Speeding up iterative applications of the BUILD supertree algorithm

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May 10, 2024

Abstract

The Open Tree of Life (OToL) project produces a supertree that summarizes phylogenetic knowledge from tree estimates published in the primary literature. The supetree construction algorithm iteratively calls Aho's BUILD algorithm thousands of times in order to assess the compatability of different phylogenetic groupings. We describe an incrementalized version of the BUILD algorithm that is able to share work between successive calls to BUILD. We provide details that allow a programmer to implement the incremental algorithm BUILDINC, including pseudo-code and a description of data structures. We assess the effect of BUILDINC on our supertree algorithm by analyzing simulated data and by analyzing a supertree problem taken from the OToL 13.4 synthesis tree. We find that BUILDINC provides up to 550-fold speedup for our supertree algorithm.

Introduction

The Open Tree of Life (OToL) project summarizes phylogenetic knowledge from tree estimates published in the primary literature. Curators for the project import published trees, associate the tip labels of the trees to standardized taxonomic labels, and correct errors in trees that occurred during the deposition of the trees into repositories. OToL also produces a synthesis tree [Hinchliff et al., 2015] that combines hundreds of input phylogenies with a comprehensive taxonomic tree from the Open Tree Taxonomy [Rees and Cranston, 2017, OTT hereafter]. This "synthetic tree" is a supertree – a tree that is produced by combining multiple input trees, and having a leaf label-set that is the union of the leaf label-sets of the input trees [Gordon, 1986].

Our supertree method is intended to summarize and transparently represent the published input trees, not to produce a phylogeny estimate that is more accurate than the inputs [Redelings and Holder, 2017]. Each edge of the supertree corresponds to a supporting branch in one of the input trees. The synthetic tree can be used as a comprehensive phylogeny of living and extinct taxa. It can also be used as a means of navigating the OToL curated collection of published input trees, and of exploring conflict between them. The OToL portal at `https://tree.opentreeoflife.org` allows browsing or downloading the latest release of the synthetic tree. It also allows for uploading and curating input phylogenies.

The OToL synthetic tree is created by an algorithm that will add a grouping from an input tree to the full tree if that grouping is compatible with the previously added groups. More specifically, the supertree algorithm iterates over branches of input phylogenies to determine if the groups subtending each internal branch can be added to the synthesis tree [Redelings and Holder, 2017]. The order in which input phylogenies are considered is an input to the algorithm, and this order is provided by data curators for the OToL project. The taxonomy tree is always the last phylogeny to be considered.

The current implementation of the supertree algorithm is fast enough to allow the full supertree to be updated periodically. A faster implementation would allow users to explore the effects of differing inputs, such as a different set of phylogenies or a different ranking of trees. This would enable constructing alternative synthetic trees on demand via the web-interface for a variety of users.

The core algorithm for determining compatibility of each potential grouping with previously added groups is the classic Build [Aho et al., 1981] algorithm. Build is invoked thousands of times during the construction of the supertree using OToL's pipeline [Redelings and Holder, 2017]. Each invocation applies Build to the set of all previously added groups (which are already known to be consistent) plus one new group. Here we describe improvements to naively calling Build iteratively. Implementing the incrementalized BuildInc algorithm has resulted in dramatic reductions in running times for the key steps in the supertree pipeline. This new algorithm will allow the OToL project to offer more frequent updates to the synthetic tree and explore features such as on-demand supertree construction under the direct control of users of the project's web-services.

While we focus on the use of Build within the OToL project, Build is an ingredient that is used in a wide range of algorithms, such as computing a consensus of equally likely trees [Sanderson et al., 2011], inferring species trees from gene trees [Roch and Warnow, 2015], determining orthology and paralogy relations between genes in a gene family [Lafond and El-Mabrouk, 2014], and hierarchical clustering [Chatziafratis et al., 2018]. In order to determine what opportunities are opened up by an incrementalized version of Build, researchers must examine each algorithm that uses Build. However, we highlight two possiblities. First, an incrementalized Build might be used to construct an "online" version of an existing algorithm – that is, an algorithm in which input is added in batches and that produces a complete result after each batch. A batch could represent a new data point, or it could represent the next gene in a genome-wide scan. Second, an incrementalized Build might aid in discovering a compatible subset of trees or bi-partitions instead of merely declaring failure when a given set is incompatible. Thus, an incrementalized version of Build has implications beyond the OToL project.

Context for Build in the current OToL pipeline

The current pipeline divides the full supertree problem into subproblems as described in Redelings and Holder [2017]. These subproblems cover regions of the taxonomy tree in such a way that adjacent sub-problems contain common nodes (higher taxa) but do not contain common edges. Each subproblem also contains the relevant region of any input tree that coincides with the region of the taxonomy tree. Repeated calls to Build produce a supertree solution to each subproblem. Solving the subproblems is a time-consuming step for the entire pipeline. Increasing the speed of the subproblem-solver would speed up the pipeline, but would also allow it to handle larger subproblems. Larger subproblems occur when OToL curators add more input phylogenies to the pipeline and this large set of inputs conflict with more groupings found in the taxonomy. Larger subproblems also occur when the final location of an *incertae sedis* taxon is far from its initial location in the taxonomy [see Redelings and Holder, 2019, for a discussion of the handling of *incertae sedis* taxa]. The increased speed might eliminate the need for decomposing the supertree problem into subproblems.

Methods

We will begin the methods description with a review of the Build algorithm and the description of the new optimizations to the algorithm that are the focus of this paper. After the algorithmic discussion, the simulation study to evaluate performance will be explained.

Overview of the Build algorithm

The Build algorithm is a recursive algorithm that determines if a set of rooted triplets of the form $x, y| \bullet z$ are jointly compatible [Aho et al., 1981]. Here, we use the symbol $\bullet$ to stand for the root of the tree to emphasize the rooting of the triple. If they are compatible it constructs a tree that displays all the triplets.

The algorithm works by creating a graph for each recursive level. If the graph forms a single connected component, then the Build algorithm has detected an incompatibility between the set of triplets. The graph contains a node corresponding to each leaf that is relevant to the current recursion level. At the root-most level of the recursion every leaf is relevant. A rooted triple is relevant to a recursion level only if each of the three leaves is relevant at that level. For each relevant triple $x, y| \bullet z$ an edge is added between x and y. Since the leaves in the more closely related pair $\{x, y\}$ are sometimes called the "cluster" of the triple, the resulting graph is called the "cluster graph" for the given set of triplets.

