SPLIT-FACETS FOR BALANCED MINIMAL EVOLUTION POLYTOPES AND THE PERMUTOASSOCIAHEDRON.

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ABSTRACT. Understanding the face structure of the balanced minimal evolution (BME) polytope, especially its top-dimensional facets, is a fundamental problem in phylogenetic theory. We show that BME polytope has a sub-lattice of its poset of faces which is isomorphic to a quotient of the well-studied permutoassociahedron. This sub-lattice corresponds to compatible sets of splits displayed by phylogenetic trees, and extends the lattice of faces of the BME polytope found by Hodge, Haws, and Yoshida. Each of the maximal elements in our new poset of faces corresponds to a single split of the leaves. Nearly all of these turn out to actually be facets of the BME polytope, a collection of facets which grows exponentially.

1. INTRODUCTION

Phylogenetics is the study of the reconstruction of biological family trees from genetic data. Results from phylogenetics can inform every facet of modern biology, from natural history to medicine. A chief goal of biological research is to find relationships between genes and the functional structures of organisms. Knowing degrees of kinship can allow us to decide whether or not an adaptation in two species is probably an inherited feature of a common ancestor, and thus help to isolate the roles of genes common to both.

Mathematically, a *phylogenetic tree* is a cycle-free graph with no nodes (vertices) of degree 2, and with a set of distinct items assigned to the degree one nodes–that is, labeling the leaves. We study a method called *balanced minimal evolution.* This method begins with a given set of n items and a symmetric (or upper triangular) square $n \times n$ *dissimilarity matrix* whose entries are numerical dissimilarities, or distances, between pairs of items. From the dissimilarity matrix, often presented as a vector of distances, the balanced minimal evolution (BME) method constructs a binary (degree of vertices ≤ 3) phylogenetic tree with the n items labeling the n leaves.

It is well known that if a distance vector is created by starting with a given binary tree T with lengths assigned to each of its edges, and finding the pairwise distances between leaves just by adding the edge lengths along the path that connects them, then the tree T is uniquely recovered from that distance vector. The distance vector (or matrix) is called *additive* in this case. One recovery process is called the *sequential algorithm*, described first in [17]. It operates by leaf insertion and is performed in polynomial time: $O(n^2)$. Another famous algorithm is *neighbor joining*, which reconstructs the tree in $O(n^3)$ time [16]. It has the advantage of being a greedy algorithm for the BME problem, when extended to the non-additive case [9].

An alternate method of recovery via minimization was introduced by Pauplin in [14] and developed by Desper and Gascuel in [4]. This BME method uses a linear functional on binary

phylogenetic trees t (without edge lengths) defined using the given distance vector. The output of the function is the length of the original tree T (assuming that the distance vector was created from T.) The function is minimized when the input tree t is identical to T, as trees without edge lengths. Thus by minimizing this functional, we recover the original *tree topology*. The latter terminology is used to describe two trees that are identical if we ignore edge lengths. The value of this approach is that the given distance vector is often corrupted by missing or incorrect data; but within error bounds we can still recover the tree topology by the minimization procedure. Furthermore, the BME method is *statistically consistent* in that as the distance vector approaches the accuracy of a true tree T, the BME method's output approaches that tree's topology [5, 1, 10].

More precisely: Let the set of n distinct species, or taxa, be called S. For convenience we will often let $S = [n] = \{1, 2, \ldots, n\}$. Let vector $\mathbf{d}$ be given, having $\binom{n}{2}$ real valued components d_{ij}, one for each pair $\{i, j\} \subset S$. There is a vector $\mathbf{c}(t)$ for each binary tree t on leaves S, also having $\binom{n}{2}$ components $c_{ij}(t)$, one for each pair $\{i, j\} \subset S$. These components are ordered in the same way for both vectors, and we will use the lexicographic ordering: $\mathbf{d} = \langle d_{12}, d_{13}, \ldots, d_{1n}, d_{23}, d_{24}, \ldots, d_{n-1,n} \rangle$.

We define, following Pauplin [14]:

$$c_{ij}(t) = \frac{1}{2^{l_{ij}(t)}}$$

where $l_{ij}(t)$ is the number of internal nodes (degree 3 vertices) in the path from leaf i to leaf j.

If a phylogenetic tree T with non-negative edge lengths is given, then we can define the distance vector $\mathbf{d}(T)$ by adding the edge lengths between each pair of leaves. Then the dot product $\mathbf{c}(T) \cdot \mathbf{d}(T)$ is equal to the sum of all the edge lengths of T, a sum which is known as the *tree length*. T is uniquely determined by $\mathbf{d}(T)$ (unless there are length zero edges, in which case there is a finite set of trees determined). Using any other tree t as the input of $\mathbf{c}(t)$ will give a sub-optimal, larger value for $\mathbf{c}(t) \cdot \mathbf{d}(T)$.

The BME tree for an arbitrary positive vector $\mathbf{d}$ is the binary tree t that minimizes $\mathbf{d} \cdot \mathbf{c}(t)$ for all binary trees on leaves S. Now this dot product is the least variance estimate of treelength, as shown in [5]. The value of setting up the question in this way is that it becomes a linear programming problem. The convex hull of all the vectors $\mathbf{c}(t)$ for all binary trees t on S is a polytope BME(S), hereafter also denoted BME(n) or $\mathcal{P}_n$ as in [6] and [11]. The vertices of $\mathcal{P}_n$ are precisely the $(2n - 5)!!$ vectors $\mathbf{c}(t)$. Minimizing our dot product over this polytope is equivalent to minimizing over the vertices, and thus amenable to the simplex method.

In Fig. 1 we see the 2-dimensional polytope $\mathcal{P}_4$. In that figure we illustrate a simplifying choice that will be used throughout: rather than the original fractional coordinates c_{ij} we will scale by a factor of 2^{n-2}, giving a new vector $\mathbf{x}(t)$ with coordinates:

$$x_{ij}(t) = 2^{n-2} c_{ij}(t) = 2^{n-2-l_{ij}(t)}.$$

The convex hull of the vectors $\mathbf{x}(t)$ is a combinatorially equivalent scaled version of the BME polytope, so we refer to it by the same name. Since the furthest apart any two leaves may be is a distance of $n - 2$ internal nodes, this scaling will result in integral coordinates for our polytope. The tree t that minimizes $\mathbf{d} \cdot \mathbf{c}(t)$ will also minimize $\mathbf{d} \cdot \mathbf{x}(t)$.

A *clade* is a subgraph of a binary tree induced by an internal (degree three) node and all of the leaves descended from it in a particular direction. In other words: given an internal

node v we choose two of its edges and all of the leaves that are connected to v via those two edges. Equivalently, given any internal edge, its deletion separates the tree into two clades. Two clades on the same tree must be either disjoint or *nested*, one contained in the other. A *cherry* is a clade with two leaves. We often refer to a clade by its set of (2 or more) leaves. A pair of *intersecting cherries* $\{a, b\}$ and $\{b, c\}$ have intersection in one leaf b, and thus cannot exist both on the same tree. A *caterpillar* is a tree with only two cherries. A *split* of the set of n leaves for our phylogenetic trees is a partition of the leaves into two parts, one part called S_1 with m leaves and another S_2 with the remaining $n - m$ leaves. A tree *displays* a split if each part makes up the leaves of a *clade*. A *facet* of a polytope is a top-dimensional face of that polytope's boundary, or a co-dimension-1 face. Faces of a polytope can be of any dimension, from 0 to that of the (improper) face which is the polytope itself.

