COSPEDTree-II: Improved Couplet based Phylogenetic Supertree

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Abstract—A Supertree synthesizes the topologies of a set of phylogenetic trees carrying overlapping taxa set. In process, conflicts in the tree topologies are aimed to be resolved with the consensus clades. Such a problem is proved to be NP-hard. Various heuristics on local search, maximum parsimony, graph cut, etc. lead to different supertree approaches, of which the most popular methods are based on analyzing fixed size subtree topologies (such as triplets or quartets). Time and space complexities of these methods, however, depend on the subtree size considered. Our earlier proposed supertree method COSPEDTree, uses evolutionary relationship among individual couplets (taxa pair), to produce slightly conservative (not fully resolved) supertrees. Here we propose its improved version COSPEDTree-II, which produces better resolved supertree, with lower number of missing branches, and incurs much lower running time. Results on biological datasets show that COSPEDTree-II belongs to the category of high performance and computationally efficient supertree methods.

Index Terms—Phylogenetic tree, Supertree, Couplet, Directed Acyclic Graph (DAG), Equivalence Relation, Transitive reduction, Internode count.

I. INTRODUCTION

Supertree methods combine the evolutionary relationships of a set of phylogenetic trees G, into a single tree T [1]. These methods differ from the consensus-based approaches [2], [3], by allowing input trees to have different but overlapping set of taxa. Supertrees are useful in combining input trees generated from completely incomparable approaches, such as statistical analysis of discrete dataset and distance analysis of DNA-DNA hybridization data [1]. Input trees often exhibit conflicting topologies, due to different evolutionary histories of respective genes, stochastic errors in site and taxon sampling, and biological errors due to paralogy, incomplete lineage sorting, or horizontal gene transfer [4]. Supertree methods quest for resolving such conflicts in order to produce a ‘median tree’, which minimizes the sum of a given distance measure with respect to the input trees [4]. Large scale supertrees are intended towards assembling the Tree of Life [5].

Our earlier work [6], and the study in [11], provide a comprehensive review of various supertree methods. Indirect supertree methods first generate intermediate structures like matrices (as in MRP [7], Minflip [8], SFIT [9]) or graphs (as in Mincut (MC) [10], modified Mincut [11]) from the input trees, and subsequently resolve these intermediate structures to produce the final supertree. These methods, especially MRP, are quite accurate, but computationally intensive. Direct methods, on the other hand, derives the supertree directly from input tree topologies. These methods may aim for minimizing either the sum of false positive (FP) branches (as in the veto approaches like PhySIC [12], SCM [13]) or the sum of Robinson-Foulds (RF) distance (as in RFS [15]) between T and G. Another approach named Superfine [16], [17] employs greedy heuristics on MRP [7] or Quartet Maxcut (QMC) [18], to derive the supertree, which may not be completely resolved. Supertrees formed by synthesizing the subtrees (such as triplets [4], [19], quartets [18], [5]) of the input trees, exhibit quite high performance. But, time and space complexities of these methods depend on the size of the subtrees used.

We have previously developed COSPEDTree [6], a supertree algorithm using evolutionary relationships among individual pair of taxa (couplets). The method is computationally efficient, but produces somewhat conservative (not fully resolved) supertrees, with low number of false positive (FP) but high number of false negative (FN) branches between T and G. Here we propose its improved version, termed as COSPEDTree-II, which produces better resolved supertree, with lower number of FN branches between T and G, keeping the FP count also low. We have also proposed a mechanism to convert a non-resolved supertree into a strict binary tree, to reduce the FN count. COSPEDTree-II requires significantly lower running time than COSPEDTree and most of the reference methods, particularly for the datasets having high number of trees or taxa.

Rest of this manuscript is organized as follows. First, we review the basics of COSPEDTree (as in [6]) in section II. The method COSPEDTree-II is then described in section III. Performance of COSPEDTree-II is summarized in section IV.

II. OVERVIEW OF COSPEDTREE

![Fig. 1. Example input phylogenetic trees. All the nodes are labeled by Newick representation.](image-url)
Let G consist of M rooted input trees $t_1, t_2, \ldots, t_M$. For an input tree $t_j$ ($1 \leq j \leq M$), let $L(t_j)$ be its set of constituent taxa. Suppose a pair of taxa $p$ and $q$ belong to $L(t_j)$. Further, let $\phi_p$ and $\phi_q$ be the parent internal nodes (points of speciation) of $p$ and $q$, respectively. COSPEDTree [6] defines four boolean relations $r^p_{kq}$ ($k \in \{1, 2, 3, 4\}$) between $p$ and $q$, with respect to $t_j$, as:

1. Earlier Speciation of $p$ than $q$ ($r^p_{1q}$) is true, if $\phi_p$ is an ancestor of $\phi_q$ in $t_j$. For the tree in Fig. 1(b), $r^p_{1q}$ is true, where $X = \{a, c\}$. Similarly, $r^{qk}_{1}$ is true for $Y = \{a, c, b\}$.

2. Later Speciation of $p$ than $q$ ($r^p_{2q}$) is true, if $\phi_p$ is a descendant of $\phi_q$. So, $r^p_{1q}$ and $r^p_{2q}$ are equivalent.

