A supertree pipeline for summarizing phylogenetic and taxonomic information for millions of species

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ABSTRACT

We present a new supertree method and software implementation that enables rapid estimation of a summary tree on the scale of millions of leaves. This software pipeline is called *"propinquity."* It uses the dependency-tracking tool *make* to direct the series of operations required to construct the tree. It relies heavily on *"otcetera"* - a set of C++ tools to performs most of the steps of the pipeline. All of the components are free software and are available on GitHub. This pipeline is currently used by the Open Tree of Life project to produce all of the versions of project's "synthetic tree" starting at version 5. The propinquity-based pipeline improves on previous supertree construction methods because it produces no unsupported branches, and it avoids unnecessary polytomies. In addition to producing a tree, the pipeline writes an annotations file that reports which grouping in the input trees support each of the groups in the supertree.

1 BACKGROUND

The Open Tree of Life project seeks to build a platform for summarizing what is known about phylogenetic relationships across all of Life (Hinchliff et al., 2015). One primary goal of the project is to build a summary tree from a comprehensive taxonomic tree and a set of published trees. The summary tree is intended to transparently and justifiably represent phylogenetic information from these inputs. The taxonomic tree is derived from the Open Tree Taxonomy (OTT hereafter, publication in preparation). The phylogenetic inputs are published trees that have been curated to align the tips to OTT and to identify the correct rooting (see McTavish et al. 2015 for further details of the curation tools). Unlike OTT, these phylogenetic trees do not include all leaf taxa. The inputs (taxonomy and phylogenetic trees) and the output summary supertree are all rooted. Here we describe the software pipeline (*propinquity*) that summarizes and integrates these smaller source trees and the taxonomy tree into a single supertree and the noteworthy tools for manipulating and solving supertrees in the *otcetera* package.

1.1 Goals

Translating the goals of the Open Tree of Life's summary tree into an explicit set of criteria is not trivial. The summary supertree should represent the phylogenetic information from source trees in a transparent and justifiable fashion. We would like to allow users to correct errors in the supertree by improving the input information rather than requiring modification to the supertree algorithm. The pipeline was designed to create a tree which:

1. displays no unsupported groups,
2. defers to groupings from higher ranked trees in the case of conflict,
3. contains no unnecessary polytomies, and
4. displays as many groupings from input trees as possible.

These goals are described more fully below. In order to accomplish transparency and justification, our pipeline also produces annotations files with information about conflict and support.

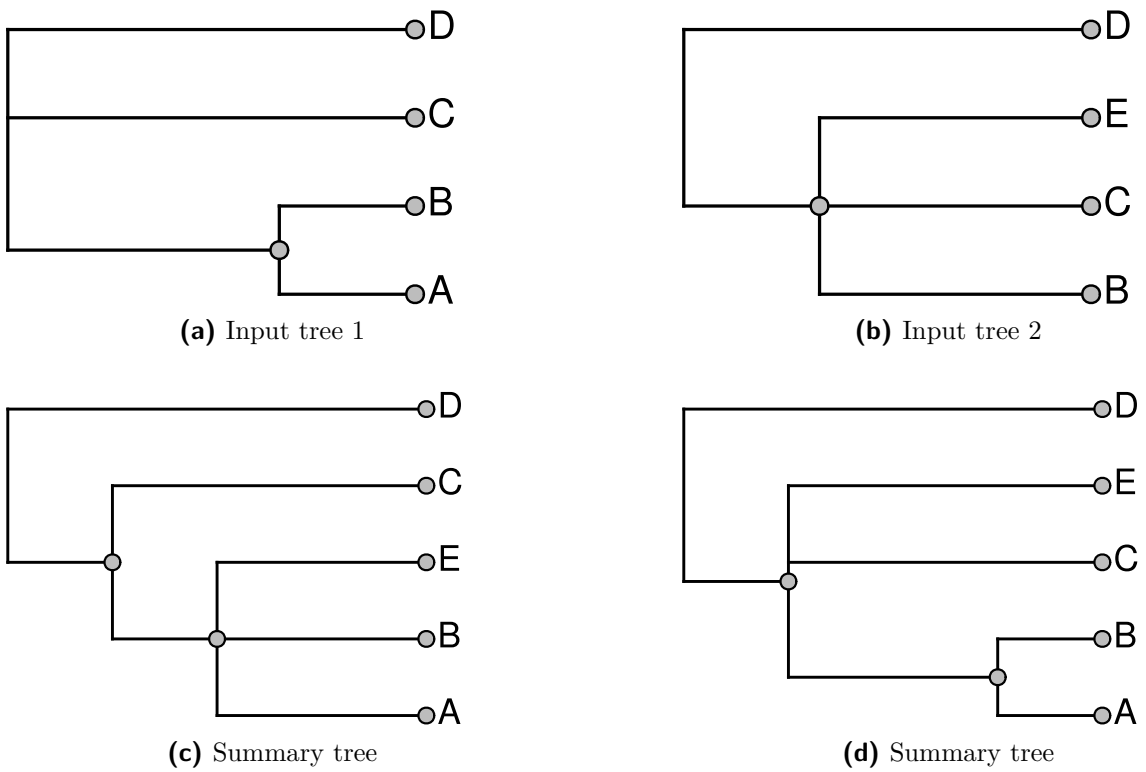
1.1.1 Goal 1: Each grouping is supported by at least one input

We require that each edge in the supertree be supported by at least one input tree edge. In addition to aiding interpretability, this requirement keeps the supertree from arbitrarily representing information that comes from none of the input trees. Of course, in a supertree analysis, the full tree will imply some relationships for subsets of the taxa that are not found in any input tree. So, the meaning of "supported by" needs some clarification.

Notation, terminology, and the definition of "supported by" Let $\mathbb{S}$ denote a supertree, and T_i denote the ith input tree. The set of taxa that are mapped to the tips of the tree T_i is $\mathcal{L}(i)$. $\mathbb{S}(i)$ denotes the summary tree induced by tip nodes that are mapped to taxa in $\mathcal{L}(i)$ and the most recent common ancestor of those leaves, and any other node that is an ancestor of some but not all of these leaves. We say that edge j of the supertree is compatible with an input tree, T_i if edge j either is not included in the induced tree $\mathbb{S}(i)$ or none of the edges in T_i are in conflict with edge j in the induced tree.

We can consider whether or not an node in an input tree is displayed by $\mathbb{S}$. For any such node j there is a set of taxa that are mapped to the tips that descend from the node. This set of taxa is the "cluster" of taxa corresponding to node j; it can be denoted $\mathcal{L}(i,j)$. It will also be referred to as the "include set" of the node. The "exclude set" of j in T_i is the set of taxa in $\mathcal{L}(i)$ but not in $\mathcal{L}(i,j)$. If the cluster of taxa for any supertree node in $\mathbb{S}(i)$ is identical to $\mathcal{L}(i,j)$, then we say that $\mathbb{S}$ displays node j of T_i. We say that the summary tree *displays* edge j if the summary tree displays the child node of edge j. Operationally, we can find the most recent common ancestor (MRCA) node of $\mathcal{L}(i,j)$ in $\mathbb{S}$; the summary tree displays j if and only if that MRCA node is not an ancestor of any member of the exclude set of j. We say that edge k of the summary tree is *supported by* node j in T_i if the summary tree displays node j, but if we contracted edge k then the modified summary tree would no longer display node j.

