Toric ideals of phylogenetic invariants for the general group-based model on claw trees $K_{1,n}$

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Abstract. We address the problem of studying the toric ideals of phylogenetic invariants for a general group-based model on an arbitrary claw tree. We focus on the group \mathbb{Z}_2 and choose a natural recursive approach that extends to other groups. The study of the lattice associated with each phylogenetic ideal produces a list of circuits that generate the corresponding lattice basis ideal. In addition, we describe *explicitly* a quadratic lexicographic Gröbner basis of the toric ideal of invariants for the claw tree on an arbitrary number of leaves. Combined with a result of Sturmfels and Sullivant, this implies that the phylogenetic ideal of *every* tree for the group \mathbb{Z}_2 has a quadratic Gröbner basis. Hence, the coordinate ring of the toric variety is a Koszul algebra.

Acknowledgment. The authors would like to thank Uwe Nagel for introducing us to the field of phylogenetic algebraic geometry and for his continuous support, motivation and guidance.

1 Introduction

Statistical models of evolution can conveniently be presented using a phylogenetic tree. A phylogenetic tree is a simple connected acyclic graph whose edges are labelled by transition matrices that reflect probabilities of moving from one vertex to another. Associated with each such tree is a set of polynomials, called phylogenetic invariants, which vanish on the statistical model. For group-based models the phylogenetic invariants form a toric ideal. Sturmfels and Sullivant ([8]) reduce the study of such invariants on an arbitrary tree to the case of claw trees. Namely, if the ideal of invariants for the claw trees is known, then the ideal of invariants for any tree is known. They also pose a conjecture that the ideal for a group-based model is generated in degree no greater than the order of the group. Their proof of the conjecture for the case \mathbb{Z}_2 is ingenious, but does not extend. We approach the problem of studying the toric ideals of invariants in a natural recursive way, which applies to other groups and gives a stronger result for \mathbb{Z}_2 .

We consider the ideal for a general group-based model for the group \mathbb{Z}_2 and an arbitrary claw tree. Section 2 contains some relevant background and further explains the motivation of our study. In section 3 we lay the foundation for our

recursive approach. The ideal of the two-leaf claw tree is trivial, so we begin with the case when the number of leaves is three. Sections 4 and 5 address the problem of describing the lattices corresponding to the toric ideals. We provide a nice lattice basis consisting of circuits. The corresponding lattice basis ideal is generated by circuits of degree two and thus in particular satisfies the Sturmfels-Sullivant conjecture.

The ideal of phylogenetic invariants is the saturation of the lattice basis ideal. However, we do not use any of the standard algorithms to compute saturation (e.g. [5], [7]). Instead, our recursive construction of the lattice basis ideals can be extended to give the full ideal of invariants, which we describe in the final section. The recursive description of these ideals depends only on the number of leaves of the claw tree and it does not require saturation. Finally, and possibly somewhat surprisingly, we show that the ideal of invariants for every claw tree admits a quadratic Gröbner basis with respect to a lexicographic term order. We describe it *explicitly*.

Combined with the main result of Sturmfels and Sullivant in [8], this implies that the phylogenetic ideal of *every* tree for the group \mathbb{Z}_2 has a quadratic Gröbner basis. Hence, the coordinate ring of the toric variety is a Koszul algebra.

2 Background

The genetic relationship between species is most conveniently presented using a phylogenetic tree, often a rooted tree T with n labeled leaves. Each node of T is a random variable with k possible states chosen from the state space S. At each leaf, we can observe any of the k states; thus there are k^n possible observations. Let p_{σ} be the probability of making a particular observation $\sigma \subset S^n$ at the leaves. Then p_{σ} is a polynomial in the model parameters. Biological applications impose restrictions on p_{σ} , such as nonnegativity and total sum 1. In phylogenetic algebraic geometry, these restrictions are ignored. Thus we consider a polynomial map ϕ that depends only on T and k and whose coordinate functions are the k^n polynomials p_{σ} :

$$\phi: \mathbb{C}^N \to \mathbb{C}^{k^n}$$
,

where N is the total number of model parameters.

A phylogenetic invariant of the model is a polynomial in the leaf probabilities p_{σ} that vanishes for every choice of model parameters. The set of these polynomials forms a prime ideal in the polynomial ring with the unknowns p_{σ} ([8]). One would like to compute this ideal.

There is a specific class of models for which the ideal is particularly nice. Namely, on each edge e of T there is a $k \times k$ transition matrix M_e whose entries represent the probabilities of transition between the states (mutation). A group-based model is one in which the matrices M_e are pairwise distinct, but it is required that certain entries coincide. For these models, transition matrices are diagonalizable by the Fourier transform of an abelian group, and the phylogenetic invariants form a toric ideal in the Fourier coordinates. The key idea behind this linear change of coordinates is to label the states (for example, A, C, G,

and T) by a finite abelian group (for example, $\mathbb{Z}_2 \times \mathbb{Z}_2$) in such a way that transitioning from one state to another depends only on the difference of the group elements. Examples of group-based models include the well-known Jukes-Cantor and Kimura's one-parameter models.