3. Simultaneous Speciation of $p$ and $q$ ($r^p_{3q}$) is true, if $\phi_p = \phi_q$. In Fig. 1(a), $r^p_{3q}$ and $r^q_{3k}$ are true.

4. Incomparable Speciation of $p$ and $q$ ($r^p_{4q}$) is true, when $\phi_p$ and $\phi_q$ occur at different (and independent) clades. For the tree in Fig. 1(a), $r^p_{4q}$ is true.

Using another taxon $s \in L(t_j)$, properties of $r_1$ to $r_4$ can be stated as the following:

**P1:** Both $r_1$ and $r_2$ are transitive. Thus,

- $r^p_{1q} \land r^q_{1s} \Rightarrow r^p_{1s}$.
- $r^p_{2q} \land r^q_{2s} \Rightarrow r^p_{2s}$.

**P2:** $r_3$ is an equivalence relation.

**P3:** $r^p_{3q} = r^q_{3k}$ and $r^p_{3s} \Rightarrow r^q_{3s}$, where $k \in \{1, 2, 4\}$.

**P4:** $r^p_{4q} = r^q_{4k}$ and $r^p_{4s} = r^q_{4s} \Rightarrow r^q_{4k}$.

**Support tree set $I_{pq}$ for a couplet $(p, q)$** is defined as:

$$I_{pq} = \{t_j : (p, q) \in L(t_j)\} \quad (1)$$

The frequency $F^p_{kq}$ ($k \in \{1, 2, 3, 4\}$) of a relation $r^p_{kq}$ between a couplet $(p, q)$ is the number of input trees $t_j$ where $t_j \in I_{pq}$ and $r^p_{kq}$ is true.

The set of allowed relations $R(p, q)$ between a couplet $(p, q)$ is defined as the following:

$$R(p, q) = \{r^p_{kq} : F^p_{kq} > 0\} \quad (2)$$

A couplet $(p, q)$ exhibits conflict if $|R(p, q)| \geq 2$ (where $|.|$ denotes the cardinality of a set). The consensus relation between $(p, q)$ is the relation having the maximum frequency.

**Priority measure $P^p_{kq}$ for a relation $r^p_{kq}$ ($k \in \{1, 2, 3, 4\}$)** between a couplet $(p, q)$ is defined as the following:

$$P^p_{kq} = F^p_{kq} - \sum_{1 \leq k' \leq 4, k' \neq k} F^p_{k'q} \quad (3)$$

COSPEDTree also defines a support score $V^p_{kq}$ for individual relations $r^p_{kq}$ as the following:

$$V^p_{kq} = F^p_{kq} \times P^p_{kq} \quad (4)$$

The consensus relation $r^p_{kq}$ between a couplet $(p, q)$ exhibits the highest $P^p_{kq}$ and $F^p_{kq}$ values. So, corresponding $V^p_{kq}$ also becomes the highest among all relations between $(p, q)$.

Final supertree $T$ resolves (assigns a particular relation to) individual couplet $(p, q)$ with a single relation $r^p_{kq}$ ($k \in \{1, 2, 3, 4\}$) between them. Maximum agreement property [15] of a supertree quests for resolving individual couplets with their respective consensus relations. But, satisfying such property is NP-hard since consensus relations among couplets can be mutually conflicting [6]. Thus, order of selection of individual candidate relations $r^p_{kq}$ (to resolve the corresponding couplet $(p, q)$) is crucial. In view of this, COSPEDTree first constructs a set of relations $S_r$, such that if a relation $r^p_{kq} \in S_r$, the couplet $(p, q)$ is resolved with $r^p_{kq}$. To construct $S_r$, COSPEDTree applies an iterative greedy approach. At each iteration, it selects a relation $r^p_{kq}$ to resolve $(p', q')$ among all unresolved couplets, provided:

$$V^p_{kq} = \max_{\forall(p,q) \forall r \in k} V^p_{kq}.$$

If the selected relation $r^p_{kq}$ does not contradict with any of the already selected relations in $S_r$, (according to the properties P1 to P4 mentioned before), it is included in $S_r$.

![Diagram](image)

Fig. 2. (a) Transitive parent problem (b) Multiple parent problem MPP. (c) No parent problem NPP. (d) solution of NPP by COSPEDTree, by inserting a hypothetical root $R$.

Suppose, $L(G) = \bigcup_{j=1}^M L(t_j)$ denotes the complete set of input taxa. Then, $N = |L(G)|$. Using the set of relations $S_r$, COSPEDTree partitions $L(G)$ into $s$ mutually exclusive taxa clusters $C_1, C_2, \ldots, C_s$, with the following rule (details are provided in [6]):

**R1:** If a pair of taxa $p$ and $q$ belong to the same cluster $C_i$ ($1 \leq i \leq s$), $r^p_{kq} \in S_r$.

**R2:** Suppose $C_i$ and $C_j$ ($1 \leq i, j \leq s$, $i \neq j$) are any two distinct taxa clusters. Then, $\forall p \in C_i$, and $\forall q \in C_j$, $r^p_{kq} \in S_r$, where $k \in \{1, 2, 4\}$. This property is denoted by saying that $r^p_{C_i C_j}$ is true, or $C_i$ is related with $C_j$ via the relation $r_k$.