Note that stating that a node in the summary tree is supported by an input does not imply that every descendant of that node must be present in the input nor that every taxon



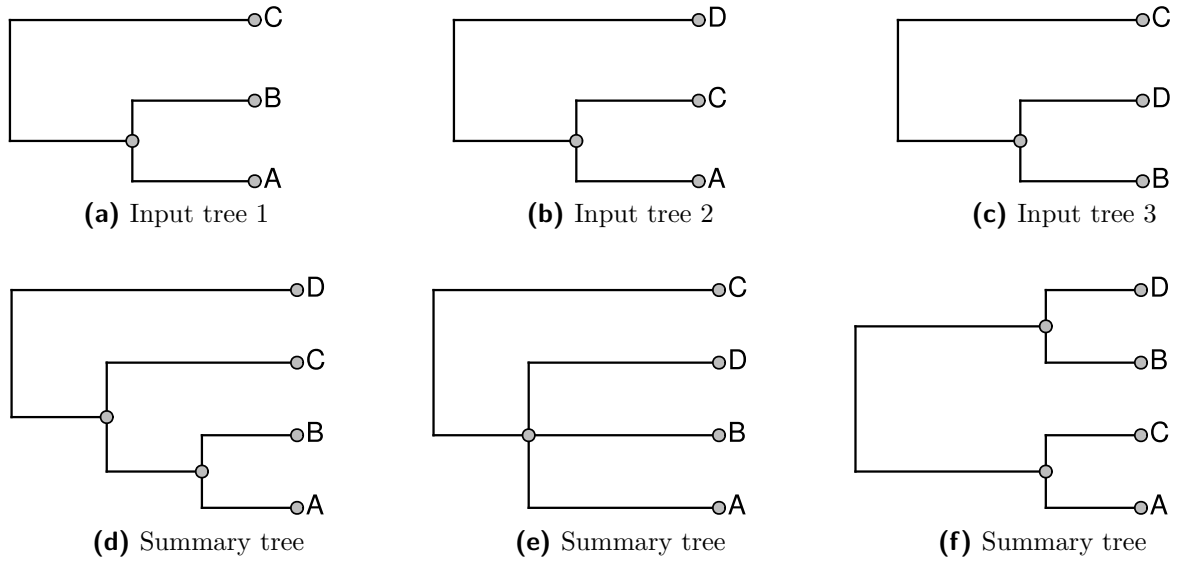
(a) Input tree 1 **(b)** Input tree 2

(c) Summary tree **(d)** Summary tree

Figure 1. An example demonstrating that our definition of "supported by" does not imply entire composition of a grouping. (a) and (b) show 2 input trees and (c) and (d) depict trees that each display each of the groupings in the input trees and which have no unsupported nodes. The BUILD algorithm (section 8) would choose tree (d) that floats taxon E closer to the root.

that is not a descendant must be excluded in order to display the node. Consider the problem shown in figure 1; panels (1a) and (1b) show two input trees. Because taxa A and E do not occur together in either input, there is some uncertainty about where to place them. By our terminology, either output shown in (1c) or (1d) would be characterized as a tree that displays all of the input groupings and which has no unsupported groups. Clearly these criteria are insufficient to specify a unique solution, and users of the output tree need to be aware that it may be possible for some taxa to "float" to multiple positions. In figure 1, taxon E floats to different positions in (1c) and (1d), whereas taxon A does not.

One of our aims in supertree construction is to minimize the amount of information in the supertree that does not come from input trees. We permit information that comes from combinations of input trees, but not any single input tree. However, we seek to exclude information that comes from none of the input trees. This motivates the criterion of not having any unsupported edges, since these edges could be removed without decreasing the support from any input tree.



(a) Input tree 1 **(b)** Input tree 2 **(c)** Input tree 3

(d) Summary tree **(e)** Summary tree **(f)** Summary tree

Figure 2. An example of 3 input trees shown in (a), (b), and (c) which do not conflict in a pairwise manner, but cannot be jointly displayed in one tree. The 3 solution trees are shown in panels (d-f). Panel (d) for ranking the tree in (c) lowest. Panel (e) shows the solution if the tree in (b) has the lowest rank. Panel (f) shows the solution if the tree in (a) is ranked lowest. Each of the solutions displays 2 of the 3 input groupings.

1.1.2 Goal 2: Tree ranking

An appealing goal for the summarization would be to find the supertree that displays the largest number of input tree edges. As discussed in Huson et al. (pages 92 and 131; 2010) the maximum compatibility problem is known to be NP-hard via a reduction to Max-Clique (Karp, 1972). In addition to being computationally daunting, this formulation of the supertree problem does not provide biologists who use the summarization tool with an obvious avenue for fixing perceived problems with the summary tree. For example, a grouping that a biologist expected may not be present in the supertree, but it may not conflict with any of the input groupings which are displayed. This can happen because displaying both node a from T_1 and node b from tree T_2 in a summary tree may only be possible by displaying a grouping that is present in no input tree. All other factors being equal, if this implied grouping conflicts with input node c in tree T_3, then c will not be displayed in the summary tree, but a biologist will not necessarily know how to fix this problem. One solution is to use a ranking of groupings. If an expert were quite confident in the c grouping, then she could assign that input node a high ranking. A supertree that used ranks could then recover this grouping even if its inclusion did not increase the total number of input nodes that are displayed by the summary tree. Figure (2) shows an example of 3 input trees for which there is no pairwise incompatibility, but no solution displays all of the input groups. Alternative rankings of inputs can result in one of three summary trees shown in panels (d-f).

Any approach to supertree construction must deal with the need to adjudicate between conflicting input trees. We choose to deal with conflict by ranking the input trees, and preferring to include edges from higher-ranked trees. The merits of using tree ranking are

questionable because the system does not mediate conflicts based on the relative amount of evidence for each alternative. However, it is a reasonable starting point. It has the benefits of making it easy to see why some groups are included or not (transparency), and it allows simpler and cleaner algorithms.

Note that if some edge c conflicts with a higher-ranked edge b, then c may still be included in the supertree. This can occur when the higher ranked edge b conflicts with a yet-higher ranked edge a, and thus b is not included. In that case, it will be possible for c to be represented in the summary tree. Thus, the fact that the summary tree displays an input edge does not imply that none of the higher ranked input trees conflict with that edge.

In order to produce a comprehensive supertree, we also require a rooted taxonomy tree in addition to the ranked list of rooted input trees. Unlike other input trees, the taxonomy tree is required to contain all taxa, and thus has the maximal leaf set. We make the taxonomy tree the lowest ranked tree. In our current formulation, the taxonomy tree is also unique in that the taxonomy is the only source of taxonomic names. Each node in the taxonomy tree corresponds to a named group. Taxonomic groups may have the same name, but each node in the taxonomy tree is identified by a unique number (its OTT Id). Taxonomic groups are identified in the summary supertree by finding a branch (or "node") that has exactly the same include|exclude relationship. The taxonomy supertree can meaningfully possess degree-two nodes. Although these nodes can be removed without affecting the relationships of the leaves, they do represent nested taxonomic groups that contain exactly one subgroup. The taxonomy is also used to determine which tips are terminal taxa.

1.1.3 Goal 3: Contain no unnecessary polytomies

The supertree should be as resolved as possible - in other words, it should have no unnecessary polytomies. Thus, for each input edge that is *not* included, we can point to a reason for non-inclusion by showing that the input edge conflicts with some edge of the summary tree. Note, that the requirement to not display unsupported groups leads to some "necessary" polytomies. For example any resolution of the polytomy shown in figure (2e) would continue to display the same two input groups, but the additional grouping would be unsupported, because the unresolved tree already displays the two input groups. Thus, the additional group would be unsupported and the unresolved tree would be preferred by our criterion. However, collapsing either internal edge of the tree shown in figure (2d) would result in a tree which displays only one input grouping. This tree would contain an unnecessary polytomy, because the polytomy would permit refinement to the depicted tree which displays more input groupings.

1.1.4 Goal 4: Display as many input nodes as feasible

We also seek to construct a supertree that represents as many input tree nodes as possible. Since non-included input tree nodes must conflict with the supertree (or they would have been added), this criterion is the same as minimizing the number of input nodes that conflict with the supertree.