Sturmfels and Sullivant in [8] reduce the computation of ideals of phylogenetic invariants of group-based models on an arbitrary tree to the case of claw trees $K_n := K_{1,n}$. The main result of [8] gives a way of constructing the ideal of phylogenetic invariants for any tree if the ideal for the claw tree is known. However, in general, it is an open problem to compute the phylogenetic invariants for a claw tree. We give a complete description of the lattice basis ideal and a quadratic Gröbner basis of the corresponding ideal of invariants for the group \mathbb{Z}_2 on $T = K_n$ for any number of leaves n. Our quadratic Gröbner basis together with the main result in [8] provides a way for constructing explicitly the ideal of invariants for any tree. In addition, these ideals are particularly nice as they satisfy the conjecture in [8] which proposes that the order of the group gives an upper bound for the degrees of minimal generators of the ideal of invariants. The case of \mathbb{Z}_2 has been solved in [8] using a technique that does not generalize. We hope to extend our recursive approach and obtain the result for an arbitrary group.

Here we consider the ideal of the general group-based model on an arbitrary claw tree. Assuming the identity labeling function and adopting the notation of [8], the ideal I of phylogenetic invariants in the Fourier coordinates for the tree $T = K_n$ is the kernel of the following homomorphism between polynomial rings:

$$\varphi: \mathbb{C}[q_{g_1,\dots,g_n}:g_1,\dots,g_n\in G] \to \mathbb{C}[a_g^{(i)}:g\in G, i=1,\dots,n+1]$$
$$q_{g_1,\dots,g_n}\mapsto a_{g_1}^{(1)}a_{g_2}^{(2)}\dots a_{g_n}^{(n)}a_{g_1+g_2+\dots+g_n}^{(n+1)},$$

where G is a finite group with k elements, each corresponding to a state. The coordinate q_{g_1,\ldots,g_n} corresponds to observing the element g_1 at the first leaf of T, g_2 at the second, and so on. The advantage of using the Fourier coordinates is that the ideal I becomes a toric ideal, thus it can be computed from the corresponding lattice basis ideal by saturation. We determine the Gröbner bases of these toric ideals.

Detailed background on phylogenetic trees, invariants, group-based models, Fourier coordinates, labeling functions and more is provided in [1], [4], [6], [8].

3 Matrix representation

Fix a claw tree $T=K_n$ on n leaves and a finite group G of order k. Soon we will specialize to the case k=2. We want to compute the ideal of phylogenetic invariants for the general group-based model on T. After the Fourier transform, the ideal of invariants (in Fourier coordinates) is given by $I=\ker\varphi$, where

$$\varphi: \mathbb{C}[q_{g_1,\dots,g_n}:g_1,\dots,g_n\in G] \to \mathbb{C}[a_g^{(i)}:g\in G, i=1,\dots,n+1]$$
$$q_{g_1,\dots,g_n}\mapsto a_{g_1}^{(1)}a_{g_2}^{(2)}\dots a_{g_n}^{(n)}a_{g_1+g_2+\dots+g_n}^{(n+1)}$$

is a map between polynomial rings in k^n and k(n+1) variables, respectively. In order to compute the toric ideal I, we first compute the lattice basis ideal $I_L \subset I$ corresponding to φ as follows. Fixing an order on the monomials of the two polynomial rings, the linear map φ can be represented by a matrix $B_{n,k}$ that describes the action of φ on the variables. Then the lattice $L = \ker(B_{n,k}) \subset \mathbb{Z}^{k^n}$ determines the ideal I_L . It is generated by elements of the form $(\prod q_{g_1,\dots,g_n})^{v^+}$ $(\prod q_{g_1,\dots,g_n})^{v^-}$ where $v=v^+-v^-\in L$. We will give an explicit description of this basis and, equivalently, the ideal I_L .

Hereafter assume that $G = \mathbb{Z}_2$. For simplicity, let us say that $B_n := B_{n,2}$.

To create the matrix B_n , first order the two bases as follows. Order the $a_q^{(i)}$ by varying the upper index (i) first and then the group element $g: a_0^{(1)}, a_0^{(2)}, \ldots$ $a_0^{(n+1)}, a_1^{(1)}, \ldots, a_1^{(n+1)}$. Then, order the q_{q_1,\ldots,q_n} by ordering the indices with respect to binary counting:

$$q_{0...00} > q_{0...01} > \cdots > q_{1...10} > q_{1...1}.$$

That is, $q_{a_1...a_n} > q_{h_1...h_n}$ if and only if $(g_1...g_n)_2 < (h_1...h_n)_2$, where

$$(g_1 \dots g_n)_2 := g_1 2^{n-1} + g_2 2^{n-2} + \dots + g_n 2^0$$

represents the binary number $g_n \dots g_n$. Next, index the rows of B_n by $a_g^{(i)}$ and its columns by q_{g_1,\dots,g_n} . Finally, put 1 in the entry of B_n in the row indexed by $a_q^{(i)}$ and column indexed by q_{q_1,\ldots,q_n} if $a_g^{(i)}$ divides the image of q_{g_1,\ldots,g_n} , and 0 otherwise.

