

Markov Bases of Binary Graph Models

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Abstract

This paper is concerned with the topological invariant of a graph given by the maximum degree of a Markov basis element for the corresponding graph model for binary contingency tables. We describe a degree four Markov basis for the model when the underlying graph is a cycle and generalize this result to the complete bipartite graph $K_{2,n}$. We also give a combinatorial classification of degree two and three Markov basis moves as well as a Buchberger-free algorithm to compute moves of arbitrary given degree. Finally, we compute the algebraic degree of the model when the underlying graph is a forest.

Keywords: Markov bases, contingency tables, graphical models, hierarchical models, toric ideals.

1 Introduction and Definitions

The study of multidimensional tables and their marginals is of central importance whenever one wishes to make inferences based on statistical samples. In general, one is presented with a nonnegative integral table of data of size $d_1 \times \cdots \times d_n$ and a simplicial complex Δ on $\{1, \dots, n\}$ which encodes the specific marginals we would like to compute; this is called a hierarchical model.

Certainly, the oldest example of such a model is the case of computing the row and column sums of a matrix. If the matrix is a square $m \times m$ matrix and we require that all the row and column sums have the same value k , one calls such a matrix a semi-magic square with magic sum k . Here, our simplicial complex consists of two isolated points.

In the more general statistical situations, each node of the simplicial complex corresponds to a feature of a population sample (e.g. eye color) and the levels of the table correspond to different states of the feature (e.g. green, brown, hazel, etc.). The faces of the simplicial complex are intended to model interactions between the features. One of the most fundamental questions in statistical analysis is: do the data appear to be satisfied by a given model? One way to test the hypothesis is to compare the sample data to the maximum likelihood estimate using the χ^2 or G^2 statistic. One problem with applying this approach directly is that the data is always an integral table, while the maximum likelihood estimate almost never is. As a result, there might be no integral table with the same marginals which has a small χ^2 statistic. This problem is especially dramatic when analyzing the large, sparse data sets which occur in real world situations (e.g. census data). To remedy this situation, one may attempt to decide whether or not a model fits the data by comparing statistics

of the data table with statistics of random integral tables with the same marginals. If the statistic of the table of data is exceptional one could hope to conclude that the table was also exceptional. For example, if the χ^2 statistic of the table of data was exceptionally small, one could conclude that the data did, in fact, fit the model.

We are now left with the problem of generating random integral tables from the set of all nonnegative integral tables with fixed marginals. One solution is to perform a random walk over the set of all nonnegative integral tables with given fixed marginal. Such a random walk can be taken by first finding a suitable set of “moves” (these are tables with integral entries which have all their marginals equal to zero) and randomly adding moves to some starting table. It is at this point in the story that computational commutative algebra enters the picture: finding such a set of moves is equivalent to finding a generating set for the associated toric ideal. For a detailed introduction to the connections between toric algebra and multidimensional contingency tables, see [2], [9], and [14].

In this paper, we restrict attention to tables where $d_i = 2$ for all i and for which the underlying simplicial complex is a graph; that is, we compute only two- and one-way marginals of our binary table. We refer to such models as binary graph models. These are generally not the usual graphical models studied so frequently in statistics, where the simplicial complex consists of the cliques of the underlying graph G [10]. Our notion of graph model coincides with the more familiar graphical model if and only if the graph has no three-cycle. Now, we will give two formal presentations of the objects of interest in this paper.

Let G be a graph on the n -element vertex set $[n] := \{1, 2, \dots, n\}$ with edge set $E(G)$. Denote by $Iso(G)$ the set of isolated vertices of G . For each edge $\{j, k\}$ of the graph G consider the linear transformations $\pi_{j,k}$

$$\begin{aligned} \pi_{j,k} : \mathbb{Z}^{2^n} &\longrightarrow \mathbb{Z}^4 \\ e_{i_1 \dots i_n} &\longmapsto e_{i_j, i_k} \end{aligned}$$

and for each isolated vertex k of G consider the linear transformations π_k

$$\begin{aligned} \pi_k : \mathbb{Z}^{2^n} &\longrightarrow \mathbb{Z}^2 \\ e_{i_1 \dots i_n} &\longmapsto e_{i_k}. \end{aligned}$$

We think of the maps $\pi_{j,k}$ as computing the 2-way marginal of a $2 \times \dots \times 2$ table corresponding to the edge $\{j, k\}$ and the maps π_k as computing the 1-way marginal of a $2 \times \dots \times 2$ table corresponding to the vertex k . We define the map π_G by taking all the marginal computations induced by a given graph as

$$\begin{aligned} \pi_G : \mathbb{Z}^{2^n} &\longrightarrow \bigoplus_{\{j,k\} \in E(G)} \mathbb{Z}^4 \oplus \bigoplus_{k \in Iso(G)} \mathbb{Z}^2 \\ v &\longmapsto \bigoplus_{\{j,k\} \in E(G)} \pi_{j,k}(v) \oplus \bigoplus_{k \in Iso(G)} \pi_k(v). \end{aligned}$$

We say that π_G is the map which computes the marginals of a $2 \times \dots \times 2$ table according to the graph G . The matrix which represents this linear transformation will be denoted A_G and the polytope which is the convex hull of the columns of A_G is denoted P_G where we consider the columns of A_G as vectors in \mathbb{R}^d for an appropriate d . A move for G is an element of the integral

kernel of π_G ; that is, a move is an integral table which does not change the G -marginals of a table it is added to. In general we are interested in sets of moves with special properties.

Definition 1.1. *A finite subset of moves $B \subset \ker_{\mathbb{Z}}(\pi_G)$ is called a **Markov basis** for the graph G if for every pair of nonnegative integral tables $v_1, v_2 \in \mathbb{N}^{2^n}$ with the same G -marginals $\pi_G(v_1) = \pi_G(v_2)$, there is a sequence of moves $\{u_i\}_{i=1}^l \subset \pm B$ such that*

$$v_1 + \sum_{i=1}^l u_i = v_2$$

and

$$v_1 + \sum_{i=1}^j u_i \in \mathbb{N}^{2^n} \quad \text{for all } 1 \leq j \leq l.$$

There is also a much shorter and more algebraic way to arrive at this definition. Recall that G is a graph on the n -element vertex set $[n] := \{1, 2, \dots, n\}$ with edge set $E(G)$, and isolated vertices $Iso(G)$. Consider the map of polynomial rings

$$\phi_G : \mathbb{C}[p_{i_1, \dots, i_n} \mid i_j \in \{0, 1\}] \longrightarrow \mathbb{C}[t_{i_j, i_k}^{(j,k)}, t_{i_l}^{(l)} \mid \{j, k\} \in E(G) \text{ and } l \in Iso(G)]$$

$$p_{i_1 \dots i_n} \longmapsto \prod_{\{j, k\} \in E(G)} t_{i_j, i_k}^{(j,k)} \prod_{l \in Iso(G)} t_{i_l}^{(l)}.$$

The object of interest in this paper is the ideal denoted $I_G = \ker(\phi_G)$, which we call the ideal of a binary graph model. It is a **toric ideal**: a prime ideal generated by monomial differences whose leading and trailing terms have disjoint support.

Markov bases and toric ideals are connected by the following fundamental theorem.

Theorem 1.2. [2] *A finite subset of moves $B = \{u_i\}_{i=1}^l \subset \ker_{\mathbb{Z}}(\pi_G)$ is a Markov basis for G if and only if the set of binomials $\{p^{u_i^+} - p^{u_i^-}\}$ is a generating set for I_G .*

Here, we write $u_i = u_i^+ - u_i^-$ as the difference of two positive vectors of disjoint support. In light of Theorem 1.2, we will use the expressions “Markov basis for G ” and “generating set for I_G ” interchangeably throughout this paper. Similarly, we can interchange the words “move” and “binomial” whenever we are discussing the Markov bases/generating sets of I_G . These definitions are best illustrated by a simple example.