1.1.5 Summary of goals

These optimality criteria help to define what it means for the supertree to represent the input trees, as well as justifying and explaining why various features of the supertree exist. The pipeline described below produces a supertree that satisfies the first three optimality

criteria and is a greedy approximation of a solution to the fourth goal. It is not guaranteed to display as many input nodes as possible. Even if the summary tree does accomplish goal 4, it is not necessarily a *unique* optimum. The pipeline takes a greedy approach to producing a summary tree by attempting to add groupings from the trees in order of the trees ranking. This can be viewed as a greedy solution to the problem of finding the tree with the maximum sum of displayed groups' weighted scores criterion (described in the appendix A) where the weights from the trees are so extreme that displaying one group from a highly ranked tree is preferred to displaying all of the groupings from lower ranked trees.

2 DESCRIPTION OF THE PROPINQUITY PIPELINE

2.1 Preprocessing steps

Propinquity was designed to function as a part of the Open Tree of Life software architecture, so the first few steps of the pipeline involve transforming artifacts from that project into a set of rooted trees and a phylogenetic taxonomy. The phylesystem API (McTavish et al., 2015) of Open Tree allows users to curate published estimates of trees and create ranked collections of these trees. Early steps in the propinquity pipeline manipulate the phylogenetic input trees to improve their usability and reliability. The first steps of the pipeline (see Figure 3) collect a list of trees to include (in the `phylo_input` subdirectory) and store copies of these files (in the `phylo_snapshot` subdirectory) to make it easier to replicate the operation (because the collection of trees and the tree files change due to curation).

2.1.1 Pruning questionable taxa from the taxonomy

OTT is a hierarchy of taxonomic names that implies a phylogenetic taxonomy. An OTT ID has a position in the hierarchy, a taxonomic name, and set of references to the same name in different taxonomies. In addition, the ID may also be associated with a set of flags that can indicate that the taxon may be questionable. These flags can either encode information taken from an input taxonomy (for example, taxa the NCBI refers to as "unplaced" are assigned an "unplaced" flag) or can arise because of some form of conflict during taxonomy construction (for example, if two taxonomies disagree on the name for a taxon, then the taxon can be merged and the name will be retained without any descendants; this name will have an OTT Id, but will be flagged as "barren"). Propinquity prunes the OTT down to a more reliable taxonomy by pruning off parts of the tree that are flagged with suspicious flags. The set of flags that lead to a subtree of the taxonomy being pruned is under the control of the user (the set of flags used by the Open Tree of Life project can be found in the `config.opentree.synth` file in the propinquity repository). For the purpose of the rest of the pipeline, an OTT Id that has been pruned from the taxonomy will be treated in the same way as invalid OTT Id. The output of this step is stored in propinquity's `cleaned_ott` subdirectory; this operation only needs to be performed when the OTT or the pruning flags change.

2.1.2 Pruning problematically mapped tips from input phylogenetic trees

Frequently, phylogenetic estimates are rooted using the outgroup criterion, which is an assumption about the monophyly of the ingroup taxa. Because the rooting of the branches in the outgroup portion of the tree is often uncertain, data curators can identify the ingroup node of the tree; propinquity uses this annotation to prune off the outgroup taxa.

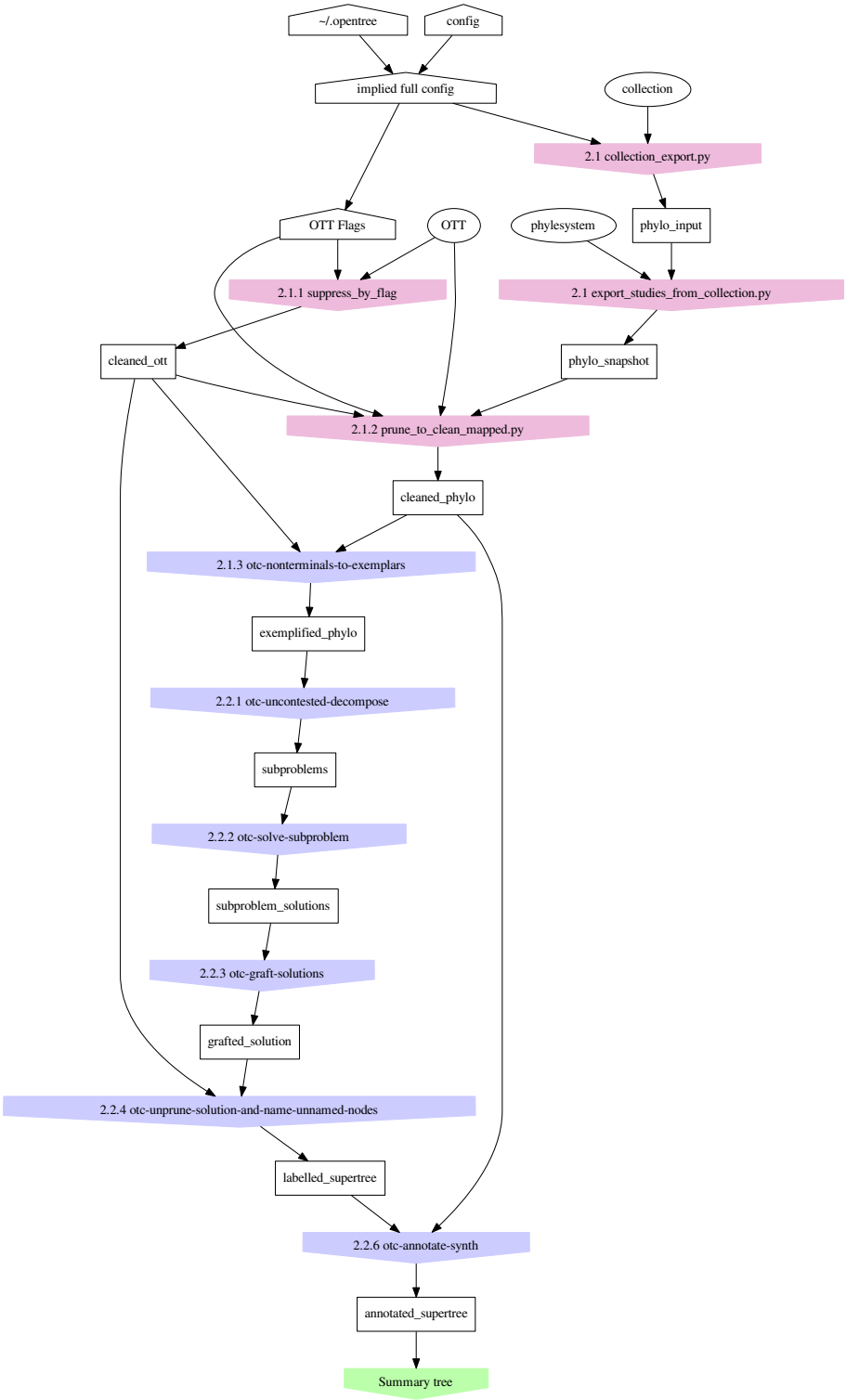


Figure 3. Organization of the *propinquity* pipeline. Each colored pentagon labels a program (blue for otcetera-based tools and red for python scripts in the propinquity or peyotl repository) that performs the important operations in each step; the number before the tool name refers to the section in this paper that describes the operation. The output of each step corresponds to a subdirectory of the propinquity system which will hold the output artifacts for the step. Ovals are resources that are required (OTT and Open Tree's phylesystem repository). White pentagons are user-controlled inputs.

