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.

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1 Introduction

Phylogenetics is concerned with determining genetic relationship between species based on their DNA sequences. First, the various DNA sequences are aligned, that is, a correspondence is established that accounts for their differences. Assuming that all DNA sites evolve identically and independently, the focus is on one site at a time. The data then consists of observed pattern frequencies in aligned sequences. This observed data are used to estimate the true joint probabilities of the observations and, most importantly, to reconstruct the ancestral relationship among the species. The relationship can be represented by a phylogenetic tree.

A phylogenetic tree $T$ is a simple, connected, acyclic graph equipped with some statistical information. Namely, each node of $T$ is a random variable with $k$ possible states chosen from the state space $S$. Edges of $T$ are labeled by transition probability matrices that reflect probabilities of changes of the states from a node to its child. These probabilities of mutation are the parameters for the statistical model of evolution, which is described in terms of a discrete-state continuous-time Markov process on the tree. Since the goal is to reconstruct the tree, the interior nodes are hidden. The relationship between the random
variables is encoded by the structure of the tree. At each of the $n$ leaves, we can observe any of the $k$ states; thus there are $k^n$ possible observations. Let $p_\sigma$ be the joint probability of making a particular observation $\sigma \subset S^n$ at the leaves. Then $p_\sigma$ is a polynomial in the model parameters.

A phylogenetic invariant of the model is a polynomial in the leaf probabilities which vanishes for every choice of model parameters. The set of these polynomials forms a prime ideal in the polynomial ring over the unknowns $p_\sigma$. The objective is to compute this ideal explicitly. Thus we consider a polynomial map $\phi : \mathbb{C}^N \to \mathbb{C}^{k^n}$, where $N$ is the total number of model parameters. The map depends only on the tree $T$ and the number of states $k$; its coordinate functions are the $k^n$ polynomials $p_\sigma$. The map $\phi$ induces a parametrization of an algebraic variety.

The study of these algebraic varieties for various statistical models is a central theme in the field of algebraic statistics ([11]). Phylogenetic invariants are a powerful tool for tree reconstruction ([2], [3], [7]).

There is a specific class of models for which the ideal of invariants is particularly nice. Let $M_e$ be the $k \times k$ transition probability matrix for edge $e$ of $T$. In the general Markov model, each matrix entry is an independent model parameter. 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. The key idea behind this linear change of coordinates is to label the states (for example, $A, C, G, \text{and } T$) by a finite abelian group (for example, $\mathbb{Z}_2 \times \mathbb{Z}_2$) in such a way that transition from one state to another depends only on the difference of the group elements. Examples of group-based models include the Jukes-Cantor and Kimura’s one-parameter models used in computational biology.

Sturmfels and Sullivant in [11] reduce the computation of ideals of phylogenetic invariants of group-based models on an arbitrary tree to the case of claw trees $T_n := K_{1,n}$, the complete bipartite graph from one node (the root) to $n$ nodes (the leaves). The main result of [11] 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 consider the ideal for a general group-based model for the group $\mathbb{Z}_2$. Let $q_\sigma$ be the image of $p_\sigma$ under the Fourier transform. Assuming the identity labeling function and adopting the notation of [11], the ideal of phylogenetic invariants for the tree $T_n$ is the kernel of the following homomorphism between polynomial rings:

$$\varphi_n : \mathbb{C}[q_{g_1,\ldots,g_n} : g_1, \ldots, g_n \in G] \to \mathbb{C}[a^{(i)}_g : g \in G, i = 1, \ldots, n+1]$$

$$q_{g_1,\ldots,g_n} \mapsto a^{(1)}_{g_1}a^{(2)}_{g_2} \cdots a^{(n)}_{g_n}a^{(n+1)}_{g_1+g_2+\cdots+g_n},$$

(*)

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 phylogenetic invariants form a toric ideal in the Fourier coordinates $q_\sigma$, which can be computed from the corresponding lattice basis ideal by saturation. The main result of this paper is a complete description.
of the lattice basis ideal and a quadratic Gröbner basis of the ideal of invariants for the group \( \mathbb{Z}_2 \) on \( T_n \) for any number of leaves \( n \).

