UNIMODULAR HIERARCHICAL MODELS  
AND THEIR GRAVER BASES

DANIEL IRVING BERNSTEIN AND CHRISTOPHER O’NEILL

Abstract. Given a simplicial complex whose vertices are labeled with positive integers, one can associate a vector configuration whose corresponding toric variety is the Zariski closure of a hierarchical model. We classify all the vertex-weighted simplicial complexes that give rise to unimodular vector configurations. We also provide a combinatorial characterization of their Graver bases.

1. Introduction

A hierarchical model consists of all joint probability distributions on discrete random variables $X_1, \ldots, X_n$ where each $X_i$ has $d_i$ states, and the $X_i$s satisfy certain interactions specified by a simplicial complex $C$. Geometrically, a hierarchical model can be viewed as the intersection of the probability simplex with a toric variety whose monomial parametrization matrix $A_{C,d}$ is determined by a simplicial complex $C$ with ground set $[n]$ and an integer vector $d \in \mathbb{Z}^n_{\geq 2}$. Since any hierarchical model is a discrete exponential family with design matrix $A_{C,d}$, it is important to study properties of the lattice $\ker \mathbb{Z} A_{C,d}$. For example, the goodness of fit of a hierarchical model specified by $(C,d)$ can be tested using a Markov basis of this lattice [9].

We are interested in properties of the matrix $A_{C,d}$ that are useful for computations in algebraic statistics. Perhaps the strongest property studied in this context is unimodularity, and this property is desirable for a number of reasons. When $A_{C,d}$ is unimodular, it is easy to solve the integer programs that arise when evaluating whether individual entries of a data table are secure [13] or when doing sequential importance sampling [8]. Additionally, Graver bases and Markov bases can be easily computed for unimodular matrices, and efficient generation of Markov basis elements is an important problem in algebraic statistics. For more about Markov bases and their uses, see the books [2][10][12].

It is also worth noting that when $A_{C,d}$ is unimodular, the semigroup spanned by its columns is saturated i.e. $A_{C,d}$ is normal. Normality was identified by Rauh and Sullivant as a key property of hierarchical models for applying the toric fiber product to construct Markov bases. There has been much recent work aiming to understand normality of $A_{C,d}$. Bruns, Hemmecke, Hibi, Ichim, Köppe, Ohsugi, and Söger classified which values of $d$ give rise to a normal $A_{C,d}$ when $C$ is the boundary of a simplex [7][11]. For binary hierarchical models (that is, when $d = 2$), Sullivant showed that when $C$ is a graph, $A_{C,d}$ is normal if and only if $C$ is free of $K_4$ minors [14]. Sullivant and the first author also classified all binary complexes $C$ on up to six vertices for which $A_{C,d}$ is normal [4]. Although several conditions ensuring the normality of $A_{C,d}$ have been identified, a complete characterization still seems out of reach.

Date: September 25, 2017.
The main contributions of this paper are twofold. First, we classify all unimodular hierarchical models (Theorem 4.3), extending the existing classification for unimodular binary hierarchical models [5]. Second, we give a combinatorial description of the Graver basis of any unimodular hierarchical model (Corollary 5.4), one that can be leveraged to obtain an algorithm for efficiently generating random Graver basis elements. In developing these results, we identify a new matrix operation which preserves unimodularity (Proposition 3.1). Similar operations, such as Lawrence lifts, have played a crucial role in identifying pairs \((C, d)\) that yield a normal or unimodular matrix \(A_{C,d}\).

2. Background

A simplicial complex \(C\) is a pair \((V, F)\) where \(V\) is a finite set and \(F\) is a set of subsets of \(V\) such that if \(G \subset F\) and \(F \in F\), then \(G \in F\). The set \(V\) is called the ground set of \(C\) and each \(F \in F\) is called a face of \(C\). Inclusion-wise maximal faces of \(C\) are called facets. We will use the notation ground\((C)\), face\((C)\) and facet\((C)\) to denote the ground set, faces and facets of a simplicial complex \(C\), respectively.

An HM pair is a pair \((C, d)\) where \(C\) is a simplicial complex on some ground set \(V\) and \(d \in \mathbb{Z}_{\geq 2}^V\) is an integer weighting of \(V\). Associated to each HM pair with ground set \([n]\) is a statistical model (i.e. a subset of a probability simplex) called a hierarchical model. It consists of the joint probability distributions on discrete random variables \(X_1, \ldots, X_n\) where each \(X_i\) has \(d_i\) states and the joint probabilities satisfy various relationships specified by \(C\). These relationships are given by polynomials which generate a toric ideal. The matrix defining the monomial parameterization of this toric ideal is denoted \(A_{C,d}\), whose construction we now describe.

Fix an HM pair \((C, d)\) with ground set \([n]\). Define \(d_F = [d_{i_1} - 1] \times \cdots \times [d_{i_k} - 1]\) for each nonempty face \(F = \{i_1, \ldots, i_k\}\) of \(C\), and define \(d_\emptyset = \{1\}\). Write \(\mathbb{R}^{d_F}\) for the vector space with coordinates indexed by \(j \in d_F\) (whose coordinates are in turn indexed by the vertices of \(F\)). For \(i \in [d_1] \times \cdots \times [d_n]\), define \(a^i \in \bigoplus_{F \in \text{face}(C)} \mathbb{R}^{d_F}\) such that

\[
a^i_{F,j} = \begin{cases} 1 & \text{whenever } F = \emptyset \text{ or } i_k = j_k \text{ for each } k \in F \\ 0 & \text{otherwise} \end{cases}
\]

and let \(A_{C,d}\) denote the matrix with columns \(a^i\) as \(i\) ranges over \([d_1] \times \cdots \times [d_n]\).

**Example 2.1.** The simplicial complex \(C\) with ground set \([3]\) and facets \([1, 2]\) and \([2, 3]\) has faces \(\emptyset, \{1\}, \{2\}, \{3\}, \{1, 2\}, \{2, 3\}\). The matrix \(A_{C,d}\) for \(d = (3, 2, 2)\) is displayed in Figure \(\text{II}\) with row and column labels. Note that \(d_F\) is a singleton unless \(F\) contains 1.