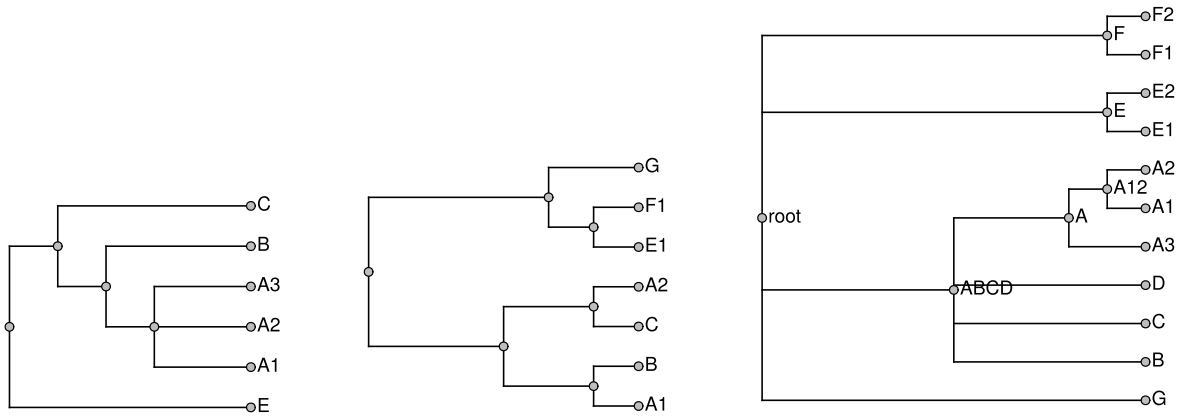
Frequently, not all tips in a phylogenetic input will have been mapped to a taxon in the current version OTT. Unmapped leaves are pruned from each phylogenetic input. In some cases, the OTT has changed and a taxon has been unambiguously mapped to another taxon. This can occur when multiple species in one version of the taxonomy are "lumped" into a single taxon in a subsequent version. OTT maintains a set of "forwarding" statements about IDs that have been removed but can be mapped to an existing taxon; propinquity uses these statements to update the OTU mapping of input trees.

Finally some leaves are mapped to taxa that occur more than once in the tree, or taxa that have ancestors represented as tips of the tree. In these cases, leaves are pruned to assure that tips are mapped to unique taxa that are not nested. In the case of nested taxa, the tip mapped to the higher level taxon is pruned, and one of the lower level tips is retained. In the case of duplicate occurrences of an OTT taxon, propinquity checks to see if a data curator has selected one of the taxa to be the exemplar for the taxon. If this selection has not been made, then the node with the lexicographically lowest ID is chosen to exemplify the taxon. This choice is arbitrary, but repeatable. The pruned phylogenetic inputs are stored in a `cleaned_phylo` subdirectory of propinquity.

2.1.3 Exemplifying tips mapped to higher taxa

Many input trees have tips that are not terminal taxa, but higher-order taxonomic groups. It is not clear how to interpret a tip in a phylogenetic estimate that is labeled with the name of a higher taxon. Several scenarios can lead to these cases: the data for the tip could have been created by merging a chimeric set of character scores from constituent taxa; the species sampled may not have been identified to the lowest taxonomic rank; or the researcher may simply have used a higher taxonomic name because he/she assumed that the taxon is monophyletic and the higher level name would be more recognizable. Rather than allowing the ambiguity about interpretation of the higher-taxon mapped tips to propagate throughout the entire pipeline, we transform the input trees by replacing higher taxa at tips with a set of terminal-taxon exemplars for each taxon. One approach would be to simply determine all descendant terminal taxa and attach them as children of the problematic tip. However, this would create a clade rather than a tip; subsequent steps in the supertree would interpret the clade as a claim of monophyly for the taxon. The input tree may not have tested monophyly of the clade, so this interpretation is unwarranted. We avoid it by attaching exemplar taxa as child nodes of the higher taxonomic tip but then collapsing the edge between the node that connected the higher taxon to its parent. Thus, if A is a non-terminal taxon containing terminal descendants a_1 and a_2 and B is a non-terminal taxon containing terminal descendants b_1 and b_2 we would replace the subtree $((A, B), c)$ with $((a_1, a_2, b_1, b_2), c)$ instead of the subtree $(((a_1, a_2)A, (b_1, b_2)B), c)$.

If a taxon is only present in the taxonomy (not in any of the input trees), then it can be pruned from the taxonomy for the construction of the supertree and then grafted back on to the summary tree later. Performing this pruning reduces the size of the supertree problem, reducing the running time of the pipeline. Similarly, when we expand a higher taxon in the exemplification step, we can omit members of the taxon if they do not occur in any of the phylogenetic inputs. If there are no members of the higher taxon sampled in any other input tree, then we arbitrarily choose one terminal taxon to represent the higher taxon. During the exemplification step, a tool from otcetera (`otc-nonterminals-to-exemplars`) reads the



(a) Tree 1 **(b)** Tree 2 **(c)** Taxonomy Tree

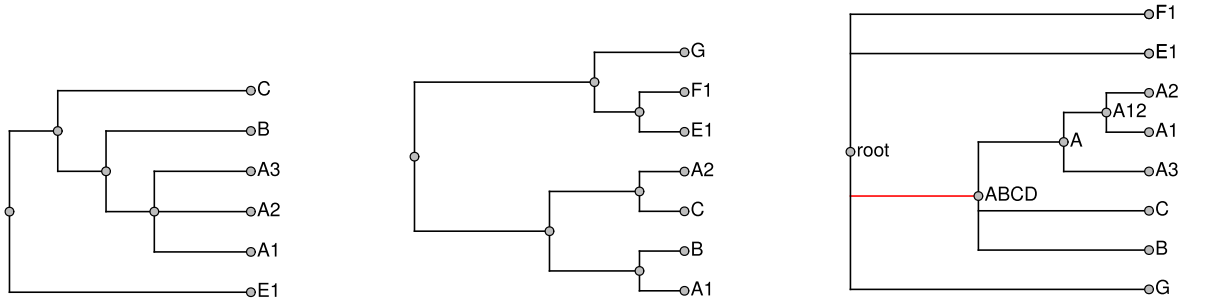
Figure 4. Input trees and taxonomy tree

taxonomy and all of the "cleaned" phylogenetic estimates from the previous step. Reading all of the inputs is necessary to assure that each higher taxon is replaced with the same set of exemplars regardless of which tree the higher taxon occurs in, and that the exemplars for a higher taxon is the union on the set of descendant terminal taxa that have been sampled in a phylogenetic input. Figure 5 shows an example of how the trees in figure 4 would be exemplified.

We prune the taxonomy by removing tips that are not present in any input tree to produce the pruned taxonomy $\mathbb{T}_p$. The tips pruned in this step will be grafted back onto the skeleton of the summary tree in a subsequent step. A terminal taxon that is represented only in the taxonomy can be pruned and then regrafted onto the solution without affecting which nodes are displayed by the final summary tree. Thus, this procedure does not impede our ability to find a good summary tree. Removing these tips produces a smaller input to the rest of the pipeline, which reduces running times. After producing the set of "exemplified" phylogenetic inputs, this tool exports a pruned down version of the taxonomy that only contains tips that are present in at least one phylogenetic input. In version 5.0 of the Open Tree of Life synthetic tree, this version of the taxonomic tree contained only 41,226 leaves (while the flag-cleaned version of OTT had 2,424,255 leaves).

2.2 Summary tree construction

After the preprocessing steps, the inputs have been converted to a set of rooted phylogenetic estimates in which each leaf is mapped to a terminal taxon in the exemplified taxonomic tree. The goal of the remainder of the pipeline is to construct a tree that maximizes the sum displayed groups' weighted scores criterion. This is accomplished in four steps: (1) dividing the full problem into subproblems based on uncontested taxa, (2) constructing a summary solution for each subproblem by greedily creating a maximally-sized list of groupings that can all be displayed simultaneously; (3) grafting the subproblem solutions into a single supertree; and (4) grafting (or "unpruning") the taxonomy-only taxa onto the solution to produce a complete summary tree.



