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Toric Geometry of Cuts and Splits

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1. Introduction

With any finite graph $G = (V, E)$ we associate a projective toric variety X_G over a field $\mathbb{K}$ as follows. The coordinates $q_{A|B}$ of the ambient projective space are indexed by unordered partitions $A|B$ of the vertex set V. The dense torus has two coordinates (s_{ij}, t_{ij}) for each edge $\{i, j\} \in E$. The polynomial rings in these two sets of unknowns are

$$\mathbb{K}[q] := \mathbb{K}[q_{A|B} \mid A \cup B = V,\ A \cap B = \emptyset],$$
$$\mathbb{K}[s,t] := \mathbb{K}[s_{ij}, t_{ij} \mid \{i, j\} \in E].$$

Each partition $A|B$ of the vertex set V defines a subset $\mathrm{Cut}(A|B)$ of the edge set E. Namely, $\mathrm{Cut}(A|B)$ is the set of edges $\{i, j\}$ such that $i \in A$, $j \in B$ or $i \in B$, $j \in A$. The variety we wish to study is specified by the following homomorphism of polynomial rings:

$$\phi_G \colon \mathbb{K}[q] \to \mathbb{K}[s,t], \qquad q_{A|B} \mapsto \prod_{\{i,j\}\in \mathrm{Cut}(A|B)} s_{ij} \cdot \prod_{\{i,j\}\in E\setminus \mathrm{Cut}(A|B)} t_{ij}. \tag{1.1}$$

One may wish to think of s and t as abbreviations for "separated" and "together". The kernel of ϕ_G is a homogeneous toric ideal I_G, which we call the *cut ideal* of the graph G. We are interested in the projective toric variety X_G that is defined by the cut ideal I_G.

Example 1.1. Let $G = K_4$ be the complete graph on four nodes, so $V = \{1, 2, 3, 4\}$ and $E = \{12, 13, 14, 23, 24, 34\}$. The ring map ϕ_{K_4} is specified by

$$\begin{aligned}
q_{|1234} &\mapsto t_{12}t_{13}t_{14}t_{23}t_{24}t_{34}, & q_{1|234} &\mapsto s_{12}s_{13}s_{14}t_{23}t_{24}t_{34},\\
q_{12|34} &\mapsto t_{12}s_{13}s_{14}s_{23}s_{24}t_{34}, & q_{2|134} &\mapsto s_{12}t_{13}t_{14}s_{23}s_{24}t_{34},\\
q_{13|24} &\mapsto s_{12}t_{13}s_{14}s_{23}t_{24}s_{34}, & q_{3|124} &\mapsto t_{12}s_{13}t_{14}s_{23}t_{24}s_{34},\\
q_{14|23} &\mapsto s_{12}s_{13}t_{14}t_{23}s_{24}s_{34}, & q_{4|123} &\mapsto t_{12}t_{13}s_{14}t_{23}s_{24}s_{34}.
\end{aligned}$$

The cut ideal for the complete graph on four nodes is the principal ideal

$$I_{K_4} = \langle q_{|1234}q_{12|34}q_{13|24}q_{14|23} - q_{1|234}q_{2|134}q_{3|124}q_{123|4} \rangle.$$

Thus the toric variety X_{K_4} defined by I_{K_4} is a quartic hypersurface in $\mathbb{P}^7$.

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EXAMPLE 1.2. Let $G = C_4$ be the 4-cycle with edges $E = \{12, 23, 34, 14\}$. The ring map ϕ_{C_4} is derived from ϕ_{K_4} in Example 1.1 by setting $s_{13} = t_{13} = s_{24} = t_{24} = 1$, and we find

$$I_{C_4} = \langle q_{|1234}q_{13|24} - q_{1|234}q_{124|3}, \\ q_{|1234}q_{13|24} - q_{123|4}q_{134|2}, q_{|1234}q_{13|24} - q_{12|34}q_{14|23}\rangle.$$

Thus the toric variety X_{C_4} is a complete intersection of three quadrics in $\mathbb{P}^7$.

We usually take the vertex set V of our graph G to be $[n] := \{1, 2, \ldots, n\}$, so that $\mathbb{K}[q]$ is a polynomial ring in 2^{n-1} unknowns and $\mathbb{K}[s, t]$ is a polynomial ring in $2|E| \leq n(n-1)$ unknowns. Each edge $\{i, j\} \in E$ corresponds to a projective line $\mathbb{P}^1$ with homogeneous coordinates $(s_{ij} : t_{ij})$, and the ring map ϕ_G represents a rational map from the product of projective lines $(\mathbb{P}^1)^{|E|}$ into the high-dimensional projective space $\mathbb{P}^{2^{n-1}-1}$. The image of this map is our toric variety X_G, which has dimension $|E| \leq n(n-1)/2$ in $\mathbb{P}^{2^{n-1}-1}$.

The geometry of X_G and the algebraic properties of its ideal I_G are determined by the *cut polytope* $\mathrm{Cut}^{\square}(G)$, which is the convex hull in $\mathbb{R}^{|E|}$ of the *cut semimetrics* $\delta_{A|B}$. Here $A|B$ runs over all unordered partitions of V, and $\delta_{A|B} \in \{0, 1\}^{|E|}$ is defined as

$$\delta_{A|B}(\{i, j\}) = \begin{cases} 1 & \text{if } |A \cap \{i, j\}| = 1, \\ 0 & \text{otherwise.} \end{cases}$$

Indeed, the convex hull of the exponent vectors in ϕ_G is affinely isomorphic to $\mathrm{Cut}^{\square}(G)$. In Example 1.1 and 1.2, respectively, we find that $\mathrm{Cut}^{\square}(K_4)$ is the cyclic 6-polytope with eight vertices and that $\mathrm{Cut}^{\square}(C_4)$ is the 4-dimensional crosspolytope (which is the dual to the 4-cube).

The cut polytope $\mathrm{Cut}^{\square}(G)$ is well studied in combinatorial optimization and is a central player in the book *Geometry of Cuts and Metrics* by Déza and Laurent [7]. The title of this paper is a reference to their book, and it reflects our desire to import this body of work into commutative algebra and algebraic statistics. In particular, we explore the extent to which the known polyhedral structure of $\mathrm{Cut}^{\square}(G)$ can be used to determine algebraic results about the cut ideals I_G. For instance, the known fact that $\mathrm{Cut}^{\square}(G)$ is full-dimensional implies that $\dim X_G = |E|$. A more significant example of such an algebraic result is derived from recent work of the second author [20], as follows.

THEOREM 1.3. *The cut ideal I_G has a squarefree reverse lexicographic initial ideal if and only if the graph G is free of K_5 minors and every induced cycle in G has length* 3 *or* 4. *In this case, every reverse lexicographic initial ideal of I_G is squarefree.*

Proof. The initial ideal of a toric ideal is squarefree if and only if the corresponding regular triangulation of the associated polytope is unimodular [18, Sec. 8]. Because the symmetry group of $\mathrm{Cut}^{\square}(G)$ is transitive on its vertices, the cut polytope $\mathrm{Cut}^{\square}(G)$ has a unimodular revlex (pulling) triangulation if and only if every revlex triangulation is unimodular [20, Cor. 2.5]. A polytope all of whose revlex triangulations are unimodular is called *compressed*. Now simply apply the classification of compressed cut polytopes given in [20, Thm. 3.2]. □

In Section 2 we describe how generating sets (Markov bases) and Gröbner bases of the cut ideal I_G can be computed when the graph G admits a certain clique-sum decomposition. The key tool here is the toric fiber product introduced in [21]. In Section 3, we summarize the results of our computational experiments and outline some conjectures that were suggested by our computations.

In the last two sections we present applications to algebraic statistics. In Section 4 we relate cut ideals to the binary graph models of [6] and to Markov random fields. In Section 5 we relate cut ideals to phylogenetic models on split systems, after Bryant [2]. These generalize the binary Jukes–Cantor models studied in [4] and [19].

2. Clique Sums and Toric Fiber Products

Our goal in this section is to relate the graph-theoretic operation of taking clique sums to the ideal-theoretic operation of taking the toric fiber product, as explained in [21]. This operation will serve as a tool for reducing the computation of the cut ideals I_G to cut ideals of smaller graphs (and that, hence, involve fewer indeterminates).

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be graphs such that $V_1 \cap V_2$ is a clique of both graphs. The new graph $G = G_1 \# G_2$ with vertex set $V = V_1 \cup V_2$ and edge set $E = E_1 \cup E_2$ is called the *clique sum* of G_1 and G_2 along $V_1 \cap V_2$. If the cardinality of $V_1 \cap V_2$ is $k+1$, this operation is also called a *k-sum* of the graphs. We suppose throughout that $k \leq 2$.