Our paper is organized as follows. In section 2 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 3 and 4 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., \[8\], \[10\]). 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 \[11\], 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. In addition, the ideals for every tree can be computed explicitly. These ideals are particularly nice as they satisfy the conjecture in \[11\] 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 \[11\] using a technique that does not generalize. We hope to extend our recursive approach and obtain the result for an arbitrary abelian group.

For a detailed background on phylogenetic trees, invariants, group-based models, Fourier coordinates, labeling functions and more, the reader should refer to \[1\], \[6\], \[9\], \[11\].

## 2 Matrix representation

Fix a claw tree \( T_n \) on \( n \) leaves and a finite abelian 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 \( T_n \). After the Fourier transform, the ideal of invariants (in Fourier coordinates) is given by \( I_n = \text{ker} \varphi_n \), where \( \varphi_n \) is a map between polynomial rings in \( k^n \) and \( k(n+1) \) variables, respectively, defined by \( (\cdot, v) \). In order to compute the toric ideal \( I_n \), we first compute the lattice basis ideal \( I_{L_n} \subset I_n \) corresponding to \( \varphi_n \) as follows. Fixing an order on the monomials of the two polynomial rings, the linear map \( \varphi \) can be represented by a matrix \( B_{n,k} \) that describes the action of \( \varphi \) on the variables. Then the lattice \( L_n = \ker(B_{n,k}) \subset \mathbb{Z}^{k^n} \) determines the ideal \( I_{L_n} \). It is generated by elements of the form \( (\prod q_1, \ldots, q_n)^{v^+} - (\prod q_1, \ldots, q_n)^{v^-} \) where \( v = v^+ - v^- \in L_n \). We will give an explicit description of this basis and, equivalently, the ideals \( I_{L_n} \).
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 $a_g^{(i)}$ 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 $q_{g_1,\ldots,g_n}$ by ordering the indices with respect to binary counting:

$$q_{0\ldots0} > q_{0\ldots01} > \cdots > q_{1\ldots10} > q_{1\ldots1}.$$

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

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

represents the binary number $g_1 \ldots g_n$.

Next, index the rows of $B_n$ by $a_g^{(i)}$ and its columns by $q_{g_1,\ldots,g_n}$. Finally, put 1 in the entry of $B_n$ in the row indexed by $a_g^{(i)}$ and column indexed by $q_{g_1,\ldots,g_n}$ 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

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

- $q_{00} \mapsto a_0^{(1)} a_0^{(2)} a_0^{(3)}$
- $q_{01} \mapsto a_0^{(1)} a_1^{(2)} a_0^{(3)}$
- $q_{10} \mapsto a_1^{(1)} a_0^{(2)} a_1^{(3)}$
- $q_{11} \mapsto a_1^{(1)} a_1^{(2)} a_1^{(3)}$.

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 $T_{n-1}$ can be considered as a subtree of $T_n$ by ignoring, for example, 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 $T_n$ with the leaf $(1)$ removed can be obtained as a submatrix of $B_n$ for the tree $T_n$ by deleting rows 1 and $(n + 1) + 1$ and taking only the first $2^{n-1}$ columns.

Divide the $n$-leaf matrix $B_n$ into a $2 \times 2$ 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 $B_{11}$, 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 $T_n$. 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.