(a) Tree 1 **(b)** Tree 2 **(c)** Pruned taxonomy tree $\mathbb{T}_P$

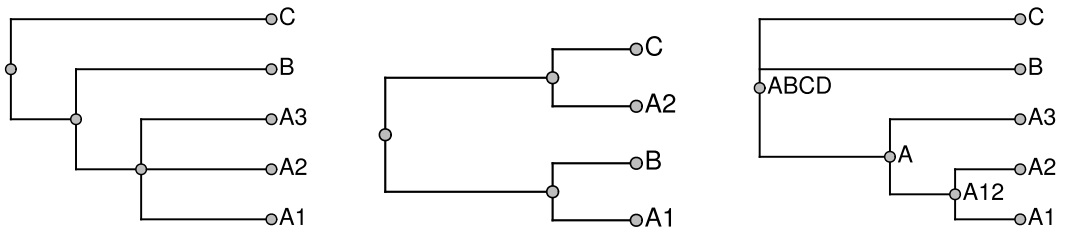
Figure 5. Exemplified input trees and taxonomy tree from figure 4. E in tree1 is exemplified by E1. Pruned taxa are E2, F2, and D. The taxa E and F are retained as monotypic taxa in the pruned taxonomy $\mathbb{T}_P$, but are not shown in panel c. The red edge in the pruned taxonomy tree is an uncontested higher taxon in the exemplified taxonomy (as explained in section 2.2.1)

2.2.1 Subproblem decomposition

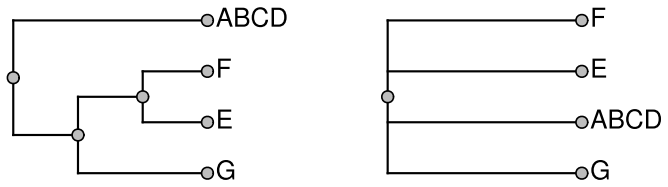
For the sake of efficiency, propinquity uses a divide-and-conquer approach to construct the supertree. Subproblems are identified by searching through the taxonomy tree to find any taxa are not contested by any single input tree. Here we say that input tree T_i contests taxon x in the pruned taxonomy, if x is not monophyletic in any resolution of tree T_i. Thus, polytomies in an input tree are treated as soft polytomies, and a taxon is not contested merely because it is not displayed by an input tree.

This operation is performed by the `otc-uncontested-decompose` tool in otcetera; see appendix B for a description of the algorithm. The output is a series of subproblems, each of which corresponds to a slice of the taxonomy and corresponding slices through each relevant input tree. Each uncontested non-terminal and non-root taxon will show up in two subproblems: it will be the root of its own subproblem and it will be tip in the subproblem that covers the next slice deeper in the tree. The red edge in figure 5c highlights the taxa that are not contested by the input shown in 5; figure 6 shows the subproblems that would be emitted as a result of this set of inputs. The supertree operation of Hinchliff et al. (2015) also used this otcetera-based decomposition step.

Note that decomposition into uncontested groups does not necessarily allow us to find the tree that maximizes the MSDGWS score. For example, see figure 7; that example is a variant of the situation shown in figure 2. In this case the groupings from each of the phylogenetic estimates, shown in panels 7a and (7b, could be displayed. That solution is shown in panel 7d, it displays two of the three input splits, but is optimal because no solution displays all three input groupings and the depicted solution displays the two highest ranked groupings. However, neither of the trees shown in panels 7a or 7b contest the taxon B shown in the taxonomy panel 7c. Thus, when using our decomposition, the branches leading to taxa $B1$ and $B2$ in the input phylogenetic trees would be sliced during the decomposition, and relabeled to refer to taxon B. This taxonomically-informed interpretation of the inputs views the two phylogenetic inputs as in conflict; so the solution returned by propinquity would defer to the higher ranked tree. The tree shown in panel 7e would be returned. This example



(a) Subproblem *ABCD*



(b) Subproblem *root*

Figure 6. Subproblems generated from the exemplified trees shown in figure 5. A trivial statemen from the first tree that a taxon labelled $ABCD$ is sister to E has been omitted, because trees with only 2 leaves do not contain phylogenetic information.

arises from the fact that the trees in 7a and 7b jointly contest taxon B, but neither contests taxon B when the trees are considered in isolation.

Despite the fact that the use of `otc-uncontested-decompose` can worsen the final score of the summary tree, we use this approach in propinquity because it makes the construction of the tree faster and it is easy for users to correct issues caused by incorrect taxa being constrained to be monophyletic. By adding a tree (even a low-ranked tree) that contests a taxon to the corpus of input trees , then the next synthetic tree will no longer consider the taxon to be uncontested. Thus the procedure encourages curation of more phylogenetic inputs as a means of improving the summary tree.

In version 5.0 of the summary tree, this decomposition procedure produced 5,545 subproblems, but only 1,586 of these were non-trivial to solve. If a subproblem contains only two tips it is trivial; 2,443 subproblems were trivial in this way. Similarly, if a subproblem contains only 2 trees it is trivial to solve because the solution will simply be all of the groupings from the first tree combined with all of the groupings from the second tree that are compatible with the first tree; 2,838 subproblems were trivial in this way. The subproblem with the largest number of tips contained 953 tips. The largest subproblem, in terms of the number of input trees (including the taxonomic tree) that were relevant, had 18 trees. Without decomposition, the supertree problem would have had 512 input trees and 41,226 leaves.

2.2.2 Subproblem solution

When solving sub-problems, we sequentially incorporate splits from trees in order of ranking, retaining splits that are compatible with the current set of splits (Alg 1). The order of splits from the same tree is not specified by this approach, and we incorporate splits using one of the possible post-order traversals of the tree. We make use of the BUILD algorithm (Aho et al., 1981) to assess compatibility. This strategy avoids unnecessary polytomies,

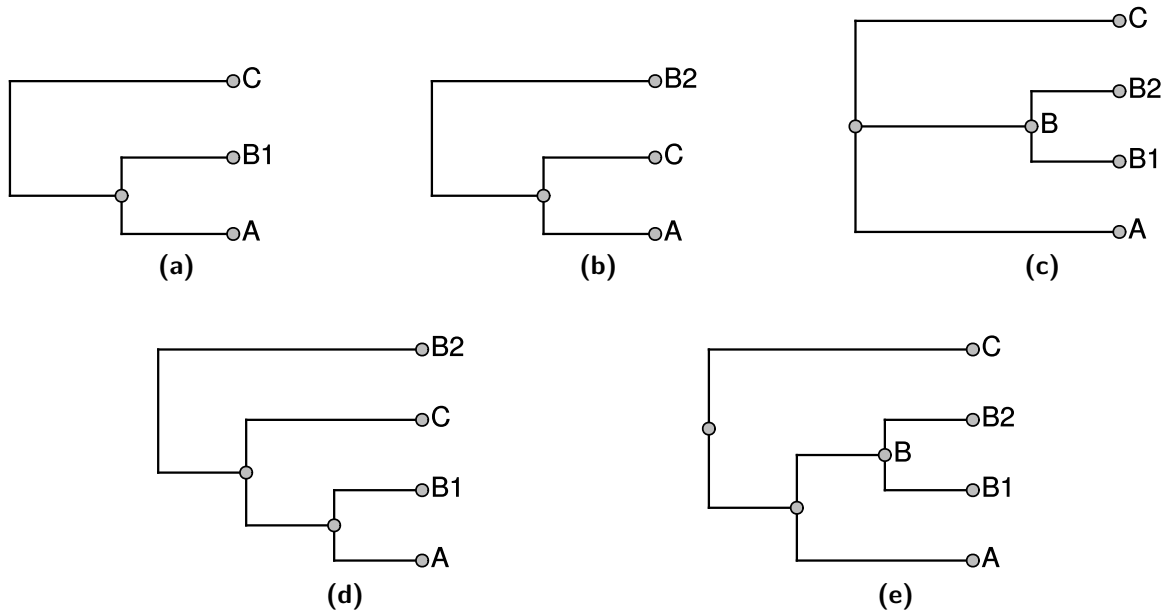


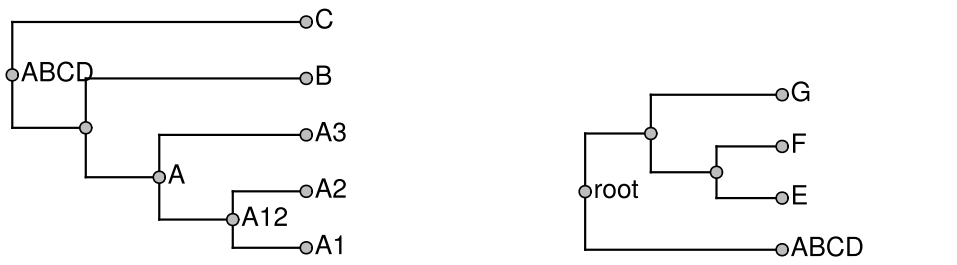
Figure 7. An example with three input trees: the highest ranked phylogenetic input panel (a), the second ranked phylogenetic input (b), and the taxonomy in panel (c). The summary tree in panel (d) has the highest possible score, but the summary shown in panel (e) would be returned from the pipeline that uses uncontested taxon decomposition.

since splits of later input trees are only rejected from the summary supertree if they conflict with higher-priority splits. Finally, we use the BUILD algorithm to construct a supertree displaying all of the splits in the set of compatible splits. Using the BUILD algorithm to construct the subproblem summary tree satisfies criterion 3, because trees from the BUILD algorithm do not contain unsupported branches.