We now explain how binomials in the cut ideal I_G can be constructed from binomials in the smaller ideals I_{G_1} and I_{G_2}. Consider an arbitrary binomial of degree d in the first smaller cut ideal I_{G_1}, say

$$\mathbf{f} = \prod_{i=1}^{d} q_{A_i|B_i} - \prod_{i=1}^{d} q_{C_i|D_i}.$$

Since $V_1 \cap V_2$ is a clique in G_1 of cardinality ≤ 3, we can permute the unknowns and partitions so that $A_i \cap V_1 \cap V_2 = C_i \cap V_1 \cap V_2$ for all i. This is a consequence of the fact that $I_{K_{k+1}}$ is the zero ideal for $k \leq 2$. For any ordered list EF of d partitions of $V_2 \backslash V_1$,

$$EF = (E_1|F_1, E_2|F_2, \ldots, E_d|F_d),$$

we define a new binomial that is easily seen to be in the cut ideal I_G of the big graph:

$$\mathbf{f}^{EF} := \prod_{i=1}^{d} q_{A_i \cup E_i|B_i \cup F_i} - \prod_{i=1}^{d} q_{C_i \cup E_i|D_i \cup F_i}.$$

This construction works verbatim if we switch the components G_1 and G_2, so that, for any binomial $\mathbf{f}$ in I_{G_2} and any ordered list EF of $\deg(\mathbf{f})$ partitions of $V_1 \backslash V_2$, we get a binomial $\mathbf{f}^{EF}$ in I_G. Moreover, if $\mathbf{F}$ is any set of binomials in I_{G_1} or in I_{G_2} then we define

$$\mathrm{Lift}(\mathbf{F}) := \{\mathbf{f}^{EF} \mid \mathbf{f} \in \mathbf{F},\ EF = \{E_i \mid F_i\}_{i=1}^{\deg \mathbf{f}}\} \tag{2.1}$$

as the union of all binomials of the form $\mathbf{f}^{EF}$ described previously.

We also define an additional set $\mathrm{Quad}(G_1, G_2)$ of quadratic binomials in I_G as follows. Let $A \mid B$ be any unordered partition of $V_1 \cap V_2$, let $C_1 \mid D_1$ and $E_1 \mid F_1$ be any ordered partitions of $V_1 \backslash V_2$, and let $C_2 \mid D_2$ and $E_2 \mid F_2$ be any ordered partitions of $V_2 \backslash V_1$. Then

$$q_{A\cup C_1\cup C_2 \mid B\cup D_1\cup D_2} \cdot q_{A\cup E_1\cup E_2 \mid B\cup F_1\cup F_2} - q_{A\cup E_1\cup C_2 \mid B\cup F_1\cup D_2} \cdot q_{A\cup C_1\cup E_2 \mid B\cup D_1\cup F_2} \tag{2.2}$$

is in $\mathrm{Quad}(G_1, G_2)$, and these are all the binomials in $\mathrm{Quad}(G_1, G_2)$. For each fixed $A \mid B$, we can express the quadrics (2.2) as the 2×2 minors of a certain matrix $(q_{\cdot|\cdot})$ of format $2^{|V_2 \backslash V_1|} \times 2^{|V_1 \backslash V_2|}$. The following theorem will be our main result in Section 2.

THEOREM 2.1. *Let $G = G_1 \# G_2$ be a* 0-, 1-, *or* 2-*sum of G_1 and G_2 and suppose that $\mathbf{F}_1$ and $\mathbf{F}_2$ are binomial generating sets for the smaller cut ideals I_{G_1} and I_{G_2}. Then*

$$\mathbf{M} = \mathrm{Lift}(\mathbf{F}_1) \cup \mathrm{Lift}(\mathbf{F}_2) \cup \mathrm{Quad}(G_1, G_2)$$

is a generating set for the big cut ideal I_G. Furthermore, if $\mathbf{F}_1$ and $\mathbf{F}_2$ are Gröbner bases for I_{G_1} and I_{G_2} then there exists a term order such that $\mathbf{M}$ is a Gröbner basis for I_G.

REMARK 2.2. If the intersection graph $G_1 \cap G_2$ is not a clique of cardinality ≤ 3, then it is generally not possible to lift every binomial in I_{G_1} and I_{G_2} to the cut ideal I_G.

Before presenting the proof of Theorem 2.1 we discuss several examples and corollaries.

EXAMPLE 2.3. If $G = G_1 \# G_2$ is a 0-sum, then its cut ideal I_G is the usual Segre product of I_{G_1} and I_{G_2}. Indeed, in this case the singleton $V_1 \cap V_2$ has only one ordered partition and $\mathrm{Quad}(G_1, G_2)$ is the ideal of 2×2 minors of the corresponding matrix $(q_{\cdot|\cdot})$. For instance, if G_1 is the graph with one edge $\{1, 2\}$ and G_2 is the graph with one edge $\{2, 3\}$, so that $V_1 \cap V_2 = \{2\}$, then $I_G = \langle \mathrm{Quad}(G_1, G_2) \rangle$ is generated by the determinant of

$$(q_{\cdot|\cdot}) = \begin{pmatrix} q_{|123} & q_{1|23} \\ q_{12|3} & q_{2|13} \end{pmatrix}.$$

Now suppose that G is any tree with n leaves. Iterating the 0-sum construction from $n = 3$ to $n > 3$, we see that X_G is the Segre embedding of $(\mathbb{P}^1)^{n-1}$ into $\mathbb{P}^{2^{n-1}-1}$.

Further generalization of Example 2.3 leads to the following result.

COROLLARY 2.4. *The toric variety X_G is smooth if and only if G is free of C_4 minors.*

Proof. We first prove the "if" direction. If G is free of C_4 minors, so that all its simple cycles have length 3, then G can be built from K_2 and K_3 by taking repeated 0-sums. Both the ideals I_{K_2} and I_{K_3} are zero and live in polynomial rings with two and four unknowns, respectively. Thus X_{K_2} is $\mathbb{P}^1$ and X_{K_3} is $\mathbb{P}^3$. The 0-sum construction amounts to taking Segre products, hence

$$X_G = \mathbb{P}^1 \times \mathbb{P}^1 \times \cdots \times \mathbb{P}^1 \times \mathbb{P}^3 \times \mathbb{P}^3 \times \cdots \times \mathbb{P}^3.$$

This Segre variety is smooth. The "only if" direction states that any smooth X_G has this special form. To prove this, suppose that G has C_4 as a minor. Then either G has an induced cycle of length $n \geq 4$ or G has, as an induced subgraph, the complete graph K_4 or the graph obtained from K_4 by removing one edge. Let H denote this induced subgraph. Using a forward reference to Lemma 3.2, we note that $\mathrm{Cut}^{\square}(H)$ is a face of $\mathrm{Cut}^{\square}(G)$. Therefore, it suffices to prove that X_H is not smooth. We saw in the Introduction that $\mathrm{Cut}^{\square}(K_4)$ and $\mathrm{Cut}^{\square}(C_4)$ are not simple. Using the familiar characterization of toric singularities [9, Sec. 2.1], this implies that the corresponding toric varieties X_H are not smooth. The same can be checked for cycles of length $n \geq 5$.

In the remaining case, $H = K_4\backslash\{14\}$ is the 1-sum of the triangle on $\{1, 2, 3\}$ and the triangle on $\{2, 3, 4\}$. Its variety X_H is the complete intersection of two quadrics in $\mathbb{P}^7$:

$$I_H = \left\langle \det\begin{pmatrix} q_{|1234} & q_{1|234} \\ q_{4|123} & q_{14|23} \end{pmatrix}, \det\begin{pmatrix} q_{2|134} & q_{12|34} \\ q_{13|24} & q_{3|124} \end{pmatrix} \right\rangle.$$

The singular locus of X_H consists of the two 3-planes in $\mathbb{P}^7$ where these matrices are zero. The cut polytope $\mathrm{Cut}^{\square}(H)$ is the free join of two squares, a nonsimple 5-polytope. $\square$

The following example naturally generalizes the graph $H = K_4\backslash\{14\}$ discussed previously.