2. New Results

Our most important new discovery is a large family of facets of the BME polytope, which we call *split − facets* in Theorem 4.7. This collection of facets is shown to exist for all n, and the number of facets in this family grows like 2^n.
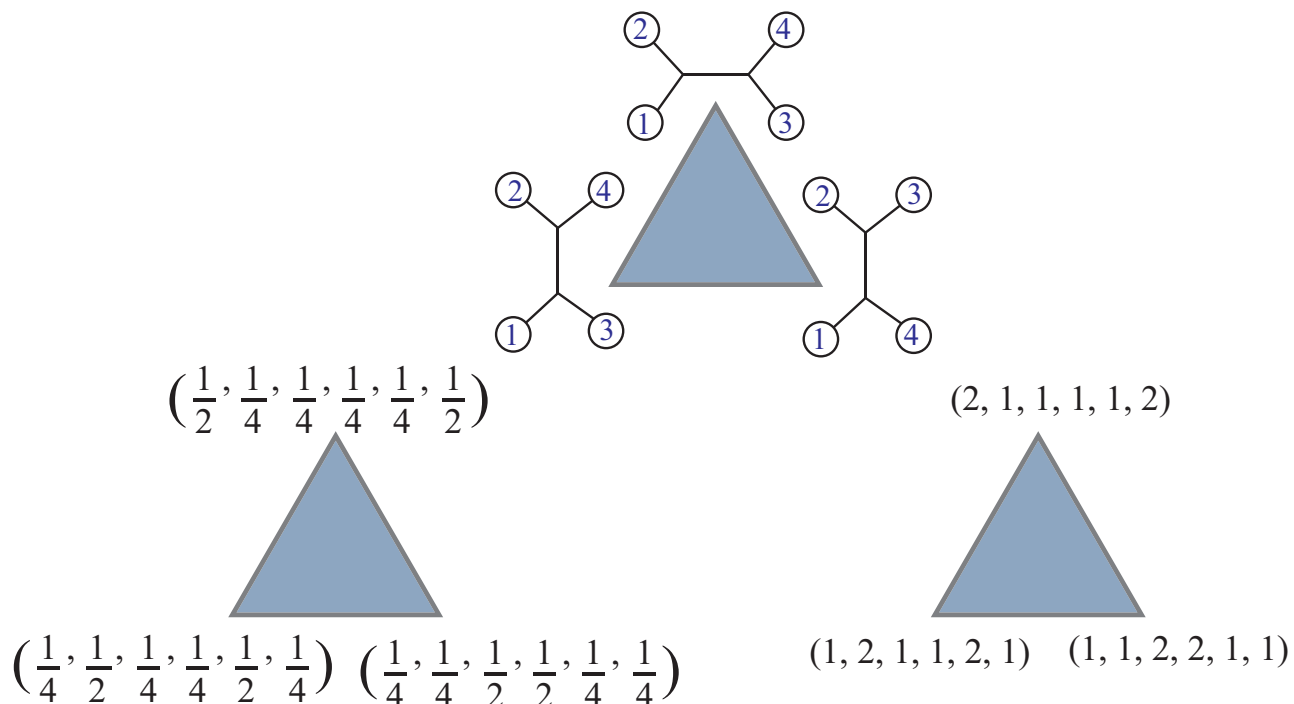

FIGURE 1. The polytope $\mathcal{P}_4$ is a triangle. At the top we label the vertices with the three binary trees with leaves $1 \ldots 4$. Each edge shows a nearest-neighbor interchange; for instance the exchange of leaves 3 and 4 on the bottom edge. At bottom left are Pauplin's original coordinates and at bottom right are the coordinates, scaled by $2^{n-2} = 4$, which we will use.

In Theorem 4.3 we show that any (non-binary) phylogenetic tree corresponds to a face of $\mathcal{P}_n$. This allows us to define a map from the permutoassociahedron to the BME polytope, taking faces to faces. In Theorem 4.6 we show that this map preserves the partial order of faces.

In Theorem 4.5 we show that a special case of these tree-faces are the clade-faces discovered earlier in [11]. In Theorem 4.7 we show that another special case of tree-faces is our new class of facets of $\mathcal{P}_n$.

3. Previous results

Until recently, little was known about the structure of the BME polytopes, but several newly discovered features were described in [12] and [11]. The coordinates of the vertices satisfy a set of n independent equalities, which we will refer to as the Kraft equalities, after an equivalent description in [3]. For each leaf i we sum the coordinates that involve it:

$$\sum_{j:j\neq i} x_{ij} = 2^{n-2}.$$

These equalities govern the dimension of the BME polytope, $\dim(\mathcal{P}_n) = \binom{n}{2} - n$.

In [11] the authors prove the first description of faces of the nth balanced minimal evolution polytope $\mathcal{P}_n$. They find a family of faces that correspond to any set of disjoint clades. In [8] we show that these clade-faces are not facets, but instead show several new familys of facets. We add to that list here with a family of facets that grows exponentially. (Our results are listed in columns 5–7 of Table 1.)

We show in [8] that any pair of intersecting cherries corresponds to a facet of $\mathcal{P}_n$. For each pair of cherries with leaves $\{a, b\}$ and $\{b, c\}$, there is a facet of $\mathcal{P}_n$ whose vertices correspond to trees that have either one of those two cherries.

In addition, any caterpillar tree with fixed ends corresponds to a facet of $\mathcal{P}_n$. Thus for each pair of species there is a facet of $\mathcal{P}_n$ whose vertices correspond to trees which are caterpillars with this pair as far apart as possible. Also shown in [8]: for $n = 5$, for each necklace of five leaves there is a corresponding facet which is combinatorially equivalent to a simplex.

4. Connection to the Permutoassociahedron

The nth permutoassociahedron $\mathcal{KP}_n$, also known as the type-A Coxeter associahedron, is defined in [13]. It is discussed in detail in [15], and related to the space of phylogenetic trees in [2]. A face of the permutoassociahedron corresponds to an ordered partition of a set S of n elements, whose parts label the leaves, left to right, of a rooted plane tree. We often use $S = \{1, \ldots, n\}$. Alternatively we may use $S = \{1, \ldots, n+1\} - \{r\}$ where $r \in S$ is the label for the root. Bijectively, one of these labeled plane trees can also be described as a partial bracketing of an ordered partition, such as $((\{3\}, \{4, 5\}), \{2\}, \{1, 6, 7\})$.

The inclusion of faces corresponds to refinement of the ordered-partition trees: refinement of the tree structure by adding branches at nodes with degree larger than 3 (so that the collapse of the added branches returns the original tree) or refinement of the ordered partition, in which parts of it are further partitioned (subdivided, with ordering). To display the subdivision, the parts of the refined partition label the ordered leaves of a new subtree: a *corolla*, which is a tree with one root, one internal node, and 2 or more leaves.

Tree refinement can also be described as adding parentheses to the bracketing, or subdividing a set in the bracketing. A covering relation is either adding a single branch (pair of parentheses) or subdividing a single part of the partition. For examples of covering relations,

$((\{3\}, \{4,5\}), \{2\}, \{1,6,7\}) > (((\{3\}, \{4,5\}), \{2\}), \{1,6,7\})$

and

$((\{3\}, \{4,5\}), \{2\}, \{1,6,7\}) > ((\{3\}, \{4,5\}), \{2\}, (\{1\}, \{6\}, \{7\}))$

or

$((\{3\}, \{4,5\}), \{2\}, \{1,6,7\}) > ((\{3\}, \{4,5\}), \{2\}, (\{1,7\}, \{6\}))$.

