *Lawrence lifting* of A [11, Chapter 7]. For $B = I_n$ but general r , this matrix is called the r th Lawrence lifting of A [10].

Remark. An integer vector in the kernel of $\Lambda(A, B, r)$ can be represented as an $r \times n$ matrix where each row is in the kernel of A , and the sum of the rows is in the kernel of B . For instance, the following 2×8 matrix is the representation of such a vector in the kernel of A_Δ in Example 2.1:

$$\begin{bmatrix} 2 & -2 & -1 & 1 & -2 & 2 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \end{bmatrix}.$$

Definition 3.4. The *type* of a vector in \mathbb{Z}^{rn} represented as an $r \times n$ matrix is the number of nonzero rows of this matrix. The *Markov complexity* $m(A, B)$ of a $d \times n$ matrix A and a $p \times n$ matrix B is the largest type of any vector in the universal Markov basis of $\Lambda(A, B, r)$ as r varies. Similarly, the *Graver complexity* $g(A, B)$ of these two matrices is defined as the largest type of any Graver basis element of $\Lambda(A, B, r)$ as r varies. Analogously, we define $g(\Delta; d_2, \dots, d_n)$ and $m(\Delta; d_2, \dots, d_n)$, the Graver and Markov complexities of the hierarchical models corresponding to Δ as d_1 varies.

We will show that the Graver complexity $g(A, B)$ is finite. This implies that the Markov complexity is also finite since $m(A, B) \leq g(A, B)$. In order to do this we relate the Graver basis $\mathcal{G}(B \cdot \mathcal{G}(A))$ to the collection of Graver bases $\mathcal{G}(\Lambda(A, B, r))$. We emphasize the “double” Graver construction: we first compute the Graver basis of A and obtain the set $\mathcal{G}(A)$. We consider each element in $\mathcal{G}(A)$ as a column vector. Then the vectors $B \cdot \mathcal{G}(A)$ are computed by multiplying each element of $\mathcal{G}(A)$ with B . Thus, $B \cdot \mathcal{G}(A)$ is a $p \times |\mathcal{G}(A)|$ matrix. Finally we compute the Graver basis of $B \cdot \mathcal{G}(A)$.

Theorem 3.5. *The Graver complexity $g(A, B)$ is the maximum 1-norm of any element in the Graver basis $\mathcal{G}(B \cdot \mathcal{G}(A))$.*

In order to prove the above theorem we need the following lemma.

Lemma 3.6. *Let $\mathbf{u} = [u^1; u^2; \dots; u^r]$ be in the Graver basis of $\Lambda(A, B, r)$. Suppose that $u^i = v^1 + v^2$ is a conformal decomposition where v^1 and v^2 are in the kernel of A . Then the element $[u^1; \dots; u^{i-1}; v^1; v^2; u^{i+1}; \dots; u^r]$ is in the Graver basis of $\Lambda(A, B, r + 1)$.*

Proof. Suppose not. Then $[u^1; \dots; u^{i-1}; v^1; v^2; u^{i+1}; \dots; u^r]$ has a conformal decomposition

$$[\bar{u}^1; \dots; \bar{u}^{i-1}; \bar{v}^1; \bar{v}^2; \bar{u}^{i+1}; \dots; \bar{u}^r] + [\hat{u}^1; \dots; \hat{u}^{i-1}; \hat{v}^1; \hat{v}^2; \hat{u}^{i+1}; \dots; \hat{u}^r]$$

where both vectors are in the kernel of $\Lambda(A, B, r + 1)$. Now since $u^i = v^1 + v^2 = (\bar{v}^1 + \hat{v}^1) + (\bar{v}^2 + \hat{v}^2)$ is a conformal decomposition of u^i , so is $(\bar{v}^1 + \bar{v}^2) + (\hat{v}^1 + \hat{v}^2)$. We note that neither the first nor the second sum is zero. But then the two nonzero vectors $[\bar{u}^1; \dots; \bar{u}^{i-1}; \bar{v}^1 + \bar{v}^2; \bar{u}^{i+1}; \dots; \bar{u}^r]$ and $[\hat{u}^1; \dots; \hat{u}^{i-1}; \hat{v}^1 + \hat{v}^2; \hat{u}^{i+1}; \dots; \hat{u}^r]$ are in the kernel of $\Lambda(A, B, r)$, and their sum forms a conformal decomposition of \mathbf{u} . This is a contradiction since \mathbf{u} is in the Graver basis of $\Lambda(A, B, r)$. \square