Algorithm 1 ConsistentSplitsFromRankedList

Require: An ordered list of M splits, $\mathcal{R} = [R_1, R_2, R_3, \ldots, R3, \ldots, R_M]$
  $\mathcal{C} = [R_1]$
  for each split i in $[2, 3 \ldots M]$ **do**
    $\mathcal{T} \leftarrow \mathcal{C} + R_i$ ▷ where '+' means concatenating 2 lists
    if BUILD($\mathcal{T}$) does not return null **then**
      $\mathcal{C} \leftarrow \mathcal{T}$
    end if
  end for
  return $\mathcal{C}$

The BUILD algorithm as originally stated by Aho et al. (1981) applies to a collection of rooted triplets. Instead of decomposing each input split into a collection of rooted triplets, we instead modify the BUILD algorithm to apply directly to larger rooted splits. The modified BUILD algorithm constructs a tree compatible with a collection of rooted splits, and returns failure if such a tree does not exist. This modified algorithm recovers the original BUILD



(a) Solution to subproblem *ABCD* **(b)** Solution to subproblem *root*

Figure 8. Solutions to the subproblems depicted in figure 6

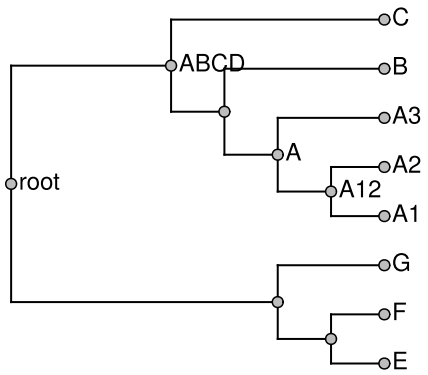


Figure 9. Grafted solution. The nodes E and F are monotypic here, but will end up being polytypic after unpruning is performed.

algorithm if only rooted triplets are supplied as input. When larger splits are supplied as input, the results are the same as if each was was decomposed into all implied triplets. The modified build algorithm has order $O(N^2 + N^2E + NL)$ where N is the number of splits passed in, E is the average size of the exclude group, and L is the total number of leaves. This simplifies to $O(N^2)$ if all splits are triplets. In this approach splits are either entirely retained or entirely discarded - consistent rooted triplets from conflicting splits are not retained. However, when unpruning taxonomy-only taxa (see below), we make an attempt to break ties in a way that preserves some partial information from conflicting splits by attaching taxa from conflicting splits at their common ancestor. Figure 8 shows the solutions that would be obtained by applying our modified version of the BUILD algorithm to the subproblems show in figure 6.

2.2.3 Solution grafting

To produce a tree that spans all of the taxa sampled in the exemplified set of input trees, we graft the subproblem solutions into a single tree (stored as the `grafted_solution/grafted_solution.tre` by propinquity). Recall that each non-root uncontested taxon used for decomposition occurs as a leaf taxon in one subproblem and as a root taxon in one other subproblem. Thus, the grafting operation simply consists of reading all of the subproblem solutions into memory and then merging the nodes that are labeled with the same OTT ID.

2.2.4 Unpruning unsampled taxa

As described above, taxa that do not have any descendants in a sampled phylogenetic input are pruned from the taxonomy for the sake of efficiency. These taxa are reattached by an "unpruning step." For those taxa that are compatible with the grafted tree, this step simply amounts to adding any unsampled taxonomic children to the node that represents the taxon in the grafted solution tree.

However, a taxon may be incompatible with the grafted solution; we refer to such taxa as "broken taxa." If a broken taxon contains some unsampled children, it is not clear where these unsampled children should be attached to the grafted solution. One approach would be to mimic the application of apply Algorithm 1 to the full (unpruned) taxonomic tree. This would be equivalent to collapsing each edge in the taxonomy that attaches a broken taxon to its parent. The unsampled children of broken taxa would attach at their least inclusive ancestral taxon which is unbroken. In cases of several adjacent taxa are broken, this can lead to polytomies of very high degree deep in the tree. This can make the summary tree difficult to navigate. Thus, we have adopted an alternative solution. The `otc-unprune-solution-and-name-unnamed-nodes` tool from otcetera attaches the unsampled children of a broken taxa to the grafted solution as children of the MRCA of the sampled children.

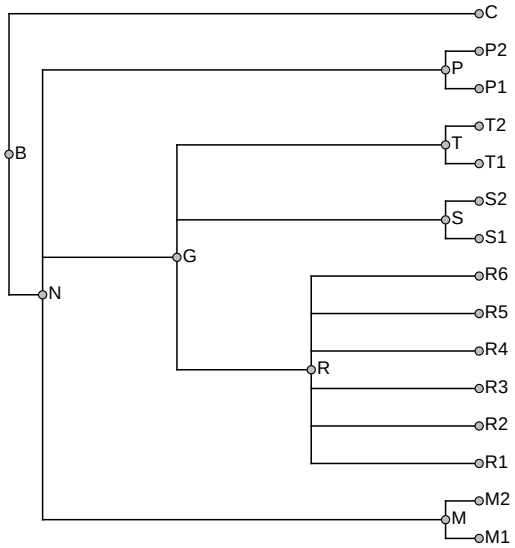
Figure 10 illustrates the two approaches to unpruning. Taxa G, M, and R (Fig 10a) are broken because they conflict with the grafted solution (Fig 10b); among these, only taxon R has children that were unsampled in the grafted solution. Ignoring all broken taxa when unpruning would cause the unsampled children (R4, R5, and R6) to attached directly at taxon N (as in the tree shown in Fig 10c), because that is the least inclusive unbroken ancestor of R. The tree illustrated in Fig 10d shows the tree that would be produced by propinquity; the children of the broken taxon R and instead attached at the MRCA of sampled children (R1, R2, and R3). Their attachment point does not correspond to a taxon in the taxonomic tree.

2.2.5 Naming unnamed nodes

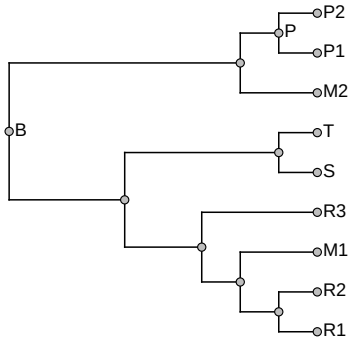
In order to annotate each node in the summary supertree, it is first necessary that each node have a unique identifier. Nodes whose include group correspond exactly to the include group of a node in the taxonomy are given the same identifier as the corresponding taxonomy node. These identifier are of the form $ottX$ where X is an integer OTT id. We generate a label of the form $mrcaottX_1ottX_2$ for an non-taxonomic node n where X_1 and X_2 are the OTT ids for two leaves, n is the MRCA of these leaves, and X_1 is the numerically smallest OTT ID that is a descendant of n, and X_2 is the next the smallest ID that can be chosen to designate n as the MRCA. Because new taxa added to OTT will be given higher OTT Ids, the use of the lowest numbered OTT Ids as designators increases the chance that a node label can be encountered in a subsequent version of the tree (though the taxonomic content may change). The deterministic choice of designators also makes the labeling insensitive to branch rotation of the grafted solution tree.