If no triplets are incompatible on a level, then the procedure applies Build to each connected component of the cluster graph. This is the recursive aspect of the algorithm. The nodes that form a connected component at one level will constitute the relevant nodes for the next recursive call. Thus the relevant leaf set is partitioned at each level. However, the edges between nodes are not passed to the next recursive level. Instead they are constructed from the set of relevant triplets at each level. A rooted triple that is relevant at one level may not be relevant at a subsequent recursion level. Thus, not all rooted triplets have a corresponding edge at the next level. A set of triplets is jointly compatible only if the BUILD algorithm finds no incompatibility at any recursive level.

Rooted Splits

The Build algorithm was originally designed to work on sets of rooted triplets. However, when working with evolutionary trees, it is more convenient to work with sets of rooted splits because each branch corresponds to a rooted split. A rooted split σ on taxon set $\mathcal{T}$ is written $\sigma = \sigma_1| \bullet \sigma_2$, where σ_1 and σ_2 are non-overlapping subsets of $\mathcal{T}$. We refer to σ_1 as the include group or "cluster", and σ_2 as the exclude group. The root of the tree is on the side of the exclude group. Note that $\sigma_1 \cup \sigma_2$ may be smaller than $\mathcal{T}$.

It is straightforward to extend Build to operate on a set of rooted splits by treating each rooted split as shorthand for all the rooted triplets that it implies. So Build is commonly modified to take a set of rooted splits Σ instead of a set of rooted triplets.

The relationship of the current optimizations to previous work

Previous approaches to speed up Build have tried to improve the order of computation for the analysis at each recursive level. Deng and Fernández-Baca [2018] decreased the order to $\mathcal{O}(M \log^2 M)$ for a set of phylogenies with $M =$ (number of edges) + (number of leaves). This is accomplished by decreasing the time for the analysis on each recursive level from $\mathcal{O}(M^2)$ to $\mathcal{O}(\log^2 M)$. It also involves sharing work between different levels of the recursive algorithm by retaining a graph between successive levels instead of creating a new graph from scratch on each level.

Our approach differs from previous work because we attempt to share work between *successive* calls to Build. When calling Build with one set of splits followed by calling Build again with one additional split, we seek to reuse work from the first call while performing the second. This requires saving work from the first call in an object that represents the solution to Build, and passing

A `Solution` object `S` contains the following fields:

> `S.T`: an array of taxon identifiers relevant to the solution level.
>
> `S.`$\mathcal{C}$: an array of Component objects - one for each non-trivial connected component of the relevant taxa for this level of Build.
>
> `S.M`: an array that maps a leaf index to the component that it is assigned to.
>
> `S.I`: an array of "implied splits". These are splits σ where σ_2 does not intersect `S.T`.

A `Component` object `C` contains the following fields:

> `C.T`: a linked list of taxon identifiers for every taxon assigned to this component.
>
> `C.`$\Delta\Sigma$: an array of splits relevant to the component.
>
> `C.S`: either Null (if no solution is possible) or a `Solution` object for the component.
>
> `C.O`: an array of pointers to original `Solution` objects subsumed by this component.

Figure 1: Definitions for the `Solution` and `Component` record types. The field `C.O` is not used by non-incremental Build.

that solution object as input to the second call. We do not attempt to decrease the order of the computation as a function of the number of leaves or edges. Instead we base our incremental approach on a naive algorithm that has total cost $\mathcal{O}(M^3)$. It may be possible to create an algorithm that is both incremental and has a more favorable order of computation for large M, but we do not attempt that here.

Data structures used to explain implementations of Build

In order to explain our incremental Build algorithm in an understandable manner, we seek to introduce the full complexity of the algorithm in stages[1]. We thus begin by describing a version of the traditional Build algorithm that saves its work in a solution data structure. This will allow us to focus on changes to the algorithm instead of changes to the data structures when we introduce the first incremental version of the algorithm at a later stage. Our version of

[1]One might even say "incrementally".

the Build algorithm constructs the connected components of the cluster graph without explicitly constructing the cluster graph. That is, our algorithm does not directly represent the edges of the cluster graph in memory.

We begin by introducing the `Solution` and `Component` record types that we will use to store temporary work during the algorithm. Using the terminology common to object-oriented programming, we will refer to an instance of these record types residing in a computer's memory as an "object." The following sections will describe the distinct steps in Build using some common programming notational conventions: (1) parentheses after the name of an algorithm denote the arguments supplied to that algorithm and (2) the period (or "dot") notation after the name of a data object is used to refer to a field within that record.

An initial `Solution` object can be created before applying the Build algorithm. Upon termination, the result of the algorithm will be emitted by storing it in that `Solution` object. As mentioned above in the overview of the algorithm, each level of Build's recursion starts with a set of taxa and a set of relevant splits. Connected components of taxa are created and merged as each input split is considered. In our object-oriented description of the algorithm, this corresponds to creation of a `Solution` object for the current level of recursion. That `Solution` object will hold a set of `Component` objects – each of which will store information about the connected components created during the algorithm. Each `Component` represents a sub-problem that needs to be solved. If no incompatibility is detected at the current level, then the algorithm recursively calls Build to create a `Solution` object for each `Component`.

Thus the `Solution` object forms a tree by indirect recursion to mirror the recursive structure of Build: each `Solution` object can contain some `Component` objects, and each `Component` object contains a `Solution` object (see Section B.1). We refer to the tree associated with a `Solution` object as a "solution data structure".

The Solution and Component objects for a level of Build

The definition of the `Solution` and `Component` record types is given in Figure 1. Creating a new `Solution` object is done with a procedure referred to as CreateBlankSolution(T), where T is a collection of taxon identifiers. A new solution object, `S`, has only its `S.T` field initialized; That field holds a copy of the taxon identifiers; thus initialization has computational complexity $\mathcal{O}(|T|)$.

Defining the Build algorithm

To start the algorithm, an initial `Solution` object can be created and initialized by filling its `S.T` field with the complete taxon set, $\mathcal{T}$. All other fields of the solution object are initially empty. We can think of the entire Build algorithm as taking a taxon set T and set of rooted splits, Σ. The full Build algorithm consists of the following steps:

1. initialize a `Solution` object, `S` to contain the taxon set T. We will refer to this set of operation as a function: CREATEBLANKSOLUTION(T);
2. call a helper algorithm BUILDA(`S`, Σ); and
3. return the result stored in object `S`.

The BUILDA algorithm describes the set of operations to be performed at a single level of recursion as well as how to call the next levels of recursion.