**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 $b_{a_j^{(j)}, q_{g_j}}$ in the row indexed by $a_j^{(j)}$ and column indexed by $q_{g_j}$ is 1 exactly when $a_j^{(j)}$ divides the image of $q_{g_j}$, one has that

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

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

### 3 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).**

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

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

**Lemma 2 (Upper bound).**

$$\text{rank}(B_n) \leq n + 2.$$  

**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).

Let \( n \geq 2 \). Then there are \( 2^n - 2(n+1) + n \) elements in the basis of the lattice \( L_n \) corresponding to \( T_n \). That is,

\[
\text{dim } \ker(B_n) = 2^n - 2(n+1) + n.
\]

Proof. We show \( \text{rank}(B_n) = 2(n+1) - n \). It can be checked directly that \( B_2 \) has full rank. Assume that the claim is true for \( n-1 \). Then by Lemmas \( \boxed{1} \) and \( \boxed{2} \),

\[
2(n+1) - n \geq \text{rank}(B_n) \geq \text{rank}(B_{n-1}) + 1 = 2n - (n-1) + 1,
\]

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

4 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 \( \boxed{1} \) 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 the rows of the following matrix:

\[
\begin{bmatrix}
0 & 0 & 1 & -1 & 1 & 0 & 0 \\
0 & 1 & 0 & -1 & 1 & 0 & 0 \\
1 & 0 & 0 & -1 & 1 & 0 & 1
\end{bmatrix}
\]

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 [The construction of \( B_n \)]

**Input:** the number of leaves \( n \) of the claw tree \( T_n \).

**Output:** \( B_n \in \mathbb{Z}^{2(n+1)\times 2^n} \).

Initialize \( B_n \) to the zero matrix.

Construct the first \( n \) rows:

for \( k \) from 1 to \( n \) do:

for \( c \) from 0 to \( 2^k - 1 \) with \( c \equiv 0 \mod 2 \) do:

for \( j \) from \( c2^n-k + 1 \) to \( (c+1)2^n-k \) do:

\( b_{k,j} := 1 \).

Construct row \( n + 1 \):

if \( n \equiv (\sum_{r=1}^{n} b_{r,j}) \mod 2 \), then \( b_{n+1,j} := 1 \).

Construct rows \( n + 2 \) to \( 2(n+1) \):

for \( i \) from 1 to \( n + 1 \) do:

for \( j \) from 1 to \( 2^n \) do:

\( b_{n+1+i,j} := 1 - b_{i,j} \).
One checks that this algorithm gives indeed the matrices $B_n$ as defined in Section 3.

The $(n + 1 + i)^{th}$ row $r_{n+1+i}$ of $B_n$ is by definition the binary complement of the $i^{th}$ row $r_i$ of $B_n$. Suppose that $r_i \cdot k = 0$ for some vector $k$. Since all entries of $B_n$ are nonnegative, a subvector of $k$ restricted to the entries where $r_i$ is nonzero must be homogeneous in the sense that the sum of the positive entries equals the sum of the negative entries. But since the ideal $I_{L_n}$ itself is homogeneous ([10]), the same must be true for the subvector of $k$ restricted to the entries where $r_i$ is zero. Hence $r_{n+1+i} \cdot k = 0$. Therefore, it is enough to analyze the top half of the matrix $B_n$ when determining the kernel elements.

**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 $T_{n-1}$ as a subtree of $T_n$. Suppose we delete leaf $(i)$ from $T_n$ to get the tree $T_n^{(i)}$ 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 $a_n^{(i)}$ (that is, observing 0 at leaf $(i)$) gives precisely the matrix $B_{n-1}$ corresponding to $T_n^{(i)}$. 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 $T_n$ 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 $\dim(\ker(B_{n-2})) - \dim(\ker(B_{n-1})) = 2^{n-2} - 1$ 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 $T_n^{(2)}$. Finally, removing any other leaf $(i)$ of $T_n$ produces a collection $V_i$ of as many new kernel elements as there are new columns involved (in terms of the submatrix structure); namely, $2^{n-i}$ new vectors. Note that every vector in $V_i$ 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 $T_n^{(i)}$.) In particular, $v = [0, \ldots, 0, 1, 0, 0, -1, -1, 0, 0, 1] \in \ker(B_n)$. 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 $\ker B_n$ in form of a $(2^n - n - 2) \times 2^n$ matrix $L_n$.

