THE DISENTANGLING NUMBER FOR PHYLOGENETIC MIXTURES

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ABSTRACT. We provide a logarithmic upper bound for the disentangling number on unordered lists of leaf labeled trees. This results is useful for analyzing phylogenetic mixture models. The proof depends on interpreting multisets of trees as high dimensional contingency tables.

For a set X of leaf labels let \mathcal{T}_X be the set of trivalent leaf labeled trees (see [5] for background on leaf labeled trees). Typically, the labels come from the set $[n] = \{1, 2, \ldots, n\}$. For $K \subseteq X$ and $T \in \mathcal{T}_X$, let $T|_K$ denote the trivalent tree $T|_K \in \mathcal{T}_K$ obtained by restricting T to the label set of leaves K, contracting vertices of degree two as necessary to obtain trivalent tree. Let $\mathcal{T}_{X,r}$ be the set of unordered lists of length r of elements of \mathcal{T}_X . Note that these elements need not be distinct. For $S \in \mathcal{T}_{X,r}$, with $S = (T_1, \ldots, T_r)$, let $S|_K = (T_1|_K, \ldots, T_r|_K)$.

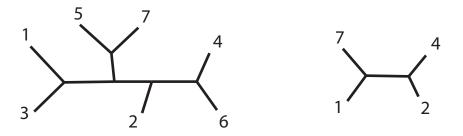


FIGURE 1. The right-hand tree is $T|_{\{1,2,4,7\}}$ for the tree T on the left.

Definition 1. Let $S_1, S_2 \in \mathcal{T}_{X,r}$ with $S_1 \neq S_2$. A subset $K \subseteq X$ is said to disentangle S_1 and S_2 if $S_1|_K \neq S_2|_K$. Let $d(S_1, S_2)$ be the cardinality of the minimum disentangling set of S_1 and S_2 . The disentangling number D(r) is

$$D(r) = \max_{n \in \mathbb{N}} \max_{S_1 \neq S_2 \in \mathcal{T}_{[n],r}} d(S_1, S_2).$$

Humphries [2] proved that the disentangling number exists, and gave the bounds

$$3(\lfloor \log_2 r \rfloor + 1) \le D(r) \le 3r$$

At present, the only exactly known values of the disentangling number are D(1) = 4 and D(2) = 6 [4]. This first value D(1) = 4, is usually stated as saying that "the quartets determine the tree" (see e.g. [5]).

The main motivation for studying the disentangling number is that it can be used as a tool in proofs of the identifiability of the tree parameters in phylogenetic mixture models. Indeed, if it can be shown, for some value $s \ge D(r)$, that the tree parameters of r class mixtures on s-leaf phylogenetic trees are (generically) identifiable under some

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phylogenetic model, then the tree parameters are (generically) identifiable for r class mixtures all trees with $t \ge s$ leaves. For example, the known value of D(2) = 6 was used in the proof of generic identifiability of the tree parameters of 2-tree Jukes-Cantor and Kimura 2-parameter mixture models [1].

We provide the following improved upper bound on the disentangling number, which is within one of the optimal possible value.

Theorem 2. $D(r) \le 3(\lfloor \log_2(r) \rfloor + 1) + 1$

To prove Theorem 2 we first reduce to rooted binary trees, as follows. Let \mathcal{RT}_X denote the set of leaf labeled rooted binary trees on leaf label set X. For $T \in \mathcal{RT}_X$ and $K \subseteq X$, let $T|_K$ be the induced binary rooted tree on leaf label set K, with edges contracted as appropriate to obtain a rooted binary tree. Let $\mathcal{RT}_{X,r}$ be the set of unordered lists of length r of elements of \mathcal{RT}_X . Note that these elements need not be distinct. For $S \in \mathcal{RT}_{X,r}$, with $S = (T_1, \ldots, T_r)$, let $S|_K = (T_1|_K, \ldots, T_r|_K)$. Define the rooted disentangling number $\mathcal{RD}(r)$ in an analogous way to the disentangling number.

Proposition 3. The disentangling and rooted disentangling numbers satisfy: $D(r) \leq RD(r) + 1$.

Proof. Let $n \geq RD(r)$, and consider a set X of cardinality n + 1, e.g. $X = \{0\} \cup [n]$. Let $S_1, S_2 \in \mathcal{T}_{X,r}$. Choosing the node 0 (or any other leaf) as a root node, we arrive at sets $\tilde{S}_1, \tilde{S}_2 \in \mathcal{RT}_{[n],r}$. By definition of the rooted disentangling number, there is a $K \subseteq [n]$ of RD(r) elements such $\tilde{S}_1|_K \neq \tilde{S}_2|_K$. This implies that the set $\{0\} \cup K$ satisfies $S_1|_{\{0\} \cup K} \neq S_2|_{\{0\} \cup K}$.