Dissecting the operations required at each level of BuildA

The operations performed in BUILDA(`S`, Σ) can be separated in several steps:

1. REMOVEIRRELEVANTSPLITS(`S`, Σ) to remove splits from Σ that are not relevant at the current level. Splits that are removed here as irrelevant are also implied by the split `S.T`$| \bullet (\mathcal{T} -$ `S.T`$)$ and are recorded on the solution in field `S.I`.
2. MERGECOMPONENTS(`S`, Σ) to find the connected components of the cluster graph by merging any two components that overlap the include group ("cluster") of a split in Σ.
3. FAIL(`S`). Return FAILURE if there is only one connected component.
4. ASSIGNSPLITSTOCOMPONENTS(`S`, Σ) to the single component on the next recursive level where they may be relevant.
5. Iterate. For each non-trivial component `C` $\in$`S`.$\mathcal{C}$:
   (a) use CREATEBLANKSOLUTION(`C.T`) to create a new solution object for each Component object and store this in `C.S`.
   (b) Recurse. Call BUILDA(`C.S`, `C.`$\Delta\Sigma$) on the sub-problem for each non-trivial component `C`, Return FAILURE if that call fails.

The REMOVEIRRELEVANTSPLITS, MERGECOMPONENTS, and ASSIGNSPLITSTOCOMPONENTS steps all have the form of a for-loop that iterates over splits in Σ and modifies `S`. This fact will be used later, when we seek to incrementalize these steps. It suggests a naive incrementalization strategy of simply iterating over any newly added splits $\Delta\Sigma$ to add their effects to `S`.

The RemoveIrrelevantSplits(`S`, Σ) step

We assume that each split in Σ has an include group fully contained in `S.T`. This means that a split is relevant at this recursive level if and only if its exclude set intersects the relevant taxon set (`S.T`).

This procedure examines each split σ in Σ. If σ is not relevant, then σ is added to the collection `S.I` of implied splits and removed from Σ. Splits removed in this step were relevant at previous recursion levels, but are irrelevant for the solution at or below the recursive level S because they do not separate any taxa in `S.T` from other taxa in `S.T`. Determining which splits to remove has computational complexity $\mathcal{O}(V \times E)$ where $V = |T|$ and $E = |\Sigma|$.

Although this is not central to the operation of the algorithm, we note the splits in `S.I` are implied by the branch of the solution tree leading to `S`. Thus the solution tree implies all the splits in Σ, and split σ is recorded on the branch that implies it.

It is not necessary to perform this step at the root level of the recursion, as all tips are inside of T for that solution object.

The MergeComponents(`S`, Σ) step

The MergeComponents step partitions taxa according to which connected component of the cluster graph they are in. This step can also be thought of as partitioning taxa in T according to an equivalence relation, where taxa are equivalent if they are in the same connected component of the cluster graph. Note in this version of Build we construct the connected components of the cluster graph without constructing the graph.

To perform the partitioning, we begin by assigning each taxon $t \in T$ to its own connected component $\{t\}$. This corresponds to a graph with no edges. We then consider each split $\sigma \in \Sigma$ and merge any components that overlap σ_1 into a single connected component. This is equivalent to adding edges to the cluster graph connecting all taxa in σ_1.

Our implementation represents the components as two related maps between components and elements: (1) the linked list of taxon identifiers included in each component (the `C.T` field of the component C), and (2) the array that maps each taxon to its component (stored in `S.M`).

Detecting mergers requires considering every taxon in every include group, and has order $\mathcal{O}(|\Sigma| \times |T|)$. There can be at most $|T|$ mergers. The cost of merging linked lists is just $\mathcal{O}(|T|)$ since merging linked lists is an $\mathcal{O}(1)$ operation. Unfortunately, when we merge two components $\mathtt{C}_1$ and $\mathtt{C}_2$ where $\mathtt{C}_2$ is smaller, we must also rewrite the array entry for taxa in $\mathtt{C}_2$. The cost per taxon is the number of times that taxon is part of a merger where it is in the smaller component. Since this can happen up to $\log_2 |T|$ times per taxon in the worst case[2], the cost is $|T| \log |T|$. The total cost is thus $\mathcal{O}(|\Sigma| \times |T| + |T| \log |T|)$. If we define $M = |\Sigma| + |T|$ following Deng and Fernández-Baca [2018], then this is $\mathcal{O}(M^2 + M \log M) = \mathcal{O}(M^2)$.

The Fail(S) step

Fail can be done in $\mathcal{O}(1)$ by having an array $\mathtt{S}.\mathcal{C}$ of active non-trivial components, and checking the size of that array. If the size is 1, and the taxon set for the single component has the same size as `S.T`, then the operation fails.

[2]The worst case is when you have a perfectly balanced merger tree for the components.

The AssignSplitsToComponents(`S`, Σ) step

For each split $\sigma \in \Sigma$ we have a guarantee that all the taxa in σ_1 are in the same component by definition of the cluster graph. We refer to the component that contains the include group of σ as its "corresponding component". We can determine the corresponding component of any split σ by simply looking up the component for the first element of σ_1 in `S.M`. We implement the assignment of a split σ to a component `C` by placing a reference to σ into `C`.$\Delta\Sigma$.

Simple optimization: Trivial and non-trivial components

In a solution object `S`, we store an array `S.M` of pointers to components. We also implement `S.T` as an array, so that if $t = T[i]$ then taxon t belongs to component `S.M`$[i]$.

Trivial components are defined as components that contain only one taxon. An optimization to improve memory usage and speed is to simply use a NULL reference in the `S.M` array to indicate that the corresponding taxon is in a trivial component, rather than creating a Component object for every trivial component. This requires only minor tweaks to the MERGECOMPONENTS step to create a new `Component` object on-the-fly whenever a set of trivial components are merged into each other with no non-trivial component involved in the merger.

Example #1: Creating a Solution

Consider calling BUILD$(\mathcal{T}, \Sigma)$ with taxa $\mathcal{T} = \{A_1, A_2, B\}$ and splits $\Sigma = \{A_1A_2|\bullet B\}$. This creates a solution data structure shown in Figure 2. BUILD begins by creating a `Solution` object $\mathtt{S}_1$ where $\mathtt{S}_1.\mathtt{T} = [A_1, A_2, B]$ and then calling BUILDA($\mathtt{S}_1$, Σ).