Example 1. Let n = 2. Then we order the q_{ij} variables according to binary counting: q_{00} , q_{01} , q_{10} , q_{11} , so that

$$\varphi : \mathbb{C}[q_{00}, q_{01}, q_{10}, q_{11}] \to \mathbb{C}[a_0^{(1)}, a_0^{(2)}, a_0^{(3)}, a_1^{(1)}, a_1^{(2)}, a_1^{(3)}]$$

$$q_{00} \mapsto a_0^{(1)} a_0^{(2)} a_{0+0}^{(3)}$$

$$q_{01} \mapsto a_0^{(1)} a_1^{(2)} a_{0+1}^{(3)}$$

$$q_{10} \mapsto a_1^{(1)} a_0^{(2)} a_{1+0}^{(3)}$$

$$q_{11} \mapsto a_1^{(1)} a_1^{(2)} a_{1+1}^{(3)}.$$

Now we put the $a_i^{(j)}$ variables in order: $a_0^{(1)},\,a_0^{(2)},\,a_0^{(3)},\,a_1^{(1)},\,a_1^{(2)},\,a_1^{(3)}$. Thus

$$B_2 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}.$$

The tree K_{n-1} can be considered as a subtree of $T = K_n$ by ignoring the leftmost leaf of T. As a consequence, a natural question arises: how does B_n relate to B_{n-1} ?

Remark 1. The matrix B_{n-1} for the subtree of T with the leaf (1) removed can be obtained as a submatrix of B_n for the tree T by deleting rows 1 and (n+1)+1 and taking only the first 2^{n-1} columnus.

Divide the *n*-leaf matrix B_n into a 2×2 block matrix with blocks of size $(n + 1) \times 2^{n-1}$:

$$B_n = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}.$$

Then, grouping together B_{11} , B_{21} without the first row of each B_{i1} , we obtain the matrix B_{n-1} . This is true because rows 1 and (n+1)+1 represent the variables $a_g^{(1)}$ for $g \in G$ associated with the leaf (1) of K_n . Note that the entries in row $a_g^{(n+1)}$ remain undisturbed as the omitted rows are indexed by the identity of the group.

Example 2. The matrix B_2 is equal to the submatrix of B_3 formed by rows 2,3,4,6,7,8, and first 4 columns.

$$B_3 = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}.$$

Remark 2. Fix any observation $\sigma = g_1, \ldots, g_n$ on the leaves. Clearly, at any given leaf $j \in \{1, \ldots, n\}$, we observe exactly one group element, g_j . Since the matrix entry $b_{a_{g_j}^{(j)}, q_\sigma}$ in the row indexed by $a_{g_j}^{(j)}$ and column indexed by q_σ is 1 exactly when $a_{g_j}^{(j)}$ divides the image of q_σ , one has that

$$\sum_{q_i \in G} b_{a_{g_j}^{(j)}, q_\sigma} = 1$$

for a fixed leaf (j) and fixed observation σ . Note that the formula also holds if j=n+1 by definition of $a_{g_{n+1}}^{(n+1)}=a_{g_1+\cdots+g_n}^{(n+1)}$. In particular, the rows indexed by $a_{g_i}^{(j)}$ for a fixed j sum up to the row of ones.

4 Number of lattice basis elements

We compute the dimension of the kernel of B_n by induction on n. We proceed in two steps.

Lemma 1 (Lower bound).

$$rank(B_n) \ge rank(B_{n-1}) + 1.$$

Proof. First note that $rank(B_n) \ge rank(B_{n-1})$ since B_{n-1} is a submatrix of the first 2^{n-1} columns of B_n . In the block $\begin{bmatrix} B_{11} \\ B_{12} \end{bmatrix}$, the row indexed by $a_1^{(1)}$ is zero, while in the block $\begin{bmatrix} B_{21} \\ B_{22} \end{bmatrix}$, the row indexed by $a_1^{(1)}$ is 1. Choosing one column from $\begin{bmatrix} B_{21} \\ B_{22} \end{bmatrix}$ provides a vector independent of the first 2^{n-1} columns. The rank must therefore increase by at least 1.

Lemma 2 (Upper bound).

$$rank(B_n) \le n+2.$$

Proof. B_n has 2(n+1) rows. Remark 2 provides n independent relations among the rows of our matrix: varying j from 1 to n+1, we obtain that the sum of the rows j and n+1+j is 1 for each $j=1,\ldots,n+1$. Thus the upper bound is immediate.

We are ready for the main result of the section.

Proposition 1 (Cardinality of lattice basis).