Example 1.3. Consider the graph G on four nodes with two edges $\{1, 2\}$ and $\{2, 3\}$ and one isolated vertex 4. The map ϕ_G is a map from a polynomial ring in sixteen variables to a polynomial ring in ten variables. It is the map of rings

$$\begin{aligned} \phi_G : \mathbb{C}[p_{ijkl} \mid i, j, k, l \in \{0, 1\}] &\longrightarrow \mathbb{C}[r_{ij}, s_{jk}, t_l] \\ p_{ijkl} &\longmapsto r_{ij} \cdot s_{jk} \cdot t_l. \end{aligned}$$

On the other hand, the marginal map π_G is given by a 10×16 matrix A_G . It is the matrix

$$A_G = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \end{pmatrix}.$$

The polytope P_G in \mathbb{R}^{10} has dimension 6 and has 10 facets. These facets are indexed naturally by the rows of A_G and the facet defining inequalities are given by $y_i \geq 0$ with one inequality for each row. The ideal I_G has a Markov basis consisting of quadratic moves. These are

$$p_{0j0l_1}p_{1j1l_2} - p_{0j1l_1}p_{1j0l_2} \text{ with } j, l_1, l_2 \in \{0, 1\}$$

and

$$p_{i_1j_1k_1l_1}p_{i_2j_2k_2l_2} - p_{i_1j_1k_1l_2}p_{i_2j_2k_2l_1} \text{ with } i_1, j_1, k_1, l_1, i_2, j_2, k_2, l_2 \in \{0, 1\}.$$

These generators are also a Gröbner basis with respect to the reverse lexicographic term order with $p_{0\dots 0} \prec \dots \prec p_{1\dots 1}$.

In general, when the underlying graph is a forest, the toric ideal I_G is relatively well understood.

Theorem 1.4. [3, 6, 15] *The ideal I_G is minimally generated by quadrics if and only if G is a forest. In this case, the set of quadratic squarefree binomials in I_G forms a Gröbner basis with respect to the reverse lexicographic term order with $p_{0\dots 0} \prec p_{0\dots 01} \prec \dots \prec p_{1\dots 1}$.*

In this paper, we are primarily concerned with investigating graphs which contain cycles. One fundamental question is to compute the following invariant of a graph.

Definition 1.5. *Let G be a graph. The **Markov width** $\mu(G)$ is the degree of the largest minimal generator of the toric ideal I_G .*

Studying the Markov width of a graph is of fundamental importance for statistical applications because it relates the complexity of analyzing data to the complexity of the underlying graphical structure. Note that, Theorem 1.4 states that the graphs with $\mu(G) = 2$ are precisely forests, which are certainly topologically simple. Indeed, the Markov width of a graph G is topological in nature, by which we mean that $\mu(G)$ can only decrease under the operations of vertex deletion and edge contraction; we will show this in Section 4. Since these operations interact nicely with the toric ideals of the initial and final graph, we will use the following definition throughout.

Definition 1.6. *Let G be a graph. By a **minor** of G , we mean a graph H which can be obtained from G via a sequence of edge contractions and vertex deletions.*

This is different from the usual definition of a graph minor in that we do not allow edge deletion, whose interaction with the toric ideal is more complicated.

The rest of the paper is organized as follows. In the next section, we discuss computational results for graphs with few vertices and suggest some conjectures based upon these data. In particular, we have computed the Markov width $\mu(G)$ for all graphs on five vertices and many of the graphs on six vertices. In the third section, we prove that the n -cycle and $K_{2,n}$ have Markov width 4. Furthermore, we are able to explicitly describe the moves needed in the Markov bases for these graph. The fourth section is devoted to the inverse problem: that is, studying which graphs may have Markov basis elements of a given degree. We give an algorithm which does not depend on computing S -pairs for computing all the minimal generators of a given degree for the ideals I_G . As a consequence of our algorithm, we give a combinatorial characterization of moves of degree two and three. In the final section, we return to the study of forests and use the reverse lexicographic Gröbner basis from Theorem 1.4 to derive combinatorial formulae for the algebraic degree of I_G whenever G is a forest.

2 Graphs with Few Vertices

In this section we discuss and display computational results about the ideals of binary graph models. In particular, we describe generating sets for the ideals I_G for all graphs G with fewer than five vertices and all the graphs on six vertices with at most eight edges. These computational results suggest many conjectures and open problems which we describe at the end of the section. All of our computations were carried out using the toric Gröbner basis program `4ti2` [8] and the computational algebra system `Macaulay 2` [7]. We limit our description to graphs which cannot be “glued” together from smaller graphs based on the following definition and theorem.

Definition 2.1. *Let (V_1, S, V_2) be a partition of the vertex set of a graph G such that*

1. *there are no edges in G between V_1 and V_2 and*
2. *S is either the empty set or S is a common vertex or edge of the induced subgraphs G_1 and G_2 with vertex sets $V_1 \cup S$ and $V_2 \cup S$, respectively.*

*Then G is called **reducible** with decomposition (V_1, S, V_2) .*

Theorem 2.2. *[4, 9] Let G be a graph which is reducible and G_1 and G_2 the induced subgraphs arising from the vertex decomposition. Then there is a degree preserving operation with which one can build generating sets and Gröbner bases for I_G from generating sets and Gröbner bases of I_{G_1} and I_{G_2} . In particular, $\mu(G) = \max(\mu(G_1), \mu(G_2))$.*

There are precisely one graph on three vertices, two graphs on four vertices, six graphs on five vertices, and six graphs with six vertices and at most eight edges which are not reducible. We will briefly describe these graphs and their Markov bases.

2.1 Three and Four Vertices

The only graph on three vertices which is not reducible is the complete graph K_3 . The Markov basis of I_{K_3} consists of the single degree four binomial

$$p_{000}p_{011}p_{101}p_{110} - p_{001}p_{010}p_{100}p_{111}.$$

The two irreducible graphs on four vertices are C_4 and K_4 . The graph C_4 is the four cycle with $E(C_4) = \{12, 23, 34, 14\}$. The Markov basis of C_4 consists of eight quadrics such as

$$p_{0000}p_{0101} - p_{0001}p_{0100}$$

and eight quartics. The complete graph K_4 has Markov basis consisting of 20 moves of degree four and 40 sextic binomials such as

$$p_{0000}^2 p_{0111} p_{1011} p_{1101} p_{1110} - p_{0001} p_{0010} p_{0100} p_{1000} p_{1111}^2.$$

2.2 Five Vertices

There are six graphs on five vertices which cannot be decomposed into subgraphs. These are the graphs we denote C_5 , $K_{2,3}$, \widetilde{K}_4 , SP , BP , and K_5 . The graph C_5 is the five-cycle $E(C_5) = \{12, 23, 34, 45, 15\}$. Its Markov basis consists of 80 quadrics and 40 quartics. The graph $K_{2,3}$ is the complete bipartite graph $E(K_{2,3}) = \{13, 14, 15, 23, 24, 25\}$. Its Markov basis consists of 44 quadrics and 420 quartics. The graph \widetilde{K}_4 is the graph obtained from K_4 by subdividing an edge, $E(\widetilde{K}_4) = \{12, 15, 23, 24, 34, 35, 45\}$. The Markov basis for $I_{\widetilde{K}_4}$ consists of 32 quadrics, 473 quartics, and 160 sextics. The graph SP is the edge graph of the square pyramid, $E(SP) = \{12, 13, 15, 23, 24, 34, 35, 45\}$. The Markov basis of SP consists of 16 quadrics, 671 quartics, and 320 sextics. The graph BP is the edge graph of the bipyramid over a triangle, $E(BP) = \{12, 13, 15, 23, 24, 25, 34, 35, 45\}$. Its Markov basis consists of 8 quadrics, 436 quartics, and 2872 sextic binomials. Finally, K_5 is the complete graph on five vertices. The Markov basis of K_5 consists of 260 degree four moves, 3952 sextic binomials, 846 binomials of degree eight such as

$$p_{00000}^3 p_{01111} p_{10111} p_{11011} p_{11101} p_{11110} - p_{00001} p_{00010} p_{00100} p_{01000} p_{10000} p_{11111}^3$$

and 480 degree ten binomials like

$$p_{00000}^2 p_{01111}^2 p_{10001}^2 p_{10010}^2 p_{10100} p_{11000} - p_{00010} p_{00101} p_{01001} p_{01110} p_{10000}^4 p_{10011} p_{11111}.$$

2.3 Six Vertices

There are a total of 29 graphs on six vertices which are not reducible. We were able to compute Markov bases for the six irreducible graphs on six vertices which have at most eight edges. It remains a major computational challenge to determine Markov bases of the other 23 irreducible graphs on six vertices. The six irreducible graphs on six vertices with less than nine edges will be denoted C_6 , $K_{2,4}$, G_{129} , G_{151} , G_{153} , and G_{154} .

The graph C_6 is the six cycle with edge set $E(C_6) = \{12, 23, 34, 45, 56, 16\}$. The graph $K_{2,4}$ is the complete bipartite graph with edge set $E(K_{2,4}) = \{13, 14, 15, 16, 23, 24, 25, 26\}$. The remaining graphs do not have special names: the labels we have chosen come from [12]. These four graphs have edge sets $E(G_{129}) = \{12, 15, 23, 26, 34, 45, 56\}$, $E(G_{151}) = \{12, 14, 23, 26, 34, 36, 45, 46\}$, $E(G_{153}) = \{12, 15, 16, 23, 24, 45, 46, 56\}$, and $E(G_{154}) = \{12, 14, 23, 25, 34, 36, 45, 56\}$. The data regarding the Markov bases of these graphs as well as all the irreducible graphs on five and fewer vertices is summarized in the following table. The columns are labeled by the particular irreducible graph, the rows are labelled by degree of minimal generators and the table entries are the number of minimal generators of a given degree.