The 2-dimensional $\mathcal{KP}_2$ is shown in Fig. 2. The 3-dimensional $\mathcal{KP}_3$ is shown in Fig. 3

number of species	dim. of $\mathcal{P}_n$	vertices of $\mathcal{P}_n$	facets of $\mathcal{P}_n$	facet inequalities (classification)	number of facets	number of vertices in facet
3	0	1	0	-	-	-
4	2	3	3	$x_{ab} \geq 1$	3	2
				$x_{ab} + x_{bc} - x_{ac} \leq 2$	3	2
5	5	15	52	$x_{ab} \geq 1$ (caterpillar)	10	6
				$x_{ab} + x_{bc} - x_{ac} \leq 4$ (intersecting-cherry)	30	6
				$x_{ab} + x_{bc} + x_{cd} + x_{df} + x_{fa} \leq 13$ (cyclic ordering)	12	5
6	9	105	90262	$x_{ab} \geq 1$ (caterpillar)	15	24
				$x_{ab} + x_{bc} - x_{ac} \leq 8$ (intersecting-cherry)	60	30
				$x_{ab} + x_{bc} + x_{ac} \leq 16$ $(3,3)$-split	10	9
n	$\binom{n}{2} - n$	$(2n-5)!!$	?	$x_{ab} \geq 1$ (caterpillar)	$\binom{n}{2}$	$(n-2)!$
				$x_{ab} + x_{bc} - x_{ac} \leq 2^{n-3}$ (intersecting-cherry)	$\binom{n}{2}(n-2)$	$2(2n-7)!!$
				$x_{ab} + x_{bc} + x_{ac} \leq 2^{n-2}$ $(m,3)$-split, $m > 3$	$\binom{n}{3}$	$3(2n-9)!!$
				$\sum_{i,j \in S_1} x_{ij} \leq (k-1)2^{n-3}$ (m,k)-split, $m > 2, k > 2$	$2^{n-1} - \binom{n}{2}$ $-n-1$	$(2m-3)!!$ $\times (2k-3)!!$

TABLE 1. Technical statistics for the BME polytopes $\mathcal{P}_n$. The first four columns are found in [12] and [11]. Our new and recent results are in the last 3 columns. The inequalities are given for any $a, b, c, \cdots \in [n]$. Note that for $n = 4$ the three facets are described twice: our inequalities are redundant.

There is a straightforward lattice map φ from the faces of $\mathcal{KP}_n$ to a sub-lattice of faces of the BME polytope. Since it preserves the poset structure, its preimages are a nice set of equivalence classes.

Definition 4.1. *Let t be a plane rooted tree with leaves an ordered partition π of S. First let t' be the tree achieved by replacing each leaf labeled by part $U \in \pi$ such that $|U| > 1$ with a corolla labeled by the elements of U. This corolla is attached at a new branch node where the leaf labeled by U was attached. Now let $\varphi(t)$ be the tree $f(t')$, where f is described as un-gluing t' from the plane in order to preserve only its underlying graph.*

An example of the map φ is shown in Fig. 4. Note that forgetting the plane structure of t' ensures that the map φ is well-defined. The corolla that replaces each leaf labeled by $U \in \pi$ is immediately seen as unordered since it is not fixed in the plane.

Fig. 5 shows the full action of φ on the 2-dimensional $\mathcal{KP}_2$.

Since our map preserves the face order, it takes vertices to vertices. It is a set projection on vertices, and the number of elements in a preimage has a nice formula:

Proposition 4.2. *Let T be a binary phylogenetic tree with n leaves. The number of ordered plane rooted binary trees t such that $\varphi(t) = T$ is 2^{n-2}.*

Proof. We note that the map is a surjection from vertices to vertices, since any leaf of a binary phylogenetic tree may be chosen as the root. By symmetry of the labeling of leaves,
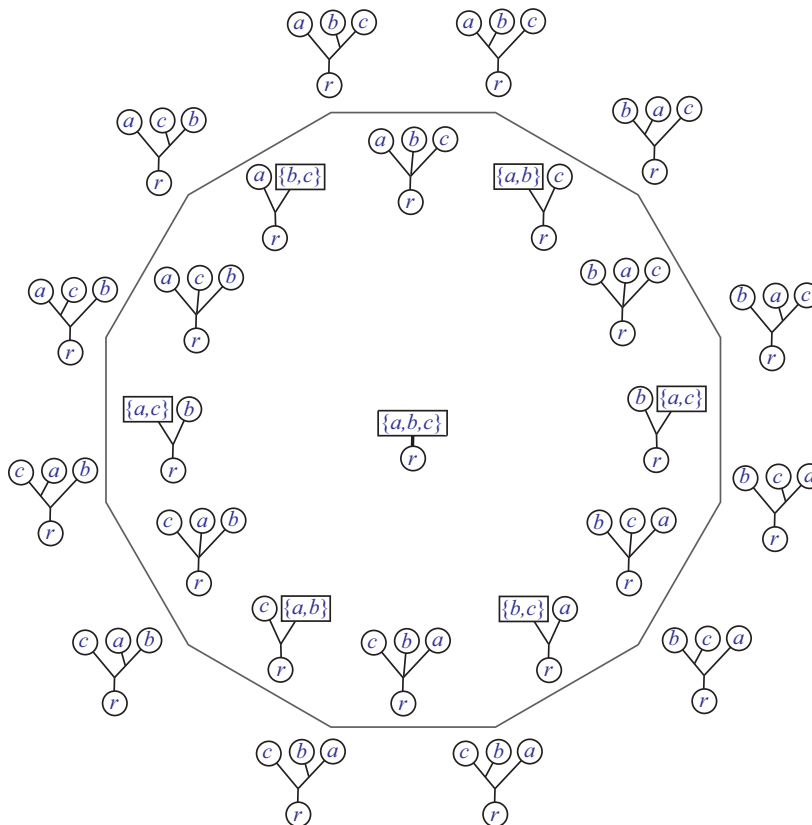

FIGURE 2. The 2-dimensional permutoassociahedron with labeled faces.

the size of each preimage must be the same. Here n is the total number of leaves, so in the permutoassociahedron vertices we are considering plane binary trees with $n-1$ leaves and a root. We divide the total numbers of vertices of the two polytopes:

$$\frac{C_{n-2}(n-1)!}{(2n-5)!!} = 2^{n-2}.$$

Here we have used the formula for Catalan numbers: $C_{n-2} = \frac{1}{n-1}\binom{2(n-2)}{n-2}$. We also use the formula $(2n-5)!! = \frac{(2n-4)!}{2^{n-2}(n-2)!}$. □ □

Now we show how the targets of the map φ are actually faces of the BME polytope. Note that the image of the (improper) face which is the entire permutoassociahedron (as well as any of its corrolla facets) is the phylogenetic tree which is a corolla, or star: it has only one node
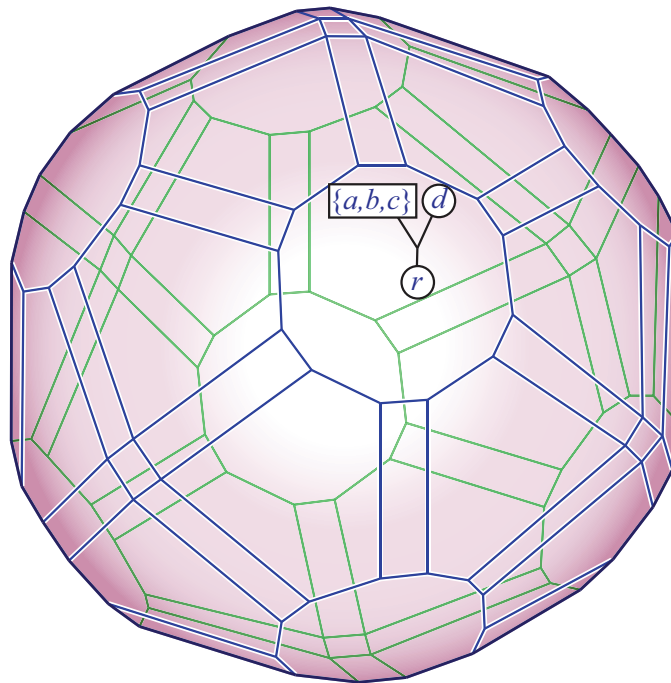