There are $2^n - 2(n+1) + n$ elements in the basis of the lattice L corresponding to $T = K_n$. That is,

$$\dim \ker(B_n) = 2^n - 2(n+1) + n.$$

Proof. We show $rank(B_n) = 2(n+1) - n$. Assume that the claim is true for n-1. Then by Lemmae (1) and (2),

$$2(n+1) - n \ge rank(B_n) \ge rank(B_{n-1}) + 1 = 2n - (n-1) + 1,$$

where the last equality is provided by the induction hypothesis. The claim follows since the left- and the right-hand sides agree. \Box

5 Lattice basis

In this section we describe a basis of the kernel of $B_n := B_{n,2}$, in which the binomials corresponding to the basis elements satisfy the conjecture on the degrees of the generators of the phylogenetic ideal. In particular, since the ideal is generated by squarefree binomials and contains no linear forms, these elements are actually circuits. By Proposition 1, we need to find $2^n - (n+2)$ linearly independent vectors in the lattice. The matrix of the tree with n=2 leaves has a trivial kernel, so we begin with the tree on n=3 leaves. The dimension of the kernel is 3 and the lattice basis is given by

$$\begin{aligned} v_1 &= [0,0,1,-1,-1,1,0,0], \\ v_2 &= [0,1,0,-1,-1,0,1,0], \\ v_3 &= [1,0,0,-1,-1,0,0,1]. \end{aligned}$$

In order to study the kernels of B_n for any n, it is useful to have an algorithmic way of constructing the matrices.

Algorithm 1 To construct B_n :

- Note that the number of columns of the n-leaf matrix is 2^n .
- Divide the first row in half. Fill the first half (2^{n-1}) entries of the first row with ones, and the second half with zeros.
- Divide the next row into blocks of size 2^{n-2} and fill it with alternating blocks of ones and zeros, starting with ones.
- Continue with each row corresponding to a leaf; ending with the n^{th} row which will look like $[1,0,1,0,\ldots,1,0]$.
- The $a_0^{(n+1)}$ row counts the number of zeros in the rows above along the same column: if n is even and the number of zeros in the first n rows is even, then the $a_0^{(n+1)}$ -row entry in that column is 1, and 0 otherwise. If n is odd and the number of zeros in the first n rows is odd, then the $a_0^{(n+1)}$ -row entry in that column is 1, and 0 otherwise.

The bottom half of the matrix is simply the binary opposite of the top half. Homogeneity of the ideal I_L shows that it is enough to analyze the top half only when determining the kernel elements.

One checks that this algorithm gives indeed the matrices B_n as defined in Section 3.

Remark 3. There are n copies of B_{n-1} inside B_n .

By deleting one leaf at a time, we get n copies of K_{n-1} as a subtree of $T = K_n$. Suppose we delete leaf (i) from T to get the tree T_i on leaves $1, 2, \ldots, i-1, i+1, \ldots, n$. Ignoring the two rows of B_n that represent the leaf (i) and taking into account the columns of B_n containing nonzero entries of the row indexed by $a_0^{(i)}$ (that is, observing 0 at leaf (i)) gives precisely the matrix B_{n-1} corresponding to T_i . Note that the entry indexed by $a_g^{(n+1)}$, for any $g \in G$, will be correct since we are ignoring the identity of the group, as in Remark 1.

This leads to a way of constructing a basis of $\ker(B_n)$ from the one of $\ker(B_{n-1})$. Namely, removing leaf (1) from T produces $\dim(\ker(B_{n-1})) = 2^{n-1} - n - 1$ independent vectors in $\ker(B_n)$. Let us name this collection of vectors V_1 . Removing leaf (2) produces a collection V_2 consisting of $\dim(\ker B_{n-1}) - \dim(\ker B_{n-2}) = 2^{n-2} - 1$ vectors in $\ker(B_n)$. V_2 is independent of V_1 since the second half of each vector in V_2 has nonzero entries in the columns of B_n where all vectors in V_1 are zero, a direct consequence of the location of the submatrix corresponding to V_2 . Finally, removing any other leaf (i) of V_2 produces a collection V_3 of as many new kernel elements as there are new columns involved (in terms of the submatrix structure); namely, V_2 is new vectors. (Note that every vector in V_2 has a nonzero entry in at least one new column so that the full collection is independent of V_1 .)

Using the above procedure, we have obtained

$$(2^{n-1}-n-1)+(2^{n-2}-1)+(2^{n-3})+\cdots+2^{n-n}$$

independent vectors in the kernel of B_n . This is exactly one less than the desired number, 2^n-n-2 . Hence to the list of the kernel generators we add one additional vector v that is independent of all the V_i , $i=1,\ldots,n$ as it has a nonnegative entry in the last column. (Note that no $v \in V_i$ has this property by the observation on the column location of the submatrix associated with each T_i .) In particular,

$$v = [0, \dots, 0, 1, 0, 0, -1, -1, 0, 0, 1] \in \ker(B_n).$$

To see this, we simply notice that the rows of the last 8-column block of B_n are precisely the rows of the first 8-column block of B_n up to permutation of rows, which does not affect the kernel.

The lattice basis we just constructed is directly computed by the following algorithm.

Algorithm 2 [Construction of the lattice basis for T_n]

Input: the number of leaves n of the claw tree T_n .

Output: a basis of ker $B_n \subset \mathbb{Z}^{2^n}$.

Begin with initializing 2^n-n-2 zero row vectors of size 2^n and organize them in a matrix K. Let P_3 be the pattern for n=3 given by the vectors v_1,v_2,v_3 : $v_1=[0,0,1,-1,-1,1,0,0],\ v_2=[0,1,0,-1,-1,0,1,0],\ v_3=[1,0,0,-1,-1,0,0,1].$ Place P_3 in the first 2^3 columns of the first $|P_3|=3$ rows of K.