Let $L_3 := \begin{bmatrix} 0 & 0 & 1 & -1 & 1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 1 & 0 & 0 \\ 1 & 0 & 0 & -1 & 1 & 0 & 1 \end{bmatrix}$.

Set $k := 4$.

The following subroutine lifts $L_{k-1}$ to $L_k$:

WHILE $k \leq n$ do:

1. Initialize $L_k$ to the zero matrix.
2. For $i$ from 1 to $k$ do:
   - $\text{cols}(i) := \{1, 2^{k-i}, (2)(2^{k-i} + 1, (3)2^{k-i}, \ldots, (2^i - 2)2^{k-i} + 1, (2^i - 1)2^{k-i}\}$.
   - Denote by $L_{k,j}[\text{cols}(i)]$ the $j$th row vector of $L_k$ restricted to columns $\text{cols}(i)$.
   - Set $i := 1$:
     - for $j$ from 1 to $2^{k-1} - k - 1$ do: $L_{k,j}[\text{cols}(i)] := L_{k-1,j}$.
   - Set $i := 2$:
     - for $j$ from 1 to $2^{k-2} - 1$ do:
       - $L_{k,(2^{k-1} - k - 1) + j}[\text{cols}(i)] := L_{k-1,(2^{k-1} - k - 1) - (2^{k-2} - 1) + j}$.
   - For $i$ from 3 to $k$ do:
     - for $j$ from 1 to $2^{k-i}$ do:
       - $L_{k,(2^{k-2} + i - 1 - k - 2) + j}[\text{cols}(i)] := L_{k-1,(2^{k-1} - k - 1) - (2^{k-i}) + j}$.
3. Finally, $L_{k,2^{k-k-2}[2^k - 7..2^k]} := [1, 0, 0, -1, 0, 0, 1]$.

RETURN $L_k$.

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

$$B_4 = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \ 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \ 0 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \ \end{bmatrix}$$

The lattice basis is given by the rows of the following matrix:
The lattice vectors correspond to the relations on the leaf observations in the natural way; namely, the first column corresponds to \(q_{0000}\), the second to \(q_{0011}\), and so on. Therefore, the lattice basis ideal for \(T_4\) in Fourier coordinates is

\[
I_{L_4} = (q_{0000}q_{1001} - q_{0011}q_{0100}, q_{0000}q_{1010} - q_{0011}q_{0100}, q_{0000}q_{1111} - q_{0011}q_{1000},
q_{0011}q_{0101} - q_{0011}q_{1000}, q_{0011}q_{0110} - q_{0011}q_{1000}, q_{0011}q_{1011} - q_{0011}q_{1000},
q_{0011}q_{1000} - q_{1001}q_{0000}, q_{0000}q_{1101} - q_{0101}q_{1000},
q_{0000}q_{1110} - q_{0110}q_{1000}, q_{1000}q_{1111} - q_{1011}q_{1100}).
\]

This ideal is contained in the ideal of phylogenetic invariants \(I_4\) 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 \(\mathbb{Z}_2\).

5 Ideal of invariants

We show that the lattice basis ideals provide basic building blocks 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. \([8],[10]\)), 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 \(I_n = \ker \varphi_n\). As we have seen, the first nontrivial ideal is \(I_3\).

5.1 The tree on \(n = 3\) leaves

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

\[
I_3 = (q_{000}q_{111} - q_{100}q_{011}, q_{011}q_{110} - q_{100}q_{011}, q_{010}q_{101} - q_{100}q_{011}).
\]
This can be verified by computation. In particular, this ideal is equal to the lattice basis ideal for the tree on three leaves; \( I_{L_3} \) 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

\[
q = q_{g_1^{(1)} g_2^{(2)} g_3^{(3)}} - q_{h_1^{(1)} h_2^{(2)} h_3^{(3)}}.
\]

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

1. Exchanging the roles of \( q_{h_1^{(1)} h_2^{(2)} h_3^{(3)}} \) and \( q_{h_1^{(1)} h_2^{(2)} h_3^{(3)}} \) if necessary,

\[
g_1^{(1)} + g_2^{(2)} + g_3^{(3)} = h_1^{(1)} + h_2^{(2)} + h_3^{(3)}
\]

and

\[
g_1^{(1)} + g_2^{(2)} + g_3^{(3)} = h_1^{(1)} + h_2^{(2)} + h_3^{(3)}
\]

2. \( g_1^{(1)} + g_2^{(2)} = 1 = h_1^{(1)} + h_2^{(2)} \) for \( 1 \leq i \leq 3 = n \).