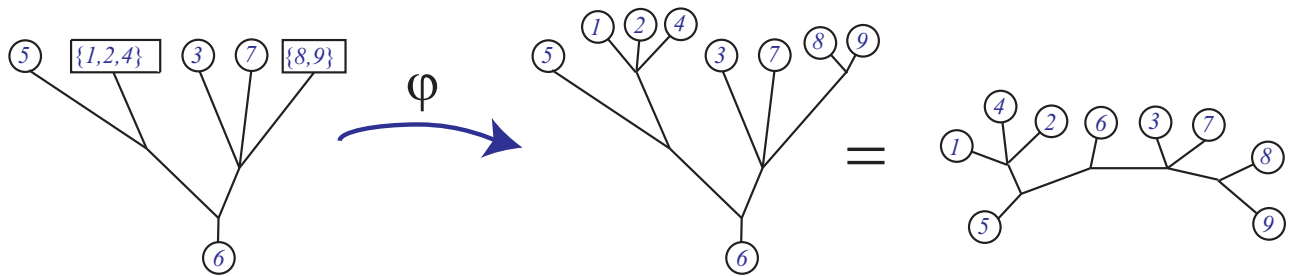FIGURE 3. The 3-dimensional permutoassociahedron with a labeled facet. This picture is redrawn from a version in [15].

FIGURE 4. Action of the map φ: the second step shows that we no longer preserve plane structure or rooted-ness.

with degree ≥ 3. This corolla corresponds to the (improper) face which is the entire BME polytope. In what follows we will assume we are speaking of proper faces.

Theorem 4.3. *For each non-binary phylogenetic tree t with n leaves there is a corresponding face $F(t)$ of the BME polytope $\mathcal{P}_n$. The vertices of $F(t)$ are the binary phylogenetic trees which are refinements of t.*

Proof. We show that for each non-binary t there is a distance vector $\mathbf{d}(t)$ for which the product $\mathbf{d}(t) \cdot \mathbf{x}(t')$ is minimized simultaneously by precisely the set of binary phylogenetic trees t' which refine t.

The distance vector $\mathbf{d}(t)$ is defined as follows: the component $d_{ij}(t)$ is the number of edges in the path between leaf i and leaf j. Next we show that, for any tree t', we have the inequality:

$$\sum_{i<j} d_{ij}(t) x_{ij}(t') \geq 2^{(n-2)} |E(t)|$$

where $E(t)$ is the set of edges of t. Moreover, we will show that the inequality is precisely an equality if and only if the tree t' is a refinement of t.

Our vector $\mathbf{d}(t)$ is constructed to be a vector of distances (of paths between leaves) for any binary tree that refines t. This is seen by assigning a length of 1 to each edge of the tree t, and calculating the distances between leaves by adding the edge lengths on the path between them for any two leaves. A binary tree t' that refines t is similarly given lengths of 1 for its edges, except for those edges whose collapse would return t' to the tree t. These latter edges are assigned a length of zero.
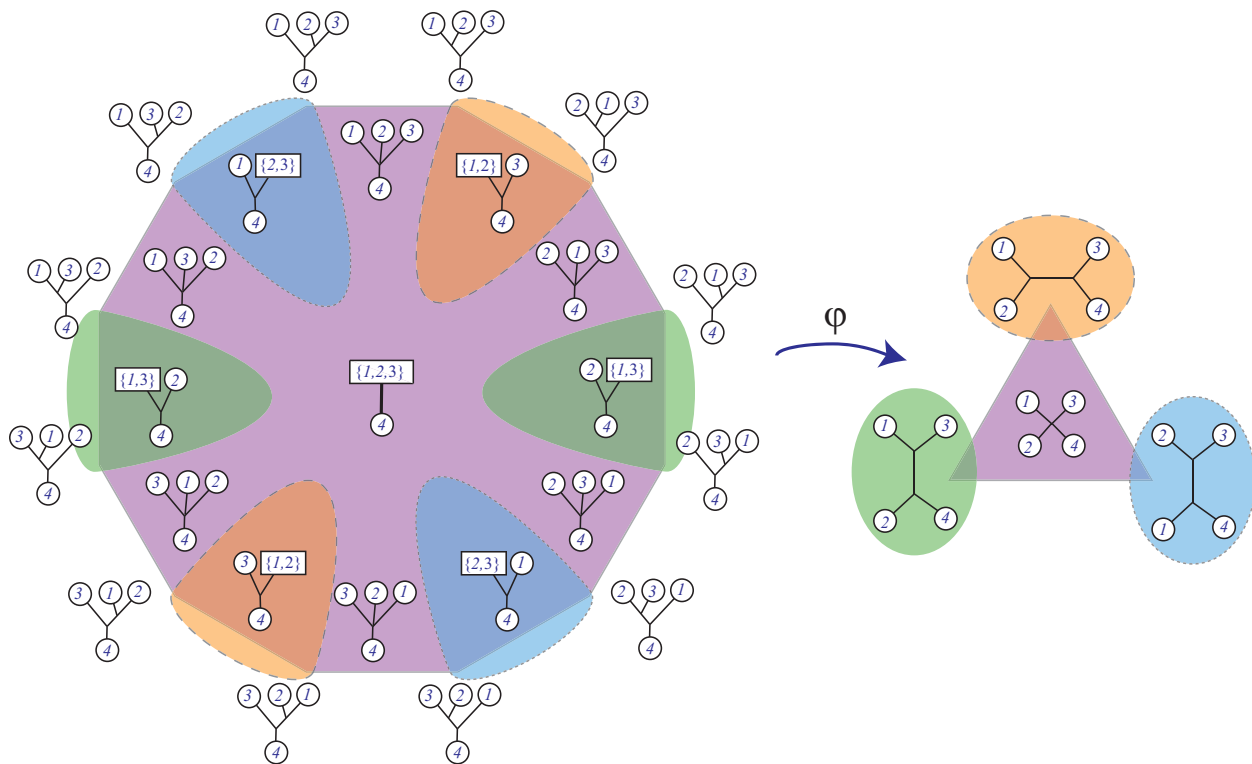

FIGURE 5. Action of the map φ: the shaded faces all map to the shaded vertices.

Now our result follows: given a distance vector whose components are the distances between leaves on a binary tree, the dot product of this vector with vertices of the BME polytope is minimized at the vertex corresponding to that tree. In our case all the binary trees t' which refine t, with their assigned edge lengths, share the distance vector $\mathbf{d}(t)$. Thus they are simultaneously the minimizers of our product, and the value of that product is $2^{(n-2)}$ times their common tree length. $\square$ $\square$

Definition 4.4. *For a non-binary phylogenetic tree t we call the corresponding face of the BME polytope the* tree-face $F(t)$.

An example of a tree-face, its vertices, and its inequality as given in the proof of Theorem 4.3, are shown in Fig. 6.

Some special cases of tree faces are important. First we mention the case in which the tree t has only one non-binary node, that is, exactly one node with degree larger than 3. Thus t can be seen as a collection of clades (and some single leaves) all attached to the non-binary node.