We pause to note that other definitions of the matrix \(A_{C,d}\) appear in the literature. However, they all share a common kernel over the integers, and thus define the same toric ideal and the same hierarchical model. The definition of \(A_{C,d}\) presented here has the added benefit of being full row-rank [14] Proposition 1].

Given an integer matrix \(A \in \mathbb{Z}^{d \times r}\), each integer vector in the integer kernel of \(A\) can be written as \(u = u^+ - u^-\) where \(u^+, u^-\) have disjoint support and nonnegative entries. The **Graver basis** of \(A\) is the set of all \(u \in \ker_{\mathbb{Z}} A\) such that there is no \(v \in \ker_{\mathbb{Z}} A\) with \(v \neq u\) and \(v^+ \leq u^+\) and \(v^- \leq u^-\). In other words, \(u\) cannot be expressed as a conformal sum of \(v, w \in \ker_{\mathbb{Z}} A\). If \(u \in \ker_{\mathbb{Z}} A\) has relatively prime entries and has minimal support
among elements of $\ker \mathbb{Z} A$, then we say that $u$ is a circuit of $A$. Equivalently, the entries of $u$ are relatively prime and the support of $u$ is a circuit in the matroid underlying the columns of $A$. It is easy to see that the set of circuits is a subset of the Graver basis. For unimodular matrices (definition below), the converse is true (Proposition 8.11 in [12]) but this fails in general.

**Definition 2.2.** A matrix $A \in \mathbb{Z}^{d \times n}$ is unimodular if the equivalent conditions below hold.

(a) Let $A'$ be any matrix obtained from $r := \text{rank } A$ linearly independent rows of $A$. Then there exists some $\lambda$ such that each $r \times r$ minor of $A'$ is $0$ or $\pm \lambda$.

(b) The Graver basis of $A$ contains only $\{0, 1, -1\}$-vectors.

(c) For any $b$ in the affine semigroup generated by the columns of $A$, the polyhedron $P_{A,b} = \{ x \in \mathbb{R}^s : Ax = b, x \geq 0 \}$ has all integral vertices.

See [5] for an explanation as to why the conditions in Definition 2.2 are equivalent. Definition 2.2 can be seen as a kernel-invariant generalization of the familiar definition of unimodularity for square integer matrices. Indeed, if $A$ is unimodular, then it is easy to construct a full-rank rational matrix $B$ such that $\ker \mathbb{Z} A = \ker \mathbb{Z} B$ and every full-rank square submatrix of $B$ has determinant $\pm 1$. To this end, Part (c) of Definition 2.2 implies that when $A$ is unimodular, integer programming problems over polyhedra $P_{A,b}$ can be solved via linear relaxation. Unimodularity (as in Definition 2.2) can also be viewed as a generalization of total unimodularity (which requires that every minor is either 0 or $\pm 1$). That said, unimodularity is an invariant of the kernel, rather than just an invariant of the matrix, and the same does not hold for total unimodularity.

Fix a simplicial complex $\mathcal{C}$ with ground set $V$ and some $v \in V$. We denote by $\mathcal{C} \setminus v$ the complex obtained by deleting $v$ from $V$ and each face of $\mathcal{C}$ containing $v$. The link of $\mathcal{C}$ about $v$, denoted $\text{link}_v(\mathcal{C})$, has ground set $V \setminus v$ and a face $F$ whenever $F \cup v$ is a face of $\mathcal{C}$. The Alexander dual of $\mathcal{C}$, denoted $\mathcal{C}^*$, is the complex on the same ground set as $\mathcal{C}$ whose facets are the complements of the minimal non-faces of $\mathcal{C}$.

An HM pair $(\mathcal{D}, d')$ is a minor of $(\mathcal{C}, d)$ if $\mathcal{D}$ can be obtained from $\mathcal{C}$ via a (possibly empty) sequence of vertex deletions and vertex links and $d'_v \leq d_v$ for every vertex of $\mathcal{D}$. The pair $(\mathcal{C}, d)$ is said to be unimodular if the matrix $A_{\mathcal{C}, d}$ is unimodular, and binary if $d = 2$. In view of Proposition 2.3 below, we say that an HM pair is minimally nonunimodular if it is not unimodular but every minor is.
Proposition 2.3. Minors of unimodular HM pairs are unimodular.

Proof. See Propositions 7.1 and 7.5 in [5].

The \( n \)-dimensional simplex will be denoted by \( \Delta_n \) and its boundary complex by \( \partial \Delta_n \).

The disjoint union of an \( m\) - and \( n\)-simplex will be denoted \( \Delta_m \sqcup \Delta_n \), and its Alexander dual will be denoted \( D_{m,n} \).

Given a simplicial complex \( C \), we say \( v \in \text{ground}(C) \) is

- a cone vertex if it appears in every facet of \( C \),
- a ghost vertex if it does not appear in any facet of \( C \), and
- a Lawrence vertex if its complement in the ground set of \( C \) is a facet.

We denote by \( \text{cone}(C) \) and \( GC \) the complex obtained by adding a cone vertex and ghost vertex to \( C \), respectively, and we denote by \( \Lambda C \) the complex obtained by adding a Lawrence vertex \( v \) to \( C \) such that \( \text{link}_v(C) = C \). Iterated application of each aforementioned operation will be denoted by superscript. For example, \( G^5C \) denotes the complex obtained by adding five ghost vertices to \( C \).

Sullivant and the first author gave a complete characterization of the set of simplicial complexes \( C \) such that the binary HM pair \( (C, 2) \) is unimodular [5]. This characterization can be expressed constructively (Theorem 2.5) or in terms of forbidden minors (Theorem 2.6). One of our main results extends Theorems 2.5 and 2.6 to non-binary HM pairs, and provides a combinatorial description of the Graver basis of the matrix \( A_{C,d} \) associated to any unimodular HM pair.

Definition 2.4. A simplicial complex \( C \) is said to be nuclear if \( C \) can be built up from \( \Delta_m \), \( \Delta_m \sqcup \Delta_n \) or \( D_{m,n} \) by applying a sequence of cone, \( G \) and \( \Lambda \) operations. The complex that \( C \) is built up from is called the nucleus of \( C \).