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 \( \varphi_2 \) of the 2-leaf tree, which is trivial.

5.2 The tree on an arbitrary number of leaves

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 \( i \)th index of each variable in \( q \).

For example,

\[
\pi_4(q_{0000 q_{1110}} - q_{0000 q_{0110}}) = q_{000 q_{111}} - q_{000 q_{011}}.
\]

Definition 2. Assume that \( n \geq 4 \).

Let \( G_n \) be the set of quadratic binomials \( q \in I_n \) that can be written as

\[
q = q^+ - q^- = q_{g_1^{(1)} \ldots g_n^{(n)}} - q_{h_1^{(1)} \ldots h_n^{(n)}}
\]

such that one of the two following properties is satisfied:
**Property (i):** For some $1 \leq i \leq n$, $j \in \mathbb{Z}_2$,

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

(1)

and

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

(2)

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

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

(3)

and

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

(4)

**Example 4.** Let $n = 4$. The set of elements $q \in G_n$ with Property (i) consists of those for which $j = 0$:

$q_0000q_0111, q_0100q_0011, q_0001q_0110, q_0100q_0011, q_0010q_0101, q_0100q_0011$.

$q_0000q_1011, q_0100q_0011, q_0001q_0110, q_0100q_0011, q_0010q_0101, q_0100q_0011$.

$q_0000q_1101, q_0100q_0011, q_0001q_0110, q_0100q_0011, q_0010q_0101, q_0100q_0011$.

$q_0000q_1110, q_0100q_0011, q_0001q_0110, q_0100q_0011, q_0010q_0101, q_0100q_0011$.

$q_0001q_1111, q_0100q_0011, q_0011q_1110, q_0100q_0011, q_0100q_0111, q_0011q_1110$.

The set of elements $q \in G_n$ with Property (ii) are:

$q_0000q_1111, q_0100q_1110, q_0001q_1110, q_0100q_1110, q_0011q_1110, q_0100q_1110$.

$q_0010q_1111, q_0100q_1110, q_0100q_1110, q_0100q_1110, q_0011q_1110, q_0100q_1110$.

$q_0000q_1111, q_0100q_1110, q_0001q_1110, q_0100q_1110, q_0011q_1110, q_0100q_1110$.

$q_0010q_1111, q_0100q_1110, q_0100q_1110, q_0100q_1110, q_0011q_1110, q_0100q_1110$.

$q_0000q_1111, q_0100q_1110, q_0001q_1110, q_0100q_1110, q_0011q_1110, q_0100q_1110$.

$q_0010q_1111, q_0100q_1110, q_0100q_1110, q_0100q_1110, q_0011q_1110, q_0100q_1110$.

**Proposition 2.** For $n \geq 4$, the set of binomials in $G_n$ generates the ideal $I_n$. That is,

$$I_n = \{ q^+ - q^- \in G_n \}.$$  

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 $1 \leq i \leq n$ and a fixed $j$,

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

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 $1 \leq i \leq n$,

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

(5)

By definition, the ideal $I_n$ is toric, so it is generated by binomials. In fact, it is generated by homogeneous binomials, because each row of the matrix $B_n$ used
for defining it has row sum \( n + 1 \) ([10], chapter 4). In addition, Sturmfels and Sullivant in [11] have shown that the ideal \( I_n \) is generated in degree 2. Hence it suffices to consider homogeneous quadratic binomials. Let \( q = q^+ - q^- \) be a binomial in \( I_n \) of degree 2. Then clearly either (11) 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 (11),

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

where the first statement holds by definition of \( \varphi_n \) and the second by definition of the projection \( \pi_i \).