Theorem 2 then follows as a corollary of the following result.

Theorem 4. $RD(r) = 3(\lfloor \log_2(r) \rfloor + 1).$

To prove the inequality $RD(r) \leq 3(\lfloor \log_2(r) \rfloor + 1)$ of Theorem 4, we use the known value RD(1) = 3 (i.e. rooted triples determined a rooted tree (see e.g. [5])) to encode multisets of trees as high dimensional contingency tables. To this end, consider the $3^{\binom{\#X}{3}}$ -dimensional space

$$Q_X := \mathbb{R}^{3^{\binom{\#X}{3}}} = \bigotimes_{\{i,j,k\} \in \binom{X}{3}} \mathbb{R} \langle e_{i|jk}, e_{j|ik}, e_{k|ij} \rangle.$$

Coordinates on this space are indexed by the lists of $\binom{X}{3}$ -rooted triplets. Each rooted X-leaf trivalent tree T gives rise to a uniquely determined standard unit vector

$$e_T := \bigotimes_{\{i,j,k\} \in \binom{X}{3}} e_{T|_{\{i,j,k\}}} \in Q_X.$$

This uniqueness is a consequence of the fact that rooted triples in a rooted tree uniquely determine the tree.

An unordered list of trees $S = (T_1, \ldots, T_r) \in \mathcal{T}_{X,r}$ gives rise to a nonnegative integer array

$$u_S = e_{T_1} + e_{T_2} + \dots + e_{T_r}$$

in Q_X , whose 1-norm is equal to r. Furthermore, the list S can be recovered from the vector u_S . We will use this encoding of sets of trees to prove Theorem 4.

Let K be a finite set. For each $k \in K$, let $d_k \in \mathbb{N}_{>1}$ and consider the space

$$\mathbb{R}^{d_K} = \bigotimes_{k \in K} \mathbb{R}^{d_k}$$

with the standard unit vectors $\otimes_{k \in K} e_{j_k}$. For each $L \subseteq K$, we get a linear map

$$\pi_L: \mathbb{R}^{d_K} \to \mathbb{R}^{d_L}, \otimes_{k \in K} e_{j_k} \mapsto \otimes_{k \in L} e_{j_k}.$$

Given $u \in \mathbb{R}^{d_K}$, $\pi_L(u)$ is called the *L*-marginal of *u*. If $\Gamma = \{L_1, \ldots, L_s\}$ is a set of subsets of *K*, we get an induced linear map

$$\pi_{\Gamma}: \mathbb{R}^{d_K} \to \bigoplus_{i=1}^{s} \mathbb{R}^{d_{L_i}}, \quad u \mapsto \pi_{L_1}(u) \oplus \cdots \oplus \pi_{L_s}(u).$$

which is the linear transformation that computes the Γ -marginals of u. Suppose now that Γ is closed downward, that is $L \in \Gamma$ and $L' \subseteq L$ implies that $L' \in \Gamma$. Such a Γ is called a simplicial complex. The elements of Γ are called the faces of Γ .

Theorem 5. [3] Let Γ be a simplicial complex, let s be the cardinality of the smallest $S \subset K$ not in Γ , and $u \in \ker_{\mathbb{Z}} \pi_{\Gamma}$ with $u \neq 0$. Then $||u||_1 \geq 2^s$.

Proof that $RD(r) \leq 3(\lfloor \log_2(r) \rfloor + 1)$. Fix r, and suppose that $D(r) > g(r) := 3(\lfloor \log_2(r) \rfloor + 1)$. Then there exists two unordered lists of rooted binary trees $S_1, S_2 \in \mathcal{T}_{[n],r}$ for n > g(r) such that for all $k \leq g(r)$ and $K \in {[n] \choose k}$, we have $S_1|_K = S_2|_K$.

Let Γ_r be the simplicial complex with ground set $\binom{[n]}{3}$ such that a set $\{K_1, \ldots, K_m\}$ forms a face of Γ_r if and only if

$$#(K_1 \cup \cdots \cup K_m) \le g(r).$$

Note that this implies that the size of the smallest $S \notin \Gamma_r$ has $\lfloor \log_2(r) \rfloor + 2$ elements (obtained by taking that many disjoint triplets).

The fact that $S_1|_K = S_2|_K$ for all $K \in {\binom{[n]}{k}}$ with $k \leq g(r)$ implies that $\pi_{\Gamma_r}(u_{S_1}) = \pi_{\Gamma_r}(u_{S_2})$. Indeed, if $L = \{K_1, \ldots, K_m\}$, then $\pi_L(e_T)$ is a table with a single nonzero entry which records which of the rooted triplets on K_1, \ldots, K_m , that tree T has. Thus, $\pi_L(u_{S_i})$ is a table which records which combinations of rooted triplets on K_1, \ldots, K_m appear in the trees in S_i . If $\#(K_1 \cup \cdots \cup K_m) \leq g(r)$, this information can be read off from $S_1|_{K_1 \cup \cdots \cup K_m} = S_2|_{K_1 \cup \cdots \cup K_m}$, and must be the same for both S_1 and S_2 .