EXAMPLE 2.5. Let $G = K_5\backslash\{15\}$ be the graph on five vertices obtained from the complete graph by deleting an edge. Thus G is the 2-sum of the complete graph G_1 on $V_1 = \{1, 2, 3, 4\}$ and the complete graph G_2 on $V_2 = \{2, 3, 4, 5\}$. Since I_{K_4} is generated by a quartic, we deduce that I_G is generated by quadrics and quartics. There are four quadrics:

$$\begin{aligned}\mathrm{Quad}(G_1, G_2) = \{&q_{15|234}q_{|12345} - q_{1|2345}q_{5|1234}, q_{34|125}q_{2|1345} - q_{12|345}q_{25|134}, \\ &q_{24|135}q_{3|1245} - q_{13|245}q_{35|124}, q_{23|145}q_{4|1235} - q_{14|235}q_{45|123}\}.\end{aligned}$$

The ideals I_{G_1} and I_{G_2} are each generated by a single quartic, as in Example 1.1, and $\mathbf{F}_1$ and $\mathbf{F}_2$ are the singletons consisting of these quartics. Now, the set $V_2\backslash V_1 = \{5\}$ has two ordered partitions, namely $5|$ and $|5$, so there are $2^4 = 16$ ordered lists of ordered partitions $E|F$. Each defines a quartic in I_G, so $\mathrm{Lift}(\mathbf{F}_1)$ consists of sixteen quartics, such as

$$\mathbf{f}_1 = q_{|12345}q_{34|125}q_{24|135}q_{23|145} - q_{1|2345}q_{25|134}q_{35|124}q_{45|123},$$
$$\mathbf{f}_2 = q_{5|1234}q_{12|345}q_{13|245}q_{14|235} - q_{15|234}q_{2|1345}q_{3|1245}q_{4|1235}.$$

Likewise, $\mathrm{Lift}(\mathbf{F}_2)$ consists of sixteen quartics, and these include

$$\mathbf{f}_3 = q_{1|2345}q_{25|134}q_{35|124}q_{45|123} - q_{15|234}q_{2|1345}q_{3|1245}q_{4|1235},$$
$$\mathbf{f}_4 = q_{|12345}q_{34|125}q_{24|135}q_{23|145} - q_{5|1234}q_{12|345}q_{13|245}q_{14|235}.$$

We conclude that the set $\mathbf{M}$ in Theorem 2.1 consists of 36 binomials and that these binomials generate I_G. However, they are not a minimal generating set, because

$$\mathbf{f}_1 - \mathbf{f}_2 + \mathbf{f}_3 - \mathbf{f}_4 = 0.$$

The set of 35 binomials obtained by removing any of the $\mathbf{f}_i$ is a minimal generating set for I_G. We also find that the minimal free resolution of I_G has the following Betti diagram:

```
total:  1 35 134 200 134 35 1
    0:  1  .   .   .   .  . .
    1:  .  4   .   .   .  . .
    2:  .  .   6   .   .  . .
    3:  . 31 128 200 128 31 .
    4:  .  .   .   .   6  . .
    5:  .  .   .   .   .  4 .
    6:  .  .   .   .   .  . 1
```

(Macaulay 2 output). Thus the toric 9-fold $X_G \subset \mathbb{P}^{15}$ is arithmetically Gorenstein. The degree of X_G is 80.

We shall derive Theorem 2.1 from the results in [21]. Specifically, we shall identify the cut ideal of $G = G_1 \# G_2$ as a toric fiber product. We begin by reviewing the setup of [21]. Let $r > 0$ be a positive integer and let $s, t \in \mathbb{N}^r$ be two vectors of positive integers. Let

$$\mathbb{K}[x] = \mathbb{K}[x^i_j \mid i \in [r],\ j \in [s_i]] \quad \text{and} \quad \mathbb{K}[y] = \mathbb{K}[y^i_k \mid i \in [r],\ k \in [t_i]]$$

be two polynomial rings with a compatible d-dimensional multigrading

$$\deg(x^i_j) = \deg(y^i_k) = \mathbf{a}^i \in \mathbb{Z}^d \quad \text{for } i = 1, 2, \ldots, r.$$

We abbreviate the collection of degree vectors by $\mathcal{A} = \{\mathbf{a}^1, \mathbf{a}^2, \ldots, \mathbf{a}^r\} \subset \mathbb{Z}^d$.

If I and J are the respective homogeneous ideals of $\mathbb{K}[x]$ and $\mathbb{K}[y]$, then the quotient rings $R = \mathbb{K}[x]/I$ and $S = \mathbb{K}[y]/J$ are also multigraded by $\mathcal{A}$. Consider the polynomial ring

$$\mathbb{K}[z] = \mathbb{K}[z^i_{jk} \mid i \in [r],\ j \in [s_i],\ k \in [t_i]],$$

and consider the $\mathbb{K}$-algebra homomorphism

$$\phi_{I,J} : \mathbb{K}[z] \to R \otimes_{\mathbb{K}} S,\ z^i_{jk} \mapsto x^i_j \otimes y^i_k.$$

The kernel of $\phi_{I,J}$ is called the *toric fiber product* of I and J and is denoted

$$I \times_{\mathcal{A}} J = \ker(\phi_{I,J}).$$

The following statement combines Theorem 2.8 and Corollary 2.10 in [21].

THEOREM 2.6. *Suppose that the set $\mathcal{A}$ of degree vectors is linearly independent. Let $\mathbf{F}_1$ be a homogeneous generating set for I and let $\mathbf{F}_2$ be a homogeneous generating set for J. Then*

$$\mathbf{M} = \mathrm{Lift}(\mathbf{F}_1) \cup \mathrm{Lift}(\mathbf{F}_2) \cup \mathrm{Quad}_{\mathcal{A}}$$

is a homogeneous generating set for $I \times_{\mathcal{A}} J$. Furthermore, if $\mathbf{F}_1$ and $\mathbf{F}_2$ are Gröbner bases for I and J, then there exists a term order such that $\mathbf{M}$ is a Gröbner basis for $I \times_{\mathcal{A}} J$.

Here $\mathrm{Quad}_{\mathcal{A}}$ is the collection of quadrics $z^i_{jk} z^i_{lm} - z^i_{jm} z^i_{lk}$ that generates $\langle 0 \rangle \times_{\mathcal{A}} \langle 0 \rangle$. The sets $\mathrm{Lift}(\mathbf{F}_i)$ have a nice description in terms of tableaux, given in [21, Sec. 2].

Proof of Theorem 2.1. Suppose $G = G_1 \# G_2$ with vertex set $V = V_1 \cup V_2$ and edge set $E = E_1 \cup E_2$, where $V_1 \cap V_2$ is a clique of size $k+1$ in both graphs. We set $d = \binom{k+1}{2} + 1$ and $r = 2^{k-1}$, and we define $\mathcal{A}$ as the vector configuration corresponding to the vertices of the cut polytope $\mathrm{Cut}^{\square}(K_{k+1})$ of the clique. The $\mathcal{A}$-grading on $\mathbb{K}[q]$ is defined by restricting the product in (1.1) to those edges $\{i, j\}$ that lie in $E_1 \cap E_2$. In other words, the degree of $q_{A|B}$ is the vertex of $\mathrm{Cut}^{\square}(K_{k+1})$ indexed by the partition $A \cap V_1 \cap V_2 \,|\, B \cap V_1 \cap V_2$.

The configuration $\mathcal{A}$ of degree vectors is linearly independent if and only if the cut polytope $\mathrm{Cut}^{\square}(K_{k+1})$ is a simplex if and only if $k \leq 2$. Theorem 2.6 requires the set $\mathcal{A}$ to be linear independent. This explains the crucial hypothesis $k \leq 2$ in Theorem 2.1.

All three cut ideals I_G, I_{G_1}, and I_{G_2} are homogeneous with respect to the indicated grading. We will show that I_G is the toric fiber product of I_{G_1} and I_{G_2}; in symbols,

$$I_G = I_{G_1} \times_{\mathcal{A}} I_{G_2}. \tag{2.3}$$

Let $A_1 | B_1$ and $A_2 | B_2$ be partitions of V_1 and V_2 such that $\deg(q_{A_1|B_1}) = \deg(q_{A_2|B_2})$. Since $V_1 \cap V_2$ is connected, this implies (possibly after relabeling) that

$$A_1 \cap V_1 \cap V_2 = A_2 \cap V_1 \cap V_2.$$

This means that $A|B$ (with $A = A_1 \cup A_2$ and $B = B_1 \cup B_2$) is a partition of V, and we have

$$\phi_{G_1}(q_{A_1|B_1}) \cdot \phi_{G_2}(q_{A_2|B_2}) = \phi_G(q_{A|B}) \cdot \phi_{G_1 \cap G_2}(q_{A_1 \cap V_1 \cap V_2 | B_1 \cap V_1 \cap V_2}). \tag{2.4}$$

This is an identity of monomials in the polynomial ring $\mathbb{K}[s,t]$ associated with the big graph G, and it is verified by plugging in the definition of the monomial map $\phi_{\bullet}$ in (1.1).