In the latter case, for each \( i \) with \( 1 \leq i \leq n \),

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

where the second statement holds by definition of \( \pi_i \) and (5). It follows that \( I_n = \{ q : q \in G_n \} \).

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 \( q \in G_{n-1} \) 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 \( 1 \leq i \leq n \) and every \( q \in G_{n-1} \). 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 \( q \in G_{n-1} \) in such a way that Property (ii) is satisfied. Namely, for every \( q = q^+ - q^- \in G_{n-1} \) 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. □

Remark 6. A different recursion has been proposed by Sturmfels and Sullivant in [12].

Recall ([10]) 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 7. The binomials in \( G_n \) 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 \( G_3 \) recursively to produce \( G_{n-1} \); that is, until the number of indices
of each generator reaches \( n - 1 \). Next, lift \( G_{n-1} \) \( n \) times so that Property (i) is satisfied for one of the \( n \) index positions. For example,

\[
q := q_{0000}q_{1111} - q_{1000}q_{0110} \in G_4
\]
can be lifted to a generator of \( I_5 \) in ten different ways: by lifting to preimages of \( \pi_1, \ldots, \pi_5 \) so that Property (i) is satisfied with either a 0 or a 1:

\[
\pi_1^{-1}(q) = \{q_{0000}q_{0111} - q_{0100}q_{0011}, q_{1000}q_{1111} - q_{1100}q_{1011}\},
\]

\[
\pi_2^{-1}(q) = \{q_{0000}q_{1011} - q_{1000}q_{0011}, q_{1000}q_{1111} - q_{1100}q_{1011}\},
\]

and so on. This will be the set of binomials in \( G_n \) 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 \( n \).

Suppose \( n \) is odd. Fix \( q^- \) in such a way to ensure that \( \text{in}_{<\omega_{eq}}(q^-) = q^+ \).

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

\[
q^- = q_{01\ldots1}q_{10\ldots0} \quad \text{and} \quad q^- = q_{01\ldots0}q_{10\ldots1}.
\]

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 receive 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 strengthen Proposition (2).

**Proposition 3.** The set \( G_n \) is a lexicographic Gröbner basis of \( I_n \), for any \( n \geq 4 \).
Proof. For the case \( n = 3 \) this is already shown. Let \( n > 3 \). Then we can partition the set of \( q \in G_n \) into those satisfying Property (i) or (ii). Note that \( I_n \) is prime by definition, and thus radical. Also, Proposition 4 shows it is generated by squarefree quadratic binomials. These facts are used in what follows.

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 \( q_1 = q_g, q_{g_2} - q_{h_1} q_{h_2} \) and \( q_2 = q_g, q_{g_3} - q_{h_3} q_{h_4} \). Then

\[
f = q_{g_2} q_{h_1} - q_{g_2} q_{h_3} q_{h_4} \in I_n.
\]

**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 \( a_s^{(n)} | \varphi_{n-1}(\pi_k(q_{g_2} q_{h_1} q_{h_2})) \) 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 \( \varphi_{n-1} \). 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 \( q_k \in G_n \) satisfying Property (ii) where both \( S(q_i, q_k) \) and \( S(q_j, q_k) \) reduce to zero. The three pairs criterion (8) 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.

\( \square \)

Proposition 4 has important theoretical consequences. Let \( S \) be a polynomial ring over the field \( K \). Recall (14) that \( S/I \) is Koszul if the field \( K \) has a linear resolution as a graded \( S/I \)-module:

\[
\cdots \to (S/I)^{\beta_3}(-2) \to (S/I)^{\beta_2}(-1) \to S/I \to K \to 0.
\]

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. 11) 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 [11] 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 $I_{L_n}$ 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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