Since $\pi_{\Gamma_r}(u_{S_1}) = \pi_{\Gamma_r}(u_{S_2})$, we see that $u_{S_1} - u_{S_2} \in \ker_{\mathbb{Z}} \pi_{\Gamma_r}$. Since $S_1 \neq S_2$, $v = u_{S_1} - u_{S_2} \neq 0$. By Theorem 5, we have $\|v\|_1 \ge 2^{\lfloor \log_2(r) \rfloor + 2} > 2r$. On the other hand each u_{S_i} has one norm r, so $\|v\|_1 \le 2r$. This is a contradiction.

Remark. Note that the same argument for the upper bound would work even if our trees were not binary, by using vector spaces of dimension $4^{\binom{[n]}{3}}$, since arbitrary rooted trees are determined by their rooted triplets (of which there are four possibilities).

The lower bound $RD(r) \ge 3(\lfloor \log_2(r) \rfloor + 1)$, can be deduced from an elegant construction of Humphries ([2] stated for unrooted trees), which we repeat here for completeness.

Proof that $RD(r) \ge 3(\lfloor \log_2(r) \rfloor + 1)$. Suppose first that $r = 2^{k-1}$. Let T be a fixed, but otherwise arbitrary rooted leaf labeled binary tree with k leaves, labeled by [k]. We will construct sets of trees on 3k leaves which prove the lower bound. Now let X be the leaf

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label set $X = \{a_1, b_1, c_1, \ldots, a_k, b_k, c_k\}$. On each triple we use two rooted trees $a_i | b_i c_i$ and $b_i | a_i c_i$, denoted t_0^i and t_1^i respectively. Given a list of trees $t_{\epsilon} = (t_{\epsilon_1}^1, \ldots, t_{\epsilon_k}^k)$ with $\epsilon \in \{0, 1\}^k$, form the tree with 3k leaves T_{ϵ} by identifying the root on tree $t_{\epsilon_i}^i$ with the label i on the leaf of T.

Now let

$$S_{k,odd} = \{T_{\epsilon} : \epsilon \in \{0,1\}^k, \quad \sum_i \epsilon_i \equiv 1 \mod 2\}$$
$$S_{k,even} = \{T_{\epsilon} : \epsilon \in \{0,1\}^k, \quad \sum_i \epsilon_i \equiv 0 \mod 2\}.$$

For any subset $K \subseteq X$, with #K = 3k - 1, we have $S_{k,odd}|_K = S_{k,even}|_K$. Indeed, this K omits one vertex, say a_k so that both triples $a_k|b_kc_k$ and $b_k|a_kc_k$ collapse to an identical cherry on b_k and c_k in all trees. Thus, the trees in both $S_{k,odd}|_K$ and $S_{k,even}|_K$ are determined by all vectors $\epsilon \in \{0,1\}^{k-1}$. Note that $\#S_{k,odd} = \#S_{k,even} = 2^{k-1}$. This implies that $RD(r) \geq 3k = 3(\log_2(r) + 1)$.

If $2^{k-1} \leq r < 2^k$, we let T' be an arbitrary tree with 3k leaves on the label set X, and let S_1 and S_2 be the multisets $S_1 = S_{k,odd} \cup \{T', \ldots, T'\}$ and $S_2 = S_{k,even} \cup \{T', \ldots, T'\}$, where we union with $r - 2^{k-1}$ copies of T'. Then by the preceding argument $S_1|_K = S_2|_K$ for all subsets $K \subseteq X$ with #K = 3k - 1.

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References

- E. Allman, S. Petrovic, J. Rhodes, and S. Sullivant. Identifiability of two-tree mixtures for groupbased models. *IEEE/ACM Transactions in Computational Biology and Bioinformatics* 8 no. 3 (2011) 710–722.
- [2] P. J. Humphries. Combinatorial Aspects of Leaf-Labelled Trees, Ph. D. Thesis, University of Canterbury, 2008.
- [3] T. Kahle. Neighborliness of marginal polytopes Contributions to Algebra and Geometry 51 (2010) 45-56.
- [4] F. A. Matsen, E. Mossel, and M. Steel. Mixed-up trees: the structure of phylogenetic mixtures. Bull. Math. Biol., 70(4):1115–1139, 2008.
- [5] C. Semple and M. Steel. Phylogenetics, volume 24 of Oxford Lecture Series in Mathematics and its Applications. Oxford University Press, Oxford, 2003.

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