2.2.6 Annotation

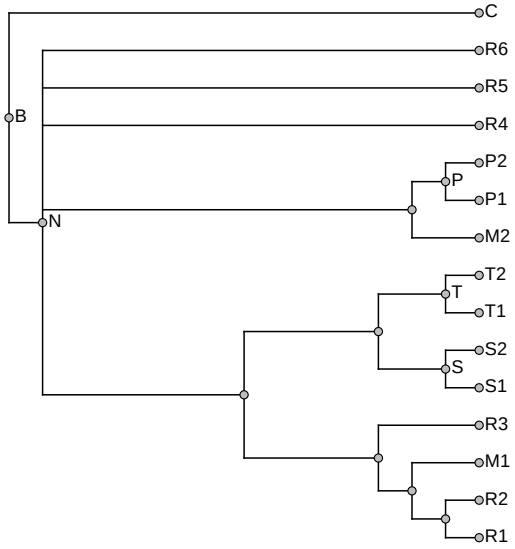
To reveal the connections between the groupings found in the a summary supertree and the input trees, propinquity uses a few Python scripts and the `otc-annotate-synth` tool from otcetera to create an annotations file describing the pipeline used and the connections



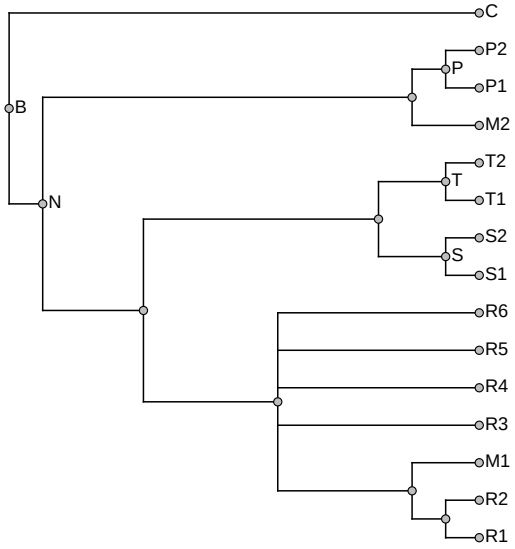
(a) Taxonomy



(b) Grafted solution



(c) Unpruned tree - broken taxa removed



(d) Unpruned tree with MRCA-attachment

Figure 10. Two approaches to unpruning. Taxa G and R in the taxonomy (a) are broken because they conflict with the grafted solution (b). Removing these broken taxa from the taxonomy before unpruning leads to taxa R4, R5, and R6 being attached directly at taxon N, as in tree (c). In tree (d), the children of the broken taxon R and instead attached at the MRCA of R1, R2, and R3.

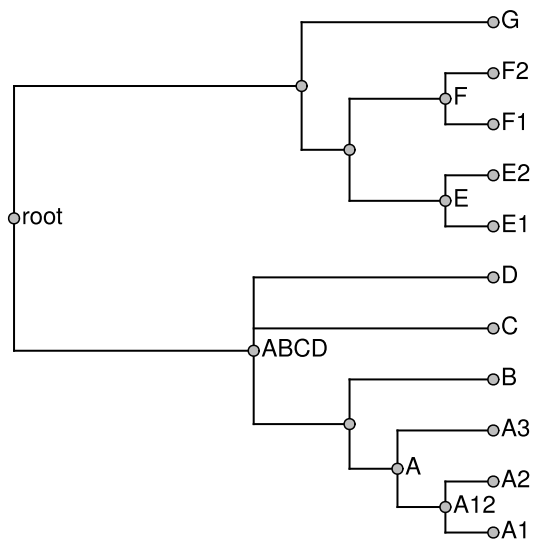
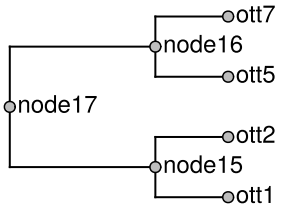


Figure 11. Unpruned tree with internal taxa. Nodes E2, F2, and D have been re-added to the tree. The nodes E and F are no longer monotypic.

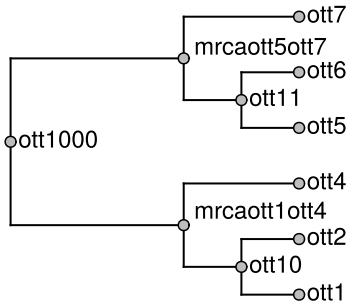
between phylogenetic information in the inputs and the summary. The JSON file produced by `otc-annotate-synth` encodes a "nodes" property that holds a mapping between a node name for the summary tree (using the naming convention described in the previous section) and a node provenance object categorizes the relationship between the node and the inputs. The node provenance object for node x uses several properties to categorize the relationship between the node and the inputs; each property in the node provenance object maps to a structure storing the tree ID and node IDs for the input tree nodes.

Conceptually, this annotation operation in equivalent to considering every node j in each input tree i and the summary tree node x. Because the vast majority of nodes in the input studies will be compatible but not directly relevant to node x we do not list all of the compatible groupings. If node x is not included in the induced tree $\mathbb{S}(i)$, then none of the nodes of tree i will be referred to in the annotations for node x. Even if x is included in $\mathbb{S}(i)$, many of the nodes of T_i will be compatible with x while being relevant to other parts of the summary tree. The only input nodes listed for node x are with rooted taxon bipartitions which conflict with, are displayed by, or are resolved by the the rooted taxonomic bipartition associated with node x. All input nodes that cannot be displayed by any supertree that contains x are stored in a "conflicts_with" property of the node provenance object. If node j of T_i is displayed by the summary tree and x is part of the path of $\mathbb{S}(i)$ that displays the split between descendants of j and other taxa, then a reference to the node j will be in the node provenance object. The exact categorization of this annotation will depend on the configuration of node x on the induced tree $\mathbb{S}(i)$:

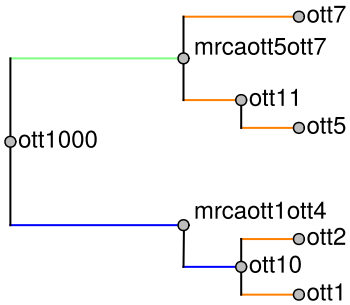
- if x is a terminal path in the induced tree then node j will be listed in the "terminal" property;
- if x is along an internal path that contains some nodes with out-degree equal to 1, then node j will be listed in the "partial_path_of" property; and



(a) Input tree T_1 named "tree1"



(b) Summary Tree $\mathbb{S}$



(c) Induced Tree $\mathbb{S}(1)$

```
{
  "nodes":  {
    "mrcaott1ott4":  { "partial_path_of":  { "tree1":  "node15", ...  } },
    "ott10":         { "partial_path_of":  { "tree1":  "node15", ...  } },
    "mrcaott5ott7":  { "supported_by":     { "tree1":  "node16", ...  } },
    "ott1":          { "terminal":         { "tree1":  "ott1", ...    } },
    "ott2":          { "terminal":         { "tree1":  "ott2", ...    } },
    "ott5":          { "terminal":         { "tree1":  "ott5", ...    } },
    "ott11":         { "terminal":         { "tree1":  "ott5", ...    } },
    "ott7":          { "terminal":         { "tree1":  "ott7", ...    } }
  },
  ...
}
```

(d) JSON annotations relating edges of (c) to edges of (a)

Figure 12. The relationship of edges in summary tree $\mathbb{S}$ (b) to edges in the input tree T_1 (a). Only edges of $\mathbb{S}$ that are present in the induced tree $\mathbb{S}(1)$ are represented by JSON annotations (d). Taxon names are here suppressed in favor of OTT ids, and edges are referenced via their tipward nodes. Edges in $\mathbb{S}(1)$ that correspond to terminal edges of T_1 are orange; edges of $\mathbb{S}(1)$ that are supported by edges of T_1 are blue; where multiple edges of $\mathbb{S}(1)$ correspond to the same edge of T_1 they are green. There is no conflict in this example. Also, if this were output from propinquity, then each internal node of $\mathbb{S}$ would be supported by other inputs trees that are not shown here.