	K_3	C_4	K_4	C_5	$K_{2,3}$	\widetilde{K}_4	SP	BP	K_5	C_6	$K_{2,4}$	G_{129}	G_{151}	G_{153}	G_{154}
2	0	8	0	80	44	32	16	8	0	528	236	360	280	320	256
4	1	8	20	40	420	473	671	436	260	160	11696	2636	4949	4149	7784
6	0	0	40	0	0	160	320	2872	3952	0	0	0	640	480	640
8	0	0	0	0	0	0	0	0	846	0	0	0	0	0	0
10	0	0	0	0	0	0	0	0	480	0	0	0	0	0	0
Total	1	16	60	120	464	665	1007	3316	5538	688	11932	2996	5869	4949	8680
$\mu(G)$	4	4	6	4	4	6	6	6	10	4	4	4	6	6	6

For these graphs, all generators are in even degree. This is not true in general, however, as we will demonstrate in Section 4. Theorem 1.4 characterizes graphs with $\mu(G) = 2$ as forests, but the next case is already quite interesting.

Problem 2.3. *Characterize those graphs with Markov width $\mu(G) = 4$.*

In the next section we will show that cycles and the complete bipartite graphs $K_{2,n}$ have Markov bases consisting of moves of degree four or less, but from the data we see that this is not yet a complete characterization.

A natural class of graphs which one would hope to understand is planar graphs. The data above suggest the following optimistic conjecture.

Conjecture 2.4. *There is a universal constant C such that the Markov width $\mu(G) \leq C$ whenever G is a planar graph. Even stronger, $C = 6$.*

On the other hand, the data also suggest the following conjecture.

Conjecture 2.5. *The invariant $\mu(G)$ is a function only of the tree width of G .*

The tree width is a topological invariant of a graph G which is equal to one less than the size of the largest clique in the chordal graph containing G which has the smallest maximal clique. For example, forests are precisely those graphs with tree width zero or one, and indeed Theorem 1.4 tells us that these graphs all have Markov width two. Conjecture 2.5 also agrees with Theorem 2.2, since the tree width of a reducible graph is the maximum of the tree widths of its components.

While the limited information we have suggests both Conjecture 2.4 and Conjecture 2.5, they cannot both be true: there are planar graphs with arbitrarily large tree width. For example, grid graphs can have arbitrarily large clique size in their minimal chordal triangulations. This suggests another research problem.

Problem 2.6. *Study the binary graph model I_G for the family of $m \times n$ grid graphs.*

We do know that $\mu(G)$ can be arbitrarily large. For example, for the complete graph K_m we can construct generators of large degree.

Proposition 2.7. *The complete graph K_m with $m \geq 3$ has Markov width $\mu(K_m) \geq 2m - 2$.*

Proof. It suffices to show that there is a minimal generator of K_m of degree $2m - 2$. For this consider the binomial

$$p_{\mathbf{0}}^{m-2} \prod_{i=1}^m p_{\mathbf{1}-e_i} - p_{\mathbf{1}}^{m-2} \prod_{i=1}^m p_{e_i}$$

where $\mathbf{0}$ is the string of all zeros, $\mathbf{1}$ is the string of all ones, and e_i is the i th unit vector. Then the monomials coming from the leading and trailing terms are the only monomials which have the given image under ϕ_{K_m} . Equivalently, the corresponding tables are the only two tables which have these same fixed marginals under π_{K_m} . Since the leading and trailing terms have disjoint support, this binomial must appear in every Markov basis for I_{K_m} . \square

Of course, this bound is already not tight for $m = 5$, where it yields $\mu(K_5) \geq 8$ despite the fact that K_5 has Markov width 10. In general we suspect that $\mu(K_m)$ grows exponentially in m .

3 Cycles and Bipartite Graphs

In this section we confirm the observations from the second section: the ideal of the cycle and the complete bipartite graph $K_{2,n}$ are generated in degrees two and four.

3.1 Cycles

For ease of notation, we will represent a binomial such as $p_{1011}p_{1110} - p_{1111}p_{1010}$ in **tableau notation** as

$$\begin{bmatrix} 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix} - \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}.$$

The tableau are obtained from a binomial by recording the indices of each variable which appears in the monomial, repeating indices when a variable appears to a power greater than one. We say that one binomial **contains** another if it does so in the Graver sense; that is, $p^u - p^v$ contains $p^a - p^b$ if $a \leq u$ and $b \leq v$ componentwise.

We first prove the following theorem bounding the degree of minimal generators for the n -cycle.

Theorem 3.1. *Let C_n be the n -cycle graph. Then $\mu(C_n) = 4$, and in particular I_{C_n} is generated in degrees 2 and 4.*

Proof. We will start with an arbitrary binomial f in the ideal, and express it as a linear combination of elements either of lower degree or of degree at most 4.

Given any binomial, take one variable from each monomial such that the two variables chosen agree in first and last index. Our strategy will be as follows: by adding multiples of ideal elements of degree 4 and less, we will eventually obtain a binomial in which both monomials have the same variable. Dividing out by this variable (which clearly does not affect membership in I_G) yields a binomial of lower degree which must still be in the ideal, completing the proof.

We now start this process. We have a variable $p_{1? \dots ?1}$ in the first term of f , and a variable $p_{1? \dots ?1}$ in the second term. We wish to eliminate all disagreements between these indices by “moving” the table entries corresponding to these binary strings using binomials of degree 4 or less.

Consider any block of disagreements, in which, without loss of generality, the indices of these variables look like $(\dots?10 \dots 01? \dots)$ and $(\dots?11 \dots 11? \dots)$. We propose to add some multiple of an ideal element of degree g at most 4 so that the resulting binomial contains the two variables in question, and is unchanged except that some of the disagreements in the block have been removed.

The two sets of index strings in g will agree on the portion of C_n outside of the block in question, counting the boundary elements. Essentially, we are performing a local move by changing indices on a subgraph of C_n . Let \tilde{f} represent the image of f in this subgraph, i.e. under the map sending $p...?I?...$ to p_I , where I is the index substring on the block we have.

Continuing in this manner, by induction on the number of disagreements we eventually obtain a binomial for which the same variable appears in both monomials, completing the proof. We now construct the ideal element g which we will add a multiple of. We first construct the part \tilde{g} which corresponds to the block in question; in the tableaux that follow, we consider only the indices corresponding to this block.

Because this element is in the ideal I_{C_n} , considering the marginal in the first two directions, since an element in the first term of f has a 10 marginal, so must an element in the second term. So \tilde{f} contains

$$\left[\begin{array}{cccccc} 1 & 0 & 0 & \cdots & 0 & 1 \end{array} \right] - \left[\begin{array}{cccccc} 1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & 0 & ? & \cdots & ? & ? \end{array} \right].$$

Now, if any of the unspecified elements is 1, we let \tilde{g} be the binomial which switches the intervening substrings, i.e. something of the form

$$\left[\begin{array}{cccccc} 1 & 1 & 1 & 1 & 1 & \\ 1 & 0 & 0 & 1 & 1 & A \end{array} \right] - \left[\begin{array}{cccccc} 1 & 0 & 0 & 1 & 1 & \\ 1 & 1 & 1 & 1 & 1 & A \end{array} \right],$$

where A is the remainder of the index string of the element that the second term of \tilde{f} contains starting with 10. We fill in the rest of both terms of g as the two index strings corresponding to the two variables contained in the second term of \tilde{f} are filled in, so that the two variables of the first term of g are contained in the second term of f . Adding g to f then has the effect of eliminating some disagreements between the two variables as desired, while leaving everything unchanged outside the block in question.