BUILDA creates a single non-trivial component $\mathtt{C}_1$ containing $\{A_1, A_2\}$ and a single trivial component containing B. BUILDA does not fail, because there is more than one component. The single split $A_1A_2| \bullet B$ is assigned to $\mathtt{C}_1$. BUILDA then creates a new solution $\mathtt{C}_1.\mathtt{S}$ where $\mathtt{C}_1.\mathtt{S}.\mathtt{T} = [A_1, A_2]$ and then calls BUILDA($\mathtt{C}_1.\mathtt{S}$, $\mathtt{C}_1.\Delta\Sigma$).

The second-level BUILDA removes the split $A_1A_2|\bullet B$ from $\mathtt{C}_1.\Delta\Sigma$ and adds it to $\mathtt{C}_1.\mathtt{S}.\mathtt{I}$. It then calls MERGECOMPONENTS, FAIL, and ASSIGNSPLITSTO-COMPONENTS with no effects. No non-trivial components are created, and the call to BUILDA succeeds because it contains the trivial components $\{A_1\}$ and $\{A_2\}$. Since there are no non-trivial components, another round of recursion is not performed.

Stepwise construction of BuildInc

The goal of the incrementalized algorithm is to reuse previous work from computing BUILD$(\mathcal{T}, \Sigma)$ when computing BUILD$(\mathcal{T}, \Sigma + \Delta\Sigma)$. The incrementalized algorithm has the signature BUILDINC$(\mathtt{S}, \Delta\Sigma)$. Although the taxon set $\mathcal{T}$ and the previously added splits Σ are not explicitly present in the signature of

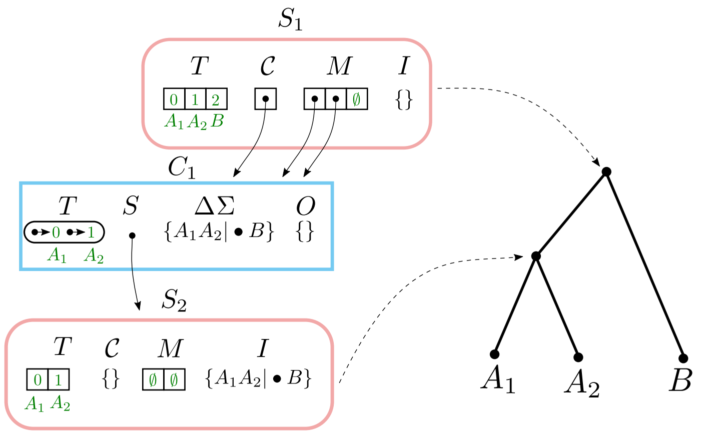


Figure 2: The `Solution` object $\texttt{S}_1$ returned by calling BUILD($[A_1, A_2, B], \{A_1A_2| \bullet B\}$). `Solution` objects have rounded edges and a pink border. `Component` objects have rectangular edges and a blue border. The temporary values $\texttt{C}_1.\Delta\Sigma$ and $\texttt{C}_1.\texttt{O}$ are shown with the values they contain before being cleared. Solid arrows indicate pointers. Dashed arrows show the correspondence between `Solution` objects and nodes on the solution tree.

BUILDINC, they are contained within `S`. `S` may also contain intermediate results from a previous BUILDINC call, so that BUILDINC can reuse previous work. If BUILDINC(`S`, $\Delta\Sigma$) succeeds, then `S` is modified in-place to contain the new splits $\Delta\Sigma$ in addition to Σ. However, if BUILDINC fails, then `S` is unmodified.

In order to simplify the description of the incrementalized algorithm BUILDINC, we first introduce two partially-incrementalized algorithms BUILDINC$'$ and BUILDINC$''$. This allows us to simplify the explanation of BUILDINC by introducing concepts in a step-wise fashion. The BUILDINC$'$ and BUILDINC$''$ algorithms both mutate the solution object even when the algorithm returns FALSE. The fully incrementalized algorithm BUILDINC adds the ability to track changes that are made to the solution object, and then roll them back if the algorithm ultimately returns FALSE. We now describe key difference in the steps of the first incrementalized algorithm BUILDINC$'$. We will use the $'$ and $''$ symbols to decorate the names of algorithms based on whether they are used in BUILDINC$'$ or BUILDINC$''$.

The incrementalized algorithm allows adding input splits either one-at-a-time, or in larger batches. We assume that the input splits have been partitioned into a series of non-overlapping subsets $\Delta\Sigma_i$ according to some strategy that is chosen in advance. Each subset constitutes a batch. The simplest strategy is to set $\Delta\Sigma_i = \{\sigma_i\}$ for some split σ_i, so that splits are added one-at-a-time. However, it is possible to incorporate input splits into the solution object in larger batches, and we explore this option in the Results section below.

Given a partition of the input splits, the general structure for all of the incrementalized algorithms is:

1. initialize a `Solution` object, `S`, to contain the taxon set T. We will refer to this set of operation as a function: CREATEBLANKSOLUTION(T);
2. BUILDINCA($\mathtt{S}, \emptyset$)
3. for each subset $\Delta\Sigma_i$
   (a) call BUILDINCA($\mathtt{S}, \Delta\Sigma_i$)
4. return the result stored in object `S`.

In the descriptions that follow, Σ will be used to denote the set of splits that have been added in previous increments of BUILDINC$'$ without failing. Thus, $\Sigma + \Delta\Sigma$ would be the set of splits included if the current round of BUILDINC$'$ succeeds, and $\Delta\Sigma$ is the set of splits that are new to the current increment of BUILDINC$'$.

BuildIncA$'$(`S`, $\Delta\Sigma$): RemoveIrrelevantSplits$'$(`S`, $\Delta\Sigma$) step

This is identical to REMOVEIRRELEVANTSPLITS except that (for reasons described below) `S.I` may already contain some splits before this step begins.

BuildIncA$'$: MergeComponents$'$(`S`, $\Delta\Sigma$) step

We seek to construct the connected components of the cluster graph for the splits $\Sigma(\mathtt{S}) + \Delta\Sigma$ from the connected components for $\Sigma(\mathtt{S})$. We will refer to connected components under the cluster graph for $\Sigma(\mathtt{S})$ as "original" components. The addition of the splits $\Delta\Sigma$ may add edges to the cluster graph, but it cannot remove any. Therefore, the addition of $\Delta\Sigma$ may merge original components, but it cannot split them. In order to compute the new connected components, we simply need to iterate over splits in $\Delta\Sigma$ and continue merging components.

Characterizing how the components for $\Sigma + \Delta\Sigma$ are related to any original components is central to our approach. The non-trivial components for $\Sigma + \Delta\Sigma$ can be characterized as *new*, *modified*, or *unmodified*.