Next, create the pattern P_4 according to the following rules. Mark columns 1 through $2^4 = 16$ of K.

- Fill columns 1-8 (and first three rows) of K with the pattern P_3 .
- Repeat for columns 1-4, 9-12 (and the next three rows).
- Place v_2 and v_3 into columns 1–2, 5–6, 9–10, 13–14 (and the following two rows)
- Place v_3 into the odd numbered columns from 1 to 16.
- Place v into the last 8 of the marked columns.

Next, create the pattern P_5 similarly: mark columns 1 through $2^5 = 32$.

- Fill columns 1–16 with the pattern P_4 .
- Take the pattern P_4 and with its vectors fill the columns $1-2^3$ and 17-24 with the last $2^3 1$ of the vectors of P_4 .
- Mark columns 1-4, 9-12, 17-20, 25-28 and fill them with the last 2^2 of the vectors of P_4 .
- Proceed marking the columns in block sizes 2^i and fill them with the last 2^i of the vectors of P_4 , until all but the last column has been filled in.
- Add one more vector by filling the last 8 of the marked columns of the zero row vector with v.

In general, create patterns P_n out of P_{n-1} recursively and fill in all the rows of K with nonzero entries in the appropriate locations.

Example 3. Consider the tree T on n=4 leaves. Then

The lattice basis is given by the rows of the following matrix:

These lattice vectors correspond to the relations on the leaf observations in the natural way; namely, the first column coresponds to $q_{0,...,0}$, the second to $q_{0,...,0,1}$, and so on. Therefore, the lattice basis ideal for T in Fourier coordinates is

```
\begin{split} I_L &= \big(q_{0010}q_{0101} - q_{0011}q_{0100}, q_{0001}q_{0110} - q_{0011}q_{0100}, q_{0000}q_{0111} - q_{0011}q_{0100}, \\ q_{0010}q_{1001} &= q_{0011}q_{1000}, q_{0001}q_{1010} - q_{0011}q_{1000}, q_{0000}q_{1011} - q_{0011}q_{1000}, \\ q_{0001}q_{1100} &= q_{0101}q_{1000}, q_{0000}q_{1101} - q_{0101}q_{1000}, \\ q_{0000}q_{1110} &= q_{0110}q_{1000}, q_{1000}q_{1111} - q_{1011}q_{1100}\big). \end{split}
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This ideal is contained in the ideal of phylogenetic invariants I for T_4 . In the next section, we compute explicitly the generators of the ideal of invariants for any claw three T_n and the group \mathbb{Z}_2 .

Ideal of invariants 6

We show that the lattice basis ideals provide a basic building block for the full ideals of invariants, as expected. However, instead of computing the ideal of invariants as a saturation of the lattice basis ideal in a standard way (e.g. [7],[5]), we use the recursive constructions from the previous section on the saturated ideals directly. We begin with the ideal of invariants for the smallest tree, and build all other trees recursively. The underlying ideas for how to lift the generating sets come from Algorithm 2.

We will denote the ideal of the claw tree on n leaves by $I_n = \ker \varphi_n$.

6.1 The tree on n=3 leaves

Claim. The ideal of the claw tree on n=3 leaves is

$$I_3 = (q_{000}q_{111} - q_{100}q_{011}, q_{001}q_{110} - q_{100}q_{011}, q_{010}q_{101} - q_{100}q_{011}).$$

This can be verified by computation. In particular, this ideal is equal to the lattice basis ideal for the tree on three leaves; I_L is already prime in this case.

Let $<:=<_{lex}$ be the lexicographic order on the variables induced by

$$q_{000} > q_{001} > q_{010} > q_{011} > q_{100} > q_{101} > q_{110} > q_{111}.$$

(That is, $q_{ijk} > q_{i'j'k'}$ if and only if $(ijk)_2 < (i'j'k')_2$, where $(ijk)_2$ denotes the binary number ijk.)

Remark 4. The three generators of I_3 above are a Gröbner basis for I_3 with respect to <, since the initial terms, written with coefficient +1 in the above description, are relatively prime so all the S-paris reduce to zero.

Remark 5. Write the quadratic binomial $q = q^+ - q^-$ as

$$q_{q_1^{(1)}q_1^{(2)}q_1^{(3)}}q_{q_2^{(1)}q_2^{(2)}q_2^{(3)}}-q_{h_1^{(1)}h_1^{(2)}h_1^{(3)}}q_{h_2^{(1)}h_2^{(2)}h_2^{(3)}}.$$

Then $q \in I_3$ if and only if the following two conditions hold:

1.
$$g_1^{(1)} + g_1^{(2)} + g_1^{(3)} = h_1^{(1)} + h_1^{(2)} + h_1^{(3)}$$
 and
$$g_2^{(1)} + g_2^{(2)} + g_2^{(3)} = h_2^{(1)} + h_2^{(2)} + h_2^{(3)},$$
 2.
$$g_1^{(i)} + g_2^{(i)} = 1 = h_1^{(i)} + h_2^{(i)} \text{ for } 1 < i < 3 = n.$$

Note that the second condition holds since otherwise the projection of q obtained by eliminating the leaf (i) at which the observations $g_1^{(i)}$ and $g_2^{(i)}$ are both equal to 0 or to 1 produces an element q' in the kernel of the map φ_2 of the 2-leaf tree, which is trivial.

The tree on an arbitrary number of leaves 6.2

Let us now define a set of maps and a distinguished set of binomials in I_n .

Definition 1. Let $\pi_i(q)$ be the projection of q that eliminates the ith index of each variable in q.

For example,

$$\pi_4(q_{0000}q_{1110} - q_{1000}q_{0110}) = q_{000}q_{111} - q_{100}q_{011}.$$

Definition 2. Let \mathcal{G}_n be the set of quadratic binomials $q \in I_n$ that can be written

$$q = q^{+} - q^{-} = q_{g_{1}^{(1)} \dots g_{1}^{(n)}} q_{g_{2}^{(1)} \dots g_{2}^{(n)}} - q_{h_{1}^{(1)} \dots h_{1}^{(n)}} q_{h_{2}^{(1)} \dots h_{2}^{(n)}}$$

such that one of the two following properties is satisfied:

Property (i): For some $1 \le i \le n, j \in \mathbb{Z}_2$,

$$g_1^{(i)} = g_2^{(i)} = j = h_1^{(i)} = h_2^{(i)}$$
 (1)

and

$$\pi_i(q) \in I_{n-1}. \tag{2}$$

Property (ii): For each $1 \le k \le n$,

$$g_1^{(k)} + g_2^{(k)} = 1 = h_1^{(k)} + h_2^{(k)}$$
 (3)

and

$$\pi_k(q) \in I_{n-1}. \tag{4}$$

Example 4. Let n=4. The set of elements $q\in\mathcal{G}_n$ with Property (i) consists of those for which j = 0:

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q_{0000}q_{1101}-q_{1000}q_{0101},\,q_{0001}q_{1100}-q_{1000}q_{0101},\,q_{0100}q_{1001}-q_{1000}q_{0101},\\
q_{0000}q_{1110} - q_{1000}q_{0110}, q_{0010}q_{1100} - q_{1000}q_{0110}, q_{0100}q_{1010} - q_{1000}q_{0110};
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 $q_{0000}q_{0111}-q_{0100}q_{0011},\,q_{0001}q_{0110}-q_{0100}q_{0011},\,q_{0010}q_{0101}-q_{0100}q_{0011},\\$ $q_{0000}q_{1011}-q_{1000}q_{0011},\,q_{0001}q_{1010}-q_{1000}q_{0011},\,q_{0010}q_{1001}-q_{1000}q_{0011},\\$

and those for which j = 1:

 $q_{1000}q_{1111}-q_{1100}q_{1011},\,q_{1001}q_{1110}-q_{1100}q_{1011},\,q_{1010}q_{1101}-q_{1100}q_{1011},\\$

 $q_{0100}q_{1111} - q_{1100}q_{0111}, q_{0101}q_{1110} - q_{1100}q_{0111}, q_{0110}q_{1101} - q_{1100}q_{0111},$

 $q_{0010}q_{1111}-q_{1010}q_{0111},\,q_{0011}q_{1110}-q_{1010}q_{0111},\,q_{0110}q_{1011}-q_{1010}q_{0111},\\$

 $q_{0001}q_{1111} - q_{1001}q_{0111}, q_{0011}q_{1101} - q_{1001}q_{0111}, q_{0101}q_{1011} - q_{1001}q_{0111}.$