The ring map that defines the toric fiber product $I_{G_1} \times_{\mathcal{A}} I_{G_2}$ can be written as

$$\phi_{I_{G_1}, I_{G_2}} \colon \mathbb{K}[q] \to \mathbb{K}[s,t], \; q_{A|B} \mapsto \phi_{G_1}(q_{A_1|B_1}) \cdot \phi_{G_2}(q_{A_2|B_2}).$$

Since (2.4) holds and since $\phi_{G_1 \cap G_2}(q_{A_1 \cap V_1 \cap V_2 | B_1 \cap V_1 \cap V_2})$ divides $\phi_G(q_{A|B})$, it follows that the unknowns s_{ij} or t_{ij} with $\{i, j\} \in E_1 \cap E_2$ can appear in $\phi_{G_1}(q_{A_1|B_1}) \cdot \phi_{G_2}(q_{A_2|B_2})$ only with exponent 2. If we replace these unknowns s_{ij}, t_{ij} by their square roots in the monomial map $\phi_{I_{G_1}, I_{G_2}}$ then the kernel remains unchanged and we obtain the monomial map $\phi_G : \mathbb{K}[q] \to \mathbb{K}[s, t]$. We conclude that $\ker(\phi_G) = \ker(\phi_{I_{G_1}, I_{G_2}})$, which is our claim (2.3). Since the configuration $\mathcal{A}$ is linearly independent, we have thus derived Theorem 2.1 from Theorem 2.6. $\square$

The proof of Theorem 2.6 given in [21] reveals the possible choices of term orders that create a Gröbner basis for I_G from given Gröbner bases $\mathbf{F}_1$ of I_{G_1} and $\mathbf{F}_2$ of I_{G_2}. First of all, the passage from a binomial $\mathbf{f}$ in $\mathbf{F}_i$ to the corresponding binomials $\mathbf{f}^{FE}$ in $\mathrm{Lift}(\mathbf{F}_i)$ is compatible with the choice of leading terms; in other words, we declare the leading term of $\mathbf{f}^{FE}$ to be the one coming from the leading term of $\mathbf{f}$. In this manner we specify a family of partial term orders on $\mathbb{K}[q]$. We then choose any tie-breaking term order on $\mathbb{K}[q]$ that makes the set $\mathrm{Quad}(G_1, G_2)$ into a Gröbner basis. Since these quadrics are the 2×2 minors of matrices $(q_{\cdot|\cdot})$ whose entries are disjoint sets of unknowns, there are many such choices of term orders. Now, the term order on $\mathbb{K}[q]$ obtained by refining the partial term order by the tie-breaker has the desired property that $\mathbf{M}$ is a Gröbner basis for I_G.

3. Computations and Conjectures

Upon encountering a new family of ideals, our first instinct is to use computer algebra to gain a better "feel" for the way the structure of the ideals depends on the parameters defining the ideals. The parameter for the cut ideal I_G is the graph G, and we are interested in how the combinatorial structure of G determines the algebraic structure of I_G. Toward this end, we undertook an exploration of the cut ideals by computing generating sets, Gröbner bases, free resolutions, and normalizations using the programs 4ti2 [11], CoCoA [5], Macaulay 2 [10], and Normaliz [1]. In this section, we summarize the results of our computations and offer a number of conjectures that arise from looking at the resulting data.

3.1. Computations

The results are summarized in Table 1, whose first column lists the graphs that we analyzed. These were all graphs on six or fewer vertices that are not clique-sum decomposable with a clique of size ≤ 3. The notation of the form G_k comes from the *Atlas of Graphs* [16]. However, if a graph has a more standard shorthand, we preferred to use the more easily identifiable abbreviations. The notations we used are:

K_l complete graph;
$K_{l_1,\ldots,l_m}$ complete m-partite graph;
C_l cycle of length l;
$\widehat{G}$ suspension of G over a point;
$G \times H$ Cartesian product graph.

Table 1 Algebraic properties of cut ideals I_G for graphs G with up to six vertices

(1) Graph	(2) 2	(3) 4	(4) 6	(5) 8	(6) 10	(7) μ	(8) codim	(9) pdim	(10) deg	(11) nor	(12) CM	(13) Gor
K_3	0	0	0	0	0	0	0	0	1	Y	Y	Y
C_4	3	0	0	0	0	2	3	3	8	Y	Y	Y
K_4	0	1	0	0	0	4	1	1	4	Y	Y	Y
C_5	30	0	0	0	0	2	10	10	52	Y	Y	N
$K_{2,3}$	19	0	0	0	0	2	9	9	72	Y	Y	Y
G_{48}	14	4	0	0	0	4	8	8	60	Y	Y	N
$\widehat{C_4}$	8	8	0	0	0	4	7	7	64	Y	Y	N
K_5	0	20	40	0	0	6	5	15	128	N	N	N
C_6	195	0	0	0	0	2	25	25	344	Y	Y	N
G_{129}	146	0	0	0	0	2	24	24	712	Y	Y	N
$K_{2,4}$	111	0	0	0	0	2	23	23	1152	Y	Y	Y
G_{151}	118	16	0	0	0	4	23	23	912	Y	Y	N
G_{153}	132	12	0	0	0	4	23	23	608	Y	Y	N
G_{154}	111	16	0	0	0	4	23	23	1280	Y	Y	Y
G_{170}	94	64	0	0	0	4	22	22	1344	Y	Y	N
G_{171}	100	28	0	0	0	4	22	22	976	Y	Y	N
G_{173}	90	52	0	0	0	4	22	22	1440	Y	Y	N
$K_2 \times K_3$	90	52	0	0	0	4	22	22	1440	Y	Y	N
$K_{3,3}$	63	72	0	0	0	4	22	22	3168	Y	Y	Y
G_{186}	72	196	0	0	0	4	21	21	1984	Y	Y	N
$\widehat{C_5}$	80	40	0	0	0	4	21	21	1232	Y	Y	N
G_{188}	64	114	0	0	0	4	21	21	1856	Y	Y	N
G_{189}	54	246	0	0	0	4	21	21	2976	Y	Y	N
G_{190}	76	128	0	0	0	4	21	21	1600	Y	Y	N
G_{194}	60	207	160	0	0	6	20		3184	N	N	N
$\widehat{K_{2,3}}$	44	420	0	0	0	4	20	20	3360	Y	Y	N
G_{198}	48	336	0	0	0	4	20	20	3040	Y	Y	N
G_{199}	44	337	80	0	0	6	20		3760	N	N	N
G_{203}	32	473	160	0	0	6	19		5696	N	N	N
$K_{2,2,2}$	24	1096	0	0	0	4	19	19	6144	Y	Y	N
G_{206}	16	671	320	0	0	6	18		11520	N	N	N
G_{207}	8	436	2872	0	0	6	17		23104	N	N	N
K_6	0	260	3952	846	480	10	16		52448	N	N	N

The columns in the table list the following features of the cut ideal I_G.

(2)–(6) number of minimal generators of I_G in degrees 2, 4, 6, 8, and 10
(7) $\mu(I_G)$ = largest degree of a minimal generator of I_G
(8) codimension (height) of I_G
(9) projective dimension of I_G
(10) degree (multiplicity) of I_G

(11) whether the semigroup algebra $\mathbb{K}[q]/I_G$ is normal
(12) whether the semigroup algebra $\mathbb{K}[q]/I_G$ is Cohen–Macaulay
(13) whether the semigroup algebra $\mathbb{K}[q]/I_G$ is Gorenstein

Blank spots in the table are entries that we were unable to compute.

If G is a small clique-sum decomposable graph then we can break it into pieces that are listed in Table 1. This tells us the degrees of the minimal generators of cut ideal I_G, but it does not list all the invariants of I_G. To be precise: Theorem 2.1 shows that

$$\mathbf{M} = \mathrm{Lift}(\mathbf{F}_1) \cup \mathrm{Lift}(\mathbf{F}_2) \cup \mathrm{Quad}(G_1, G_2)$$

generates the cut ideal I_G, but the set $\mathbf{M}$ need not generate minimally when $\mathbf{F}_1$ and $\mathbf{F}_2$ are minimal generating sets of I_{G_1} and I_{G_2}. This happens in Example 2.5. Furthermore, we do not know how taking toric fiber products affects the Cohen–Macaulay type. For instance, the usual Segre product of two Gorenstein ideals need not be Gorenstein.

3.2. Conjectures

We now present some conjectures inspired by our computations. Our main observation is that many of the coarse invariants of the cut ideals seem to be preserved under taking minors of the underlying graph. Recall that a graph H is a minor of G if H can be obtained from G by deleting and contracting edges. By the Robertson–Seymour theorem on graph minors [17], we may hope to characterize the class of graphs whose cut ideals satisfy some algebraic property by a finite list of excluded minors.

The protypical example of such a conjecture concerns the maximal degree of a binomial appearing in a minimal generating set of the cut ideal I_G. This number is $\mu(I_G)$.

CONJECTURE 3.1. *The set of graphs G such that $\mu(I_G) \le k$ is minor-closed for any k.*

As evidence for Conjecture 3.1, note that two operations related to taking graph minors amount to taking faces of the corresponding cut polytopes.

LEMMA 3.2. (1) *If H is an induced subgraph of G, then* $\mathrm{Cut}^{\square}(H)$ *is a face of* $\mathrm{Cut}^{\square}(G)$.

(2) *If H is obtained from G by contracting an edge, then* $\mathrm{Cut}^{\square}(H)$ *is a face of* $\mathrm{Cut}^{\square}(G)$.

Proof. For part (2), intersect $\mathrm{Cut}^{\square}(G)$ with the hyperplane $x_{ij} = 0$, where ij is the contracted edge. For part (1), intersect $\mathrm{Cut}^{\square}(G)$ with the hyperplanes $x_{ij} = 0$ for all edges ij in G not incident to H, together with one extra condition $x_{ij} = 0$ for each connected component of $G \setminus H$, where ij is an edge incident to said connected component and H. $\square$

This implies that generating degrees can only go down when passing to an induced subgraph or when contracting an edge.