COSPEDTree creates a directed acyclic graph (DAG), whose nodes are individual taxa clusters $C_i$ ($1 \leq i \leq s$). A directed edge from $C_i$ to $C_j$ means $r^i_{C_i C_j}$ is true. However, the occurrence of one or more of the following properties means this DAG needs to be refined to form a tree:

1. **Transitive parent problem (TPP):** For three nodes A, B, and C, when $r^B_{AC}$, $r^B_{BC}$, and $r^B_{AB}$ are simultaneously true, as indicated in Fig. 2(a).

2. **Multiple parent problem (MPP):** When $r^A_{BC}$, $r^B_{BC}$, and $r^A_{AB}$ are simultaneously true, as shown in Fig. 2(b).

3. **No parent problem (NPP) (Fig. 2(c)):** when a node A does not have any parent, i.e., there exists no node B such that $r^A_{B}$ is true. COSPEDTree [6] applies transitive reduction to resolve TPP. The problem MPP is solved by arbitrary parent assignment, while NPP is resolved by assigning one hypothetical
root node to the isolated node (as shown in Fig. 2(d)). Finally, a depth first traversal of this DAG produces the supertree $T$. As there is no restriction regarding the number of taxa in individual taxa clusters (partitions with respect to the relation $r_3$), $T$ may not be strictly binary (completely resolved).

**III. PROPOSED METHODOLOGY**

COSPEDTree-II extends COSPEDTree by incorporating the following modifications:

1. COSPEDTree-II skips the formation of $S_r$. Rather, the taxa clusters (containing one or more taxon) are first derived, solely by the frequencies of different relations between individual couples. Subsequently, directed edges between individual pairs of clusters are assigned, according to the properties of individual couples contained within these cluster pairs. Such processing on the taxa clusters, rather than the couples, achieves high speedup and much lower running time.

2. In COSPEDTree, if a relation $r_{pq}^k$ (1 $\leq$ $k$ $\leq$ 4) between a couplet $(p, q)$ is supported in a tree $t_j \in T_{pq}$, the frequency $F_{pq}^k$ is incremented by 1. COSPEDTree-II, on the other hand, uses fractional and dynamic frequency values. In the above case, COSPEDTree-II increments $F_{pq}^k$ with a weight $W_{pq}^j$ (0 $<$ $W_{pq}^j$ $\leq$ 1), which varies for individual couplets $(p, q)$, and also for individual trees $t_j \in T_{pq}$.

3. For the problem MPP, COSPEDTree-II proposes a deterministic selection of the parent, for the node having multiple parents.

4. COSPEDTree-II also suggests a mechanism to convert a non-binary supertree into a binary tree.

Subsequent sections describe all such improvements.

**A. Fractional frequency value for relations**

![Diagram](image)

Fig. 3. (a) to (c) shows three input trees. Fig. (d) shows the corresponding supertree.

COSPEDTree-II applies a fractional frequency value $W_{pq}^j$ if an input tree $t_j$ supports the relation $r_{pq}^k$ between a couplet $(p, q)$. Value of $W_{pq}^j$ depends on the set $L(t_j)$. Utility of such a dynamic (and fractional) frequency measure is explained by Fig. 2, which shows three input trees (Fig. 3(a) to Fig. 3(c)) and corresponding supertree (Fig. 3(d)). For the couplet (A,C), all of the relations $r_2$, $r_3$ and $r_4$ are supported. However, we observe that the relation $r_3$ is supported only because corresponding tree does not include taxa B and D. Similarly, the relation $r_2$ occurs due to the absence of the taxon D. When both B and D are present (Fig. 3(c)), the relation $r_4$ (which is the ideal relation between (A,C)) is satisfied. So, the relation $r_4$ should be given higher weight, since the corresponding tree has higher taxa coverage. So, our proposed dynamic frequency measure varies according to the coverage of taxa of different input trees.

Considering an input tree $t_j$ (1 $\leq$ $j$ $\leq$ $M$) and a couplet $(p, q)$ in $L(t_j)$, first we define the following notations:

- $V(t_j)$: set of nodes (leaf or internal) of $t_j$.
- $LCA_{pq}^j$: lowest common ancestor (LCA) of $p$ and $q$ in $t_j$.
- $Clade_{t_j}(v)$: subtree rooted at an internal node $v \in (V(t_j) - L(t_j))$.
- $Cluster_{t_j}(v)$: Set of taxa underlying $Clade_{t_j}(v)$.