Theorem 2.5 ([5, Theorem 6.3]). The matrix \( A_{C,2} \) is unimodular if and only if \( C \) is a nuclear simplicial complex.

Theorem 2.6 ([5, Theorem 6.3]). A simplicial complex \( C \) is nuclear if and only if it has no minors isomorphic to any of the following:

1. the disjoint union of the boundary of a simplex and an isolated vertex,
2. the boundary complex of the octahedron or its Alexander dual,
3. the path on four vertices, or
4. a complex on ground set \( \{1, 2, 3, 4, 5\} \) with facet(\( C \)) equal to
   - \( \{1, 2\}, \{1, 5\}, \{2, 3, 4\}, \{3, 4, 5\} \),
   - \( \{1, 3, 4\}, \{2, 3, 5\}, \{2, 4, 5\} \), or
   - \( \{1, 2\}, \{2, 3, 5\}, \{3, 4\}, \{1, 4, 5\} \).

3. A NEW UNIMODULARITY-PRESERVING OPERATION

In this section we describe a new unimodularity-preserving operation that is key in the proof of Theorem 4.3. We also describe how this operation acts on the Graver basis in the case that is relevant to us. The results in this section are about general integer matrices and do not depend on any specific properties of hierarchical models.
Given a matrix $A \in \mathbb{Z}^{d \times n}$, denote by $G_qA$ and $\Lambda_pA$ the matrices
\[
G_qA = \begin{pmatrix} A & \cdots & A \end{pmatrix} \quad \text{and} \quad \Lambda_pA = \begin{pmatrix} A & 0 & \cdots & 0 \\ 0 & A & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A \\ I & I & \cdots & I \end{pmatrix}.
\]

Note that $G_qA_{C,d} = A_{G(d,q)}$ and that $\Lambda_pA_{C,d}$ has the same kernel as $A_{\Lambda(d,p)}$. The operations $A_2$ and $G_q$ for $q \geq 1$ are unimodularity-preserving, in the sense that applying them to a unimodular matrix produces a unimodular matrix (for $A_2$, this follows from [12 Theorem 7.1]). In this section, we add a new unimodularity preserving operation to the list: inserting a ghost vertex operation immediately before a Lawrence lift (Proposition 3.1). This operation provides the last crucial step in generalizing Theorem 2.5 to arbitrary unimodular HM pairs.

**Proposition 3.1.** Let $A \in \mathbb{Z}^{d \times n}$ be a matrix and let $p \geq 2$ be a fixed integer. Then $\Lambda_pA$ is unimodular if and only if $\Lambda_pG_qA$ is unimodular for all integers $q \geq 2$.

**Proof.** Assume $A$ has full row-rank $d$. It follows that $\Lambda_pG_qA$ and $\Lambda_pA$ do as well. So, it suffices to show that any maximal square submatrix of $\Lambda_pG_qA$ has determinant $\pm 1$ or 0 whenever any maximal square submatrix of $\Lambda_pA$ does. We proceed by showing that the possible values of a determinant of such a sub-matrix is independent of $q$. To this effect, we claim that the absolute value of any such determinant is equal to the absolute value of a determinant of the form
\[
\begin{pmatrix}
\cdots & A_1^R & 0 & \cdots & 0 & A_1^S & 0 & \cdots & 0 \\
\vdots & 0 & A_2^R & \cdots & 0 & 0 & A_2^S & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & A_{p-1}^R & 0 & 0 & \cdots & A_{p-1}^S & \cdots & 0 \\
\cdots & 0 & \cdots & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & 0 & \cdots & 0 & \vdots & \vdots & 0 & \cdots & 0 \\
S & 0 & 0 & \cdots & 0 & I_1^R & I_2^R & \cdots & I_{p-1}^R & 0 & 0 & \cdots & 0 \\
T & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 \\
[p-1] & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 & \cdots & 0
\end{pmatrix}
\]

where in the block corresponding to each $S \subseteq [p-1]$, if $i \notin S$ then $A_i^S = I_i^S$ is the unique $0 \times 0$ matrix, and if $i \in S$, then $A_i^S$ is some constant matrix $A_i^S$ and $I_i^S$ is the identity matrix with the same number of columns as $A_i^S$. To see this, note that a square column submatrix of $\Lambda_pG_qA$ will have a (possibly empty) submatrix of an identity matrix for its final columns. We can find the determinant by applying Laplace expansion about these columns. Each column of the resulting matrix is obtained by padding a column of $A$ either with all zeros, or all zeros and a single 1. We move all columns of the former description to the rightmost side of the matrix and rearrange them to match the right hand part of the block structure shown above. For the rest of the block structure, note
that these remaining columns are naturally partitioned into \( p - 1 \) blocks of the form 
\[
\begin{pmatrix}
0 & A_i^T & 0 & I
\end{pmatrix}^T
\]
where \( i = 1, \ldots, p - 1 \) and \( A_i \) is a column submatrix of \( A \). Each column 
\( a_j \) of \( A \) appears in some subset of these blocks which we can index by a subset of \([p - 1]\).
We can then organize the columns of this submatrix according to this subset indexing 
and then organize the bottom block of rows to get the desired block structure.

Now if \( S \) is a singleton, then every row in the block of rows labeled \( S \) has exactly 
one 1 and all the remaining entries 0. Therefore, we can remove all those blocks using 
Laplace expansion along these rows. Using the identity matrices in the bottom half of our 
matrix, we can apply row operations to turn each row-block of the form \( \begin{pmatrix} 0 & \cdots & 0 & A^S \end{pmatrix} \)
into \( \begin{pmatrix} -A^S & \cdots & -A^S & 0 \end{pmatrix} \). This leaves several columns that have a single 1 and all other 
entries 0. Applying Laplace expansion along these columns leaves the matrix
\[
\begin{bmatrix}
\cdots & A^R & \cdots & 0 & A^S & \cdots & 0 & \cdots & B_1 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\
\cdots & 0 & \cdots & A^R & 0 & \cdots & A^S & \cdots & 0 & \cdots & B_{p-2} & 0 \\
\cdots & -A^R & \cdots & -A^R & -A^S & \cdots & -A^S & \cdots & 0 & \cdots & 0 & B_{p-1}
\end{bmatrix}.
\]

Note that each \( A^S \) is either the \( 0 \times 0 \) matrix, or a column submatrix of \( A \) (possibly with 
repeated columns). So the set of possible nonzero determinants is independent of \( q \). \( \square \)

We conclude this section by demonstrating how to recover the Graver basis of \( \Lambda_3 G_q A \)
from the Graver basis of \( \Lambda_3 A \), for use in Corollary 5.4. In what follows, we write each 
\( v \in \ker \Lambda_3 G_q A \) in the form \( v = (a, b, c) \) with \( a, b, c \in \ker G_q A \). Additionally, we let 
\( v_i = (a_i, b_i, c_i) \in \mathbb{Z}^{3q} \) denote the restriction of \( v \) to coordinates corresponding to the \( i \)-th 
column of \( A \) (in particular, these columns are not sequential above).