COROLLARY 3.3. (1) *If H is an induced subgraph of G, then $\mu(I_H) \leq \mu(I_G)$.*
(2) *If H is obtained from G by contracting an edge, then $\mu(I_H) \leq \mu(I_G)$.*

Proof. For any two toric ideals, we always have $\mu(I_{\mathcal{B}}) \leq \mu(I_{\mathcal{A}})$ whenever $\mathcal{B}$ is a face of $\mathcal{A}$. Thus, the desired inequalities are a direct consequence of Lemma 3.2. □

Therefore, to prove Conjecture 3.1, it would suffice to show that generating degrees are nonincreasing after deletion of edges. Observe that the face property does not hold when deleting an edge, as seen by comparing Examples 1.1 and 1.2.

CONJECTURE 3.4. *Let H be obtained from G by deleting an edge. Then $\mu(I_H) \leq \mu(I_G)$.*

The smallest instance of Conjecture 3.1 (namely, $k = 2$) concerns those graphs G whose cut ideal I_G is generated by quadrics. We propose the following simple characterization.

CONJECTURE 3.5. *The cut ideal I_G is generated by quadrics if and only if G is free of K_4 minors* (*i.e., if and only if G is series-parallel*).

If a graph G has K_n as a minor, then that minor can be realized by a sequence of edge contractions only. By Corollary 3.3(2), the cut ideal of every graph with a K_4 minor has a minimal generator of degree 4. Thus, to prove Conjecture 3.5 we must show that graphs without K_4 minors have quadratically generated cut ideals. Graphs free of K_4 minors are known as *series-parallel graphs.* Every series-parallel graph can be built from K_2 by successive series and parallel extensions. The series extensions are just 0-sums. Hence, to prove Conjecture 3.5, it would suffice to show that $\mu(I_G)$ does not increase when performing a parallel extension.

Another conjecture, along the same lines as Conjecture 3.5, concerns quartic generators.

CONJECTURE 3.6. *The cut ideal I_G is generated in degree ≤ 4 if and only if G is free of K_5 minors.*

In algebraic statistics, minimal generators of toric ideals are called *Markov bases* [6; 8; 22]. Therefore Conjectures 3.1, 3.4, 3.5, and 3.6 concern the complexity of Markov bases for moves among the $\mathbb{N}$-valued functions on the cuts of a graph G. As we shall see in Sections 4 and 5, the underlying toric models [15, Sec. 1.2] are important in statistics, which gives added relevance to our computations and conjectures in this section.

From the more theoretical perspective of commutative algebra, it appears that Conjecture 3.6 also captures the class of graphs having normal and Cohen–Macaulay cut ideals.

CONJECTURE 3.7. *The semigroup algebra $\mathbb{K}[q]/I_G$ is normal if and only if $\mathbb{K}[q]/I_G$ is Cohen–Macaulay if and only if G is free of K_5 minors.*

That $\mathbb{K}[q]/I_{K_5}$ is not normal and not Cohen–Macaulay can be seen in Table 1. The gap between the codimension (5) and the projective dimension (15) is remarkably large in this case (we note that the associated semigroup Q and its saturation Q_{sat} differ by only one point). The property of being normal is preserved when passing from a semigroup algebra to a facial subalgebra. Hence we can deduce from Lemma 3.2 that every graph with a K_5 minor has a nonnormal cut ring $\mathbb{K}[q]/I_G$. Thus, to prove a large part of Conjecture 3.7 it would be sufficient to prove that graphs G that are free of K_5 minors have normal semigroup algebras $\mathbb{K}[q]/I_G$. Here we are using Hochster's theorem, which states that normal implies Cohen–Macaulay among semigroup algebras [12].

One question that remains is to characterize those K_5-free graphs G whose cut ideal I_G is Gorenstein. Being Gorenstein seems to depend in a complicated way on the structure of the graph G. In general, the Gorenstein property is not preserved under taking toric fiber products and, in particular, is not preserved under taking clique sums of graphs. We do not have a firm conjecture on the structure of those graphs whose cut ideal is Gorenstein.

4. From Cut Ideals to Binary Graph Models

We now explain the correspondence between certain cut ideals and the toric ideals of binary graph models. These are statistical models for $2 \times 2 \times \cdots \times 2$ contingency tables, whose algebraic properties were studied by Develin and Sullivant in [6]. Our main result in this section (Theorem 4.1) states that binary graph models on n nodes coincide with cut ideals of those graphs on $n+1$ nodes where one node is connected to all others.

Let G be a graph with vertex set $V = [n] = \{1, 2, \dots, n\}$ and edge set E, and suppose that G has no isolated vertices. We introduce a polynomial ring with 2^n unknowns,

$$\mathbb{K}[p] = \mathbb{K}[p_{i_1 i_2 \cdots i_n} \mid i_1, i_2, \dots, i_n \in \{0, 1\}],$$

and a polynomial ring with $4 \cdot |E|$ unknowns,

$$\mathbb{K}[b] = \mathbb{K}[b^e_{ij} \mid i, j \in \{0, 1\},\ e \in E].$$

The binary graph model is defined by the following homomorphism of polynomial rings:

$$\psi_G \colon \mathbb{K}[p] \to \mathbb{K}[b],\ \ p_{i_1 \cdots i_n} \mapsto \prod_{\{k,l\} \in E} b^{kl}_{i_k i_l}.$$

The kernel of ψ_G is a toric ideal that we denote by J_G. The *binary graph model* of G is the 0-set of J_G in $\mathbb{P}^{2^n - 1}$. In statistics, this toric variety corresponds to the hierarchical model for $2 \times 2 \times \cdots \times 2$ contingency tables, where the 2×2 margins on the edges of G are fixed. The Markov basis for this model consists of the minimal generators of J_G.

The *suspension* of the graph $G = (V, E)$ is the new graph $\widehat{G}$ whose vertex set equals $[n+1] = V \cup \{n+1\}$ and whose edge set equals $E \cup \{\{i, n+1\} \mid i \in V\}$. Given any binary string $\mathbf{i} = i_1 i_2 \cdots i_n \in \{0, 1\}^n$, we define the associated partition $A(\mathbf{i})|B(\mathbf{i})$ of $[n+1]$ by the condition $k \in B(\mathbf{i})$ if and only if $i_k = 1$. Similarly, if $A|B$ is a partition of $[n+1]$ with $n+1 \in A$, we obtain a binary string $\mathbf{i}(A|B)$ by reversing the procedure. This specifies a natural bijection between the 2^n unknowns $p_{\mathbf{i}}$ in $\mathbb{K}[p]$ and the 2^n unknowns $q_{A|B}$ in $\mathbb{K}[q]$.

THEOREM 4.1. *Let γ be the ring isomorphism $\mathbb{K}[p] \to \mathbb{K}[q]$ defined by $p_{\mathbf{i}} \mapsto q_{A(\mathbf{i})|B(\mathbf{i})}$. Then*

$$\gamma(J_G) = I_{\widehat{G}}.$$

We remark that Theorem 4.1 is already known at the level of the underlying convex polytopes; this is the content of [7, Chap. 5]. The polytope underlying the toric ideal J_G is the *marginal polytope* or *covariance polytope* of the graph G. It is isomorphic to the cut polytope of the suspension $\widehat{G}$ under the *covariance mapping,* as explained in [7, Sec. 5.2]. The identification of J_G with $I_{\widehat{G}}$ in Theorem 4.1 lifts the covariance mapping to the setting of toric algebra. Before presenting the proof, we discuss a few examples.

EXAMPLE 4.2. Let $G = K_3$ be the complete graph on three nodes. The homomorphism ψ_G takes the polynomial ring $\mathbb{K}[p_{000}, p_{001}, p_{010}, p_{011}, p_{100}, p_{101}, p_{110}, p_{111}]$ to the polynomial ring $\mathbb{K}[b_{00}^{12}, b_{01}^{12}, b_{10}^{12}, b_{11}^{12}, b_{00}^{13}, b_{01}^{13}, b_{10}^{13}, b_{11}^{13}, b_{00}^{23}, b_{01}^{23}, b_{10}^{23}, b_{11}^{23}]$ by sending p_{ijk} to $b_{ij}^{12}b_{ik}^{13}b_{kl}^{23}$. The kernel J_G is the principal ideal generated by $p_{000}p_{011}p_{101}p_{110} - p_{001}p_{010}p_{100}p_{111}$. The isomorphism γ sends $p_{000} \mapsto q_{1234|}$, $p_{001} \mapsto q_{124|3}$, $p_{010} \mapsto q_{134|2}$, $p_{011} \mapsto q_{14|23}$, $p_{100} \mapsto q_{1|234}$, $p_{101} \mapsto q_{13|24}$, $p_{110} \mapsto q_{12|34}$, and $p_{111} \mapsto q_{123|4}$. The image of J_{K_3} under γ is the principal ideal I_{K_4} discussed in Example 1.1. Note that K_4 is the suspension of K_3.