The set of elements $q \in \mathcal{G}_n$ with Property (ii) are:

 $q_{0000}q_{1111}-q_{1001}q_{0110},\,q_{0001}q_{1110}-q_{1000}q_{0111},\,q_{0011}q_{1100}-q_{1001}q_{0110},\\$

 $q_{0010}q_{1101}-q_{1000}q_{0111},\,q_{0101}q_{1010}-q_{1001}q_{0110},\,q_{0100}q_{1011}-q_{1000}q_{0111}.$

Proposition 2. The set of binomials in \mathcal{G}_n generates the ideal I_n . That is,

$$I_n = (q: q^+ - q^- \in \mathcal{G}_n).$$

In addition, this set of generators can be obtained inductively by lifting the generators corresponding to the various phylogenetic ideals on n-1 leaves.

Proof. Condition (3) is simply the negation of (1). Condition (1) can be restated as follows: for some $1 \le i \le n$ and a fixed j,

$$(a_j^{(i)})^2 |\varphi_n(q^+)|$$
 and $(a_j^{(i)})^2 |\varphi_n(q^-)|$.

Therefore, Property (i) translates to having an observation j fixed at leaf (i) for each of the variables in q. On the other hand, condition (3) means that for any k, not all the k^{th} indices are 0 and not all are 1. Thus Property (ii) means that no leaf has a fixed observation, and can be restated as follows: for every $1 \le i \le n$,

$$a_0^{(i)} a_1^{(i)} | \varphi_n(q^+) \text{ and } a_0^{(i)} a_1^{(i)} | \varphi_n(q^-).$$
 (5)

Let $q \in I_n$ with $\deg(q) = 2$. Then clearly either (1) or (3) holds; that is, either the index corresponding to one leaf is fixed for all the monomials in q, or none of them are.

In the former case, for the index i from equation (1),

$$q \in I_n \iff \varphi_n(q^+) = \varphi_n(q^-)$$
$$\iff \varphi_{n-1}(\pi_i(q^+)) = \varphi_{n-1}(\pi_i(q^-)) \iff \pi_i(q) \in I_{n-1},$$

where the first statement holds by definition of φ_n and the second by definition of the projection π_i .

In the latter case, for each i with $1 \le i \le n$,

$$q \in I_n \iff \varphi_n(q^+) = \varphi_n(q^-)$$
$$\iff \varphi_{n-1}(\pi_i(q^+)) = \varphi_{n-1}(\pi_i(q^-)) \iff \pi_i(q) \in I_{n-1},$$

where the second statement holds by definition of π_i and (5).

Since Sturmfels and Sullivant have shown that the ideal I_n is generated in degree 2, it follows that $I_n = (q : q \in \mathcal{G}_n)$.

In particular, the set of generators for I_n with Property (i) can be obtained from those of I_{n-1} by inserting first 0 at the i^{th} index position for each monomial of $q \in \mathcal{G}_{n-1}$ and then repeating the same process by inserting 1. This operation corresponds to lifting to all the possible preimages of $\pi_i(q)$ that satisfy Property (i) for each $1 \le i \le n$ and every $q \in \mathcal{G}_{n-1}$. The set of generators for I_n with Property (ii) can be obtained from those of I_{n-1} by a similar lifting to all preimages of $\pi_i(q)$ for each $q \in \mathcal{G}_{n-1}$ in such a way that Property (ii) is satisfied. Namely, for every $q = q^+ - q^- \in \mathcal{G}_{n-1}$ with Property (ii), one inserts 0 at the i^{th} index position for one monomial of q^+ and for one monomial of q^- , and inserts 1 at the i^{th} index position for the remaining monomials of q^+ and q^- . In addition, by definition of Property (ii), it suffices to lift to the preimages of $\pi_n(q)$ only. \square

Remark 6. A different recursion has been proposed by Sturmfels and Sullivant in [9].

Remark 7. The generators for the ideal I_3 all satisfy Property (ii), since the matrix for the 2-leaf tree has a trivial kernel.

Recall ([7]) that a binomial $q = q^+ - q^- \in I$ is said to be *primitive* if there exists no binomial $f = f^+ - f^- \in I$ with the property that $f^+|q^+$ and $f^-|q^-$. A *circuit* is a primitive binomial of minimal support.

Remark 8. The binomials in \mathcal{G}_n are circuits of I_n , since the ideal is generated by squarefree binomials and contains no linear forms.

In general, we can describe the generators of I_n as follows: given n, begin by lifting \mathcal{G}_3 recursively to produce \mathcal{G}_{n-1} ; that is, until the number of indices of each generator reaches n-1. Next, lift \mathcal{G}_{n-1} n times so that Property (i) is satisfied for one of the n index positions. For example,

$$q := q_{0000}q_{1111} - q_{1001}q_{0110} \in \mathcal{G}_4$$

can be lifted to a generator of I_5 in ten different ways: by lifting to preimages of π_1, \ldots, π_5 so that Property (i) is satisfied with either a 0 or a 1:

$$\pi_1^{-1}(q) = \{q_{00000}q_{01111} - q_{01001}q_{00110}, q_{10000}q_{11111} - q_{11001}q_{10110}\},$$

$$\pi_2^{-1}(q) = \{q_{00000}q_{10111} - q_{10001}q_{00110}, q_{01000}q_{11111} - q_{11001}q_{01110}\},$$

and so on. This will be the set of binomials in \mathcal{G}_n with Property (i). Clearly, some generators will repeat during the recursive lifting: lifting by inserting 0 at position (i) allows the 0 to occur at the previous i-1 positions. Also, fixing 1 at any leaf allows 0 to appear on any of the other leaves.

To construct $q^+ - q^-$ with Property (ii), we need not proceed inductively, as all projections of binomials that satisfy this property must satisfy it, too. Instead, we consider two cases corresponding to the parity of n. Namely, recalling the definition of Property (ii), first we fix q^- in such a way to ensure that $in_{<_{lex}}(q) = q^+$.

Suppose n is odd. Fix q^- by taking

$$q^- = q_{01...1}q_{10...0}$$