- new (a component composed entirely of previously-trivial components)
- unmodified (a non-trivial component present in the original $\mathtt{S}.\mathcal{C}$)
- modified (a non-trivial component that contains at least one original non-trivial component)

If `S` is initially empty, then all non-trivial components will be new. If `S` is not initially empty, then all three types of non-trivial components can occur. If an original component `C`$'$ is a subset of a component `C`, then we say that `C`$'$ is *subsumed* by `C`. We now describe how these three classes of non-trivial components retain original solutions.

A *new* (non-trivial) component `C` will have an empty solution `C.S`. There is no original solution to retain, since all its subsumed components are trivial.

For *unmodified* (non-trivial) components, we retain the single original `Solution` object in the field `C.S`. We will modify the retained solution if any splits from $\Delta\Sigma$ are assigned to `C`.

Modified (non-trivial) components have a taxonomic set `C.T` that was not a connected component in the previous iteration of BuildIncA$'$. However, the `Component` object does not need to be created *de novo*; instead, we repurpose the `Component` object from one of the subsumed non-trivial components to represent the new, larger equivalence class. The previous solution in `C.S` is not the solution for the enlarged taxon set. However, we retain all the solutions for all subsumed non-trivial components in an additional field for in the component data structure, `C.O`.

BuildIncA$'$: AssignSplitsToComponents$'$(`S`, $\Delta\Sigma$) step

Splits in $\Delta\Sigma$ must be assigned to their corresponding components by placing them in `C.`$\Delta\Sigma$, just as in BuildIncA. However, splits in Σ are treated differently depending on which original component they were previously assigned to.

Splits from Σ(`S`) that were assigned to an unmodified component `C` are still associated with that component. This is because they were contained in `C.S`, and it has been retained.

Splits from Σ(`S`) that were assigned to a modified component `C` are no longer associated with `C` because `C.S` has been discarded. We therefore iterate over original components `C`$'$ that were subsumed by `C` and append their splits to `C.`$\Delta\Sigma$ (see Section B.2).

New components cannot contain any splits from Σ(`S`), so we do not need to do anything extra for them.

BuildIncA$'$: recursive call to BuildIncA$'$step

We seek to construct a solution for each of the components `C` $\in$ `S.`$\mathcal{C}$ using BuildIncA$'$. In all cases we do this by calling BuildIncA$'$(`C.S`, `C.`$\Delta\Sigma$) to add splits in `C.`$\Delta\Sigma$ to the solution `C.S`. For unmodified components, `C.S` is the original solution for `C`, so previous work is re-used. Any corresponding splits from $\Delta\Sigma$ are added to this original solution.

For modified components, `C.S` is a Null reference indicating that no solution has been calculated. We construct an empty `Solution` with taxa `C.T`. The set `C.`$\Delta\Sigma$ contains splits corresponding to `C` from both Σ(`S`) and $\Delta\Sigma$. Therefore, despite the existence of previous work in `C.O`, we do not manage to re-use any of it.

For new components, `C.S` is also Null. We also construct an empty `Solution` with taxa `C.T`. The set `C.`$\Delta\Sigma$ contains only splits from $\Delta\Sigma$. There is no previous work that could be re-used here.

Example #2: Adding a split to an unmodified component

When incrementally adding a split that resolves a node below the top level, BuildIncA$'$passes the split down the tree until it reaches the level of the resolved node. At levels higher than the resolved node, the split is assigned to one of the components, but does not modify it. At the resolved node, the split either modifies components or causes the creation of a new non-trivial component.

To see this, let's consider incrementally adding the split $\sigma_2 = a_1 a_2 | \bullet a_3$ to a `Solution` object that contains $\sigma_1 = a_1 a_2 a_3 | \bullet b$ (Fig. 3). Here the split σ_2 resolves a node in the original solution data structure.

Running BuildIncA$'$($\mathtt{S}_1$,$\{\sigma_2\}$) leaves the only non-trivial `Component` $\mathtt{C}_1$ at the top level unchanged. σ_2 is AssignEd to $\mathtt{C}_1$ and ends up in $\mathtt{C}_1.\Delta\Sigma$.

This leads to a call to BuildIncA$'$($\mathtt{S}_2$, $\{\sigma_2\}$). σ_2 is not removed, so $\mathtt{S}_2.\mathtt{I}$ is unchanged. However, σ_2 leads to the creation of a new non-trivial component $\mathtt{C}_2$ in Merge. σ_2 is AssignEd to $\mathtt{C}_2$ and ends up in $\mathtt{C}_2.\Sigma$.

Finally, we get a call to BuildIncA$'$($\mathtt{S}_3$,$\{\sigma_3\}$). Here σ_2 is finally removed, and placed into $\mathtt{S}_3.\mathtt{I}$. No non-trivial components are created, so we are done.

Example #3: Merging two components

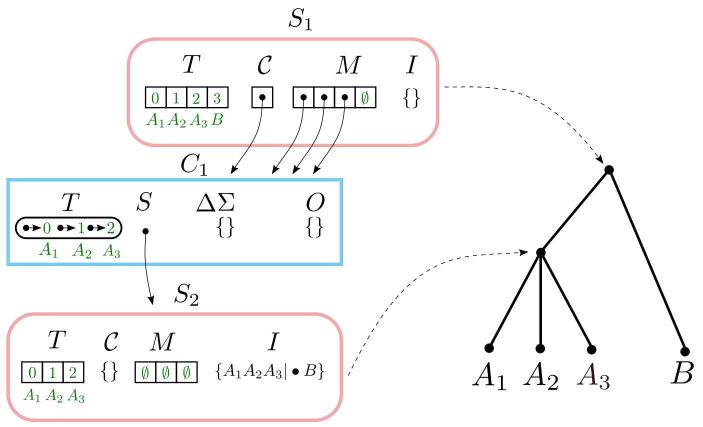
When incrementally adding a split that groups two children of a node in the solution tree, the components that correspond to the grouped children tend to re-emerge at a lower level. However, BuildIncA$'$is not able to recognize this, and so must solve each of these re-emergent components from scratch.

To see this, let's consider incrementally adding the split $a_1 b_1 | \bullet c$ to a `Solution` object that contains $a_1 a_2 | \bullet b_1$ and $b_1 b_2 | \bullet c$ (Fig. 4). The new split merges the original components $\mathtt{C}_1$ (containing and $\{A_1, A_2\}$) and $\mathtt{C}_2$ (containing $\{B_1, B_2\}$). The new component $\{A_1, A_2, B_1, B_2\}$ is then stored in the modified `Component` object for $\mathtt{C}_1$.