EXAMPLE 4.3. Theorem 4.1 explains some of the coincidences between rows in our Table 1 and the table in [6, p. 447]. For instance, the ideal $J_{K_4} \cong I_{K_5}$ is minimally generated by 20 quartics and 40 sextics. And if G is the edge graph of the bipyramid (denoted BP in [6]), then its suspension $\widehat{G}$ is the graph G_{207} in our Table 1 and the ideal $J_{BP} \cong I_{G_{207}}$ is minimally generated by eight quadrics, 436 quartics, and 2872 sextics.

The results in [6, Sec. 3] imply the following corollary for cut ideals. Note that it is consistent with Conjecture 3.6 because the relevant suspensions $\widehat{G}$ have no K_5 minors.

COROLLARY 4.4. *Let G be a cycle C_n or a complete bipartite graph $K_{2,n}$. Then the cut ideal $I_{\widehat{G}}$ of the suspension $\widehat{G}$ is generated by binomials of degrees* 2 *and* 4.

The results in [6, Sec. 4] provide counterexamples to a conjecture that seems to be implied by Table 1—namely, there exist graphs whose cut ideals have minimal generators of odd degree. The smallest such example for a binary graph model involves the graph $G = K_2 \times K_3$, the edge graph of the triangular prism, whose graph ideal J_G has a minimal generator of degree 3. The suspension of this graph, which has seven vertices, has a cut ideal with an odd-degree minimal generator.

Proof of Theorem 4.1. It suffices to show that there exist a pair of homomorphisms $\alpha\colon \mathbb{K}[b] \to \mathbb{K}[s,t]$ and $\beta\colon \mathbb{K}[s,t] \to \mathbb{K}[b]$ such that $\phi_{\widehat{G}} \circ \gamma = \alpha \circ \psi_G$ and

$\psi_G \circ \gamma^{-1} = \beta \circ \phi_{\widehat{G}}$. The maps α and β (restricted to $\mathbb{K}[p]/J_G$ and $\mathbb{K}[q]/I_{\widehat{G}}$, respectively) will then lift to the isomorphism γ. In order to do this correctly, we extend $\mathbb{K}[s,t]$ and $\mathbb{K}[b]$ to allow fractional powers of the unknowns. Which fractional powers are needed will be clear from the context.

We define the map $\alpha\colon \mathbb{K}[b] \to \mathbb{K}[s,t]$ as follows:

$$b_{00}^{kl} \mapsto t_{kl} t_{k,n+1}^{1/\deg(k)} t_{l,n+1}^{1/\deg(l)}, \qquad b_{01}^{kl} \mapsto s_{kl} t_{k,n+1}^{1/\deg(k)} s_{l,n+1}^{1/\deg(l)},$$
$$b_{10}^{kl} \mapsto s_{kl} s_{k,n+1}^{1/\deg(k)} t_{l,n+1}^{1/\deg(l)}, \qquad b_{11}^{kl} \mapsto t_{kl} s_{k,n+1}^{1/\deg(k)} s_{l,n+1}^{1/\deg(l)}.$$

Here $\deg(k)$ denotes the degree of the node k in the graph G, and similarly for the node l.

We wish to show that α satisfies $\phi_{\widehat{G}} \circ \gamma = \alpha \circ \psi_G$. Toward that end, we look at which unknowns s_{kl}, t_{kl} appear to what powers in the monomials $\alpha(\psi_G(p_{\mathbf{i}}))$ and $\phi_{\widehat{G}}(\gamma(p_{\mathbf{i}}))$. An unknown s_{kl} appears in $\alpha(\psi_G(p_{\mathbf{i}}))$ with multiplicity 1 if and only if $i_k i_l \in \{01, 10\}$ if and only if $\{k,l\} \in \mathrm{Cut}(A(\mathbf{i})\,|\,B(\mathbf{i}))$ if and only if s_{kl} appears in $\phi_{\widehat{G}}(\gamma(p_{\mathbf{i}}))$ with multiplicity 1. A similar argument shows that t_{kl} appears with the same multiplicity in both $\alpha(\psi_G(p_{\mathbf{i}}))$ and $\phi_{\widehat{G}}(\gamma(p_{\mathbf{i}}))$. To check the multiplicity of $s_{k,n+1}$ (and similarly for $t_{k,n+1}$), note that the fractional powers guarantee that $s_{k,n+1}$ appears in $\alpha(\psi_G(p_{\mathbf{i}}))$ if and only if it has multiplicity 1 in $\alpha(\psi_G(p_{\mathbf{i}}))$. This happens if and only if $i_k = 1$ if and only if $(k, n+1) \in \mathrm{Cut}(A(\mathbf{i})\,|\,B(\mathbf{i}))$ if and only if s_{kl} appears in $\phi_{\widehat{G}}(\gamma(p_{\mathbf{i}}))$ with multiplicity 1.

We now define our second ring homomorphism $\beta\colon \mathbb{K}[s,t] \to \mathbb{K}[b]$ as follows:

$$s_{k,n+1} \mapsto \prod_{l:\{k,l\}\in E} (b_{00}^{kl} b_{01}^{kl})^{-1/2} \cdot B, \qquad t_{k,n+1} \mapsto \prod_{l:\{k,l\}\in E} (b_{10}^{kl} b_{11}^{kl})^{-1/2} \cdot B$$
$$s_{kl} \mapsto (b_{01}^{kl} b_{10}^{kl})^{1/2}, \qquad t_{kl} \mapsto (b_{00}^{kl} b_{11}^{kl})^{1/2}.$$

Here B denotes the product of all unknowns in $\mathbb{K}[b]$ raised to the power $1/2n$,

$$B = \prod_{\{k,l\}\in E} \prod_{i,j\in\{0,1\}} (b_{ij}^{kl})^{1/2n}.$$

To prove that β satisfies $\psi_G \circ \gamma^{-1} = \beta \circ \phi_{\widehat{G}}$ we compare the multiplicity of b_{ij}^{kl} in $\psi_G(\gamma^{-1}(q_{A|B}))$ and $\beta(\phi_{\widehat{G}}(q_{A|B}))$. By symmetry, it suffices to analyze the case $ij = 00$. For fixed k,l, the unknown b_{00}^{kl} has multiplicity 1 in $\psi_G(\gamma^{-1}(q_{A|B}))$ if and only if $\{k,l\} \notin \mathrm{Cut}(A\,|\,B)$ and $k,l \in A$. Here, b_{01}^{kl}, b_{10}^{kl}, b_{11}^{kl} all occur with multiplicity 0.

Now we analyze the multiplicity of b_{ij}^{kl} in $\beta(\phi_{\widehat{G}}(q_{A|B}))$. Suppose $\{k,l\} \notin \mathrm{Cut}(A\,|\,B)$ and $k,l \in A$. This means that $t_{kl} t_{k,n+1} t_{l,n+1}$ is a factor of $\phi_{\widehat{G}}(q_{A|B})$. Looking at the expansion of $\beta(\phi_{\widehat{G}}(q_{A|B}))$ shows that, aside from the factor of B^n, the only multiplicands that could possibly contain b_{00}^{kl} are t_{kl}, $t_{k,n+1}$, and $t_{l,n+1}$. The first contributes $(b_{00}^{kl})^{1/2}$, the second and third contribute nothing, and the factor of B^n contributes $(b_{00}^{kl})^{1/2}$ for a grand total of b_{00}^{kl}. On the other hand, b_{01}^{kl} appears with multiplicity 0 because t_{kl} and $t_{k,n+1}$ contribute nothing, $t_{l,n+1}$ contributes $(b_{01}^{kl})^{-1/2}$, and B^n contributes $(b_{00}^{kl})^{1/2}$. A similar argument shows that b_{10}^{kl} and b_{11}^{kl} also appear with multiplicity 0. This agrees with the multiplicity of b_{ij}^{kl} in $\psi_G(\gamma^{-1}(q_{A|B}))$ and so completes the proof of Theorem 4.1. $\square$

5. From Jukes–Cantor Phylogenetic Models to Cut Ideals

In this section we apply cut ideals to phylogenetics. Our main result (Theorem 5.5) states that cut ideals of graphs with n nodes are precisely the binary Jukes–Cantor models on cyclic split systems on n taxa. This class includes the Jukes–Cantor models on phylogenetic trees whose algebraic properties were studied in [4] and [19]. We re-derive the quadratic Gröbner basis for these ideals by relating Theorem 2.1 to [19, Thm. 21].

The extension of statistical models of evolution from phylogenetic trees to split systems is due to David Bryant, who described these models in [2]. This extension has the double advantage of being useful for biological applications and leading to a richer mathematical theory. We next give an algebraic introduction to Jukes–Cantor models for arbitrary split systems. Later on, we specialize to split systems that are cyclic and hence most relevant for the NeighborNet method [3]. This will take us back to cut ideals.