with n indices in each of the two variables. Then n-1 being even provides that $a_0^{(n+1)}a_1^{(n+1)}|\varphi_n(q^-)$. Thus every choice of q^+ must satisfy the same. To find q^+ , we need to choose pairs of n-digit binary numbers with digits complementary to each other, and thus there are $2^{n-1}-1$ choices for q^+ . Specifically, listing the smallest $2^{n-1}-1$ n-digit binary numbers and pairing them with the largest $2^{n-1}-1$ n-digit binary numbers in reverse order produces all choices for q^+ , and we have a complete list of generators. For example, the first such generator in the list would be $q_{0...0}q_{1...1}-q_{01...1}q_{10...0}$.

If n is even, then we can create q^- such that $(a_0^{(n+1)})^2$ or $(a_1^{(n+1)})^2$ divides $\varphi_n(q^-)$ and $\varphi_n(q^+)$. Namely, the two choices for q^- are

$$q^- = q_{01...1}q_{10...0}$$

and

$$q^- = q_{01...10}q_{10...01}$$
.

The list of all possible q^+ is obtained in the manner similar to the case when n is odd, except that the odd pairs in the list receive the first choice of q^- , while the even pairs recieve the second. The number of such generators $q^+ - q^-$ is $2^{n-1} - 2$, since there are 2^n n-digit binary numbers and thus half as many pairs, and 2 choices are taken by the q^- .

In summary, the number of generators of I_n that satisfy Property (ii) is

$$(2^{n-1}-2)+(n \mod 2).$$

Next we strenghten Proposition (2).

Proposition 3. The set \mathcal{G}_n is a lexicographic Gröbner basis of I_n , for any n.

Proof. For the case n=3 this is already shown. Let n>3. Then we can partition the set of $q \in \mathcal{G}_n$ into those satisfying Property (i) or (ii).

Let $q_i, q_j \in I_n$. If $(q_i^+, q_j^+) = 1$, the S-pair $S(q_i, q_j)$ reduces to zero. Also, if q_i^- and q_j^- are not relatively prime, the cancellation criterion provides that the corresponding S-pair also reduces to zero. Therefore we consider $f := S(q_i, q_j) \in I_n$ with $(q_i^+, q_j^+) \neq 1$ and $(q_i^-, q_j^-) = 1$. In particular, $\deg(f) = 3$. Let us write $q_i = q_{g_1}q_{g_2} - q_{h_1}q_{h_2}$ and $q_j = q_{g_1}q_{g_3} - q_{h_3}q_{h_4}$. Then

$$f = q_{g_3}q_{h_1}q_{h_2} - q_{g_2}q_{h_3}q_{h_4} \in I_n.$$

Case I. Suppose q_i satisfies Property (i) and q_j satisfies Property (ii). Then there exists a k such that $\pi_k(q_i) \in I_{n-1}$. Furthermore, Property (ii) implies that $\pi_k(q_j) \in I_{n-1}$. A very technical argument shows that

$$\pi_k(f) \in I_{n-1}$$

and furthermore, this projection preserves the initial terms. In summary, to check that $\pi_k(f) \in I_{n-1}$, it suffices to ensure that $a_s^{(n)}|\varphi_{n-1}(\pi_k(q_{g_3}q_{h_1}q_{h_2}))$ if and only if $a_s^{(n)}|\varphi_{n-1}(\pi_k(q_{g_2}q_{h_3}q_{h_4}))$, where s is the sum of the observations on the leaves of the (n-1)-leaf tree obtained from T by deleting leaf (k). There are two cases corresponding to the parity of n. If n is odd, there are additional subcases determined by the correspondence of the images of the variables in the two monomials of f under φ_{n-1} . The facts that q_i and q_j satisfy Properties (i) and (ii), respectively, play a crucial role in the argument. Checking all the cases then shows that $\pi_k(f) \in I_{n-1}$ and that initial terms are preserved under this projection.

Applying the induction hypothesis then finishes the proof.

Case II. Suppose both q_i and q_j satisfy Property (i). Then there is a $q_k \in \mathcal{G}_n$ satisfying Property (ii) where both $S(q_i, q_k)$ and $S(q_j, q_k)$ reduce to zero. The three-pair criterion ([5]) provides the desired result.

Case III. If both q_i and q_j satisfy Property (ii), then it can be seen from the construction preceding this Proposition that the initial terms are relatively prime, so their S-polynomial need not be considered.

Proposition 3 has important theoretical consequences. Let S be a polynomial ring over the field K. Recall ([2]) that S/I is Koszul if the field K has a linear resolution as a graded S/I-module:

$$\cdots \to (S/I)^{\beta_2}(-2) \to (S/I)^{\beta_1}(-1) \to S/I \to K \to 0.$$

An ideal $I \subset S$ is said to be quadratic if it is generated by quadrics. S/I is quadratic if its defining ideal I is quadratic, and it is G-quadratic if I has a quadratic Gröbner basis. It is known (e.g. [2]) that if S/I is G-quadratic, then it is Koszul, which in turn implies it is quadratic. The reverse implications do not hold in general. We have just found an infinite family of toric varieties whose coordinate rings S/I are G-quadratic.

Corollary 1. The coordinate ring of the toric variety whose defining ideal is I_n is Koszul for every n.

The approach developed here produces the list of generators for the kernel of B_n all of which are of degree two. In addition, by constructing the toric ideals of invariants inductively, we are able to explicitly calculate the quadratic Gröbner bases. In light of the conjecture posed in [8] that the ideal of phylogenetic invariants for the group of order k is generated in degree at most k, we are working on generalizing the above approach to any abelian group of order k. In particular, we want to give a description of the lattice basis ideal I_L and the ideal of invariants I for $G = \mathbb{Z}_2 \times \mathbb{Z}_2$ with generators of degree at most 4. These phylogenetic ideals are of interest to computational biologists.

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