Proof of Theorem 3.5: Lemma 3.6 implies that in order to compute the Graver complexity $g(A, B)$ we only need to consider elements $\mathbf{u} = [u^1; \dots; u^r]$ where u^i is in the Graver basis $\mathcal{G}(A) = \{v_1, \dots, v_k\}$. Given any such \mathbf{u} , we construct a vector $\Gamma \in \mathbb{Z}^k$ where the i th entry counts how many times v_i appears in \mathbf{u} . The 1-norm of Γ is the type of \mathbf{u} . Hence we need to show that Γ is in the Graver basis of $B \cdot \mathcal{G}(A)$ if and only if \mathbf{u} is in the Graver basis of $\Lambda(A, B, r)$. If Γ is not in the Graver basis of $B \cdot \mathcal{G}(A)$, then it has a conformal decomposition $\Gamma_1 + \Gamma_2$ such that $B \cdot \mathcal{G}(A) \cdot \Gamma_i = 0$ for $i = 1, 2$. Reversing the operation that produced Γ from \mathbf{u} , Γ_1 and Γ_2 yield vectors $\mathbf{v}_1, \mathbf{v}_2 \in \ker_{\mathbb{Z}}(\Gamma(A, B, r))$ such that $\mathbf{u} = \mathbf{v}_1 + \mathbf{v}_2$ and this decomposition is conformal. Thus \mathbf{u} could not be in the Graver basis of $\Lambda(A, B, r)$.

Conversely, a conformal decomposition of \mathbf{u} translates into a conformal decomposition of Γ since none of $u^1, \dots, u^r \in \mathcal{G}(A)$ have conformal decompositions. \square

Proof of Theorem 1.1: The hierarchical model defined by Δ and d gives rise to A_{Δ} which is of the form $\Lambda(A_{\text{link}(\Delta)}, A_{\Delta \setminus \{1\}}, d_1)$ by Lemma 2.2. Theorem 3.5 implies that the Markov complexity $m(A_{\text{link}(\Delta)}, A_{\Delta \setminus \{1\}})$ is bounded by the finite Graver complexity $g(A_{\text{link}(\Delta)}, A_{\Delta \setminus \{1\}})$. This means that for all $d_1 \geq m(A_{\text{link}(\Delta)}, A_{\Delta \setminus \{1\}})$ the universal Markov basis $\mathcal{M}_{\Delta, d}$ will consist of tables of the format $r \times d_2 \times \dots \times d_n$ where $r \leq m(A_{\text{link}(\Delta)}, A_{\Delta \setminus \{1\}})$. \square

In practice, the Graver complexity and the Markov complexity may vary a lot, as the following examples illustrate. All of our examples were computed using `4ti2` [7] and the results for Markov bases of reducible models using [6, 9].

Example 3.7. Let $\Delta = \{\{1, 2\}, \{1, 3\}, \{2, 3\}\}$. Then for $d_2 = d_3 = 3$, the Markov complexity is $m(\Delta; 3, 3) = 5$ (the main result in [1]), while the Graver complexity is $g(\Delta; 3, 3) = 9$.

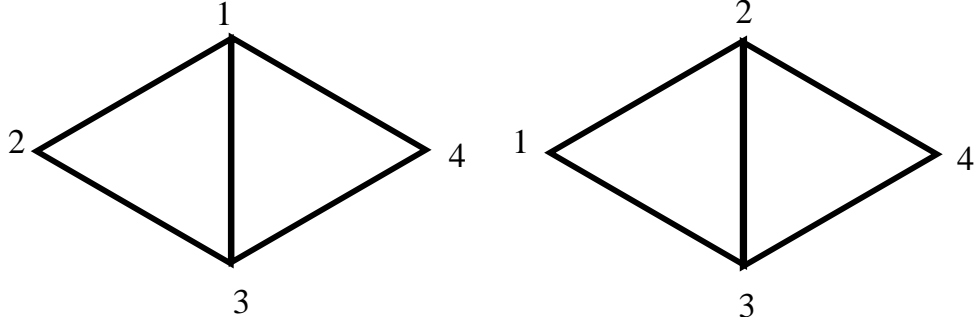


Figure 1: Renaming the vertices in Δ can change the Markov complexity

Example 3.8. Let $\Delta = \{\{1, 2\}, \{1, 3\}, \{1, 4\}, \{2, 3\}, \{3, 4\}\}$. Then for $d_2 = d_3 = d_4 = 2$ the Markov complexity is $m(\Delta; 2, 2, 2) = 2$ while $g(\Delta; 2, 2, 2) = 4$. On the other hand, for the same complex in a different orientation (see Figure 1) $\Delta' = \{\{1, 2\}, \{1, 3\}, \{2, 3\}, \{2, 4\}, \{3, 4\}\}$ and $d_2 = d_3 = d_4 = 2$, the Markov complexity is $m(\Delta'; 2, 2, 2) = 4$ while $g(\Delta'; 2, 2, 2) = 16$.