5.1. The One-Parameter Model Associated with a Single Split

We consider a set of n taxa labeled by $[n] = \{1, 2, \ldots, n\}$. Each Jukes–Cantor model is a subvariety of the $(2^n - 1)$-dimensional projective space $\mathbb{P}^{2^n-1}$ whose coordinates we denote by $p_{i_1\cdots i_n}$. The coordinate $p_{i_1\cdots i_n}$ represents the probability of observing the states $i_1, \ldots, i_n \in \{0, 1\}$ at the taxa. We shall employ a linear change of coordinates known as the *Fourier transform* or *Hadamard conjugation*; see [15, Sec. 4.4] and [19, Sec. 2]. The Fourier coordinates are here denoted $f_{j_1\cdots j_n}$, and they are related to the probability coordinates as follows:

$$f_{j_1\cdots j_n} = \sum (-1)^{i_1 j_1 + \cdots + i_n j_n} \cdot p_{i_1\cdots i_n}, \tag{5.1}$$

where the sum is over all elements $(i_1, \ldots, i_n)$ of the abelian group $(\mathbb{Z}/2\mathbb{Z})^n$. It is easy to invert this linear transformation:

$$p_{i_1\cdots i_n} = \frac{1}{2^n} \sum (-1)^{j_1 i_1 + \cdots + j_n i_n} \cdot f_{j_1\cdots j_n}, \tag{5.2}$$

where the sum is over $(j_1, \ldots, j_n) \in (\mathbb{Z}/2\mathbb{Z})^n$.

A *split* $\{C, D\}$ is a partition $C \cup D = \{1, \ldots, n\}$ of the set of taxa such that $n \in D$. We fix a split $\{C, D\}$ and introduce one free parameter u. In statistical applications, this parameter u would range over real numbers between 0 and $\frac{1}{2}$. In algebraic geometry we allow any point $(u_0 : u_1)$ on the complex projective line $\mathbb{P}^1$, where $u_0 = 1$ and $u_1 = u$.

We map the u-line $\mathbb{P}^1$ into the probability space $\mathbb{P}^{2^n-1}$ by setting

$$f_{j_1\cdots j_n} = \begin{cases} 0 & \text{if } j_1 + \cdots + j_n \text{ is odd,} \\ u_0 & \text{if } \sum_{k\in C} j_k \text{ and } \sum_{k\in D} j_k \text{ are both even,} \\ u_1 & \text{if } \sum_{k\in C} j_k \text{ and } \sum_{k\in D} j_k \text{ are both odd.} \end{cases}$$

This line in $\mathbb{P}^{2^n-1}$ is the Jukes–Cantor model associated with the split $\{C, D\}$. Using the transformation (5.1), we can express the parameterization in probability coordinates:

$$p_{i_1\cdots i_n} = \begin{cases} (u_0+u_1)/4 & \text{if } i_1 = \cdots = i_n, \\ (u_0-u_1)/4 & \text{if } i_k = 1 \text{ for all } k \in C \text{ and } i_l = 0 \text{ for all } l \in D, \\ (u_0-u_1)/4 & \text{if } i_k = 0 \text{ for all } k \in C \text{ and } i_l = 1 \text{ for all } l \in D, \\ 0 & \text{otherwise.} \end{cases}$$

In sum, the Jukes–Cantor model for a single split is a straight line in $\mathbb{P}^{2^n-1}$. Given two points in this model, we can multiply their Fourier coordinates, one coordinate at a time, and so derive a new point in the model. Thus the model is a semigroup with respect to multiplication of Fourier coordinates. The model is a line that is also a toric curve.

5.2. The Jukes–Cantor Model Defined by an Arbitrary Split System

A *split system* is simply a collection of r distinct splits of $[n] = \{1, \ldots, n\}$ for some positive integer r:

$$\Sigma = \{\{C_1, D_1\}, \{C_2, D_2\}, \ldots, \{C_r, D_r\}\}.$$

Each split $\{C_i, D_i\}$ specifies a one-parameter Jukes–Cantor model, which is a semigroup under multiplication of Fourier coordinates. We define the *Jukes–Cantor model of* Σ to be the semigroup generated by the r one-parameter models of the splits $\{C_i, D_i\} \in \Sigma$.

Explicitly, the parameterization of this Jukes–Cantor model is given as follows. The parameter space is the direct product of r copies of the projective line $\mathbb{P}^1$. The homogeneous coordinates of the ith projective line $\mathbb{P}^1$ are denoted $(u_0^i : u_1^i)$. There are precisely 2^{n-1} nonzero Fourier coordinates $f_{j_1\cdots j_n}$, which are indexed by the group

$$(\mathbb{Z}/2\mathbb{Z})^n_{\text{even}} = \{(j_1, \ldots, j_n) \in (\mathbb{Z}/2\mathbb{Z})^n : j_1 + \cdots + j_n \text{ is even}\}.$$

Each nonzero Fourier coordinate is expressed as a monomial of degree r in the parameters

$$f_{j_1\cdots j_n} = \prod_{\{C_i, D_i\} \in \Sigma} u^i_{\sum_{k \in C_i} j_k}. \tag{5.3}$$

Because this parameterization is given by monomials, the ideal of algebraic invariants of the Jukes–Cantor model is a toric ideal in the Fourier coordinates. This toric ideal is the kernel of the ring map (5.3), and we denote it by JC_Σ. It lives in the polynomial ring $\mathbb{K}[f]$ whose generators are the 2^{n-1} Fourier coordinates $f_{j_1\cdots j_n}$ indexed by $(\mathbb{Z}/2\mathbb{Z})^n_{\text{even}}$.

It is important to understand that Jukes–Cantor models are toric varieties (since JC_Σ is a toric ideal in the Fourier coordinates) but are *not* toric models (i.e., log-linear models or discrete exponential families) in the sense of [15, Sec. 1.2] because JC_Σ is not a toric ideal when rewritten in the probability coordinates $p_{i_1\cdots i_n}$ via the Fourier transform (5.1).

PROPOSITION 5.1. *If* Σ *consists of* r *splits, then the Jukes–Cantor model is* r*-dimensional.*

Proof. We can write the 2^{n-1} nonzero monomials in the parameterization (5.3) as the columns of a 0–1 matrix A with $2r$ rows—one for each unknown u_0^i and u_1^i—as in [18] or in [15, Sec. 1.2]. The rows of this matrix span an $(r+1)$-dimensional linear space. This implies that the semigroup algebra $\mathbb{K}[f]/JC_\Sigma$ has Krull dimension $r+1$, and hence the associated projective variety (which is our Jukes–Cantor model) has dimension r. □

Jukes–Cantor models for split systems do indeed generalize the familiar models associated with trees. Let T be a tree with leaves labeled by $[n]$. Every edge of T defines a split $\{C, D\}$ of $[n]$. We write $\Sigma(T)$ for the set of splits coming from all the edges of T.

PROPOSITION 5.2. *$JC_{\Sigma(T)}$ equals the usual Jukes–Cantor model associated with the tree T.*

Proof. This is seen by comparing the parameterization for split systems in (5.3) with that given in [19, Sec. 3] for group based models on trees. The condition that $\sum_{k\in C_i} j_k$ be even in the split system representation is replaced with the condition that $\sum_{k\in\Lambda(e)} j_k$ be even, where $\Lambda(e)$ is the set of leaves below the edge e. The concept of being a "leaf below an edge" is equivalent to being on one side of a split. □

5.3. Cyclic Split Systems

We now turn our attention to the family of cyclic split systems. These split systems are particularly useful for representing and analyzing metric spaces in biology, since they can be drawn in the plane using NeighborNet [3].

Formally, we define cyclic split systems as follows. We draw a convex n-gon in the plane and label the vertices by $1, \ldots, n$ in clockwise order. Every line in the plane that does not pass through any of the vertices defines a split $\{C, D\}$. The *complete cyclic split system* $\Sigma^{(n)}$ is the collection of all splits of $[n] = \{1, \ldots, n\}$ that arise in this manner.

REMARK 5.3. The number of nontrivial cyclic splits in $\Sigma^{(n)}$ equals $n(n-1)/2$.

A *cyclic split system* is any subset of $\Sigma^{(n)}$. In other words, a split system Σ is cyclic if, for each split $\{C, D\} \in \Sigma$, the set C is an interval of integers $C = [k, l] = \{k, k+1, \ldots, l\}$.

Now we will show that every cyclic split ideal JC_Σ is a cut ideal. We associate to each cyclic split system Σ a graph G_Σ with vertex set $[n]$ as follows. For each cyclic split $\{C, D\} \in \Sigma$, where $n \in D$ and $C = [k, l]$, we introduce the edge $\{k-1, l\}$ in G_Σ (here $0 := n$). Hence G_Σ is a graph with one edge for each split in Σ. The representation of a cyclic split system Σ by its graph G_Σ is quite natural, as the following proposition shows.