**Proposition 3.2.** Let \( A \in \mathbb{Z}^{d \times n} \) be a matrix and fix \( q \geq 1 \). Assume \( \Lambda_3 G_q A \) is unimodular. 
Then the Graver basis of \( \Lambda_3 G_q A \) consists of vectors \( v = (a, b, c) \) obtained in the following 
ways (up to scaling by \(-1\) and permutation of \( a, b \) and \( c \)):

(a) for some \( i \leq n \) and \( j, k \leq q \), \( a_{i,j} = b_{i,k} = 1 \) and \( a_{i,k} = b_{i,j} = -1 \) are the only nonzero 
entries in \( v \);

(b) for every \( i \leq n \), each vector \( a_i, b_i, \) and \( c_i \) has at most 1 nonzero entry, and writing \( a'_i, b'_i, \) and \( c'_i \) for the sum of the entries of \( a_i, b_i, \) and \( c_i \) respectively, the vector 
\( (a'_1, \ldots, a'_n, b'_1, \ldots, b'_n, c'_1, \ldots, c'_n) \) lies in the Graver basis of \( \Lambda_3 A \); or

(c) for some \( i \leq n \) and \( j, k \leq q \), \( a_{i,j} = 1, a_{i,k} = -1, b_{i,j} = -1, \) and \( c_{i,k} = 1 \), and the 
vector \( v' = (a', b', c') \) with all coordinates the same as in \( v \), aside from 
\[ a'_{i,j} = a'_{i,k} = 0, \quad c'_{i,j} = 1, \quad \text{and} \quad c'_{i,k} = 0 \]
also lies in the Graver basis of \( \Lambda_3 G_q A \).

We clarify the statement of Proposition 3.2 with an example before giving the proof.

**Example 3.3.** Consider the matrix
\[
A = \begin{bmatrix}
1 & 1 & 0 \\
0 & 1 & 1
\end{bmatrix},
\]
whose Graver basis consists of \( v = e_1 - e_2 + e_3 \) and its negative. One can compute the 
Graver basis of \( \Lambda_3 A \) using the software 4ti2 \( \square \) to check unimodularity. It follows from
Proposition 3.1 that $\Lambda_3 G_q A$ is unimodular for all $q$. Up to reordering, every vector in the Graver basis of $\Lambda_3 A$ has the form $(v, -v, 0)$. Using Proposition 3.2 we can obtain Graver basis vectors for $\Lambda_3 G_q A$ in the following ways.

- Vectors of the form $(a, -a, 0)$ for some $a$ in the Graver basis of $G_3 A$, yielding type (i) vectors such as $((e_1, -e_1, 0), (e_1, e_1, 0), (0, 0, 0))$, and type (ii) vectors such as $((e_1 + e_3, -e_2, 0), (e_1 - e_3, e_2, 0), (0, 0, 0))$

obtained by “spreading” the vector $v$ across $G_3 A$. Writing the latter vector in the form $(a, b, c)$ and using the notation introduced above Proposition 3.2, we have $a_1 = (1, 0, 0), b_1 = (-1, 0, 0)$ and $c_1 = (0, 0, 0)$, whose entries correspond to the columns of $\Lambda_3 G_q A$ containing the first column of $A$.

- Vectors obtained from another Graver basis vector $(a, b, c)$ by (up to reordering of $a$, $b$ and $c$) moving a single nonzero entry of $a$ to an unoccupied entry of $a$ corresponding to the same column of $A$, and then adding a 1 and a -1 to $c$ appropriately. This yields Graver basis vectors such as $((e_1, -e_1, 0), (e_1, 0, e_1), (0, e_1, -e_1))$ and $((e_1 + e_3, -e_2, 0), (e_3, e_2, -e_1), (-e_1, 0, e_1))$

obtained from the each of the vectors above. Notice that vectors obtained in this way are always of type (iii), and that this process applied can be applied to each type (i) and type (ii) vector at most once for each column of $A$.

Proof of Proposition 3.2. Suppose $v$ lies in the Graver basis of $\Lambda_3 G_q A$. Since $\Lambda_3 G_q A$ is unimodular, the first $qn$ rows of $\Lambda_3 G_q A$ ensure that $\{a_{i,j}, b_{i,j}, c_{i,j}\}$ is $\{0, 0, 0\}$ or $\{1, 0, -1\}$ for all $i \leq n$ and $j \leq q$. We first prove that $a_i$, $b_i$, and $c_i$ each have no repeated nonzero entries for $i \leq n$. To this end, suppose after appropriately scaling $v$ and relabeling $a$, $b$ and $c$ that $a_{i,j} = a_{i,k} = 1, b_{i,j} = -1, c_{i,j} = 0$ for some $j, k \leq q$. Then $\{b_{i,k}, c_{i,k}\} = \{0, -1\}$, and in either case, the vector $v' = (a', b', c')$ obtained from $v$ by setting

$$a'_{i,j} = a_{i,j} + a_{i,k} = 2, \quad b'_{i,j} = b_{i,j} + b_{i,k}, \quad c'_{i,j} = c_{i,j} + c_{i,k}, \quad \text{and} \quad a'_{i,k} = b'_{i,k} = c'_{i,k} = 0,$$

is a conformal sum of nonzero vectors in $\text{ker}_{\mathbb{Z}} A$ if and only if $v$ is, which contradicts the unimodularity of $\Lambda_3 G_q A$.