Otherwise, all of the elements marked ? must be 0. We can apply the same argument to the terminal string and to the other binomials to obtain g in all cases except where \tilde{f} contains

$$\left[\begin{array}{cccccc} 1 & 0 & \cdots & 0 & 1 & \\ 1 & 1 & \cdots & 1 & 0 & \\ 0 & 1 & \cdots & 1 & 1 & \end{array} \right] - \left[\begin{array}{cccccc} 1 & 1 & \cdots & 1 & 1 & \\ 1 & 0 & \cdots & 0 & 0 & \\ 0 & 0 & \cdots & 0 & 1 & \end{array} \right].$$

In this case, because we have a 00 marginal in the first two coordinates of the second term of \tilde{f} , we must have one in the first term. If that element contains any 1, by adding a multiple of a binomial of degree 2 involving it and the third element in the first term, and then another multiple of a binomial of degree 2 involving the third element and the first element in the first term, we can construct a g essentially as before which reduces disagreements. The only case where we cannot apply this argument to this fourth element is when \tilde{f} contains

$$\left[\begin{array}{cccccc} 1 & 0 & \cdots & 0 & 1 & \\ 1 & 1 & \cdots & 1 & 0 & \\ 0 & 1 & \cdots & 1 & 1 & \\ 0 & 0 & \cdots & 0 & 0 & \end{array} \right] - \left[\begin{array}{cccccc} 1 & 1 & \cdots & 1 & 1 & \\ 1 & 0 & \cdots & 0 & 0 & \\ 0 & 0 & \cdots & 0 & 1 & \\ 0 & 1 & \cdots & 1 & 0 & \end{array} \right].$$

In this case, we let \tilde{g} be this binomial of degree 4, corresponding to switching the middle substrings of all 0's and all 1's. Again, we extend this to g by copying the indices from f outside this block to the relevant variables, and we can add this element to f to eliminate this patch of

disagreements between the variables in question. This completes the proof by induction. Note that we did not use any elements of degree 3 in this process, so I_{C_n} is in fact generated in degrees 2 and 4. \square

This theorem not only shows that the minimal generators are all of degree 2 or 4, but it also gives a complete description of these generators. The degree-2 generators come from separations of the graph; we will prove a general statement characterizing degree-2 generators of graph ideals in Section 5. As for the minimal generators of degree four, we have the following categorization.

Theorem 3.2. *The minimal generators of degree 4 in the graph ideal I_{C_n} are those elements of the form*

$$\begin{bmatrix} A_1 & 1 & B & 1 \\ A_2 & 1 & 1-B & 0 \\ A_3 & 0 & 1-B & 1 \\ A_4 & 0 & B & 0 \end{bmatrix} - \begin{bmatrix} A_1 & 1 & 1-B & 1 \\ A_2 & 1 & B & 0 \\ A_3 & 0 & B & 1 \\ A_4 & 0 & 1-B & 0 \end{bmatrix},$$

where the columns correspond to V_1, x_1, V_2 , and x_2 , V_1 and V_2 are contiguous blocks of elements, and these elements in this order comprise the n -cycle. Here, $1-B$ represents the opposite string of B .

Note that these generators of degree 4 are very similar to the generator of degree 4 in K_3 , namely

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} - \begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix}.$$

We will prove a general similarity theorem in this vein in Section 4, when we classify generators of a given degree.

3.2 Complete Bipartite Graphs

Another nice class of models is the $K_{m,n}$ model, where $K_{m,n}$ is the complete bipartite graph with partite sets of m and n vertices. We first prove the following theorem.

Theorem 3.3. *The graph ideal for $G = K_{2,n}$ is generated in degrees 2 and 4 (for $n \geq 2$).*

Proof. As in the proof of Theorem 3.1, we use binomials of small degree (≤ 4) to transform a binomial in this ideal to one whose two terms share a variable, completing the proof by induction. Let the vertices of the two-element partite set be $V = \{v_1, v_2\}$, and let the vertices of the n -element partite set be $W = \{w_1, \dots, w_n\}$.

For each monomial M , we define the submonomial M_{ij} , $i, j \in \{0, 1\}$, to be the product of the variables with ij in the index string corresponding to the two-element partite set; we will write that index string first. For a monomial M , we define $a_{ij}(M)$ to be the total degree of M_{ij} , and $b_{ij,k,l}(M)$ to be the number of appearances of the digit k in the w_l -position of the index strings of the variables in M_{ij} . Here $k \in \{0, 1\}$ and $l \in \{1, \dots, n\}$. In other words, these function values enumerates the marginal in the direction (v_1, v_2, w_l) with the set values (i, j, k) . We can of course recover $a_{ij}(M) = b_{ij,0,l} + b_{ij,1,l}$ for any l .

Then we have the following easy lemma.

Lemma 3.4. *If M_1 and M_2 are monomials such that $b_{ij,k,l}(M_1) = b_{ij,k,l}(M_2)$ for all i, j, k, l , then their difference can be expressed as a sum of multiples of quadratic elements of I_G .*

We do this simply by, for each M_{ij} , using quadratic generators corresponding to the separation $(w_l, V, W \setminus \{w_l\})$ to move around the $b_{ij,1,l}(M)$ 1's in the l th column. Consequently, we need only to connect monomials with the same marginals and different F -values. We introduce an additional definition.

Given a monomial M , the function $c_{ij,l}(M)$ is defined to be the subset of $0, 1$ which appears in the w_l -position in the variables of M_{ij} . Explicitly, this contains 0 when $b_{ij,0,l}(M) > 0$, and 1 when $b_{ij,1,l}(M) > 0$.

We now unspool a series of moves designed to connect all of the remaining F -values of monomials with the same marginals.

Lemma 3.5. *Suppose we have a monomial M and a column l such that $1 \in c_{01,l}(M), c_{10,l}(M)$ and $0 \in c_{00,l}(M), c_{11,l}(M)$. Then M is equivalent by adding a multiple of a binomial of degree 4 to a monomial with the following changes to the a_I 's and b_I 's:*

$$\begin{aligned} +1 &: b_{01,0,l}, b_{10,0,l}, b_{11,1,l}, b_{00,1,l}, \\ -1 &: b_{01,1,l}, b_{10,1,l}, b_{11,0,l}, b_{00,0,l}. \end{aligned}$$

Proof. This corresponds merely to adding a multiple of the degree 4 binomial

$$\begin{bmatrix} 1 & 1 & 1 & I_1 \\ 1 & 0 & 0 & I_2 \\ 0 & 0 & 1 & I_3 \\ 0 & 1 & 0 & I_4 \end{bmatrix} - \begin{bmatrix} 1 & 0 & 1 & I_1 \\ 1 & 1 & 0 & I_2 \\ 0 & 1 & 1 & I_3 \\ 0 & 0 & 0 & I_4 \end{bmatrix},$$

where the columns are v_1, w_l , and v_2 , and all other vertices in some order. This binomial comes from the minor K_3 given by contracting all the $w_i, i \neq l$, into either v_1 or v_2 . \square

Lemma 3.6. *Suppose we have a monomial M such that for each column l , there exists some index i_l such that $i_l \in c_{01,l}(M), c_{10,l}(M)$. Then M is equivalent by adding a multiple of a binomial of degree 2 to a monomial with the following changes to the a_I 's and b_I 's:*

$$\begin{aligned} +1 &: a_{11}, a_{00}, b_{11,i_l,l}, b_{00,i_l,l}, \\ -1 &: a_{10}, a_{01}, b_{01,i_l,l}, b_{10,i_l,l}, \end{aligned}$$

for all $l \in \{1, \dots, n\}$.

Proof. If I is the index string composed of the i_l , this corresponds to adding a multiple of the degree 2 binomial

$$\begin{bmatrix} 1 & 1 & I \\ 0 & 0 & I \end{bmatrix} - \begin{bmatrix} 1 & 0 & I \\ 0 & 1 & I \end{bmatrix},$$

where the columns are indexed by v_1, v_2 , and the w_l . \square

Now, suppose we have two monomials with the same marginals, that is the same image under ϕ_G . Add multiples of the binomials from Lemma 3.5 and Lemma 3.6 until one can no longer apply these; since both increase $a_{11} + \sum b_{11,l}$, one will not go around in circles. Our monomials M and N are now in ‘‘reduced’’ form, in the sense that neither move can be applied. We break the situation down into cases.

Case 1. Suppose that M_{11} and N_{11} are both not equal to 1, so that both M and N have an entry which is 11 in the (v_1, v_2) direction.

If, for each l , there exists an index i_l such that $i_l \in c_{11,l}(M)$ and $i_l \in c_{11,l}(N)$, then, as desired, we can simply extract the variable $p_{11,(i_l)}$ from both M and N ; in other words, for both M and N , we can find a monomial with the same values of a and b containing this variable.

If this is not the case, then there exists an l for which without loss of generality $c_{11,l}(M) = \{1\}$ and $c_{11,l}(N) = \{0\}$. Looking at the (v_1, w_l) marginal, there exists at least one marginal 11 because of the first condition; consequently, there must exist at least one of these marginals in N . Since $c_{11,l}(N) = \{0\}$, the only other option is that $1 \in c_{10,l}(N)$. Similarly, considering the (v_2, w_l) marginal, we must have $1 \in c_{01,l}(N)$.