The Graver complexity $g(A, B)$ gives an upper bound for the Markov complexity $m(A, B)$, in terms of the Graver basis of B times the Graver basis of A . There is an analogous lower bound for the Markov complexity in terms of the Graver basis of B times the Markov basis of A . To describe this lower bound, we introduce the notion of semiconformal decompositions.

Definition 3.9. Let \mathbf{u} , \mathbf{v} , and \mathbf{v}' be nonzero vectors in $\ker_{\mathbb{Z}}(A)$. We say that $\mathbf{u} = \mathbf{v} + \mathbf{v}'$ is a *semi-conformal decomposition* if $v_i > 0$ implies that $v_i \leq u_i$ and $v'_i < 0$ implies $u_i \leq v'_i$ for all $1 \leq i \leq n$. Note that if the first condition holds ($v_i > 0$ implies that $v_i \leq u_i$ for all i) the second condition ($v'_i < 0$ implies $u_i \leq v'_i$ for all i) is satisfied automatically. The set $\mathcal{S}(A) \subset \ker_{\mathbb{Z}}(A)$ is the set of vectors in $\ker_{\mathbb{Z}}(A)$ which have no semi-conformal decomposition.

A useful fact about vectors in the kernel of a matrix which have no semi-conformal decomposition is that they must belong to the Markov basis.

Lemma 3.10. *Let $A \in \mathbb{N}^{d \times n}$ with no zero columns. If \mathcal{M} is any Markov basis of A , then $\mathcal{S}(A) \subseteq \mathcal{M}$. In particular, $\mathcal{S}(A) \subseteq \mathcal{M}(A)$.*

Proof. Suppose that $\mathbf{u} \in \mathcal{S}(A)$ has no semiconformal decomposition but there is some Markov basis \mathcal{M} of A that does not contain \mathbf{u} . Write $\mathbf{u} = \mathbf{u}^+ - \mathbf{u}^-$ as the difference of two nonnegative integer vectors with disjoint support. Note that \mathbf{u}^+ and \mathbf{u}^- belong to the same fiber. Since \mathcal{M} is a Markov basis for A there is a sequence of elements from \mathcal{M} , $\{\mathbf{v}^1, \mathbf{v}^2, \dots, \mathbf{v}^s\}$

with $s \geq 2$ which connects \mathbf{u}^- to \mathbf{u}^+ where intermediate summands are always nonnegative. In other words, we can write

$$\mathbf{u}^+ = \mathbf{u}^- + \sum_{k=1}^s \mathbf{v}^k,$$

and the set of indices where \mathbf{v}^1 is negative is a subset of the set of indices where \mathbf{u}^- is nonzero, and $u_i^- \geq |v_i^1|$ for this subset of indices. But this implies that

$$\mathbf{u} = \mathbf{v}^1 + \sum_{k=2}^s \mathbf{v}^k$$

is a semiconformal decomposition of \mathbf{u} . This contradicts our assumption that $\mathbf{u} \in \mathcal{S}(A)$ and hence $\mathbf{u} \in \mathcal{M}$. \square

Theorem 3.11. *The Markov complexity $m(A, B)$ is bounded below by the maximum 1-norm of any element in the Graver basis $\mathcal{G}(B \cdot \mathcal{S}(A))$.*

Proof. Let $\Gamma \in \mathcal{G}(B \cdot \mathcal{S}(A))$. Following the proof of Theorem 3.5, Γ translates into a vector $\mathbf{u} = [u^1; \dots; u^r]$ with each $u^i \in \mathcal{S}(A)$. Furthermore, we know that \mathbf{u} lies in the Graver basis of $\Lambda(A, B, r)$. We wish to show that it lies in some minimal Markov basis of $\Lambda(A, B, r)$. To do this, we show that \mathbf{u} has no semiconformal decompositions. Suppose, to the contrary that there was some semiconformal decomposition of \mathbf{u} . Since \mathbf{u} is in the Graver basis of $\Lambda(A, B, r)$, any semiconformal decomposition $\mathbf{u} = \mathbf{v} + \mathbf{v}'$ induces a semiconformal decomposition of (at least) one of the vectors u^i . However, this is a contradiction, because $\mathcal{S}(A)$ consists of vectors with no semiconformal decompositions. Thus r , which is the 1-norm of Γ is a lower bound for the Markov complexity $m(A, B)$. \square