Next, if for all $i$, the vectors $a_i$, $b_i$, and $c_i$ each have at most one nonzero entry, then we are in case (ii) above. Otherwise, after appropriate scaling of $v$ and relabeling of $a$, $b$ and $c$, we have $a_{i,j} = 1, a_{i,k} = -1, b_{i,j} = -1, c_{i,j} = 0$ for some $i \leq n$ and $j, k \leq q$. If $b_{i,k} = 1$, then these 4 nonzero entries form a primitive vector in the kernel of $\Lambda_3 G_q A$, so $v$ has no other nonzero entries and we are in case (i) above. In all remaining cases, $b_{i,k} = 0$ and $c_{i,k} = 1$, meaning we are in case (iii) above. Note that the vector $v'$ constructed from $v$ still yields 0 in the $j$-th and $k$-th rows of the identity blocks portion of $\Lambda_3 G_q A$, as well as each row of $\Lambda_3 G_q A$ consisting of copies of $A$. As such, $v'$ still lies in the kernel of $\Lambda_3 G_q A$. This completes the proof. \qed

4. THE CLASSIFICATION

In this section, we present the complete classification of the unimodular HM pairs. Just as in the characterization of unimodular binary HM pairs that appeared in [5],
our classification comes in two forms: a recipe for constructing any unimodular HM pair, and a list of forbidden minors.

**Observation 4.1.** Different HM pairs may yield the same matrix. Let \( C \) be a complex on ground set \( V \). Assume \( C \) has a face \( E \) such that any for any facet \( F, E \cap F \neq \emptyset \) implies \( E \subseteq F \). Let \( C' \) denote the complex on ground set \( V' := (V \cup \{v_0\}) \setminus E \) with facets

\[
\text{facet}(C') = \{ F \in \text{facet}(C) : F \cap E = \emptyset \} \cup \{ F \cup \{v_0\} : E \subset F \}.
\]

Let \( d \in \mathbb{Z}_{\geq 2}^V \) and define \( d' \in \mathbb{Z}_{\geq 2}^{V'} \) such that \( d'_v = d_v \) for all \( v \in V \cap V' \) and \( d'_v = \prod_{v \in F} d_v \). Then \( \ker Z \mathcal{A}_{C,d} = \ker Z \mathcal{A}_{C',d'} \).

**Proposition 4.2.** The following HM pairs are minimally nonunimodular:

1. any of the complexes listed in Theorem 2.6 with \( d = 2 \),
2. \( \Lambda(\Delta_0 \sqcup \Delta_0) \) with facets \( \{12, 23, 13\} \) and \( d = (3, 3, 3) \),
3. \( \Lambda(\Delta_1 \sqcup \Delta_1) \) with facets \( \{125, 345, 1234\} \) and \( d = (2, 2, 2, 2, 3) \),
4. \( \Lambda(\Delta_1 \sqcup \Delta_0) \) with facets \( \{124, 34, 123\} \) and \( d = (2, 2, 3, 3) \),
5. \( D_{1,1} \) with facets \( \{12, 23, 34, 14\} \) and \( d = (2, 2, 2, 3) \),
6. \( \Lambda \Gamma(\Delta_0 \sqcup \Delta_0) \) with facets \( \{12, 13, 234\} \) and \( d = (4, 2, 2, 2) \),
7. \( \Lambda D_{1,1} \) with facets \( \{1234, 125, 235, 345, 145\} \) and \( d = (2, 2, 2, 2, 3) \), and
8. \( \Lambda \Lambda \Gamma(\Delta_0 \sqcup \Delta_0) \) with facets \( \{1234, 1235, 145, 245\} \) and \( d = (2, 2, 2, 3, 3) \).

**Proof.** [5] Proposition 4.1] gives minimal nonunimodularity of the complexes listed in Theorem 2.6. The Graver basis for [8] was too large to compute, but selecting a large enough random sample of the matrix’s columns enabled 4ti2 [11] to produce Graver basis elements with entries of absolute value strictly greater than 1. Computations are available on our website [3]. In light of Observation 4.1, we see that the matrix for [3] has the same integer kernel as the matrix for the HM pair \( \{12, 23, 13\}, (4, 4, 3) \) and the matrix for [11] has the same integer kernel as the matrix for the HM pair \( \{12, 23, 13\}, (4, 3, 3) \) which both have [2] as a minor. Minimal nonunimodularity of the remaining HM pairs are given by [5] Proposition 7.9]. \( \square \)

**Theorem 4.3.** The following are equivalent:

(a) \((C, d)\) is unimodular;
(b) \((C, d)\) contains no minor isomorphic to any HM pair listed in Proposition 4.2 and
(c) \( C \) is nuclear. If \( C \) has nucleus \( D_{m,n} \), then \( d_v = 2 \) for each Lawrence vertex \( v \) and each vertex \( v \) from the nucleus \( D_{m,n} \). Otherwise, we can choose the vertices of \( C \) to make nucleus \( \Delta_m \sqcup \Delta_n \) so that either

1. \( d_v = 2 \) for each Lawrence vertex \( v \), or
2. \( \min\{m, n\} = 0, d_v = 2 \) for the unique vertex \( v \) of \( \Delta_0 \) and \( d_v \leq 3 \) for each Lawrence vertex \( v \) with equality attained at most once.

**Proof.** The implication \((a) \Rightarrow (b)\) follows from Propositions 4.2 and 2.3. Now, if \((C, d)\) satisfies \((b)\), then via the minors in \((b)\), Theorems 2.5 and 2.6 imply \( C \) is nuclear. So \((c)\) follows once we show that the remaining minors in Proposition 4.2 ensure \( d \) satisfies the necessary requirements.