Now, we have $b_{11,0,l}(N) = k > 0$. Since $b_{11,0,l}(M) = 0$, looking at the 10-count in the (v_1, w_l) direction, we must have $b_{10,0,l}(M) = b_{10,0,l}(N) + k$. However, looking at the 00-count in the (v_2, w_l) direction, it now follows that we must have $b_{00,0,l}(N) = b_{00,0,l}(M) + k$, and in particular $0 \in c_{00,l}(N)$. This is a contradiction, since we can now apply a move as in Lemma 3.5 to N , contradicting the assumption that N is reduced.

Case 2. Exactly one of M_{11} and N_{11} is equal to 1.

Suppose without loss of generality that $M_{11} \neq 1$ and $N_{11} = 1$. Take any $i_l \in c_{11,l}(M)$; this i_l must be in $c_{10,l}(N)$ and $c_{01,l}(N)$. This means that we can apply a move as in Lemma 3.6 to N , again contradicting the hypothesis that N is reduced.

Case 3. Both M_{11} and N_{11} are empty.

In this case, it follows immediately that $b_{10,i,l}(M) = b_{10,i,l}(N)$ for all i and l by considering the (v_1, w_l) marginals equal to $(1, i)$. If $M_{10} \neq 1$, this means that we can find an i_l for all l such that this number is nonzero, and we can then pull the corresponding variable out of both M and N . Similarly, if $M_{01} \neq 1$, we can find a shared variable there, and if both of these are 1 then applying the same argument to $M_{00} = M$ and $N_{00} = N$ finishes the job.

Our litany of cases has come to an end, completing the proof of Theorem 3.3. Note again that we have not only shown that $\mu(K_{2,n}) = 4$, but also given an explicit generating set in degrees 2 and 4 for $I_{K_{2,n}}$. \square

For $K_{m,n}$ where $m, n > 2$, the answer is less clear. The statement and proof of Theorem 3.3 indicate that for m fixed, as n gets large, the maximum degree of an element in the Markov basis of the graph ideal of $K_{m,n}$ stabilizes. The degree, on the other hand, certainly goes up as $\min(m, n)$ does; for instance, there is an element of degree $2m$ in the Markov basis of $K_{m,m}$, and we have the following result.

Proposition 3.7. *Fix $m \geq 2$. Then for $n \geq \binom{m}{2}2^{m-2}$, there is an element of degree 2^{m-1} in the graph ideal of $K_{m,n}$.*

Proof. Let the vertices of $K_{m,n}$ be $\{v_1, \dots, v_m\} \cup \{w_I\}$, where $I = (i_1, \dots, i_m)$ is an index string of length m , consisting of precisely two 1's, and some number of 0's and 2's. There are precisely $\binom{m}{2}2^{m-2}$ such strings.

Specify the marginals as follows: between v_j and w_I , insist upon i_j marginals of 11, $2 - i_j$ marginals of 01, $2^{m-2} - i_j$ marginals of 10, and $2^{m-2} - 2 + i_j$ marginals of 00. What this means is that exactly two variables with coordinate w_I equal to 1 occur, and that the sum of the v -coordinates (considered as vectors) is precisely I ; it furthermore specifies that each of 0 and 1 occurs 2^{m-2} times in each v_j -coordinate.

For each w_I , there are only two ways to express the vector I as the sum of two 0-1 vectors. Since we consider all index strings I , we obtain that for each diamond in the natural Boolean

partial order of binary strings of length m , either the top and bottom elements are in the set of v -coordinates of table entries, or the middle two entries are. By an easy induction, it follows that the set of v -coordinates, which numbers only 2^{m-1} , must consist of either all strings with an even number of 1's, or all strings with an odd number of 1's. From here, we can easily compute the w -coordinates of each of these entries.

These resulting tables are the only two which satisfy these marginals, and thus their difference, an element of degree 2^{m-1} , must be in the Markov basis of $I_{K_{m,n}}$ as desired. For all $n \geq \binom{m}{2}2^{m-2}$ there is a move of degree 2^{m-1} by Corollary 4.2. \square

We suspect that the following conjecture, an extension of the result for $K_{2,n}$, holds.

Conjecture 3.8. *The graph ideal for $G = K_{m,n}$ is generated in degree at most $2^{\min\{m,n\}}$.*

4 Combinatorial Classification of Minimal Generators of Low Degree

In this section, we give algorithms for computing all generators of a given degree in the graph ideal I_G . For degrees two and three, we give an explicit combinatorial characterization of these generators, giving a generating set which generates I_G in degree less than or equal to 3; for arbitrary degree d , we categorize these generators as pullbacks of a distinguished generator in the graph ideal of a fundamental graph X_d . The key lemma is the following, relating generators in I_G to generators in a minor of G .

Lemma 4.1. *Let G be a graph, and let $f = \Pi p_{I_j} - \Pi p_{I_k}$ be a binomial contained in I_G . Then we have the following.*

(a) *If v_i corresponds to a column where all the index strings I_j have the same value, then f is a minimal generator if and only if \tilde{f} is a minimal generator of the graph ideal $G \setminus v_i$, where \tilde{f} is the natural image of f with the column v_i deleted from each index string.*

(b) *If v_i and v_j are adjacent and correspond to columns where for each index string I_j or I_k , the value of that string in each column is identical, then f is a minimal generator if and only if \tilde{f} is a minimal generator, where \tilde{f} is the natural image of f with the two columns v_i and v_j fused. Here, \tilde{f} is an element of the graph ideal of G with those two vertices fused.*

(c) *Suppose v_i and v_j are any two vertices and correspond to columns where for each index string I_j or I_k , the value of that string in each column is identical. In this case, if f is a minimal generator of the graph ideal of G , then \tilde{f} is a minimal generator of the graph ideal of G with those two vertices fused.*

Proof. In each case, a decomposition of \tilde{f} into generators of lower degree can be lifted via the obvious method to a decomposition of f . In (a), this is simply inserting the shared value of v_i into each index string to form a valid index string for G ; in (b) and (c), this is simply duplicating the value of each index string in the obvious manner.

In cases (a) and (b), any decomposition of f must necessarily satisfy the property that each binomial used has the property in question, by considering in (a) any marginal containing v_i and in (b) the marginal corresponding to the edge $v_i v_j$. Therefore, a decomposition of f naturally yields a decomposition of \tilde{f} , so if \tilde{f} is a minimal generator f must be also. \square

This lemma has a corollary legitimizing our notion of minor.

Corollary 4.2. *If H is a minor of G , then $\mu(H) \leq \mu(G)$.*

Proof. It suffices to show $\mu(H) \leq \mu(G)$ if H is obtained from G by a single vertex deletion or edge contraction. However, if it is obtained by a vertex deletion, then by part (a) of Lemma 4.1, every minimal generator of a given degree in I_H lifts to a minimal generator of the same degree in I_G . Similarly, part (b) of Lemma 4.1 guarantees that $\mu(H) \leq \mu(G)$ if H is obtained from G via an edge contraction. \square

A natural extension of this is the following, which agrees with the data in Section 2, but which we have been unable to prove.

Conjecture 4.3. *If H is obtained from G by deleting an edge, then $\mu(H) \leq \mu(G)$.*

This set of minimal generators comes with a group action. In particular, the group $(\mathbb{Z}/2)^n$ acts naturally on $\mathbb{C}[p_I]$, via the element (c_1, \dots, c_n) sending a variable $p_{i_1 \dots i_n}$ to p_{j_1, \dots, j_n} , where $j_r = i_r + c_r$; the sum is evaluated in $\mathbb{Z}/2$. This action consists merely of flipping 0's and 1's in some positions.

Furthermore, the automorphism group $\text{Aut}(G)$ acts naturally on $\mathbb{C}[p_I]$ as well, by permuting the indices according to the permutation of the vertices of the graph, so we have a natural action of $(\mathbb{Z}/2)^n \oplus \text{Aut}(G)$ on $\mathbb{C}[p_I]$. This action maps I_G onto itself; we make the following natural definition.

Definition 4.4. *Two generators are **equivalent** if they lie in the same orbit of $\mathbb{C}[p_I]$ under the action of $(\mathbb{Z}/2)^n \rtimes \text{Aut}(G)$.*

If two generators of graph ideals I_{G_1} and I_{G_2} reduce to equivalent generators in a basic graph H by means of the above manipulations, we say that they are **weakly similar**. If they furthermore reduce to equivalent generators using only manipulations of type (a) and (b), we say that they are **strongly similar**. We are now prepared to define the object pivotal in our categorization of generators of degree d .