Example 3.12. Applying Theorem 3.11 for the simplicial complex $\Delta = \{\{1, 2\}, \{1, 3\}, \{2, 3\}\}$ we have $m(\Delta; 3, 3) \geq 5$, $m(\Delta; 3, 4) \geq 8$, and $m(\Delta; 3, 5) \geq 12$. It is interesting to note that in the first two of these cases our lower bound for the Markov complexity is equal to the value reported in [1, 2]. The Markov complexity $M(\Delta; 3, 5)$ remains undetermined.

4 Generalizations and Extensions

Given Theorem 1.1, it is natural to ask to what extent this result is the best possible. In particular, do there exist any bounds on the complexity of Markov basis elements if we fix Δ and allow d_1 and d_2 to vary? The answer to this question is negative if we allow arbitrary Δ .

Example 4.1. Let $\Delta = \{\{1, 2\}, \{1, 3\}, \{2, 3\}\}$ and fix $d_3 \geq 2$. There are no bounds m_1 and m_2 such that every Markov basis element has format strictly contained in a $m_1 \times m_2 \times d_3$ table. A well-known example of such a move of large format is shown in [4]. Denote by e_{ijk} the 3-way table with a 1 in the (i, j, k) position and zeroes elsewhere. For each $m > 1$ the vector

$$\begin{aligned} \mathbf{u} = & e_{111} + e_{221} + \cdots + e_{mm1} \\ & + e_{122} + e_{232} + \cdots + e_{m-1m2} + e_{m12} \\ & - e_{112} - e_{222} - \cdots - e_{mm2} \\ & - e_{121} - e_{231} - \cdots - e_{m-1m1} - e_{m11} \end{aligned}$$

belongs to the universal Markov basis $\mathcal{M}(A_\Delta)$ that has format $m \times m \times 2$.

On the other hand, for reducible models, we can prove more general finiteness results. These are based on the structural theorems for building Markov bases for reducible models in [6, 9]. Recall that for a simplicial complex Δ , $|\Delta| = \cup_{F \in \Delta} F$ is the underlying set of Δ .

Definition 4.2. A simplicial complex Δ is called *reducible* with decomposition (Δ_1, S, Δ_2) , if $S \in \Delta_1$, $S \in \Delta_2$, $|\Delta_1| \cap |\Delta_2| = S$, and $\Delta = \Delta_1 \cup \Delta_2$.

If Δ is reducible we use the notation d^1 and d^2 to denote the substrings of d that are indexed by $|\Delta_1|$ and $|\Delta_2|$ respectively.

Example 4.3. The simplicial complex $\Delta = \{\{1, 2\}, \{1, 3\}, \{2, 3\}, \{2, 4\}, \{3, 4\}\}$ pictured in Figure 1 is reducible with $S = \{2, 3\}$, $\Delta_1 = \{\{1, 2\}, \{1, 3\}, \{2, 3\}\}$, and $\Delta_2 = \{\{2, 3\}, \{2, 4\}, \{3, 4\}\}$. The vectors d^1 and d^2 are (d_1, d_2, d_3) and (d_2, d_3, d_4) , respectively.

One of the main results from [6, 9] is the constructive version of the following.

Theorem 4.4. *Let Δ be a reducible simplicial complex and let d be given. Let l_1 and l_2 be the maximum 1-norm of any element of $\mathcal{M}_{\Delta_1, d^1}$ and $\mathcal{M}_{\Delta_2, d^2}$, respectively. Then the maximum 1-norm of any element of $\mathcal{M}_{\Delta, d}$ is $\max\{4, l_1, l_2\}$.*

This allows us to deduce that reducible models have Markov bases of finite complexity as many levels vary.