If \( C \) has nucleus \( D_{m,n} \), then minors \((5)\) and \((7)\) ensure that \((c)\) is satisfied, so assume \( C \) has nucleus \( \Delta_m \sqcup \Delta_n \) and that \( C \) has a Lawrence vertex \( v \) such that \( d_v \geq 3 \). If \( d_v \geq 4 \),
then minor (3) ensures that in the iterative construction of $C$ as a nuclear complex, $v$ must have been added before any ghost vertices. Therefore $C$ is built up from $\Lambda^k(\Delta_m \sqcup \Delta_n)$. Perturbing the order in which we add a Lawrence vertex does not change the resulting vertex-labeled complex so we may assume $k = 1$. Minor (3) ensures we can assume without loss of generality that $n = 0$. So at this point, we know $(C, d)$ has been built from an HM pair $(C', d')$ where $C' = \Lambda(\Delta_m \sqcup \Delta_0)$. Minor (4) ensures that $d'_u = 2$ for the vertex $u$ from $\Delta_0$. However, we can realize this same complex where $u$ is the Lawrence vertex and $v$ is the unique vertex in $\Delta_0$, so we could have chosen a different set of vertices to play the role of the nucleus that would not require $v$ to be added as a Lawrence vertex.

To complete the proof of $(\mathfrak{a}) \Rightarrow (\mathfrak{b})$, it remains to consider the case where $d_v \in \{2, 3\}$ for each Lawrence vertex $v$. Using a similar argument as before, we can see that if all the Lawrence vertices with $d_v = 3$ are added before any ghost vertices in the construction of $C$ as a nuclear complex, then by choosing different vertices to play the role of the nucleus we could have $d_v = 2$ for all Lawrence vertices $v$. So assume all non-binary Lawrence vertices are added after a ghost vertex. Minor (5) ensures that at most one Lawrence vertex $v$ can have $d_v = 3$, and minors (2), (3), and (4) imply the remaining conditions.

It remains to show (2) $\Rightarrow$ (1) so assume $(C, d)$ satisfies (2). If $C$ has nucleus $D_{m,n}$, then [5 Theorem 7.10] implies $(C, d)$ is unimodular if and only if it satisfies (2). Since the operation cone commutes with $\Lambda$ and $G$ and unimodularity of $(C, d)$ is independent of $d_v$ for all cone vertices $v$, we may assume that $C$ can be obtained without using the cone operation. We may also assume that $G$ is never applied twice in a row, as doing so yields the same matrix as simply adding a single ghost vertex with a larger vertex label.

If, on the other hand, $C$ has nucleus $\Delta_m$, then since $\Lambda G \Delta_m = \text{cone}^{m+1}(\Delta_0 \sqcup \Delta_0)$, we may restrict attention to the final case, namely where $C$ has nucleus $\Delta_m \sqcup \Delta_n$. In particular,

$$C = \Lambda^0 G \Lambda^1 G \Lambda^2 G \cdots G \Lambda^k (\Delta_m \sqcup \Delta_n).$$

If $(C, d)$ satisfies the first case of (3) then unimodularity of $(C, d)$ follows from unimodularity of $(\Delta_m \sqcup \Delta_n, d')$ and the fact that adding Lawrence vertices with label 2 and ghost vertices of any vertex label preserves unimodularity. So it only remains to show unimodularity of pairs $(C, d)$ that satisfy the second case of (3).

Let $(C', d')$ be a hierarchical model. We claim that if $(\Lambda C', (d', 3))$ is unimodular, then $(\Lambda G C', (d', q, 3))$ and $(\Lambda \Lambda C', (d', 2, 3))$ are unimodular as well. Indeed, unimodularity of $(\Lambda G C', (d', q, 3))$ follows from Proposition [3.1] and $\ker_Z(\mathcal{A}_{\Lambda G C', (d', q, 3)}) = \ker_Z(\Lambda_3 G q \mathcal{A}_{C', d'})$ and $\ker_Z(\mathcal{A}_{\Lambda C', (d', 3)}) = \ker_Z(\Lambda_3 \mathcal{A}_{C', d'})$. Additionally, $(\Lambda \Lambda C', (d', 2, 3))$ has the same defining matrix as $(\Lambda \Lambda C', (d', 3, 2))$, which is unimodular if and only if $(\Lambda C', (d', 3))$ is. At this point, unimodularity of $(C, d)$ follows by induction if we show unimodularity of the HM pair $(\Lambda(\Delta_m \sqcup \Delta_0), e)$ where $e_v = 3$ for the Lawrence vertex and $e_v = 2$ for the vertex of $\Delta_0$. Letting $p$ be the product of the vertex labels in $\Delta_m$, this HM pair has the same matrix as the HM pair $\{(12, 13, 23), (3, 2, p)\}$ which was shown to be unimodular in [11].

As a corollary of Theorem 4.3, we obtain a classification of the unimodular discrete undirected graphical models, that is, hierarchical models whose simplicial complex is the clique complex of a graph. For a given graph $G$, we let $\mathcal{C}(G)$ denote the clique complex of $G$. A suspension vertex of $G$ is a vertex that shares an edge with every other vertex. Let $S^k G$ denote the graph obtained by adding $k$ suspension vertices to $G$. 


Corollary 4.4. The matrix $\mathcal{A}_{\mathcal{C}(G),d}$ is unimodular if and only if one of the following holds:

(a) $G$ is a complete graph;
(b) $G = S^kC_4$, where $C_4$ is the four-cycle and $d_v = 2$ for each vertex from $C_4$; or
(c) $G$ is obtained by gluing two complete graphs along a (possibly empty) common clique.

Proof. The constraints on $G$ follow immediately from [5, Lemma 5.3]. When $G = S^kC_4$, Theorem 4.3 implies the constraints on $d$. □

5. The Graver basis of a unimodular hierarchical model

In the final section of this paper, we present a combinatorial characterization of the Graver basis of any unimodular hierarchical model’s defining matrix. Following the constructive characterization of unimodular hierarchical models in Theorem 4.3, our characterization comes in two steps: (i) a description of the Graver basis of each nucleus, and (ii) a description of how to obtain the Graver basis of a matrix produced by one of the unimodularity preserving operations allowed by Theorem 4.3(c) given the Graver basis of its input matrix.

Proposition 5.1 characterizes the Graver basis of each possible nucleus. For any unimodular matrix, the Graver basis consists of vectors with entries in $\{0, 1, -1\}$ and coincides with the set of circuits (see Proposition 8.11 in [12]). As such, the characterization presented in Proposition 5.1 simply describes the signed circuits of the oriented matroid underlying each given hierarchical model. We remind the reader how to construct oriented matroids from signed circuits and cuts of a directed graph; for a more thorough introduction to oriented matroids, see [6].