Definition 4.5. *Fix a degree $d \geq 2$. The **fundamental graph** X_d has vertex set (S_i, T_i) , where S_i and T_i are subsets of $\{1, \dots, d\}$ with cardinalities $|S_i| = |T_i| \leq d/2$, and if $|S_i| = d/2$ then $1 \in S_i$. Two vertices (S_1, T_1) and (S_2, T_2) are connected by an edge if $|S_1 \cap S_2| = |T_1 \cap T_2|$.*

To this fundamental graph is associated a distinguished element of I_{X_d} .

Definition 4.6. *Fix a degree $d \geq 2$. Then the **distinguished generator** $f_d \in I_{X_d}$ is the binomial*

$$\begin{bmatrix} I_1 \\ \dots \\ I_d \end{bmatrix} - \begin{bmatrix} J_1 \\ \dots \\ J_d \end{bmatrix},$$

where $I_{ji} = 1$ if $j \in S_i$ and 0 otherwise, and similarly $J_{ji} = 1$ if $j \in T_i$ and 0 otherwise.

It is clear that the distinguished generator is actually in I_{X_d} , since for all adjacent v_i and v_j , the number of 11-marginals in I is equal to $S_i \cap S_j$, while the number of 11-marginals in J is equal to $T_i \cap T_j$. By definition of X_d , these are equal, and furthermore, the number of 11-marginals determines the numbers of all other marginals (along with the numbers of 1's in each column of I and J , which are of course identical.)

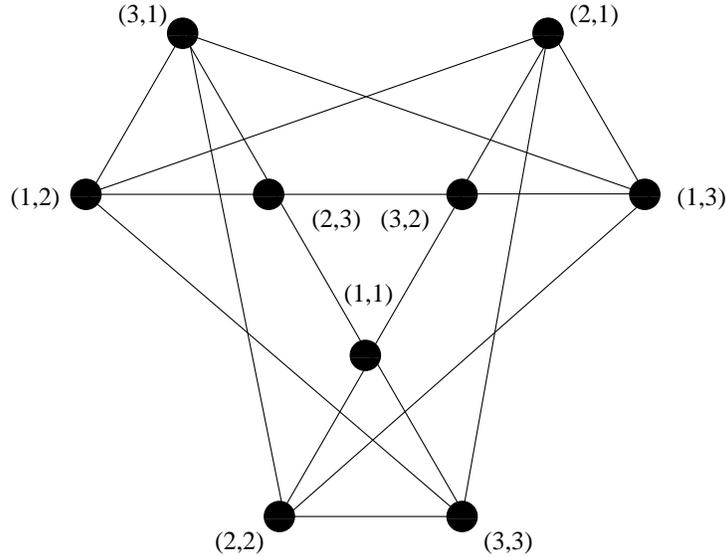


Figure 1: The fundamental graph X_3

Example 4.7. The fundamental graph X_2 has two vertices $(1, 1)$ and $(1, 2)$ which are not connected by an edge. The distinguished generator of I_{X_2} is the binomial

$$\begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

which is just as 2×2 determinant. The fundamental graph X_3 has nine vertices which are $(1, 1), (1, 2), \dots, (3, 3)$. Two vertices (i, j) and (k, l) are connected if and only if $i \neq k$ and $j \neq l$. Each vertex has degree four: X_3 is the edge graph of the 4-polytope $\Delta_2 \times \Delta_2$, the product to two triangles pictured in Figure 1. Note the six triangular prisms which appears as minors of X_3 . The fundamental generator of I_{X_3} is the binomial

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix} - \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}.$$

With these definitions, we can formulate the main theorem of this section, categorizing all generators of degree d .

Theorem 4.8. *Let G be any graph. Then the minimal generators of degree d in I_G can be enumerated by the following procedure.*

1. Consider all graph homomorphisms ϕ from minors H of G to X_d .
2. Determine if the natural image of the fundamental generator \tilde{f}_d is a minimal generator on the image subgraph.
3. If so, consider the pullback $\phi^* \tilde{f}_d$, a binomial of degree d in I_G . We can pull this back to H using Lemma 4.1 part (b) and (c), and then to G using Lemma 4.1 part (a) and (b).

A graph homomorphism $G \rightarrow H$ is simply a map ϕ from vertices of G to vertices of H such that if u and v are adjacent in G , $\phi(u)$ and $\phi(v)$ are adjacent in H . Note that since we have used Lemma 4.1 part (c), the pullback will not always be a minimal generator but the set of moves calculated in this way contains all minimal generators I_G of degree d .

Proof. Suppose we have a generator f of degree d in I_G , written in tableau notation as

$$\begin{bmatrix} I_1 \\ \dots \\ I_d \end{bmatrix} - \begin{bmatrix} J_1 \\ \dots \\ J_d \end{bmatrix},$$

where I and J are 0-1 matrices. Each column of I has the same number of 1's as the corresponding column of J . If this number is either 0 or d , we can delete that vertex via Lemma 4.1 (a) to obtain an equivalent generator in a minor of G , proving the theorem by induction.

Therefore, by flipping 0 with 1 if necessary, we can assume that each column has at most $d/2$ 1's, and if it has $d/2$ 1's then I_i has a 1 in that column. To each vertex v_i associate the pair (S_i, T_i) , where $j \in S_i$ if I_j has a 1 in the column corresponding to v_i , and $j \in T_i$ if J_j has a 1 in that column. If two adjacent vertices have the same pair, we can contract the edge between them via Lemma 4.1 (b) to again obtain an equivalent generator in a minor of G .

If this is not the case, then we claim that the map given by sending v_i to the vertex (S_i, T_i) in X_d is a graph homomorphism. Indeed, all that we need to check is that if v_i and v_j are connected by an edge, $S_i \cap S_j = T_i \cap T_j$ (and it is not the case that $(S_i, T_i) = (S_j, T_j)$, which is true since no two adjacent vertices have the same pair.) But this must be true, since each is just the number of 11-marginals along the edge $v_i v_j$ in the corresponding tables I and J , which are equal since f is in I_G .

Furthermore, this map fuses two vertices v_i and v_j only if the corresponding columns of I and of J are identical. Therefore, by Lemma 4.1 (c), the image of f in I_R , where R is the image subgraph of X_d , must be a minimal generator of X_{I_R} . However, this generator is precisely the natural image of the distinguished generator in the graph ideal I_R . If this is irreducible, then f is produced by the procedure in Theorem 4.8, which we have just done in reverse. If not, then f cannot be a minimal generator by the contrapositive of Lemma 4.1. \square

In this manner, we have reduced the computation of all generators of degree d to the process of determining which images of the distinguished generator in subgraphs of X_d are minimal generators, and of enumerating graph homomorphisms from G to X_d . While the problem of computing graph homomorphisms is a difficult one, we can use symmetry techniques to greatly aid us in many cases. Theorem 4.8 also divulges which generators are weakly similar: those whose corresponding graph homomorphisms have images which are isomorphic subgraphs of X_d .

We now apply Theorem 4.8 to degrees 2 and 3. Consider first generators of degree 2. The fundamental graph X_2 has two vertices, $(1,1)$ and $(1,2)$, which are not connected by an edge. Given a minor of G , it has a homomorphism onto X_2 if and only if there are no edges between the vertices mapped to $(1,1)$ and the vertices mapped to $(1,2)$. In this case the homomorphisms correspond to partitions of the vertices into V_1 and V_2 . Extracting the definition of minor yields the following Corollary.

Corollary 4.9. *Let G be a graph. Then equivalence classes of generators of degree 2 of I_G correspond to partitions $V_1 \cup V_2 \cup V_3$, where there are no edges between V_1 and V_2 . The generator corresponding to this is precisely*

$$\begin{bmatrix} 101 \\ 011 \end{bmatrix} - \begin{bmatrix} 111 \\ 001 \end{bmatrix},$$

where the three columns correspond to V_1, V_2 , and V_3 .

Readers familiar with the study of graphical models and their induced independence statements will recognize this as a theorem which says that the only independence statements induced by a graphical model are the global independence statements. See, for example [10].

Next, we turn our attention to the case of generators of degree 3, using the methods of Theorem 4.8 to obtain a combinatorial classification of all such cubic minimal generators of I_G . The fundamental graph X_3 has nine vertices $\{(1,1), \dots, (3,3)\}$, with (i,j) connected to (k,l) if $i \neq k$ and $j \neq l$. By direct computation, the image of the fundamental generator d_3 in I_R , R a subgraph of X_3 , is a minimal generator if and only if R contains one of the six triangular prism subgraphs of X_3 . Therefore, we can classify cubic generators by finding all homomorphisms from minors of G to the fundamental graph X_3 whose image contains a triangular prism. In particular, if no such homomorphism exists, then I_G cannot have a generator of degree 3. This yields the following corollary.