PROPOSITION 5.4. *Let T be a planar tree with leaves labeled cyclically* $1, \ldots, n$, *and let $\Sigma(T)$ be the associated cyclic split system. Then the graph $G_{\Sigma(T)}$ consists of the edges in the subdivision of the convex n-gon that is dual to the tree T.*

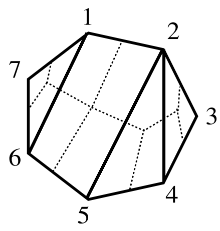

Figure 1 Tree with seven leaves and corresponding subdivision of the 7-gon

Proof. The proof of this result is straightforward. The idea is illustrated in Figure 1. □

We now come to the main result of this section. We define a bijection between the set of all 2^{n-1} cuts of $[n]$ and the set $(\mathbb{Z}/2\mathbb{Z})^n_{\text{even}}$ of binary strings that sum to zero. If $A\,|\,B$ is any cut, then the corresponding binary string $j_1 j_2 \cdots j_n$ is defined as

$$j_k = \begin{cases} 1 & \text{if } \{k-1, k\} \in \operatorname{Cut}(A\,|\,B), \\ 0 & \text{otherwise.} \end{cases}$$

It is easy to see that $j_1 + \cdots + j_n$ is even and that the cut $A\,|\,B$ is uniquely encoded in the string $j_1 j_2 \cdots j_n$. This bijection defines an isomorphism of polynomial rings $\tau : \mathbb{K}[q] \to \mathbb{K}[f]$ by sending the unknown $q_{A|B}$ to $f_{j_1 \cdots j_n}$.

THEOREM 5.5. *Let Σ be a cyclic split system and let G_Σ be the associated graph. Then the Jukes–Cantor model JC_Σ equals the image of the cut ideal I_{G_Σ} under the isomorphism τ.*

Proof. To see that the preceding bijection between cut coordinates and Fourier coordinates gives an isomorphism between the cut model for G_Σ and the Jukes–Cantor model JC_Σ, we must define an appropriate bijection between the parameters. This bijection between parameters is induced by the map that sends a cyclic split in Σ to an edge of the graph G_Σ. Namely, we identify the $\mathbb{P}^1$ parameter space associated to the split $\{C_i, D_i\}$, where $C_i = [k+1, l]$, with the $\mathbb{P}^1$ parameter space associated to the edge $\{k, l\}$ in G_Σ via

$$(u_0^i : u_1^i) = (t_{kl} : s_{kl}). \tag{5.4}$$

Now, the unknown s_{kl} appears in the squarefree monomial $\phi_{G_\Sigma}(q_{A|B})$ if and only if $\{k, l\} \in \operatorname{Cut}(A\,|\,B)$ if and only if $j_{k+1} + \cdots + j_l$ is odd if and only if $\sum_{\nu \in C_i} j_\nu$ is odd if and only if the unknown u_1^i appears in the squarefree monomial on the right-hand side of (5.3). Likewise, t_{kl} appears in $\phi_{G_\Sigma}(q_{A|B})$ if and only if u_0^i appears in the right-hand side of (5.3). This shows, modulo the identification (5.4), that the image of the cut coordinate $q_{A|B}$ under the map ϕ_{G_Σ} equals the image of the Fourier coordinate $f_{j_1 \cdots j_n}$ under the map (5.3). Therefore, both maps have the same kernel, and we conclude that $JC_\Sigma = \tau(I_{G_\Sigma})$. □

EXAMPLE 5.6. Let $\Sigma = \Sigma^{(4)}$ be the complete cyclic split system on four taxa:

$$\Sigma = \{\{12, 34\}, \{23, 14\}, \{1, 234\}, \{2, 134\}, \{3, 124\}, \{123, 4\}\}. \tag{5.5}$$

The associated graph G_Σ is the complete graph on $\{1,2,3,4\}$. With the ordering of the splits as in (5.5), the map τ and the Jukes–Cantor parameterization (5.3) are given by

$$\begin{aligned}
q_{|1234} &\mapsto f_{0000} \mapsto u_0^4 \cdot u_0^2 \cdot u_0^3 \cdot u_0^5 \cdot u_0^1 \cdot u_0^6,\\
q_{4|123} &\mapsto f_{1001} \mapsto u_0^4 \cdot u_0^2 \cdot u_1^3 \cdot u_0^5 \cdot u_1^1 \cdot u_1^6,\\
q_{3|124} &\mapsto f_{0011} \mapsto u_0^4 \cdot u_1^2 \cdot u_0^3 \cdot u_1^5 \cdot u_0^1 \cdot u_1^6,\\
q_{2|134} &\mapsto f_{0110} \mapsto u_1^4 \cdot u_0^2 \cdot u_0^3 \cdot u_1^5 \cdot u_1^1 \cdot u_0^6,\\
q_{1|234} &\mapsto f_{1100} \mapsto u_1^4 \cdot u_1^2 \cdot u_1^3 \cdot u_0^5 \cdot u_0^1 \cdot u_0^6,\\
q_{12|34} &\mapsto f_{1010} \mapsto u_0^4 \cdot u_1^2 \cdot u_1^3 \cdot u_1^5 \cdot u_1^1 \cdot u_0^6,\\
q_{13|24} &\mapsto f_{1111} \mapsto u_1^4 \cdot u_0^2 \cdot u_1^3 \cdot u_1^5 \cdot u_0^1 \cdot u_1^6,\\
q_{14|23} &\mapsto f_{0101} \mapsto u_1^4 \cdot u_1^2 \cdot u_0^3 \cdot u_0^5 \cdot u_1^1 \cdot u_1^6.
\end{aligned}$$

Under the identification (5.4), this coincides with the parameterization in Example 1.1. The Jukes–Cantor ideal for the complete split system on four taxa equals

$$J_\Sigma = \langle f_{0000} f_{0101} f_{1010} f_{1111} - f_{0011} f_{0110} f_{1001} f_{1100} \rangle.$$

The ordering of the factors u_j^i in the preceding monomials coincides with the lexicographic ordering of the edges of K_4. If we set $u_0^1 = u_1^1 = u_0^2 = u_1^2 = 1$ in the parameterization then we get the 4-cycle in Example 1.2, which represents the Jukes–Cantor model for the star tree. This model is the same as the rooted claw tree $K_{1,3}$ in [13, Ex. 14].

5.4. Algebraic Invariants for Jukes–Cantor Models on Cyclic Split Systems

The polynomials in the ideal J_Σ are known as *algebraic invariants* in phylogenetics. When expressed in terms of the coordinates $p_{i_1 \cdots i_n}$ via (5.1), these polynomials are the algebraic relationships that hold among the joint probabilities for all distributions in the model. Using Theorem 5.5, we can now translate our results and conjectures about cut ideals to the setting of Jukes–Cantor models. We begin by giving a new proof of a known result.

COROLLARY 5.7 [19, Thm. 2(a)]. *Consider the Jukes–Cantor model for any trivalent tree T with taxa $[n]$. Then the ideal $JC_{\Sigma(T)}$ has a Gröbner basis consisting of quadrics.*

Proof. By Proposition 5.4 and Theorem 5.5, we have $JC_{\Sigma(T)} = I_G$, where G is the edge graph of a triangulation of the n-gon. Such a planar graph can be decomposed into triangles using 2-sums. The result then follows from Theorem 2.1. □

We now discuss the Jukes–Cantor ideals JC_Σ for some other cyclic split systems. Each of the graphs G in Table 1 corresponds to such a split system. Namely, for each edge $\{k,l\}$ of G we introduce the cyclic split $\{C,D\}$, where $C = \{k+1, k+2, \ldots, l\}$ and $D = [n]\backslash C$.

The complete graph K_n corresponds to the complete split system $\Sigma^{(n)}$. Table 1 reveals that the algebraic invariants for $\Sigma^{(5)}$ are generated in degree ≤ 6 and that the algebraic invariants for $\Sigma^{(6)}$ are generated in degree ≤ 10. Conjectures 3.5 and 3.6 translate into conjectures about which Jukes–Cantor ideals JC_Σ are generated by quadrics and which are generated by quartics. Whether the generating degree $\mu(JC_\Sigma)$ for a cyclic split system can only decrease upon removal of a split is still unknown (cf. Conjecture 3.4).

Huson and Bryant [14] have shown that cyclic split systems, even if they do not arise from trees, always have useful representations by phylogenetic networks. However, this representation is generally not unique [14, Fig. 5]. These *split networks* on n taxa are thus in many-to-one correspondence—via Theorem 5.5, to graphs with n vertices—and our results here shed light on the algebraic invariants of the associated statistical model [2]. One concrete application of this correspondence to phylogenetics will be the exact computation of maximum likelihood parameters for models of splits as described in [13, Sec. 6].

EXAMPLE 5.8. Let $n = 6$ and consider the bipartite graph $K_{3,3}$, where the bipartition separates $\{1,3,5\}$ from $\{2,4,6\}$. The corresponding split system Σ consists of the six trivial splits $\{\{i\},[6]\backslash\{i\}\}$ and the three nontrivial splits $\{123,456\}$, $\{234,156\}$, and $\{345,126\}$. This is the smallest split system whose split network is not unique (and is depicted in [14, Fig. 5]). Using our Table 1, we see that the corresponding Jukes–Cantor ideal JC_Σ is minimally generated by 63 quadrics and 72 quartics. The semigroup algebra $\mathbb{K}[f]/JC_\Sigma$ is also normal and hence, by Hochster's theorem [12], Cohen–Macaulay.

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