Proposition 4.5. *For t an n-leaved phylogenetic tree with exactly one node ν of degree $m > 3$, the tree-face $F(t)$ is precisely the clade-face $F_{C_1,\dots,C_p}$, defined in [11], corresponding to the collection of clades $C_1,\dots,C_p$ which result from deletion of ν. Thus $F(t)$ is combinatorially equivalent to the smaller dimensional BME polytope $\mathcal{P}_m$.*

Proof. Any tree t' which is a binary refinement of t can be constructed by attaching the clades $C_1,\dots,C_p$ to p of the leaves of a binary tree $\hat{t}$. Note that since we don't consider single leaves to be clades, we need to say that $\hat{t}$ has m leaves where $m - p$ is the number of single leaves attached to ν.

$$x(t) = (4,2,1,1,2,1,1,2,2,4)$$

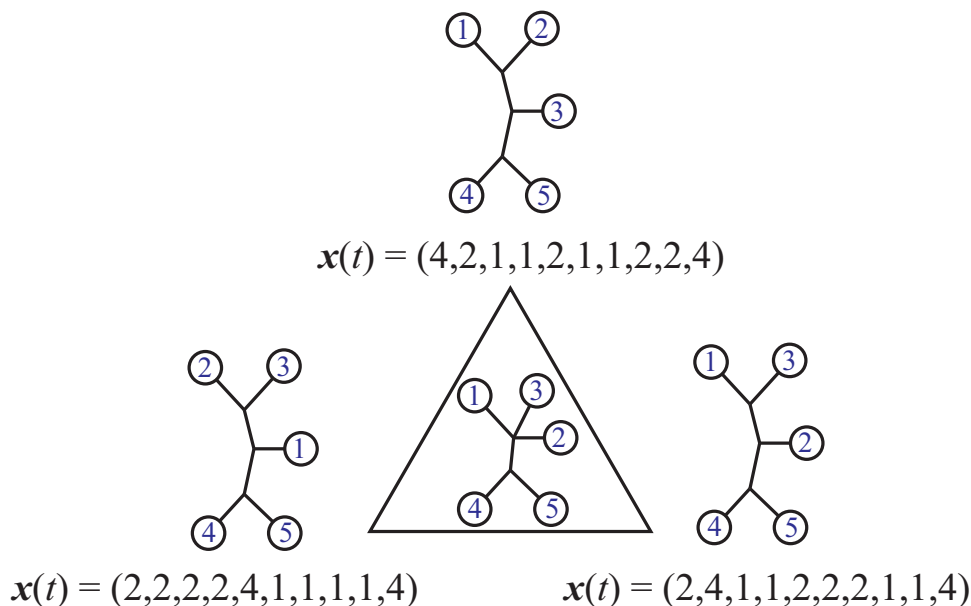$$x(t) = (2,2,2,2,4,1,1,1,1,4) \qquad x(t) = (2,4,1,1,2,2,2,1,1,4)$$

FIGURE 6. The three binary trees shown are the vertices of the tree-face corresponding to the tree in the center. The inequality which defines this face is:
$2x_{12} + 2x_{13} + 3x_{14} + 3x_{15} + 2x_{23} + 3x_{24} + 3x_{25} + 3x_{34} + 3x_{35} + 2x_{45} \geq 48$

Recall from [11] that the face $F_{C_1,\dots,C_p}$ is the image of an affine transformation of the BME polytope $\mathcal{P}_m$. As stated by those authors, this combinatorial equivalence follows since every tree in $F_{C_1,\dots,C_p}$ can be constructed by starting with a binary tree on m leaves and attaching the clades $F_{C_1,\dots,C_p}$ to p of the m leaves.   □   □

See Fig. 6 for an example of a clade-face, in fact a *cherry clade-face*, where the single clade in question is the cherry $\{4,5\}$.

In [11] it is pointed out that the clade-faces form a sub-lattice of the lattice of faces of $\mathcal{P}_n$. Containment in that sublattice is simply refinement, where a sub-clade-face of a clade-face $F(t)$ can be found by refining the tree t, as long as the result still has only a single non-binary node.

Now it is straightforward to see that refinement of trees in general gives a partial ordering of tree-faces, and indeed another sub-lattice of faces of the BME polytope which contains the clade-faces as a sub-lattice. We note that the map φ from the permutoassociahedron is a lattice map.

Proposition 4.6. *If $x \leq y$ (thus containment as faces in the face lattice of $\mathcal{KP}_n$,) then $\varphi(x) \leq \varphi(y)$ (so containment as faces in the face lattice of $\mathcal{P}_n$, the BME polytope).*

Proof. The refinement of a labeled plane rooted tree t, or the refinement of the ordered partition labeling the leaves, both correspond to the refinement of $\varphi(t)$. The former is direct, the latter is seen via the replacement of parts in the partition by the corresponding corollas, before and after subdivision.   □   □

Next we look at what are perhaps the most important tree-faces: those which correspond to facets of the BME polytope. It turns out that these facets correspond to trees t which have exactly two adjacent nodes with degree larger than 3.

Theorem 4.7. *Let t be a phylogenetic tree with $n > 5$ leaves which has exactly one interior edge $\{\nu, \mu\}$, with ν and μ each having degree larger than 3. Then the trees which refine t are the vertices of a facet of the BME polytope $\mathcal{P}_n$.*

The proof is in Section 6. Note that this implies that there are clade-faces which are not contained in any tree-face facet, as seen in Fig. 7.

It is clarifying to refer to the new family of facets in Theorem 4.7 as *split-facets*. The binary phylogenetic trees which display a given split correspond precisely to the trees which refine a tree as described in that theorem.

In fact we can see all the tree-faces in terms of displayed splits, since a split always corresponds to an internal edge. Thus we have that requiring 2 or more splits which the binary trees must all display simultaneously corresponds to specifying a tree-face, all of which are subfaces of split-facets.

5. Enumeration

5.1. **Number of split-facets.** For $n = 6$ there are 31 splits in all, but only 10 splits which obey the requirement that there are at least three leaves in each part. For n leaves the number of splits is $2^{(n-1)} - 1$. (This is half the number of nontrivial, proper subsets.) Discarding the

splits with only one leaf and discarding the cherry clade-faces, we are left with:

$$2^{(n-1)} - \binom{n}{2} - n - 1$$

split facets.

5.2. **Number of vertices in a split-facet.** For $n = 6$ each facet of this type has 9 vertices since there are three choices of binary structure on each side of the split. Thus the facet itself must be an 8-dimensional simplex.

We also found a formula for the number of vertices in a split-face with parts of the split being S_1 of size k and S_2 of size $m = n - k$. The number of vertices is:

$$(2m - 3)!!(2k - 3)!! .$$

This formula is found via the multiplication principle, in which all possible clades are counted for each part of the split.

5.3. **Number of facets that a given tree belongs to, in the Splitohedron.** The split-faces, intersecting-cherry facets, and caterpillar facets together outline a relaxation of the BME polytope. We define a new polytope:

Definition 5.1. *The* splitohedron $Sp(n)$ *is defined as the intersection of the half-spaces of* $\mathbb{R}^{\binom{n}{2}}$ *given by the following inequalities listed by name: the intersecting-cherry facets, the split-facets, the caterpillar facets and the cherry clade-faces– and also obeying the n Kraft equalities.*

FIGURE 7. Examples of chains in the lattice of tree-faces of the BME polytope $\mathcal{P}_7$.

The splitohedron is a bounded polytope because the cherry clade-faces, where the inequality is $x_{ij} \leq 2^{n-3}$, and the caterpillar facets, where the inequality is $x_{ij} \geq 1$, show that it lies inside the hypercube $[1, 2^{n-3}]^{\binom{n}{2}}$. It has the same dimension as the BME polytope, and often has many of the same vertices.