With such definitions, the set of excess taxa (excluding the couplet itself) underlying the LCA node of $(p, q)$ in $t_j$, is defined as the following:

$$U_{pq}^j = Cluster_{t_j}(LCA_{pq}^j) - \{p, q\}$$

For $(p, q)$, union of all excess taxa underlying the respective $LCA_{pq}^j$ nodes for all $t_j \in T_{pq}$, is:

$$U_{pq}^G = \bigcup_{t_j \in T_{pq}} U_{pq}^j$$

We assign the weight of a relation $r_{pq}^k$ (1 $\leq$ $k$ $\leq$ 4) between $(p, q)$ in an input tree $t_j$, as:

$$W_{pq}^j = \frac{|U_{pq}^G \cap L(t_j)|}{|U_{pq}^G|}$$

where $W_{pq}^j = 1$ if $U_{pq}^G = \phi$.

Thus, the weight equals the proportion of taxa within $U_{pq}^G$, that is covered in the input tree $t_j$. Frequency $F_{pq}^j$ of the relation $r_{pq}^k$, is now redefined as the following:

$$F_{pq}^j = \sum_{t_j \text{ supports } r_{pq}^k} W_{pq}^j$$

**B. Generating taxa clusters**

COSPEDTree [6] creates taxa clusters after formation of the set of resolving relations $S_r$. COSPEDTree-II, on the other hand, creates taxa clusters before resolving any couplets at all. Rather, for individual couplets $(p, q)$, COSPEDTree-II inspects the values of $F_{pq}^k$ for individual relations $r_{pq}^k$ ($k \in \{1, 2, 3, 4\}$). Creation of taxa clusters requires identifying couplets which can be resolved by the relation $r_3$. COSPEDTree-II places a pair of taxa $p$ and $q$ in the same taxa cluster (thereby resolving the couplet $(p, q)$ with the relation $r_3$), provided:

1. Either $|R(p, q)| = 1$ and $r_{pq}^3 \in R(p, q)$ ($R(p, q)$ is already defined in Eq. 2).
2. Or $|R(p, q)| = 2$ and $r_{pq}^3$ is majority consensus. In such a case, $F_{pq}^3 \geq 0.5 \times \{ \sum_{k \neq 3} F_{pq}^k \}$.
3. If $|R(p, q)| > 2$, the couplet $(p, q)$ is not placed in the same taxa cluster, even if $r_{pq}^3$ is majority consensus. This is because, as the couplet exhibits high degree of conflict, we check the relations between $p$, $q$, and other taxa set.

The first condition is obvious. A couplet having only $r_3$ as its allowed relation would be preferably resolved with it. On the other hand, if there exists one more relation $r_{pq}^{k'}$ ($k' \neq 3$)
within \( R(p,q) \), we check whether \( F_{pq}^{i} \) > \( F_{pq}^{j} \), which ensures that \( r_{pq}^{i} \) is the majority consensus relation of \((p,q)\). In such a case, the couplet is highly probable of being resolved with \( r_{3} \) in the final supertree.

Above mentioned heuristics are applied for individual couplets, to perform the equivalence partitioning (taxa clusters) of the input taxa set \( L(G) \).

C. Connectivity between taxa clusters to form DAG

Creation of the taxa clusters is followed by the assignment of directed edges between them. As mentioned in section II, directed edge from a cluster \( C_{i} \) to a cluster \( C_{j} \) corresponds to the relation \( r_{C_{i}C_{j}}^{1} = r_{C_{i}C_{j}}^{2} \) being true. In such a case, the cluster pair \((C_{i}, C_{j})\) is said to be resolved by the relation \( r_{1} \). In general, a pair of clusters can be resolved via one of the relations \( r_{1}, r_{2} \) or \( r_{4} \) (no directed edge in this case). For individual relations \( r_{k} \ (k \in \{1,2,4\}) \), we define its frequency \( F_{k}^{C_{i}C_{j}} \) with respect to the pair of cluster \((C_{i}, C_{j})\), as the following:

\[
F_{k}^{C_{i}C_{j}} = \sum_{\forall p \in C_{i}, \forall q \in C_{j}} F_{pq}^{k}
\]

(9)

Priority of individual relations \( r_{k} \ (k \in \{1,2,4\}) \) for the cluster pair \((C_{i}, C_{j})\) is defined as the following:

\[
F_{k}^{C_{i}C_{j}} = F_{k}^{C_{i}C_{j}} - \sum_{k' \in \{1,2,4\}, k \neq k'} F_{k'}^{C_{i}C_{j}}
\]

(10)

Support score of a relation \( r_{k} \) between the cluster pair \((C_{i}, C_{j})\) is defined as:

\[
V_{k}^{C_{i}C_{j}} = F_{k}^{C_{i}C_{j}} + F_{k}^{C_{i}C_{j}}
\]

(11)

Note that we have used sum, rather than the product, of the priority and frequency measures. This is due to the disparity of signs of frequency (which is always non-negative) and the priority (which can be negative even for a consensus relation) measures. Higher support score of a relation (between a pair of clusters) indicates higher frequency and priority of the corresponding relation.