Corollary 4.10. *For all n , the graph ideal I_{K_n} has no minimal generators of degree 3.*

Proof. The only minors of K_n are copies of K_m for $m \leq n$. Furthermore, all homomorphic images of complete graphs are again complete graphs (indeed, of the same degree.) The only complete graphs occurring in X_3 are K_2 and K_3 , neither of which contains a triangular prism. \square

Corollary 4.10 shows why edge deletion does not behave well with respect to the graph ideal I_G and its Markov basis; this operation obviously can introduce elements of new degrees, since there exist graphs with cubic minimal generators, and every graph can be obtained from a complete graph by edge deletion. The same technique can be used to show that there are no minimal generators of degree 5 in the graph ideal I_{K_n} , since the largest clique in X_5 has size 5, and the distinguished generator cannot be minimal in the graph ideal of these subgraphs since in fact there are no minimal generators of degree 5 in K_i for $i \leq 5$.

In addition to the description of Theorem 4.8, we can obtain a more straightforward combinatorial characterization of minimal generators of degree 3 in graph ideals. We start with a pair of definitions.

Definition 4.11. *Let G be any graph. Then the **3-coloring graph** $C_3(G)$ has vertices equal to the set of proper 3-colorings of G . Two 3-colorings are connected by an edge if one can be obtained from the other by the following (reversible) procedure: pick a color $i \in \{1, 2, 3\}$, pick a connected component of the induced subgraph consisting of all vertices with colors not equal to i , and switch the other two colors on this component.*

Definition 4.12. *A graph G is **3-rigid** if the coloring space $C_3(G)$ is disconnected.*

The crucial example of a 3-rigid graph is the same triangular prism that arose in the analysis of degree 3 via Theorem 4.8. This graph is 3-rigid, since there are only two proper 3-colorings up to permutation of the colors: one triangle (v_1, v_2, v_3) is colored $(1, 2, 3)$, and the other triangle (w_1, w_2, w_3) must be colored either $(2, 3, 1)$ or $(3, 1, 2)$. Here, the vertex labels are chosen so that v_i is adjacent to w_i . It is easy to check that these colorings lie in different connected components of

$C_3(G)$; the connected component of each consists of the colorings obtained from it by permutation of the colors.

We now present a complete description of cubic generators of G based on these combinatorial objects.

Proposition 4.13. *Let G be any graph. Then we can enumerate the (equivalence classes of) cubic minimal generators of the graph ideal I_G as follows.*

- (a) Find all the 3-rigid minors of G .
- (b) For each such 3-rigid minor H , consider all of the connected components of the 3-coloring graph of H_3 . For each connected component, pick a representative 3-coloring R_i .
- (c) For each R_i , $i > 1$, take the element

$$f = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} - \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix},$$

where $a_{jk} = 1$ if either the vertex k of G is deleted in obtaining H or its image in H is colored with color j in R_1 , and $b_{jk} = 1$ if either k is deleted or its image in H is colored with color j in R_i .

Each of these elements f is a minimal generator of I_G in degree 3, and these elements together with the quadratic elements described above generate I_G up to degree 3.

Proof. Suppose we have a cubic minimal generator of I_G , given by

$$f = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} - \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}.$$

We construct two 3-colorings C_A and C_B of a minor of G as follows. For the vertex v_j , consider the j -th column of A and B . If this consists of all 1's or all 0's, delete v_j . If not, exchange 0's and 1's if necessary so that it has exactly one 1. Then, in C_A (resp. C_B), color v_j with the position in which this 1 appears in A (resp. B).

Next, if two adjacent vertices have the same color in A (equivalent to having the same color in B by counting 11-marginals along this edge), then contract that edge. What remains is two proper 3-colorings of a minor H , and when these 3-colorings are converted to a binomial in I_G via the method in part (c), we recover precisely the element f . By Lemma 4.1, the image \tilde{f} in I_H is a minimal generator if and only if f is a minimal generator of I_G .

We claim that the image \tilde{f} is a minimal generator of I_H , i.e. inexpressible as a sum of multiples of quadrics, if and only if C_A and C_B are in different connected components of $C_3(H)$. Indeed, consider a multiple of a binomial generator, say

$$g = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} - \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix}.$$

If we convert the two monomials of g into colorings, the same set of vertices will have color 3 in these colorings. Therefore, the difference between these colorings consists of changing colors from 1 to 2 or vice versa. The only way this can be done while preserving the properness of the coloring is if the change consists of switching the colors 1 and 2 on some connected components of the induced subgraph of H consisting of vertices not colored 3. Therefore, when we add a multiple

of a binomial generator, we end 1 up with an element corresponding to a 3-coloring in the same component of $C_3(H)$, and any two elements connected by an edge in $C_3(H)$ differ by a multiple of a binomial generator.

Consequently, the colorings C_A and C_B are in the same component of $C_3(H)$ if and only if \tilde{f} is not expressible as the sum of multiples of binomials in I_H , which is equivalent to \tilde{f} being a minimal generator of I_H , as desired. \square

Classifying 3-rigid graphs is an interesting problem; the graph $C_3(G)$ has been studied in connection with the problem of picking a random 3-coloring of a graph [16]. Indeed, the flip interchanging two colors on a connected component is precisely the move used in the Wang-Swendsen-Kotecký algorithm to pick a random k -coloring of a graph, and this scheme has ties to mathematical physics [17]. There are simple operations to produce 3-rigid graphs from other ones, but the triangular prism seems to be the only 3-rigid graph without a proper 3-rigid minor.

This method, paralleling Theorem 4.8, can be extended to higher degrees. However, it rapidly becomes unwieldy, as the vertices can now be colored with sets of $d/2$ colors, and the moves are more complicated, consisting of all moves keeping one of the colors fixed. For instance, the fundamental graph X_4 has 34 vertices and understanding the homomorphisms to this graph seems difficult.

5 Algebraic Degree of Forests

A recent series of results gave a very thorough description of the family of ideals of decomposable models [3, 6, 15]. A special case of these results is the following fundamental theorem.

Theorem 5.1. *The ideal I_G is minimally generated by quadrics if and only if G is a forest. In this case, the set of quadratic squarefree binomials in I_G forms a Gröbner basis with respect to the reverse lexicographic term order with $p_{0\dots 0} \prec p_{0\dots 01} \prec \dots \prec p_{1\dots 1}$.*

Sturmfels [14] posed the natural follow-up problem of calculating the degree of the toric ideal I_G . The degree of the toric ideal is interesting in statistics because it provides a natural upper bound for the maximum likelihood degree of the toric ideal [14]. In this section we give combinatorial formulae for the degree of the graph model ideal I_G when G is a forest. As the maximum likelihood degree of a forest is always 1, we see that the degree can be arbitrarily far from the maximum likelihood degree. To perform these degree computations, we first recall a result about the degree of a general toric ideal. This result can be found in [13].

Theorem 5.2. *Let A be a $d \times n$ matrix whose toric ideal I_A is homogeneous in the standard \mathbb{Z} -grading. Then the degree of the ideal I_A (= degree of the projective toric variety defined by I_A) is equal to the normalized volume of the lattice polytope $Q = \text{conv}(A)$.*

Henceforth, the normalized volume of a lattice polytope Q will be denoted $\text{Vol}(Q)$. This theorem reduces the problem of calculating degree to computing the normalized volume of polytope. We now record some basic facts about the polytope P_G when the underlying graph is a forest.

Lemma 5.3. *The polytope P_G has dimension equal to the sum of the number of vertices and the number of edges of the graph (this is true for any graph). There are precisely $4 \cdot |E(G)| + 2 \cdot |\text{Iso}(G)|$ facets of P_G when G is a forest. If the variables in marginal space are labelled $y_{i_j, i_k}^{(j,k)}$ for the variables coming from an edge and $y_{i_l}^{(l)}$ for the variables coming from an isolated vertex, then the facets are given by the inequalities*

$$y_{i_j, i_k}^{(j,k)} \geq 0 \text{ and } y_{i_l}^{(l)} \geq 0.$$

Proof. The dimension formula appears in [9]. The polyhedral results are a direct consequence of the closed form expressions for maximum likelihood estimates in decomposable models in [10]. \square

The following lemma implies that to compute the degree of I_G when G is a forest, one need only describe a formula which is valid for trees. Furthermore, this lemma is important for carrying out the recursive computations implied by Theorem 5.5.