Theorem 5.2. *For an n-leaved binary phylogenetic tree, if the number of cherries is at least $n/4$ then the tree represents a vertex in the BME polytope that is also a vertex of the splitohedron. For $n \leq 11$ the tree represents a vertex regardless of the number of cherries.*

Proof. For a given binary phylogenetic tree t it is straightforward to count how many distinct facets of the splitohedron it belongs to. If that number is as large as the dimension, we know that the tree lies at a vertex of the polytope $Sp(n)$. First we note that an inequality which defines a facet of the BME polytope and which is also obeyed by the splitohedron therefore defines a facet of the splitohedron as well, by the nature of relaxation.

For each cherry $\{a, b\}$ of t we have that t lies within $2(n-2)$ facets, an intersecting-cherry facet for each choice of either a or b and a third leaf that is neither. For each interior edge that does not determine a cherry clade, we have that t lies within a split-facet. There are $n - 3 - p$ such interior edges, where p is the number of cherries. Finally, if t is a caterpillar then it lies within 4 caterpillar facets, determined by a choice of one leaf from each cherry to fix.

All together t lies within $p(2n-4)+n-3-p = (2n-5)p+n-3$ facets of the splitohedron, if it is not a caterpillar. For any n this number increases with p, as p ranges from 2 to $\lfloor \frac{n}{2} \rfloor$. The dimension of the polytope is $\binom{n}{2} - n = \frac{1}{2}(n^2 - 3n)$. Comparing the two expressions shows that the tree t will represent a vertex of $Sp(n)$ as long as $p \geq \frac{n^2 - 5n + 6}{4n - 10}$. This is true, for instance, when $p \geq n/4$.

In the worst case scenario for non-caterpillar trees, we have $p = 3$ and t is a vertex when $n^2 \leq 17n - 36$, or for $n \leq 14$. For caterpillar trees, where $p = 2$, we have the extra four facets so t is a vertex when $n^2 \leq 13n - 22$, or for $n \leq 11$.

Thus for $n \leq 11$ we have all the binary phylogenetic trees represented as vertices of the splitohedron. $\qquad \square \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \square$

6. PROOF OF THEOREM 4.7

First we prove that the split-facet is always a face of the BME polytope. This is implied by Theorem 4.3. However it is more useful to prove the following simpler linear inequality.

Lemma 6.1. *Consider the split $\pi = \{S_1, S_2\}$ of the set of leaves. Let $|S_1| = k \geq 3$ and $|S_2| = m \geq 3$. Then the following inequality becomes an equality precisely for the trees which display the split, and a strict inequality for all others.*

$$\sum_{i < j, \text{ leaves } i, j \, \in \, S_1} x_{ij} \leq (k-1)2^{n-3}.$$

Proof. (of the face inequality.) It follows directly from the fact that the sum of all coordinates for any tree with n leaves is $n2^{n-3}$. Thus, if we double-sum over the leaves, we have $\sum_i (\sum_j x_{ij}) = n2^{n-2}$; twice the total since we add each coordinate twice. Now consider a tree with $k + 1$ leaves (anticipating a clade with k leaves) and the double sum is $(k+1)2^{k-1}$. If we only sum over the first k leaves, thereby ignoring all the coordinates involving the $k + 1$st

leaf, the smaller double sum totals to $(k-1)2^{k-1}$. (Note that the additional internal node connecting to the $k+1$st leaf is causing the perceived difference in results for our clade of k leaves from an entire tree of n leaves.) Next consider the actual situation of interest, where there is a clade of size k whose coordinates we double-sum over, but we have replaced the extra leaf with another clade of size $n-k$. Here each coordinate in the double sum is multiplied by the power of 2 achieved by adding $n-k-1$ leaves, so our total becomes

$$2^{n-k-1}(k-1)2^{k-1} = (k-1)2^{n-2}.$$

Recall that we have been double counting, so our result is 2 times too much: the actual sum of the coordinates in any clade with leaves from S_1 is

$$\sum_{i < j, \text{ leaves } i,j \in S_1} x_{ij} = (k-1)2^{n-3}.$$

It is clear that for any tree which does not contain a clade consisting only of the leaves in S_1, it instead must contain a collection of clades whose leaves together make up the set S_1 (some of which may be singletons.) Since some of these must be further apart (separated by more internal nodes from each other) than if they formed a single clade, then summing all the coordinates using indices only from S_1 will give a total strictly smaller than in the case where S_1 makes up the leaves of a single clade. $\qquad\square$ $\qquad\qquad\square$

Notice that using the second part of the split, S_2, as the basis for the sum works just as well. In practice the smaller part of the split is chosen in order to provide a shorter inequality. Now we prove the dimension of these faces.

Proof. of Theorem 4.7: *Base case.* The proof is inductive. We start by proving the base case in which one of the parts of the split has exactly $k = 3$ leaves, and the other has size $m \geq 3$.

To do this, we fill in the flag which goes from this facet down to the clade face for a fixed combination of the 3-leaved section of the split.

The first inequality is that of the facet itself, where we simply have a split. If we label the leaves in our $k = 3$-leaf section a,b,c; then our simplified inequality from above is $x_{a,b} + x_{a,c} + x_{b,c} \leq 2^{n-2}$. Let the leaves in the m-leaf section be labeled as $1, 2, ..., m$. We now rely on the fact that to show a chain of subfaces, our subsequent face inequalities only need to be strict on trees which obey the previous face inequality exactly, as an equality. This raises a caveat: the inequalities used for subfaces of the flag in our proof may not be actual face inequalities of the entire polytope.

Our next inequality is:

$$3x_{a,1} - x_{b,1} - x_{c,1} + 2x_{a,b} + 2x_{a,c} \leq 3 \cdot 2^{n-3}.$$

This is intended to include all trees with a in a cherry, and to require the leaf 1 to be near the leaf a when a is not in the cherry. See the set pictured in part (ii) of Fig. 8.

In the case when a is in the cherry, $x_{b,1}$ or $x_{c,1}$ will be the size of $x_{a,1}$ and the other will be twice its size. So the sum $3x_{a,1} - x_{b,1} - x_{c,1}$ will be 0. Then, $x_{a,b}$ or $x_{a,c}$ must be 2^{n-3} and the other 2^{n-4}. These add to $3 \cdot 2^{n-4}$. So $2x_{a,b} + 2x_{a,c} = 3 \cdot 2^{n-3}$.

When a is not in the cherry, for out inequality to be maximal we must have $x_{a,1} = 2^{n-4}$ and hence $x_{b,1}$ and $x_{c,1}$ as 2^{n-5}. So $3x_{a,1} - x_{b,1} - x_{c,1} = 3 \cdot 2^{n-4} - 2 \cdot 2^{n-5} = 2^{n-3}$. Then, since a is near b and c but not in the cherry, we have $2x_{a,b} + 2x_{a,c} = 2 \cdot 2^{n-3}$. So, the left hand side of

our equation is $3 \cdot 2^{n-3}$ when 1 is close to a, as wanted. If 1 were to be further, it is easy to see the expression would be smaller.

Our next set of steps is dependent upon the size of m. The intent here is to build off of previous steps by forcing specific leaves to be far from the k-leaf cluster in each step. See the sets pictured in parts $(iii) - (v)$ of Fig. 8. Our inequalities will be:

$$3x_{a,i} - x_{b,i} - x_{c,i} + \frac{2^{i-1}}{2^{n-4}}(x_{a,b} + x_{a,c}) \geq 3 \cdot 2^{i-1}$$

when $i \geq 3$. When $i = 2$, we use the inequality:

$$3x_{a,2} - x_{b,2} - x_{c,2} + \frac{2^{3-1}}{2^{n-4}}(x_{a,b} + x_{a,c}) \geq 3 \cdot 2^{3-1}.$$

This is because 2 is in a cherry with 3 so they must satisfy the same inequality, albeit with different coordinates.