The set \( Q \) of support scores for different relations between individual cluster pairs is defined as follows:

\[
Q = \{ F_{k}^{C_{i}C_{j}} : C_{i} \neq C_{j}, k \in \{1,2,4\}, F_{k}^{C_{i}C_{j}} > 0 \}
\]

(12)

Individual taxa clusters are now resolved by an iterative algorithm, using the set \( Q \). Each iteration extracts a relation \( r_{k'}^{C_{i}C_{j}} \ (k' \in \{1,2,4\}) \) from \( Q \), provided the following:

\[
V_{k'}^{C_{i}C_{j}} = \max\left( V_{C_{i}C_{j}}, V_{k}^{C_{i}C_{j}} \right)
\]

(13)

Following conditions are checked to see whether the extracted relation \( r_{k'}^{C_{i}C_{j}} \) can resolve the cluster pair \((C_{x}, C_{y})\).

1) If \((C_{x}, C_{y})\) is already resolved with a different relation, \( r_{k'} \) is not applied.

2) If \( k' = 1 \) or \( 2 \), resolving \((C_{x}, C_{y})\) with \( r_{k'} \) would create a directed edge between the cluster pair. If such an edge forms a cycle with the existing configuration of the taxa clusters, \( r_{k'} \) is not applied.

For no such above mentioned conflicts, the relation \( r_{k'} \) is applied between \( C_{x} \) and \( C_{y} \).

The set \( Q \) is implemented as a max-priority queue \([21]\), to achieve \( O(1) \) time complexity for extracting the cluster pair having the maximum support score. Iterations continue until \( Q \) becomes empty. However, the final DAG may still have the problems TPP, MPP, and NPP (as defined in Fig. [2]). The problem TPP is removed by transitive reduction (already described in COSPEDTree \([6]\)). COSPEDTree-II employs a better solution for the problem MPP, which is described in the following section.

D. Solving Multiple Parent Problem (MPP)

As shown in Fig. \([20]\) the problem MPP corresponds to a cluster \( C_{x} \) having \( k \ (k \geq 2) \) other clusters \( C_{1}, C_{2}, \ldots, C_{k} \) as its parent, which are not themselves connected by any directed edges. The objective is to assign a unique parent \( C_{p} \ (1 \leq p \leq k) \) to the cluster \( C_{z} \). Such assignment was arbitrary in COSPEDTree \([6]\). COSPEDTree-II proposes a deterministic selection of \( C_{p} \), by a measure called the internode count \( I_{t_{j}}(p,q) \) between a couplet \((p,q)\), with respect to a rooted tree \( t_{j} \). The measure was introduced in \([22]\) for unrooted trees. Here, the measure is adapted for a rooted tree \( t_{j} \), as the number of internal nodes between \( p \) and \( q \) through the node \( LCA_{t_{j}}^{pq} \).

As individual trees \( t_{j} \) carry overlapping taxa subsets of \( L(G) \), we define a normalized internode count distance between \( p \) and \( q \) in \( t_{j} \) as:

\[
I_{t_{j}}^{N}(p,q) = \frac{I_{t_{j}}(p,q)}{W_{pq}^{t_{j}}}
\]

(14)

where \( W_{pq}^{t_{j}} \) is defined in the Eq. \([7]\). So, \( I_{t_{j}}^{N}(p,q) \) becomes low only when both \( I_{t_{j}}(p,q) \) is low and \( W_{pq}^{t_{j}} \) is high (when the tree \( t_{j} \) carries higher proportion of the taxa subset belonging to \( U_{pq}^{G} \)).

Significance of the internode count distance can be explained by considering a rooted triplet \((r, (p,q))\) (shown in the Newick \([20]\) format), consisting of three taxa \( p \), \( q \) and \( r \). Here, \( I^{N}(p,q) < I^{N}(p,r) = I^{N}(q,r) \). In general, lower internode count means corresponding couplet is evolutionarily closer, compared to the other couplets.

Average internode count of a couplet \((p,q)\), with respect to \( G \), is defined by the following expression:

\[
I_{avg}(p,q) = \frac{1}{|I_{pq}|} \sum_{t_{j} \in I_{pq}} I_{t_{j}}^{N}(p,q)
\]

(15)

The internode count distance between a pair of cluster \( C_{x} \) and \( C_{y} \) is defined by the following equation:

\[
I(C_{x}, C_{y}) = \frac{\sum_{\forall p \in C_{x}, q \in C_{y}} I_{avg}(p,q)}{|C_{x}||C_{y}|}
\]

(16)

where \(|C_{x}|\) denotes the cardinality of the taxa cluster \( C_{x} \).

For the MPP problem, COSPEDTree-II selects the cluster \( C_{p} \ (1 \leq p \leq k) \) as the parent of \( C_{z} \), provided that \( C_{p} \) has the lowest internode count distance to \( C_{z} \):

\[
C_{p} = \arg \min_{1 \leq i \leq k} I(C_{z}, C_{i})
\]

(17)
Such condition is based on the assumption that the cluster pair having lower internode count, is possibly closer in the evolutionary tree, compared to other cluster pairs.

**E. Binary supertree generation**

![Diagram](image)

Fig. 4. (a) Example of a multifurcation, containing the taxa subset $X = A \cup B \cup C \cup D$. (b) an input tree $t_{j|X}$, restricted to the taxa subset $X$. (c) Tree $t'_{j|X}$ created from $t_{j|X}$.