BuildIncA$'$handles merged components by extracting the splits from subsumed solutions. Therefore, $\mathtt{C}_1.\Delta\Sigma$ contains *all three* splits, and not just the incrementally added split. We can see that the original component $\{A_1, A_2\}$ re-emerges at a lower level as $\mathtt{C}_3$. However, BuildIncA$'$solves it from scratch. The component $\{B_1, B_2\}$ does *not* re-emerge at a lower level. This is because the split $b_1 b_2 | \bullet c$ can be satisfied on the same level, and is not passed down.

The partially incrementalized algorithm BuildInc$''$

The BuildInc$'$ algorithm can only reuse work for unmodified components; modified components must be recomputed from scratch. Figuring out how to re-use previous work for modified components was one of the most difficult steps in designing BuildInc. The key insight is that a solution data structure can be regarded as a collection of splits (see section B.2). Thus, instead of extracting the splits from original solutions that were subsumed by a modified component, we may simply pass down the original solutions themselves.



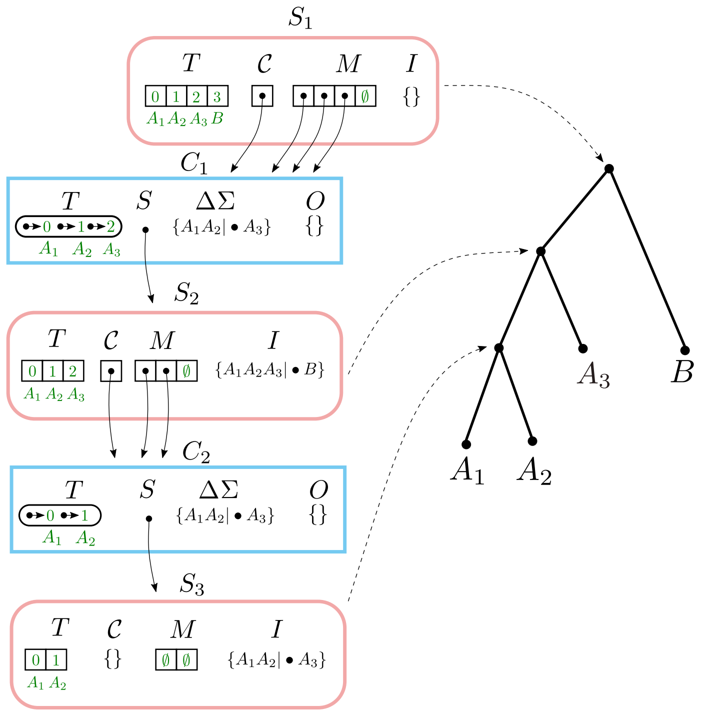
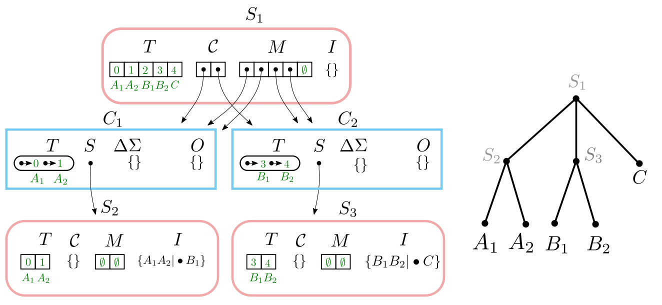
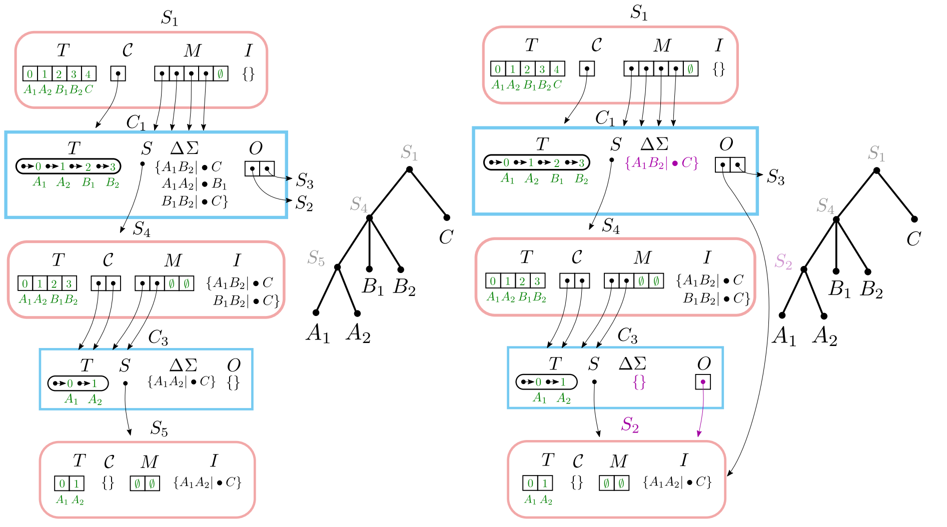


Figure 3: Adding a split to an unmodified component. Top: the result of adding the split $A_1A_2A_3|\bullet B$. Bottom: the result of incrementally adding the split $A_1A_2|\bullet A_3$, starting with the top Solution.



(a) Original solution



(b) BUILDINCA′ (c) BUILDINCA″

Figure 4: Merging two components. (a) The initial solution contains the splits $A_1A_2|\bullet B_1$ and $B_1B_2|\bullet C$. In both (b) and (c), when $A_1B_1|\bullet C$ is incrementally added, the original components $\mathtt{C}_1$ and $\mathtt{C}_2$ are merged and stored in the modified `Component` object for $\mathtt{C}_1$.The original component $\{A_1, A_2\}$ re-emerges at a lower level as $\mathtt{C}_3$. (b) In BUILDINCA′, $\mathtt{C}_1.\Delta\Sigma$ contains *all three* splits, and not just the incrementally added split. The re-emergent component $\{A_1, A_2\}$ is solved from scratch. (c) In BUILDINCA″, $\mathtt{C}_1.\Delta\Sigma$ contains only the new split $A_1B_2|\bullet C$. The original solution $\mathtt{S}_3$ is punctured, and its split $B_1B_2|\bullet C$ is added to $\mathtt{S}_4.\mathtt{I}$. However, the original solution $\mathtt{S}_2$ for $\{A_1, A_2\}$ is passed down to $\mathtt{C}_3$ and can be re-used, saving work.