Corollary 4.5. *Let Δ be a reducible simplicial complex with induced sub-complexes Δ_1 and Δ_2 and suppose that $1 \in |\Delta_1| \setminus |\Delta_2|$ and $2 \in |\Delta_2| \setminus |\Delta_1|$. Let d_3, \dots, d_n be given. Then there exists constants $(m_1, m_2) = m(\Delta; d_3, \dots, d_n)$ such that every element in the universal Markov basis $\mathcal{M}_{\Delta, d}$ has format smaller than $m_1 \times m_2 \times d_3 \times \cdots \times d_n$.*

Proof. Restricting to Δ_1 and Δ_2 and allowing d_1 and d_2 to vary respectively, we know by Theorem 1.1 there is a bound on the format of Markov basis elements that appear in $\mathcal{M}_{\Delta_1, d^1}$ and $\mathcal{M}_{\Delta_2, d^2}$. However, a bound on the format also implies that these vectors have bounded 1-norm (one such bound is the Markov complexity times the largest 1-norm of any element in $\mathcal{G}(A_{\text{link}(\Delta)})$). Applying Theorem 4.4, we deduce that every element of $\mathcal{M}_{\Delta, d}$ has 1-norm bounded by some fixed constant. But bounded 1-norm implies bounded format and completes the proof. \square

Besides the condition that Δ is reducible, the crucial requirement to prove the preceding corollary was that 1 and 2 were not adjacent to each other in Δ . We conjecture that this property is enough to guarantee bounded Markov complexity in general.

Conjecture 4.6. *Suppose that $\{1, 2, \dots, j\}$ is an independent subset of the underlying graph of Δ . Then for fixed d_{j+1}, \dots, d_n , there exists numbers $(m_1, \dots, m_j) = m(\Delta; d_{j+1}, \dots, d_n)$ such that every element in the universal Markov basis $\mathcal{M}_{\Delta, d}$ has format smaller than $m_1 \times \dots \times m_j \times d_{j+1} \times \dots \times d_n$.*

Unfortunately, we do not know if Conjecture 4.6 is true even in the simplest nonreducible case, namely the four-cycle $\Delta = \{\{1, 3\}, \{2, 3\}, \{2, 4\}, \{1, 4\}\}$ with $j = 2$. If a proof exists, it must depend on techniques different from those developed here, because if $j > 1$ and Δ satisfies the hypotheses of Conjecture 4.6 there is no bound on the formats of the Graver basis elements for A_Δ .

5 Computations

The following table displays computational results of the Markov complexity and Graver complexity of all binary hierarchical models where one of the dimensions of the tables is allowed to vary. In the notation of Theorem 1.1 this is the Markov complexity $m(\Delta; 2, 2, 2)$ and the Graver complexity $g(\Delta; 2, 2, 2)$. Note that all the entries which are marked with a star are Markov and Graver complexities which were not known, or could not have been determined, without the use of Theorem 1.1. All of the computations described in this section were performed using the toric Gröbner basis program `4ti2` [7]. The second and fifth column m correspond to the computed Markov complexity and the third and sixth column g is the Graver complexity. We use the bracket notation from multivariate statistics [8] for denoting simplicial complexes. Thus $[12][23][34]$ represents the simplicial complex $\{\{1, 2\}, \{2, 3\}, \{3, 4\}\}$.

Model	m	g	Model	m	g
[123][124][134][234]	2	2	[12][13][23][34]	2	10*
[123][124][134]	2	2	[12][13][23][14]	2	2*
[123][124][234]	2	2	[12][23][24][34]	4	8*
[123][124][34]	2	2	[12][14][23][34]	4*	5*
[123][234][14]	4	4	[123][4]	2	2
[123][14][24][34]	4*	4*	[234][1]	2	8
[234][12][13][14]		12*	[12][13][23][4]	2	8*
[12][13][14][23][24][34]		10*	[23][24][34][1]	4	16*
[123][124]	2	2	[12][23][34]	2	6*
[123][234]	2	2	[12][14][23]	2	4*
[123][24][34]	4	4*	[12][23][4]	2	6*
[234][12][13]	2	10*	[12][13][4]	2	3*
[123][14][24]	2	2*	[23][34][1]	2	14*
[12][13][23][24][34]	4	16*	[12][34]	2	4
[12][13][14][23][24]	2	4*	[12][3][4]	2	4*
[123][34]	2	2	[34][1][2]	2	12*
[123][14]	2	2	[1][2][3][4]	2	10*
[234][12]	2	4			

Finally, we used the Theorem 3.11 to compute some lower bounds for the Markov complexity.

$$m([12][13][23], 3, 5) \geq 12$$

$$m([12][13][23], 4, 4) \geq 16$$

$$m([123][124][134][234], 3, 3, 3) \geq 19$$

These lower bounds are benchmark values for extending the types of results pursued in [1] and [2] in which the values $m([12][13][23], 3, 3) = 5$ and $m([12][13][23], 3, 4) = 8$ were explicitly computed.

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