After resolving the problem MPP, the refined DAG is converted to the supertree $T$, by a depth first traversal procedure (as described in COSPEDTree [6]). However, the generated supertree $T$ may not be completely resolved. COSPEDTree-II proposes a refinement strategy which converts $T$ into a strict binary tree.

Suppose, the tree contains an internal multi-furcating node of degree $n > 2$. Let $X_1, X_2, \ldots, X_n$ denote the taxa subsets descendant from it, where each taxa subset $X_i (1 \leq i \leq n)$ consists of one or more taxa named as $X_{i1}, X_{i2}, \ldots$, etc. Union of these taxa subsets is represented by $X = \bigcup_{i=1}^{n} X_i$. Suppose, $t_{j|X}$ represents the input tree $t_j (1 \leq j \leq M)$ restricted to the set of taxa $X$. Thus, $L(t_{j|X}) = L(t_j) \cap X$. Considering Fig. 4(a) as an example, the node $R$ represents a multi-furcation with degree 4. Four taxa subsets $A, B, C$, and D, descend from $R$. Here, $X = A \cup B \cup C \cup D$. Generation of a binary tree requires introducing bifurcations among these taxa subsets. So, for individual input trees $t_j$, corresponding restricted input tree $t_{j|X}$ is produced, as shown in Fig. 4(b).

Our proposed binary refinement first generates a tree $t'_{j|X}$ from the tree $t_{j|X}$, such that the leaves of $t'_{j|X}$ represent individual taxa subsets $X_i (1 \leq i \leq n)$. In other words, individual taxon in $t_{j|X}$ is replaced by the name of its corresponding taxa subset (without any duplicate). For example, both the taxa $A_2$ and $A_3$ (belonging to the taxa subset $A$) are present in the tree $t_{j|X}$ (as shown in Fig. 4(b)). So, in $t'_{j|X}$, a leaf node labeled $A$ is first inserted as a child of the LCA node of $A_2$ and $A_3$. Subsequently, the leaves $A_2$ and $A_3$ are deleted from $t'_{j|X}$. This process is repeated for other taxa subsets $B, C$ and $D$ as well. Fig. 4(c) shows the tree $t'_{j|X}$.

For the current set of taxa $X$, each of the input trees $t_j$ are processed to generate the corresponding $t'_{j|X}$. These trees are then used as input to an existing triplet based supertree approach thTBR [19], to generate a supertree $T_X$ consisting of the taxa subsets $X_i$ as its leaves. The supertree method is selected since it processes rooted triplets, and generates a rooted output tree. The tree $T_X$ is used as a template, such that its order of bifurcation among individual taxa subsets $X_i$ is replicated to the original multi-furcating node $R$ and its descendants. As the degree of multifurcation ($n$ in this case) is much lower than the total number of taxa ($N$), construction of $T_X$ is very fast. This process is continued until all the multi-furcating nodes are resolved.
TABLE IV
RESULTS FOR THPL [27] DATASET (M = 19, N = 558)

| Method          | FP | FN | RF | MAST | Runtime |
|-----------------|----|----|----|------|---------|
| MnlTpr [18]     | 114| 149| 291| 4.93 | 1.1h    |
| MRP PAUP [7]    | 75 | 176| 551| 6.27 | 31m     |
| PhySIC [12]     | 0  | 279| 279| 1.19 | 5.7m    |
| RFS [15]        | 106| 66 | 172| 11.9 | 4.5m    |
| SCM* [13]       | 13 | 128| 141| 4.64 |         |
| Superfine(MBB)* [15] | 85 | 50 | 135| 6.39 | 1m      |
| Superfine(QMC)* [16] | 62 | 43 | 105| 6.5  | 1.5m    |
| thSPR, thTBR [19] | ER | ER | ER | ER    |         |
| Supertriplet II | F  | F  | F  |       |         |
| COSPEDTree     | 88 | 162| 250| 4.21 | 4.5m    |
| COSPEDTree-II  | 96 | 137| 233| 5.74 | 2s+9s+1.2m |
| COSPEDTree-II+B| 166| 114| 180| 8.22 | 2s+9s+1.2m |

TABLE V
RESULTS FOR CETARTIODACTYLA [28] DATASET (M = 201, N = 299)

| Method          | FP | FN | RF | MAST | Runtime |
|-----------------|----|----|----|------|---------|
| MMC [11]        | 1181| 1438| 2619| 83.84 |         |
| MRP PAUP [7]    | 860| 964| 1824| 120.84|         |
| PhySIC [12]     | ER | ER | ER | ER    |         |
| RFS [15]        | ER | ER | ER | ER    |         |
| thSPR, thTBR [19] | 969| 1006| 1975| 118.39| 5.5m    |
| thTBR [19]      | 969| 1006| 1975| 118.09| 4.5m    |
| Supertriplet II | 125| 2178| 2300| 595   |         |
| COSPEDTree     | 510| 1001| 1511| 80.43 | 11.7m   |
| COSPEDTree-II  | 732| 864| 1566| 95.2  | 2s+1s+43s |
| COSPEDTree-II+B| 1240| 667| 1907| 102.18| 2s+1s+43s |

F. Computational complexity of COSPEDTree-II

For M input trees covering a total of N taxa, both COSPEDTree [6] and COSPEDTree-II incurs $O(MN^2)$ time complexity for extracting the couplet based measures from the trees. These methods differ in their subsequent steps. COSPEDTree first resolves individual couples in $O(N^2 \log N)$ time (as shown in [6]), and subsequently partitions the taxa set according to the relation $r_3$, to form a DAG containing $N_C$ ($< N$) nodes (taxa clusters). Formation of a supertree from this DAG involves $O(N^3)$ time complexity [6].