Performing operations such as MergeComponents, AssignSplitsToComponents, and RemoveIrrelevantSplits turns out to be more efficient when the input splits are packaged in original solutions. These operations frequently do not break apart the collections of splits.

Most importantly, passing down original solutions can sometimes allow us to reuse solutions instead of recomputing them from scratch. When an original component $\mathtt{C}'$ is subsumed by merging, it may sometimes re-emerge deeper in the recursion stack as a descendant of the merged component. If the original solution $\mathtt{S}$ manages to percolate down the tree to the new location of $\mathtt{C}'$ then we can re-use $\mathtt{S}$. However, if any of the splits in $\Sigma(\mathtt{S})$ is satisfied at an earlier recursion level, then $\mathtt{S}$ must be broken up and cannot be re-used. This will be described in further detail below and illustrated in Example #4.

We therefore modify the signature of BuildIncA$'(\mathtt{S}, \Delta\Sigma)$ to BuildIncA$''(\mathtt{S}, \Delta\Sigma, \mathtt{O})$, where $\mathtt{O}$ is a set of original solutions. The call BuildIncA$''(\mathtt{S}, \Delta\Sigma, \mathtt{O})$ indicates an attempt to add both splits in $\Delta\Sigma$ and splits in $\mathtt{O}$ to the splits in $\mathtt{S}$. We will write $\Sigma(\mathtt{O})$ to indicate the splits contained in $\mathtt{O}$, where

$$\Sigma(\mathtt{O}) = \bigcup_{\mathtt{S}' \in \mathtt{O}} \Sigma(\mathtt{S}')$$

These original solutions in $\mathtt{O}$ satisfy three properties that we will prove in Appendix A:

1. If $\mathtt{O}$ is non-empty, then $\mathtt{S}$ contains no splits.

2. Each original solution in $\mathtt{O}$ has a taxon set that is a subset of $\mathtt{S.T}$.

3. All the original solutions in $\mathtt{O}$ have non-overlapping taxon sets.

BuildIncA$''$: MergeComponents$''(\mathtt{S}, \Delta\Sigma, \mathtt{O})$ step

We seek to construct the connected components of the cluster graph for the splits $\Sigma(\mathtt{S}) \cup \Delta\Sigma \cup \Sigma(\mathtt{O})$ from the connected components for $\Sigma(\mathtt{S})$. In addition to iterating over $\Delta\Sigma$ and merging components, BuildIncA$''$ must additionally handle splits in $\Sigma(\mathtt{O})$. One possible approach would be to iterate over splits in $\Sigma(\mathtt{O})$ and merge components that overlap each split. However, it turns out that there is a more efficient way.

We note that each original solution $\mathtt{S}' \in \mathtt{O}$ is a connected component of the original cluster graph for some higher recursive level. Additionally, the taxa in $\mathtt{S}'.\mathtt{T}$ are connected solely by edges corresponding to splits in $\Sigma(\mathtt{S}')$ (see Section B.3). This is because any split whose include group overlaps the component is assigned to (and only relevant to) that component. Therefore, the effect of the splits $\Sigma(\mathtt{S}')$ is only to connect the taxa in $\mathtt{S}'.\mathtt{T}$. We may therefore iterate over original solutions $\mathtt{S}' \in \mathtt{O}$ and merge any two components that both overlap $\mathtt{S}'.\mathtt{T}$. This makes it unnecessary to extract the splits $\sigma \in \mathtt{S}'$.

BuildIncA$''$: AssignSplitsToComponents$''$($\mathtt{S}$, $\Delta\Sigma$, $\mathtt{O}$) step

BuildIncA$''$ needs to assign splits in $\Sigma(\mathtt{S})$, $\Delta\Sigma$, and $\Sigma(\mathtt{O})$ to their corresponding components. Each split in $\Delta\Sigma$ is assigned to a component $\mathtt{C}$ and stored in $\mathtt{C}.\Delta\Sigma$, just as as in BuildA and BuildIncA$'$. However, there are two major differences from BuildIncA$'$.

First, BuildIncA$''$ does not need to do anything for splits in $\Sigma(\mathtt{S})$, because they are already assigned to their correct component. BuildIncA$'$needed to extract splits from $\mathtt{C.O}$ and add them to $\Delta\Sigma$ if $\mathtt{C}$ was a merged component. However, BuildIncA$''$ passes $\mathtt{C.O}$ down to the next recursive level directly, so this is unnecessary. Note that since BuildIncA$''$ no longer assigns splits from $\Sigma(\mathtt{S})$ to $\mathtt{C}.\Delta\Sigma$, $\mathtt{C}.\Delta\Sigma$ will consist only of splits from $\Delta\Sigma$.

Second, BuildIncA$''$ must assign splits in $\Sigma(\mathtt{O})$ that were recieved from the previous recursive level to their corresponding component. However, all splits for a subsolution $\mathtt{S}' \in \mathtt{O}$ have to end up in the same component. This is because $\mathtt{S}'.\mathtt{T}$ must be entirely contained in one component. The splits of $\mathtt{S}'$ must then be in the same component. Therefore, we may simply assign original solutions $\mathtt{S}'$ to components in their entirety. We can determine which component a solution $\mathtt{S}'$ goes to by looking up the component for any element in $\mathtt{S}'.\mathtt{T}$.

BuildIncA$''$: recursive call to BuildIncA$''$

As before, BuildIncA$''$($\mathtt{S}$, $\Delta\Sigma$, $\mathtt{O}$) must iterate over the non-trivial components $\mathtt{C} \in \mathtt{S}.\mathcal{C}$ and construct a solution $\mathtt{C.S}$ for each of them. In all cases this is done by calling BuildIncA$''$($\mathtt{C.S}$, $\mathtt{C}.\Delta\Sigma$, $\mathtt{C.O}$). Passing original solutions from modified components down the tree in $\mathtt{C.O}$ allows us to reuse previous work, as described in the section on RemoveIrrelevantSplits$''$ below. The only difference from BuildIncA$'$is the third argument, the set of original solutions, $\mathtt{O}$.

BuildIncA$''$: RemoveIrrelevantSplits$''$($\mathtt{S}$, $\Delta\Sigma$, $\mathtt{O}$) step

There are two differences between BuildIncA$'$($\mathtt{S}$, $\Delta\Sigma$) and BuildIncA$''$($\mathtt{S}$, $\Delta\Sigma$, $\mathtt{O}$). First, $\mathtt{O}$ might contain a solution $\mathtt{S}'$ to the problem we are trying to solve. In that case, we would like to reuse that solution. Second, when checking for implied splits, we need to check inside each original solution $\mathtt{S}' \in \mathtt{O}$ as well as inside $\Delta\Sigma$. We now discuss these differences in greater detail.