- if x is along an internal path without any node of out-degree 1, then node j will be listed in the "supported_by" property, because node j supports the existence of grouping x in the sense that collapsing the edge that separates x from its parent would cause the summary tree to no longer display node j.

These three relationships are illustrated in Figure 12. Finally, if T_i does not display x from $\mathbb{S}(i)$, but there exists an unresolved node j in T_i which could be resolved such that the tree would then display x, then a reference to node j will be listed in the "resolves" property of node x.

The otcetera annotation tool can also detect cases in which including information from node j in T_i could further resolve a polytomy x in the summary tree; such a case would be annotated using the "resolved_by" property of x. However, because of our goal of excluding unnecessary polytomies, none of the nodes in propinquity's summary tree will use this annotation when they are annotated with the set of input trees.

2.2.7 Self-documentation

An optional step in the propinquity pipeline (triggered by the executing the "make html" target) can compose an "index.html" file for each directory created during the pipeline to explain the artifacts held in that directory and report summary statistics about the summarization run.

3 CONCLUSIONS

Here we have described the motivation and methodology used by the propinquity tool that is currently used by the Open Tree of Life project to build its summary tree. A modified version of the treemachine software which built the summary tree described in the Hinchliff et al. (2015) paper is used by the project to serve the tree produced by propinquity via Open Tree of Life APIs. The migration of summary tree construction from treemachine (used for version 4) to propinquity (for all versions from v5.0 to present) has decreased the computational time required to construct a supertree from several hours to about 8 minutes (after some preprocessing steps which only have to be performed when the input taxonomy changes). The amount of RAM required during tree construction has also decreased substantially. We ran propinquity on the same input trees used to construct version Open Tree version 4. Unlike the version 4 tree, the tree from propinquity contained no unsupported nodes or unnecessary polytomies. The number of displayed input splits increased from 35,518 (for version 4) to 39,639; an 11.2% increase. The number of input splits that do not conflict with the summary tree, but are not incorporated dropped from 2718 to 0. The number of input splits that conflict with the phylogeny dropped from 2760 to 1357, a decrease of 1357, or 49.2%.

4 ACKNOWLEDGEMENTS

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A THE MAXIMUM SUM DISPLAYED GROUPS' WEIGHTED SCORES CRITERION

Let $\mathcal{W}$ is a weighting function that maps any input tree's internal node to a non-negative number. If $I(\mathbb{S}, i, j)$ is an indicator function that is 1 if summary tree $\mathbb{S}$ displays the node $V(i, j)$ and 0 otherwise then: $SDGWS(\mathbb{S}) = \sum_i \sum_j I(\mathbb{S}, i, j)\mathcal{W}(i, j)$ is the "sum of displayed groups' weighted scores" for a tree where i indexes all of the input trees and j indexes each non-root internal node in tree i. Preference for this tree is referred to as the maximum sum displayed groups' weighted scores criterion (MSDGWS criterion). The summary tree constructed by the propinquity pipeline is a greedy heuristic for finding a tree that maximizes this score when the weights for a node are determined by the tree's weight and the difference in weighting is so large that displaying one node from a highly ranked tree is preferred to displaying all of the nodes in the trees with lower rank.

B DESCRIPTION OF THE DECOMPOSITION ALGORITHM OF OTC-UNCONTESTED-DECOMPOSE

The input is the a ranked list of input trees and comprehensive taxonomy.

B.1 Creation of multigraph of the taxonomy with embedded trees

The tool creates a multigraph by starting with a graph is isomorphic to the taxonomic tree. The nodes and edges created in this step will be referred to as the "taxonomic graph." Next, we add nodes and edges to that graph in a procedure that we refer to as "embedding" the input trees into the taxonomy. A node is introduced for each node in an input tree, and these nodes are mapped the MRCA nodes in the taxonomic graph. In other words, for any node y in an input tree with a cluster of descendants, $\mathcal{C}$, we find the most tipward node

z in the taxonomic graph that is an ancestor to all of the taxa in $\mathcal{C}$; let $m(y) = z$ refer to this mapping, and $m'(z) = y$ refer to the reverse mapping. Each edge e_{ij} in a source tree i connects ancestor to its descendant, $a(e_{ij}) \rightarrow d(e_{ij})$. The edges are introduced into the graph. We also introduce new edges to create a from $m(a(e_{ij}))$ through its descendants to $m(d(e_{ij}))$; we denote this path $p(e_{ij})$ and refer to the edges in the path as "embedding edges for tree i". Note, that this is a path through the taxonomic nodes, while the edge e_{ij} connects source tree nodes. The mapping between e_{ij} and $p(e_{ij})$ is stored, and the edges are labelled with the index i so that it is clear which tree created them. Because the taxonomic tree is highly unresolved, it is frequently the case that $m(a(e_{ij}))$ is the same node as $m(d(e_{ij}))$; in these cases the embedding edge is a loop. This situation occurs whenever edge e_{ij} can resolve part of the polytomy represented by a taxon.

We treat the taxonomy as the lowest ranked input tree. The next step will collapse contested edges in the taxonomic graph. To retain all of the information from the taxonomy we embed the taxonomy into the taxonomic graph as if it were another input tree

B.2 Detection of uncontested higher taxa

After every input tree and the taxonomy tree have been embedded into the taxonomic graph, we perform postorder traversal over the taxonomic graph that underlies the multi-graph. For any internal node (each of which corresponds to a non-terminal taxon) we determine whether or not it is contested by examining each input tree. We can determine tree i contests the taxon represented by taxonomic node x by looking at the parents of all of the "exiting" embedding edges for tree i. These are the set of embedding edges that have x as a daughter and have a parent node that is not x (ergo a parent node that is taxonomically higher than x). If there are more than one parent nodes in this set of exiting embedding edges, then tree i contests that taxon. If there is only parent node, then the all of the constituent taxa belonging to this taxon that are present in tree i have one parent that is more inclusive; this means that the input tree does not contest monophyly of the taxon.

If the taxon is uncontested, then it may be the case that some input trees do not contest the taxon, but contain polytomies that could be resolved to display the taxon. The cases can be identified by finding multiple exiting embedding edges that have the same taxon y as their parent node. In these cases, a pseudo input tree node is created and becomes the parent node for these edges; this new node is then connected to y as if it had been an input edge. This operation is equivalent to resolving an input tree's polytomy in favor of the monophyly of the uncontested taxon. This is the only way in which the input trees are modified during the decomposition.

B.3 Collapsing contested taxa from the taxonomic graph

If a taxonomic node x fails the "uncontested" test described in the previous section, then the node corresponding to the taxon is removed from the taxonomic graph and the set of edges (and mappings between input edges and embedded paths) is updated as if this taxon had not been present in when the taxonomic graph was created. This consists of detecting changing any edge in an embedding path that is adjacent to x by replacing the reference to x with a reference to its parent $a(x)$. Note that we do not collapse the edge corresponding to this taxon in the part of the graph that represents the embedding of the taxonomy into the taxonomic graph. Thus, the taxonomy will still claim the monophyly of the taxon. This is

relevant if the input grouping that contests taxon x is overruled (in the subproblem solution step) by a higher ranked split. In other words, the fact that the a taxon is contested during the decomposition is not a guarantee that the taxon will not be monophyletic in the final supertree.

B.4 Emitting subproblems

Whenever an uncontested taxon is identified, the appropriate slice of each input trees that intersect with the taxon is written to a file. Then the multigraph is simplified by slicing any off the taxon. This slicing is accomplished by examing all of the exiting embedding edges for the taxon. The descendant taxa of each input tree is relabeled with the identifier of the contested taxa and all of that node's descendants are removed. Thus this input node will act as as if it were a leaf mapped to the uncontested taxon. All descendants of the taxonomic graph are also pruned off.