COSPEDTree-II, on the other hand, first forms the taxa clusters in $O(N^2)$ time (processing time for all couplets). Subsequently, support scores for individual relations between each pair of taxa clusters are placed in the max-priority queue $Q$. Here, size of $Q$ is $O(N^2)$, considering $N_C$ as the number of taxa clusters. During each iteration, maintaining the max-priority property of $Q$ requires $O(\log N_C)$ time. So, the complete iterative stage to resolve all pairs of clusters (assigning connectivities between them) involves $O(N_C^2 \log N_C)$ time complexity. As in general, $N_C$ is considerably lower than $N$, this iterative step in COSPEDTree-II is much faster than COSPEDTree.

Resolving individual pair of clusters, rather than the couplets, enables COSPEDTree-II to achieve a significant speedup. Suppose, $|X|$ denotes the cardinality of a taxa cluster $X$. So, for a pair of taxa clusters $X$ and $Y$, COSPEDTree [6] resolves all $|X| \times |Y|$ couplets, and maintains their relations (and the transitive connectivities inferred from these relations). But COSPEDTree-II resolves $X$ and $Y$ by processing only one relation between them. So, for this cluster pair, speedup achieved by COSPEDTree-II is $\approx |X| \times |Y|$. For a total of $N_C$ taxa clusters, number of cluster pairs is $\binom{N_C}{2}$. Thus, overall speedup achieved by COSPEDTree-II is $\approx \sum_{X,Y \in \binom{N_C}{2}} |X| \times |Y|$.

To derive the time complexity associated with the binary refinement of COSPEDTree-II, suppose $m$ is the number of internal nodes in $T$ having degree $\geq 2$. Further, suppose $n$ ($> 2$) denotes the maximum degree of multi-furcation among all of these nodes. In such a case, applying $\text{th}TBR$ [19] for a particular internal node involves maximum $O(Mn^3)$ time complexity. So, overall complexity of the binary refinement stage is $O(Mn^3m)$.

COSPEDTree [6] involves a storage complexity of $O(N^2)$, to store the couplet based measures. COSPEDTree-II uses additional storage space for storing the set of excess taxa $(|U|_a^G)$ for individual couplets ($p,q$). As $0 \leq |U|_a^G \leq (N-2)$, the space complexity of COSPEDTree-II is $O(N^3)$.

IV. EXPERIMENTAL RESULTS

Both COSPEDTree and COSPEDTree-II are implemented in Python (version 2.7). Tree topologies are processed by the phylogenetic library Dendropy [20]. A desktop having Intel® Quad Core i5-3470 CPU, with 3.2 GHz processor and 8 GB RAM, is used to execute these methods.

A. Dataset

COSPEDTree-II is tested with the datasets like Marsupials (267 taxa and 158 input trees) [23], Placental Mammals (726 trees and 116 taxa) [24], Seabirds (121 taxa and 7 trees) [26], Temperate Herbaceous Papilionid Legumes (THPL) (19 trees and 558 taxa) [27]. Work in [16] modified these datasets by removing duplicate taxon names and few infrequent taxa information. We have also experimented with Mammal dataset [12], [4] consisting of 12958 trees and 33 taxa [3]. In addition, the dataset Cetartiodactyla (201 input trees and 299 taxa) [28] is also tested [4].

B. Performance measures

Performance comparison between COSPEDTree-II and the reference approaches, employs the following measures:

1. Datasets are downloaded from the link http://www.cs.utexas.edu/~phylo/software/superfine/submission/.
2. Downloaded from the link http://www.supertriplets.univ-montp2.fr.
3. Maintained in TreeBASE [29], and is downloaded from the link https://treebase.org/treebase-web/search/study/summary.html?id=1271.
1) **False positive distance** $FP(T, t_j)$: Number of internal branches present in the supertree $T$, but not in the input tree $t_j$ ($1 \leq j \leq M$).
2) **False negative distance** $FN(T, t_j)$: Number of internal branches present in $t_j$ but not in $T$.
3) **Robinson-Foulds distance** $RF(T, t_j)$: Defined as $FP(T, t_j) + FN(T, t_j)$.
4) **Maximum agreement subtree** $MAST(T, t_j)$: Let $N_j$ be the number of taxa contained in the maximum agreement subtree (MAST) common to $T$ and $t_j$. Then, $MAST(T, t_j) = \frac{N_j}{|L(t_j)|}$. This measure is computed using Phylonet [30].

Above measures are accumulated for all the input trees $t_j$ ($1 \leq j \leq M$), to be used as the final performance measures. Supertree producing lower values of the sum of FP, FN, and RF values is considered better. On the other hand, supertree having higher sum of MAST score is considered superior.