This works since $3x_{a,i} - x_{b,i} - x_{c,i}$ is 0 when a is in the cherry, and it is half the size of $\frac{2^{i-1}}{2^{n-4}}(x_{a,b} + x_{a,c})$ when it is not in the cherry. Also, $\frac{2^{i-1}}{2^{n-4}}(x_{a,b} + x_{a,c})$ is $\frac{3}{2}$ the size when a is in the cherry as when a is not in the cherry. So in both cases, when we have what we want,
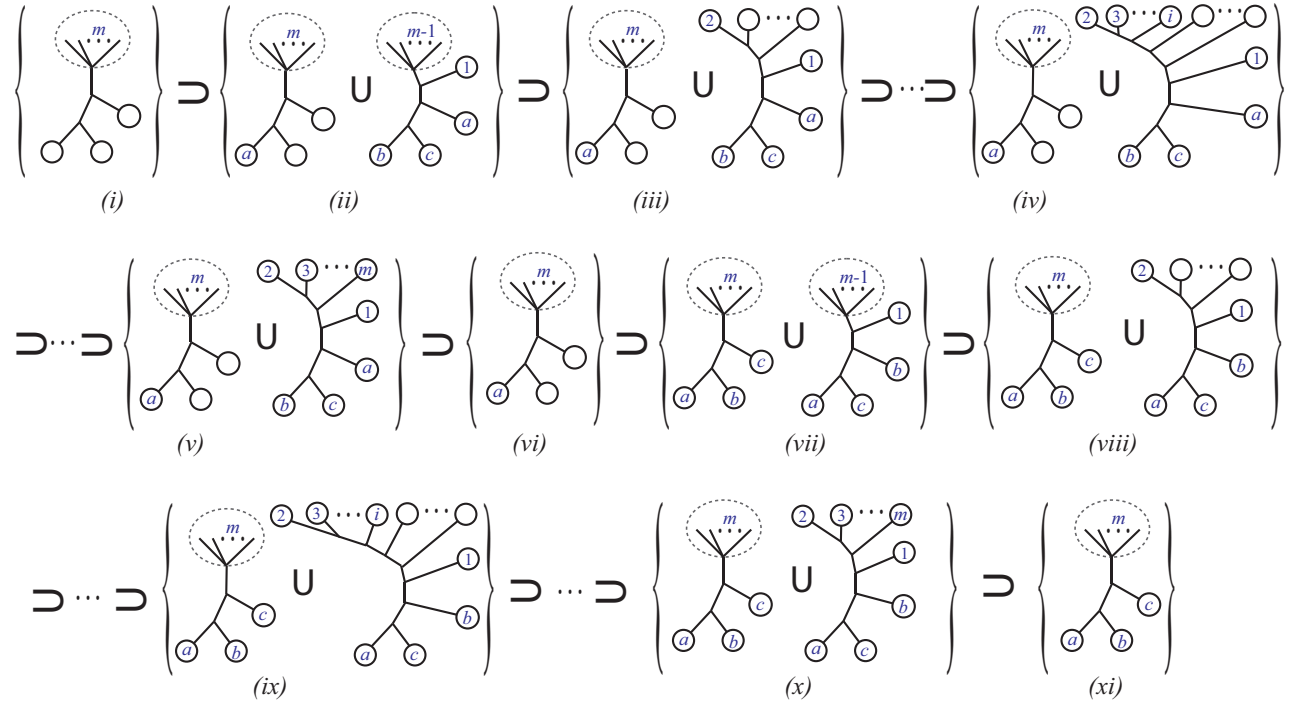

FIGURE 8. Flag for the base case in proof of Theorem 4.7. The sets include all the trees that can be formed by completing the pictures with additional leaf labels. Dashed-circled corollas denote all possible binary structures on the leaves (which are not always shown). Dots between labeled leaves denote an ordered caterpillar structure, while dots between unlabeled leaves denote an unordered caterpillar.

we have equality. If the leaf i moves at all when a is in the cherry, we still have equality. If it moves when a is not in the cherry, $3x_{a,i} - x_{b,i} - x_{c,i}$ will become larger.

After this chain, we have a simple inequality which forces a to be in the cherry, as in the set pictured in part (vi) of Fig. 8. It looks like:

$$2x_{a,b} + 2x_{a,c} \leq 3 \cdot 2^{n-3}.$$

Next, for the set pictured in part (vii) of Fig. 8, we have $3x_{b,1} - x_{a,1} - x_{c,1} + 2x_{a,b} + 2x_{b,c} \leq 3 \cdot 2^{n-3}$. This works like the inequality for the face below the facet. This meaning that, it forces 1 to be close to b when b is not in the cherry, and has no effect on the tree when b is in the cherry. We then have the same i-indexed chain after it with the roles of a and b reversed, since we are trying to achieve the same result as with a but with b. See the sets pictured in part $(viii) - (x)$ of Fig. 8. So, the inequalities are:

$$3x_{b,i} - x_{a,i} - x_{c,i} + \frac{2^{i-1}}{2^{n-4}}(x_{b,a} + x_{b,c}) \geq 3 \cdot 2^{i-1}$$

when $i \geq 3$ and when $i = 2$,

$$3x_{b,2} - x_{a,2} - x_{c,2} + \frac{2^{3-1}}{2^{n-4}}(x_{b,a} + x_{b,c}) \geq 3 \cdot 2^{3-1}.$$

To finish, we use the fixed clade face of dimension $\binom{m+1}{2} - (m+1)$ as described in [11] where c is not in the cherry. See the set pictured in part (xi) of Fig. 8. The total length of our chain is $\binom{n}{2} - n - 1$, proving that the (m,3)-split face is a facet.
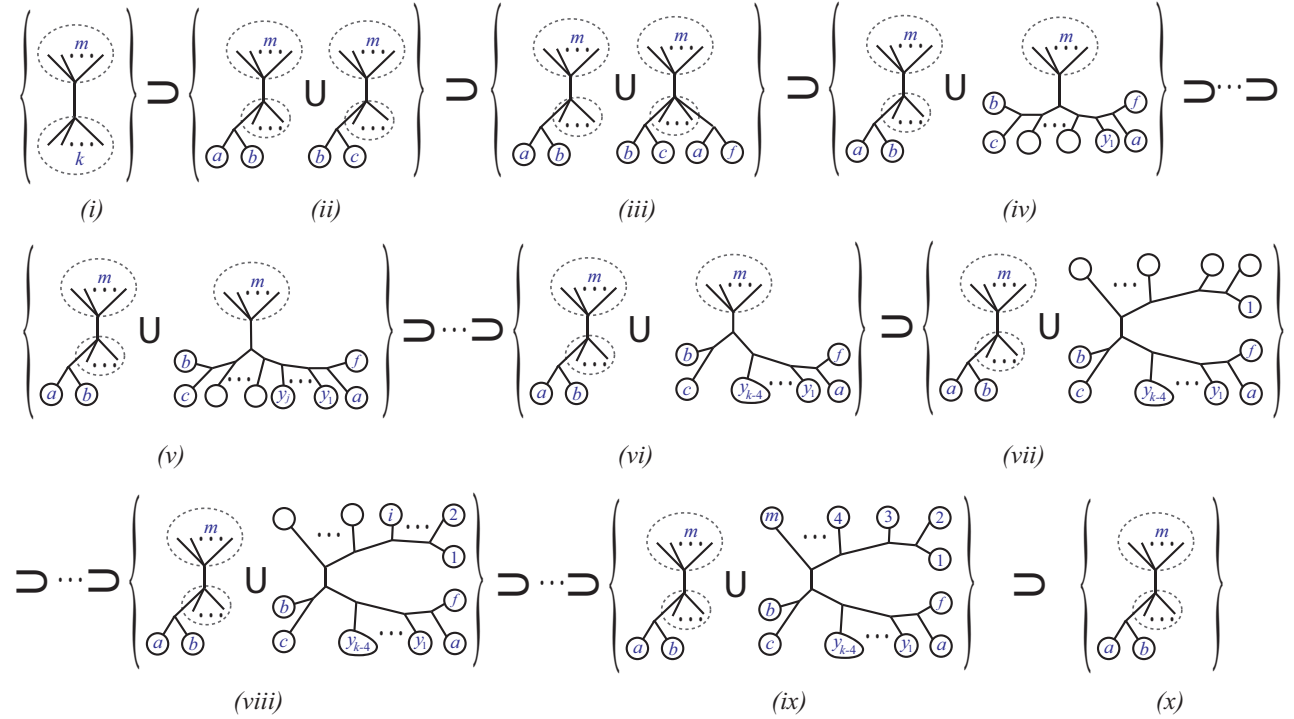