A signed circuit of a directed graph $G$ is a bipartition of the set of edges in a simple cycle $v_1, \ldots, v_n, v_1$ of the undirected graph underlying $G$ according to whether or not the edge $v_i v_{i+1}$ agrees with $G$’s orientation. The edges that agree are called positive while those that disagree are called negative. A signed bond of $G$ is a bipartition of the set of edges in a bond (i.e. minimal cut) of $G$ that splits $G$ into connected components $A$ and $B$ according to whether or not the edge $e$ is directed from $A$ to $B$. The edges pointing from $A$ to $B$ are called positive while those pointing from $B$ to $A$ are called negative. The set of signed circuits and the set of signed bonds of $G$ each are the signed circuits of an oriented matroid. These two oriented matroids are dual to each other.

Let $K_{2^{m+1}, 2^{n+1}}$ denote the complete bipartite graph on partite sets $2^{[m+1]}$ and $2^{[n+1]}$. Label the vertices in each partite set by the binary $(m+1)$- and $(n+1)$-tuples in $\{1, 2\}^{m+1}$ and $\{1, 2\}^{n+1}$, respectively. Each edge is naturally labeled with the $(m + n + 2)$-tuple obtained by concatenating the labels of its vertices. Let $G_1^{m,n}$ be the directed graph with underlying undirected graph $K_{2^{m+1}, 2^{n+1}}$ where all edges are directed from the partite set $2^{[m+1]}$ to the partite set $2^{[n+1]}$. Let $G_2^{m,n}$ be the directed graph obtained from $G_1^{m,n}$ by reversing the orientation of the edges whose $(m + n + 2)$-tuple has an odd number of twos.

Proposition 5.1. The set of signed circuits of the oriented matroid underlying the columns of $\mathcal{A}_{\Delta_m}$ is empty. The signed circuits of the oriented matroid underlying the columns of $\mathcal{A}_{\Delta_m \cup \Delta_n, 2}$ are the signed circuits of $G_1^{m,n}$. The signed circuits of the oriented matroid underlying the columns of $\mathcal{A}_{\Delta_m \cup \Delta_n, 2}$ are the signed bonds of $G_2^{m,n}$. 
Proof. For the first statement, note that the matrix $A_{\Delta m}$ is square with determinant 1 and therefore has trivial kernel. For the second statement, recall that row operations do not affect the underlying oriented matroid. Then note that after multiplying the appropriate rows of $A_{\Delta m \sqcup \Delta n, 2}$ by $-1$, we obtain the vertex-arc incidence matrix of $G_{1, m, n}^n$.

By Proposition 3.6 in [5] and its proof, $A_{D, m, n, 2}$ can be obtained from a particular Gale dual $B$ of $A_{\Delta m \sqcup \Delta n, 2}$ by negating the columns of $B$ corresponding to the binary $(m + n + 2)$-tuples with an odd number of twos, then negating all negative rows of the resulting matrix. The oriented matroid underlying the columns of $B$ is dual to the oriented matroid underlying the columns of $A_{\Delta m \sqcup \Delta n, 2}$. Therefore, the signed circuits of the oriented matroid underlying the columns of $B$ are the signed bonds of $G_{1, m, n}^n$. On the oriented matroid level, the process of turning $B$ into $A_{D, m, n, 2}$ by negating the appropriate rows and columns has the effect of reversing the orientation of the edges of $G_{1, m, n}^n$ corresponding to binary $(m + n + 2)$-tuples with an odd number of twos. This gives us $G_{2, m, n}^n$. □

Example 5.2. We illustrate Proposition 5.1 in the case $m = 1$ and $n = 0$. We can draw the relevant simplicial complexes as follows. Note that $D_{1, 0}$ has a ghost vertex which we indicate pictorially with an open circle.

$$
\Delta_1 \sqcup \Delta_0 = \begin{array}{c}
1 \bullet \\
\text{1} \\
2 \bullet \\
\text{2} \\
3 \bullet \\
\text{3}
\end{array}
D_{1, 0} = \begin{array}{c}
1 \bullet \\
\text{1} \\
2 \bullet \\
\text{2} \\
\circ \text{3}
\end{array}

$$

Figure 2 depicts $A_{\Delta_1 \sqcup \Delta_0, 2}$ and $A_{D_{1, 0}, 2}$ alongside the directed graphs $G_{1, 0}^1$ and $G_{2, 0}^1$.

The edges corresponding to the binary 3-tuples 221, 222, 212, 211 form a cycle in $G_{1, 0}^1$ with 221 and 212 having positive orientation, and 222 and 211 both having negative orientation. Therefore the vector $e_{221} + e_{212} - e_{222} - e_{211}$ is in the Graver basis of $A_{\Delta_1 \sqcup \Delta_0, 2}$. The edges corresponding to the binary 3-tuples 221, 211, 121, 111 form a minimal cut in $G_{2, 0}^1$, partitioning the vertices into $\{1\}$ and its complement. Calling these sets $A$ and $B$ respectively, note that the edges corresponding to 221 and 111 point from $A$ into $B$ whereas the edges corresponding to 211 and 121 point from $B$ into $A$. Therefore, the vector $e_{221} + e_{111} - e_{211} - e_{121}$ lies in the Graver basis of $A_{D_{1, 0}, 2}$.

We now state the obvious extension of Proposition 5.1 to the case where $C = \Delta_m \sqcup \Delta_n$ but $d = 2$ need not hold.

Proposition 5.3. Let $C = \Delta_m \sqcup \Delta_n$ with vertex set $\{1, \ldots, m + n + 2\}$ and facets $\{1, \ldots, m + 1\}$ and $\{m + 2, \ldots, m + n + 2\}$. Fix $d \in \mathbb{Z}^{m+n+2}$ and let $G_{d, m, n}^d$ be the complete bipartite graph with partite vertex sets $[d_1] \times \cdots \times [d_{m+1}]$ and $[d_{m+2}] \times \cdots \times [d_{m+n+2}]$, with edges oriented so that they all point towards the same partite set. Label each edge by the element of $[d_1] \times [d_{m+n+2}]$ obtained by concatenating its vertices. Then the signed circuits of the oriented matroid underlying the columns of $A_{C, d}$ are the signed circuits of $G_{d, m, n}^d$.