**C. Performance comparison**

We have reported the results for the following two variations of COSPEDTree-II:

1) **COSPEDTree-II**: Produces supertree with possible multi-furcations.
2) **COSPEDTree-II + B**: Produces completely resolved binary supertrees, by applying the binary refinement suggested in section III-E.

Tables II to VI compare the performances of both of these variants, and with the reference approaches as well. Reference methods marked with a symbol “*”, could not be executed in all datasets, either due to the unavailability of corresponding source code, or due to their very high computational complexity. In such a case, we have used their results (both topological performance and running time) published in the existing studies [16]. The approaches MRP and superfine require PAUP* [31] to execute, which is a commercial tool and not available to us. So, these methods could not be tested in all datasets. Missing entries are indicated by ‘-’.

The methods RFS [15] and Supertriplet [4] produced errors in parsing few of the input datasets. Entries showing ‘ER’ indicate these errors. Supertrees generated by Supertriplet [4] could not be parsed by Phylonet [30]. So, we could not compute the MAST scores for these trees. Finally, a symbol ‘F’ indicates that corresponding method could not produce a valid supertree for that dataset.

Results show that COSPEDTree-II produces better resolved supertrees than COSPEDTree, as indicated by lower FN, and mostly lower RF values for individual datasets. COSPEDTree-II also achieves higher MAST scores for these datasets. COSPEDTree-II+B produces completely resolved binary supertrees. So, the number of FN branches reduces. However, as the input trees may not be fully resolved (may contain multi-furcating nodes), number of FP branches increases considerably. As COSPEDTree-II+B produces completely resolved supertrees, corresponding MAST scores are much higher than COSPEDTree-II.

Comparison with reference approaches shows that only RFS [15] produces supertrees with consistently lower RF and higher MAST scores than COSPEDTree-II. The method Superfine [16] performs better than COSPEDTree-II for the datasets Seabirds and THPL, while our methods perform slightly better (in terms of lower RF and higher MAST score) for the Marsupials and Placental Mammals dataset. Superfine does not always generate strictly binary (completely resolved) supertrees (for example, in the THPL dataset), unlike COSPEDTree-II+B. Such a supertree exhibits much lower RF, but also much lower MAST score (compared to COSPEDTree-II+B).

Matrix based methods like Minflip, SFIT, MMC, are outperformed by COSPEDTree-II. Veto approaches like SCM, PhySIC, produce supertrees with the lowest (mostly zero) FP branches, by not including any conflicting clades. In such a case, the number of FN branches becomes very high, and MAST scores of these trees also become much lower. COSPEDTree-II also produces significantly better results than MRP PAUP for all the datasets except Cetartiodactyla. Subtree decomposition based approaches like thSPR, thTBR, produce slightly higher MAST score values than COSPEDTree-II, since these methods directly synthesize input triplets, or in general, subtree topologies. Considering the measure RF, on the other hand, these methods are mostly outperformed by COSPEDTree-II.

**D. Runtime Comparison**

Tables II to VI express the running time of COSPEDTree-II and COSPEDTree-II+B for different datasets, in the formats $(A+B)$ or $(A+B+C)$, respectively, where:

1) $A =$ Time to extract the couplet based measures from the input trees.
2) $B =$ Time to process the couplets and cluster pairs, to produce a (possibly not binary) supertree.
3) $C =$ Time required to refine the non-resolved supertree into a strict binary tree.

We observe that COSPEDTree-II incurs a significant fraction of its running time in the stages A and C. The stage A depends on the processing speed of the python based phylogenetic library Dendropy [20]. On the other hand, running time for the stage $C$ depends both on the construction of $t'_{j/X}$ from individual $t_j$, for all the multi-furcating nodes, and on the execution of thTBR [19]. Results show that COSPEDTree-II incurs much lower running time than COSPEDTree. Excluding the binary refinement stage, the running time is decreased by a factor from 2 (for the dataset Mammal [12], [4]) to 135 (for the dataset Cetartiodactyla [28]).

When the number of taxa is high (such as Marsupials [23], Cetartiodactyla [28]), COSPEDTree-II exhibits much lower running time than the triplet based methods [19], [4], due to its lower time complexity. For datasets with large number of trees, COSPEDTree-II incurs slightly higher running time than these methods, due to the time associated in extracting the couplet based measures.
V. Conclusion

We have proposed COSPEDTree-II, an improved couplet based supertree construction method (extending our earlier proposed method COSPEDTree). COSPEDTree-II produces supertrees with lower topological errors, and incurs much lower running time (compared to COSPEDTree). A binary refinement to generate a fully resolved supertree, is also suggested. Due to its high performance and much lower running time, COSPEDTree-II can be applied in large scale biological datasets.

EXECUTABLE

Executable and the results of COSPEDTree-II are provided in the link [http://www.facweb.iitkgp.ernet.in/~jay/phtree/cospedtree2/cospedtree2.html](http://www.facweb.iitkgp.ernet.in/~jay/phtree/cospedtree2/cospedtree2.html).

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