Lemma 5.4. *Let G be a graph with a partition of the vertices $\{V_1, V_2\}$ such that there is no edge in G between the V_1 and V_2 . Let G_1 and G_2 be the corresponding induced subgraphs. Let d_1 and d_2 be the corresponding dimensions of the polytopes P_{G_1} and P_{G_2} ; that is, $d_i = |V_i| + |E(G_i)|$. Then we have*

$$\text{Vol}(P_G) = \binom{d_1 + d_2}{d_1} \cdot \text{Vol}(P_{G_1}) \cdot \text{Vol}(P_{G_2}).$$

Proof. With these restrictions on the graph G , we have $P_G = P_{G_1} \times P_{G_2}$. Equation 5.4 is then the usual formula for the normalized volume of the direct product in terms of the normalized volumes of the components of the product. \square

We now come to the main theorem of this section.

Theorem 5.5. *Let G be a tree with n -vertices. Then the degree of the toric ideal I_G can be calculated by the formula*

$$\text{deg}(I_G) = \frac{1}{2} \sum_{e \in E(G)} \text{deg}(I_{G \setminus e})$$

where the notation $G \setminus e$ denotes the graph G with the edge e removed.

Proof. As previously indicated, we prove the theorem by calculating the volume of the corresponding polytope P_G . Theorem 5.1 implies that the pulling triangulation of P_G induced by the reverse lexicographic term order above is unimodular. This in turn, implies that the normalized volume of P_G is equal to the sum of the normalized volumes of the facets of P_G which do not contain the vertex indexed by the variable $p_{1 \dots 1}$ (see [13] for all the definitions and relevant theory). This is where the polyhedral description of P_G when G is a forest becomes essential. We see from the polyhedral characterization that there are exactly $n - 1$ facets of P_G which do not contain this “last” vertex, and that they are indexed by the edges of G . We will show that the normalized volume of the facet F_e of P_G which is indexed by the edge e has volume precisely $\frac{1}{2} \text{Vol}(P_{G \setminus e})$ which will complete the proof.

There are two cases to consider: either the edge in question has one node a leaf or not (the case of the graph on two vertices with a lone edge is clear, by a direct calculation). We will handle the two cases separately.

Case 1: We may suppose without loss of generality that our edge e is $\{1, 2\}$, the vertex 1 is a leaf and the vertex 2 has the edge $\{2, 3\}$ incident to it. Then the matrix whose columns correspond to the vertices of P_G has the top eight rows which look like

$$\begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{pmatrix}$$

with this 8×8 block repeated 2^{n-3} times across the first eight rows. We claim that the facet which corresponds to the inequality $y_{1,1}^{(1,2)} \geq 0$ (corresponding to the fourth row of the above matrix) has volume equal to $\frac{1}{2} \text{Vol}(P_{G \setminus \{1,2\}})$. Note the the vertices of P_G which lie on this facet are precisely the $3 \cdot 2^{n-2}$ vertices of P_G which have a zero in the fourth row. First we show that this facet is naturally isomorphic to a sub-configuration of $P_{G \setminus \{1,2\}}$. Consider the matrix $A_{G \setminus \{1,2\}}$ whose columns give the vertices of $P_{G \setminus \{1,2\}}$. This matrix has two fewer rows than the matrix A_G above and is almost the same: its first six rows look like

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

To show the natural isomorphism mentioned above, it suffices to show that there is a unimodular linear transformation from the first six columns of the first matrix above to the first six columns of the second matrix above. Such a linear transformation is obtained by replacing the first row by the sum of the first and second rows, and then deleting the second and fourth rows. We can delete the second and fourth rows because they are linear combinations of other rows and hence do not change the polyhedral description. Such a transformation is clearly unimodular.

Now that we have shown that our configuration of $3 \cdot 2^{n-2}$ points sits naturally inside $P_{G \setminus \{1,2\}}$, we wish to compute its volume. For this, we show that there is a hyperplane which divides $P_{G \setminus \{1,2\}}$ into two congruent pieces, one of which is the convex hull of our new configuration of $3 \cdot 2^{n-2}$ points. This hyperplane is given by the equation

$$y_0^{(1)} - y_1^{(1)} + y_{0,0}^{(2,3)} + y_{0,1}^{(2,3)} - y_{1,0}^{(2,3)} - y_{1,1}^{(2,3)} = 0.$$

Note that exactly 2^{n-1} vertices of $P_{G \setminus \{1,2\}}$ lie on this hyperplane (these are the ones corresponding to the middle four columns of the submatrix of $A_{G \setminus \{1,2\}}$ displayed above) and the remaining 2^{n-1} vertices are split equally on each side of the hyperplane. In particular, all of the vertices from our configuration of $3 \cdot 2^{n-2}$ points lie on the nonnegative side of this hyperplane and the remaining 2^{n-2} points are on the negative side. Furthermore, there is a natural reflexive symmetry across this hyperplane. To complete the proof, we must show more: not only is the point configuration naturally “cut in half” by this hyperplane, but so is the polytope $P_{G \setminus \{1,2\}}$. This follows from a direct computation with the eight points listed above. We performed the computation using the program PORTA [1].

Case 2: The argument is very similar to case 1; we will sketch the relevant details. We may assume that our edge is the edge $\{2,3\}$. Since neither 2 nor 3 is a leaf we may assume G also

contains the edges $\{1, 2\}$ and $\{3, 4\}$. With these conditions, the first 12 rows of our matrix looks like

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{pmatrix}$$

with this block repeated 2^{n-4} times. We wish to show that the facet defined by the inequality $y_{1,1}^{(2,3)} \geq 0$ (corresponding to the eighth row in the above matrix) has volume equal to $\frac{1}{2} \text{Vol}(P_{G \setminus \{2,3\}})$. The vertices which lie on this facet are precisely the $3 \cdot 2^{n-2}$ vertices with a zero in the eighth row in this matrix representation. First we show that this facet naturally appears as a sub-configuration of $P_{G \setminus \{2,3\}}$. This can be achieved by applying a unimodular transformation to the configuration: the key point is that once we restrict attention to the facet, the middle 4 rows of the above configuration can be written as linear combinations of the other rows and hence are redundant in terms of the polyhedral description.

Now we show that there is a hyperplane which divides the polytope $P_{G \setminus (2,3)}$ in half. This is just the hyperplane given by

$$y_{0,0}^{(1,2)} - y_{0,1}^{(1,2)} + y_{1,0}^{(1,2)} - y_{1,1}^{(1,2)} + y_{0,0}^{(3,4)} + y_{0,1}^{(3,4)} - y_{1,0}^{(3,4)} - y_{1,1}^{(3,4)} = 0.$$

Note that our configuration of $3 \cdot 2^{n-2}$ points are precisely the points on the nonnegative side of this hyperplane. Furthermore, there is a natural reflexive symmetry across the hyperplane. A direct calculation shows that this hyperplane not only separates the point configuration, but also divides the polytope into two symmetric pieces with the the desired integral points as vertices. Thus we deduce the desired equation of volumes. \square

For some special families of trees we use this recurrence relation to deduce simple formulae for the degree. These appear in the following corollaries.

Corollary 5.6. *Let $K_{1,n}$ denote a star graph with n leaves. Then $\text{deg}(I_{K_{1,n}}) = (n!)^2$.*

Proof. Removing any edge of the graph $K_{1,n}$ produces the graph consisting of the disjoint union of a $K_{1,n-1}$ and an isolated point. Hence from theorem 5.5 and lemma 5.4 we deduce that

$$\text{deg}(I_{K_{1,n}}) = n \cdot \frac{1}{2} \binom{2n}{1} \cdot \text{deg}(I_{K_{1,n-1}}) = n^2 \cdot \text{deg}(I_{K_{1,n-1}}).$$

Since $\text{deg}(I_{K_{1,1}}) = 1$ we have the desired result. \square

Corollary 5.7. *Let T_n denote the graph of the n -chain and $d_n = \deg(I_{T_n})$. Then d_n satisfies the recurrence*

$$d_{n+1} = \frac{1}{2} \sum_{i=1}^n \binom{2n}{2i-1} d_i d_{n+1-i}$$

with $d_1 = 1$. Furthermore, we have the equality of generating functions

$$\sum_{n=1}^{\infty} \frac{d_n}{(2n-1)!} x^{2n-1} = \sqrt{2} \tan\left(\frac{x}{\sqrt{2}}\right).$$

Proof. The recurrence relation 5.7 follows immediately from the formula in Theorem 5.5 and by applying Lemma 5.4 to the graph consisting of two disjoint chains of length i and $n+1-i$.

To deduce the equality of generating functions, let $y = \frac{1}{2} \sum_{n=1}^{\infty} \frac{d_n}{(2n-1)!} x^{2n-1}$. The recurrence relation implies that $2y' - 2 = y^2$. Solving the differential equation yields the desired formula. \square

The recurrence relation and generating function in the case of the n -chain also appears in a paper by Poupard [11], but we do not know how to show that the objects we are counting (simplices in a regular unimodular triangulation) are in bijection with the objects she was counting (types of binary trees).

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