Having now characterized the Graver basis of each nucleus, it remains to describe how each of the operations cone($\cdot$), $G$, $A_2$ and $A_3$ affect the Graver basis of a unimodular matrix $A_{C, d}$. Adding ghost vertices changes $A_{C, d}$ by $A_{G(d \ q)} = G_q(A_{C, d})$. Therefore,
every element in the Graver basis of $A_{CC,(d,q)}$ is either of the form
\[
(0 \ldots 0 e_i 0 \ldots 0 - e_i 0 \ldots 0)
\]
where $e_i$ is the $i^{th}$ standard basis vector, or $(u_1 \ u_2 \ldots \ u_q)$ where $u_1 + u_2 + \cdots + u_q$ is a conformal sum which lies in the Graver basis of $A_{C,d}$. Keeping in mind the representation of $A_{C,d}$ given in [5], it is easy to see that the kernel of $A_{cone(C),(d,q)}$ is the same as the kernel of the following matrix
\[
\begin{pmatrix}
A_{C,d} & 0 & \ldots & 0 \\
0 & A_{C,d} & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & A_{C,d}
\end{pmatrix}
\]

The Graver basis of $A_{cone(C),(d,q)}$ consists of elements of the form $(0 \ldots 0 \ u \ 0 \ldots 0)$ where $u$ is in the Graver basis of $A_{C,d}$. Again, considering the representation of $A_{C,d}$ given in [5], the kernel of $A_{A(C),(d,p)}$ is the same as the kernel of $\Lambda_p A_{C,d}$. From this it easily follows that the Graver basis of $A_{A(C),(d,q)}$ consists of elements of the form $(u - u)$ where $u$ is in the graver basis of $A_{C,d}$.

This leaves the operation $\Lambda_3$. Theorem 4.3 tells us that we only need to consider $\Lambda_3$ when applied to $A_{C,d}$ where $C$ is nuclear with nucleus $\Delta_m \cup \Delta_0$ and $d_v = 2$ for the vertex of the $\Delta_0$ and every Lawrence vertex. The operation $cone(-)$ commutes with each other operation, and $\Lambda_2$ commutes with $\Lambda_3$, so it suffices to describe the Graver basis of complexes of the form
\[
C = \Lambda_3 G A^{k_1} G_{q_1} A^{k_2} G_{q_2} \cdots A^{k_i} G_{q_i} A^{k_{i+1}} (\Delta_m \cup \Delta_0).
\]
Using Proposition 3.2, a Graver basis for the matrix corresponding to $C$ can be obtained inductively, starting with the Graver basis for the matrix corresponding to the labeled complex $\Lambda_3(\Delta_m \sqcup \Delta_0)$, whose matrix is the same as for the HM pair ($\{12, 13, 23\}, (3, 2, p)$).

**Corollary 5.4.** The Graver basis of any unimodular HM pair can be obtained by way of Propositions 5.1 and 5.3 and the discussion thereafter.

**ACKNOWLEDGMENTS**

This work began at the 2016 AMS Mathematics Research Communities in Algebraic Statistics which was supported by the National Science Foundation under Grant Number DMS 1321794. Daniel Irving Bernstein was partially supported by the US National Science Foundation (DMS 0954865) and the David and Lucille Packard Foundation.

**REFERENCES**

[1] 4ti2 team. 4ti2—a software package for algebraic, geometric and combinatorial problems on linear spaces. Available at www.4ti2.de.

[2] Satoshi Aoki, Hisayuki Hara, and Akimichi Takemura. *Markov bases in algebraic statistics*, volume 199. Springer Science & Business Media, 2012.

[3] Daniel Irving Bernstein and Christopher O’Neil. Supplementary materials. http://www4.ncsu.edu/~dibernst/Supplementary_materials/Unimodular.html 2017.

[4] Daniel Irving Bernstein and Seth Sullivant. Normal binary hierarchical models. *Experimental Mathematics*, 26(2):153–164, 2017.

[5] Daniel Irving Bernstein and Seth Sullivant. Unimodular binary hierarchical models. *Journal of Combinatorial Theory, Series B*, 123:97–125, 2017.

[6] Anders Björner, Michel Las Vergnas, Neil White, Bernd Sturmfels, and Gunter M Ziegler. Oriented matroids. 1999.

[7] Winfried Bruns, Raymond Hemmecke, Bogdan Ichim, Matthias Köppe, and Christof Söger. Challenging computations of Hilbert bases of cones associated with algebraic statistics. *Exp. Math.*, 20(1):25–33, 2011.

[8] Yuguo Chen, Ian H Dinwoodie, and Seth Sullivant. Sequential importance sampling for multiway tables. *The Annals of Statistics*, pages 523–545, 2006.

[9] Persi Diaconis and Bernd Sturmfels. Algebraic algorithms for sampling from conditional distributions. *Ann. Statist.*, 26(1):363–397, 1998.

[10] Mathias Drton, Bernd Sturmfels, and Seth Sullivant. *Lectures on algebraic statistics*, volume 39. Springer Science & Business Media, 2008.

[11] Hidefumi Ohsugi and Takayuki Hibi. Toric ideals arising from contingency tables. *Commutative Algebra and Combinatorics, Ramanujan Mathematical Society Lecture Note Series*, (4):91–115, 2007.

[12] Bernd Sturmfels. *Gröbner Bases and Convex Polytopes*, volume 8 of *University Lecture Series*. American Mathematical Society, Providence, RI, 1996.

[13] Seth Sullivant. Compressed polytopes and statistical disclosure limitation. *Tohoku Math Journal*, 58(3):433–445, 2006.

[14] Seth Sullivant. Normal binary graph models. *Ann. Inst. Statist. Math.*, 62(4):717–726, 2010.

**Mathematics, North Carolina State University, Box 8205, Raleigh, NC 27695**

_E-mail address: dibernst@ncsu.edu_

**Mathematics, University of California, Davis, One Shields Ave, Davis, CA 95616**

_E-mail address: coneill@math.ucdavis.edu_