FIGURE 9. Flag for the inductive step in proof of Theorem 4.7. Picture notation is as above.

Inductive step. Next we assume the theorem for splits of respective sizes $k-1$ and m, both larger than 3, and inductively prove it for all k, m. We consider all the trees which display a given split π into leaves $S_1 = \{1, \ldots, m\}$ and leaves $S_2 = \{a, b, c, f\} \cup \{y_1, \ldots, y_{k-4}\}$.

The inductive assumption allows us to use Theorem 4.5 in our proof. We can calculate the dimension of a face which has as its vertices all the binary phylogenetic trees that both display the split π and also have a cherry $\{a, b\}$. These trees are a subset of the set of all the trees with the cherry $\{a, b\}$, which describes a clade-face of the BME polytope. That clade-face is equivalent to $\mathcal{P}_{n-1}$, and using the argument of the proof of Theorem 4.5 as found in [11], the cherry can be considered as a leaf of the trees of $\mathcal{P}_{n-1}$. Thus the trees that both display our split and also have a cherry $\{a, b\}$ display a split π' into m and $k-1$ "leaves" which gives, by induction, a facet of $\mathcal{P}_{n-1}$. The dimension of this face is thus $\binom{n-1}{2} - (n-1) - 1$, and so it is the top-dimensional face in a flag of length $\binom{n-1}{2} - (n-1)$.

Next we show the existence of a chain of faces of length $n-2$, beginning with the face of all trees that display our split π and ending with the face that has all trees displaying π and possessing the cherry $\{a, b\}$. Concatenating this chain to the flag shown by induction gives a flag of length $\binom{n}{2} - n$, which implies that our split-face is indeed a facet.

After the split face, the second face in our flag is described by all the trees that both display the split π and possess either cherry $\{a, b\}$ or cherry $\{b, c\}$. These trees, as a sub-face of the split face, have the face inequality:

$$x_{ab} + x_{bc} - x_{ac} \leq 2^{(n-3)}.$$

Note that this is a face by virtue of being the intersection of the split-facet and the intersecting-cherry facet: in fact the proof from here is inspired by the proof of Theorem 4 (the intersecting-cherry facet) in [8]. Indeed the next face in our flag is described by containing the trees which both display the split π and possess either cherry $\{a, b\}$ or the two cherries $\{b, c\}$ and $\{a, f\}$. Again this is an intersection of faces: the split-face and the second face of the flag shown in the proof of Theorem 4 in [8]. For completeness, the inequality obeyed by this third face is:

$$x_{bc} + x_{bf} - x_{ac} - x_{af} \geq 0.$$

Next we have a chain of $k-4$ faces which correspond to ordering the remaining $k-4$ leaves of S_2. For $j \in 1 \ldots k-4$ we take the set of trees that have the split π and the cherry $\{a, b\}$, or which have the cherries $\{b, c\}$ and $\{a, f\}$ as the two cherries of a caterpillar clade made from S_2, and for which the leaves $y_1 \ldots y_j$ are attached in that order starting as close as possible to the cherry $\{a, f\}$. See the pictures of sets (iv) - (vi) in Fig. 9, noting how the caterpillar clade is attached to S_1 at any point among its unordered nodes. The jth term in this list of faces obeys the inequality:

$$(2^{n-3} - 2^{m-1})(x_{ay_j} - x_{by_j}) \leq (2^{n-3} - x_{ab})(2^{n-3-j} - 2^{m+j-1}).$$

To see that this is an equality for the sets of trees in question, note first that when $\{a, b\}$ is a cherry then $x_{ab} = 2^{n-3}$ and $x_{ay_j} = x_{by_j}$. Also, when S_2 is fixed as a caterpillar clade, then $x_{ab} = 2^{m-1}$ and $x_{ay_j} - x_{by_j} = 2^{n-3-j} - 2^{m+j-1}$. Finally, when y_j is found in a location on the caterpillar clade closer to leaf b, (which is the only way to be in the previous face while avoiding being in the current face), then $x_{ay_j} - x_{by_j}$ is forced to be a lesser value.

After the chain of caterpillar clades using S_2, we add a chain using caterpillar clades on S_1. This chain begins with the set pictured in part $(viii)$ of Fig. 9, where the leaf 1 is in the cherry

at the far end of the flag. This face obeys the equality:

$$(2^{n-3} - 2^{m-1})(x_{a1} - x_{b1}) \leq (2^{n-3} - x_{ab})(2 - 2^{k-3}).$$

The comments just made about the previous faces also apply here, to show that the equality holds on the face and that when S_2 is fixed as a caterpillar clade, then $x_{ab} = 2^{m-1}$. Now though we see that if the leaf 1 is any closer to b, then both x_{a1} and x_{b1} increase. However, since they are both powers of two then increasing both by a factor of another power of two means their difference will be even larger–and we are subtracting in the order that ensures the inequality.

The remaining links in the chain are formed by fixing the leaves $2, \ldots, m$ in order along the caterpillar clade in S_1, as in pictured sets $(viii)$ and (ix) of Fig. 9. When the leaf i is fixed, the face obeys the inequality:

$$(2^{n-3} - 2^{m-1})(x_{ai} - x_{bi}) \leq (2^{n-3} - x_{ab})(2^{i-1} - 2^{i+k-5}).$$

This inequality is an equality on the face and strict on the trees of the previous face excluded from the current face, by the same arguments as above.

Finally we exclude all the trees displaying the split except for those with the cherry $\{a, b\}$, as shown by the pictured set (x) in Fig. 9. This completes the proof by induction, as explained above. $\square$ $\square$

7. Future work

We have shown that (for $n \leq 11$) the splitohedron contains among its vertices all the possible phylogenetic trees. Therefore if the BME linear program is optimized in the splitohedron at a valid tree vertex for $n \leq 11$, it is also optimized in the BME polytope.

More importantly, however, the binary phylogenetic trees for any n all lie on the boundary of several facets of the splitohedron which are also facets of the BME polytope. Our continuing research program involves writing code that uses various linear programming methods in sequence, with a branch-and-bound scheme, to find the BME tree.

Then by finding further facets we will improve this theorem, hopefully to a version that holds for all $n > 11$.

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