Reusing previous work in BuildIncA$''$($\mathtt{S}$, $\Delta\Sigma$, $\mathtt{O}$)

Suppose that $\mathtt{O}$ contains a solution $\mathtt{S}'$ with the same taxon set as $\mathtt{S}$. In that case, we would like to re-use the previous work in $\mathtt{S}'$ instead of solving the problem from scratch.

We first note that $\Sigma(\mathtt{S})$ must be empty, since $\mathtt{O}$ was non-empty, so it is safe to discard $\mathtt{S}$ and use $\mathtt{S}'$ instead. Second, $\mathtt{O}$ is empty after removing $\mathtt{S}'$. This is because $\mathtt{S}'$ contains all the taxa in $\mathtt{S.T}$ and there are no remaining taxa in $\mathtt{S.T}$ for any other solutions to contain.

We therefore replace the call to BuildIncA$''$(S, $\Delta\Sigma$, O) with BuildIncA$''$(S$'$, $\Delta\Sigma$, $\emptyset$). This preserves the invariant that S and O cannot both be non-empty.

Removing implied splits from original solutions

Recall that a split σ should be placed into S.I if and only if σ_2 does not intersect S.T. For an original solution S$' \in$ O, we claim that only splits in S$'$.I can satisfy this condition. If a split σ from S$'$ is not in S$'$.I, then σ_2 must intersect S$'$.T. But S$'$.T is a subset of S.T, so σ_2 intersects S.T as well and cannot go into S.I. Therefore, for each original solution S$'$, we only need to check the splits in S$'$.I.

If any split in S$'$.I meets the criterion, then we remove it from S$'$.I (conceptually) and move it to S.I. However, if one of the splits *is* removed from a solution, then the solution no longer has the property that its splits are all in the same connected component. It is no longer a solution. In such a case, we say that the solution is "punctured".

In order to retain our invariants, we remove punctured solutions from O. However, we must retain the splits that they contain. For each punctured original solution S$'$, we copy the splits in S$'$.I that were *not* moved to S.I into the set $\Delta\Sigma$. We move the child solutions S$'$.$\mathcal{C}_i$.S into O. In this way, all the splits of S$'$ are retained — some in S.I, some in $\Delta\Sigma$, and some in O.

Original solutions in O that are not punctured may be retained unmodified.

Note that replacing an original solution S$' \in$ O with its child solutions retains the invariants that solutions in O (i) have non-overlapping taxon sets and (ii) are contained within S.T. The taxon sets of child solutions to a solution S$'$ are contained within S$'$.T and are non-overlapping. Since S$'$.T is contained within S.T and does not overlap with any other solutions in O, its child solutions must also be contained within S.T and not overlap any other solutions in O.

Example #4: Merging two components and re-using original solutions

When incrementally adding a split that groups two children of a node, the components that correspond to the grouped children tend to re-emerge at a lower level. While BuildIncA$'$solves the solutions from scratch, BuildIncA$''$ is able to re-use the original solutions to these components.

To see this, we show how BuildIncA$''$ solves the same problem that BuildIncA$'$solved in Example #3 (Fig. 4). Unlike BuildIncA$'$, BuildIncA$''$ leads to C$_1$.$\Delta\Sigma$ containing only the single incrementally-added split $A_1B_1|\bullet C$. Instead of extracting the splits $A_1A_2|\bullet B_1$ and $B_1B_2|\bullet C$ from the original solutions S$_2$ and S$_3$, BuildIncA$''$ passes down the original solutions themselves.

The original component $\{A_1, A_2\}$ re-emerges at a lowever level, and is solved by re-using the original solution S$_2$. The other original solution S$_3$ is punctured, and its split $B_1B_2|\bullet A$ is added to S$_4$.I.

The fully incrementalized algorithm BuildInc

The BuildInc$'$ and BuildInc$''$ algorithms modify the original solution data structure as they execute. When these algorithms discover that the additional splits are incompatible with the previous solution, we cannot simply revert to the previous solution, because it has been modified. We must therefore recreate the previous solution data structure from scratch, discarding all of the saved work.

We address this problem by extending BuildInc$''$ to record any change that it makes to the original solution. We can then reverse these changes in the case of failure. We call the extended algorithm BuildInc. Much of the description of BuildInc thus boils down to (i) specifying just what information must be recorded to reverse changes made by BuildIncA$''$ and (ii) some optimizations that avoid spending time recording information that will never be used.

An overview of the Rollback approach

All modifications to each `Solution` object `S` are complete before any modifications are made to its children. We can therefore represent modifications to the solution data structure as a sequence R of modifications to individual `Solution` objects. If BuildIncA returns failure at the top level, we can then walk this sequence in reverse order, and roll back the changes that it describes. We create the record type `RollbackInfo` to record modifications made to an individual `Solution` object (Figure 5).

Component mergers are the most interesting type of modifications that BuildIncA$''$ makes to `Solution` objects. We can represent component mergers for each `Solution` object as a sequence of individual mergers of two components. For each component merger, we record enough information about the two original components to reverse the merger. It is then possible to reverse the mergers by walking the sequence in reverse order, and undoing each merger in turn. We create the record type `MergeRollbackInfo` to record modifications made to an individual `Solution` object (Figure 5).

Mergers are of two types: mergers of two non-trivial components, or mergers of a non-trivial component with a trivial component. We handle mergers of two trivial components, by creating an empty "non-trivial component" data structure, and merging it with each trivial component in turn.

Details of rollback info

The `RollbackInfo` record type

Changes that occur to `S` during BuildIncA$(\mathtt{S}, \Delta\Sigma)$ include (i) appending additional implied splits to `S.I`, (ii) modifying the component list $\mathtt{S}.\mathcal{C}$, and (iii) merging components. We can therefore record the changes that occur to `S` in terms of (i) the original set of implied splits `S.I`, (ii) the original list of components $\mathtt{S}.\mathcal{C}$, and (iii) a sequence of records that describe individual merges of two

A `RollbackInfo` object `r` contains the following fields:

`r.S`: a pointer to the `Solution` object that this rollback info is about.

`r.n_old_implied_splits`: the previous number of implied splits `S.I`.

`r.merge_rollback_info`: the sequence of MergeRollbackInfo objects

`r.n_orig_components`: the original number of components

`r.old_components`: the array of pointers to components *after* merging but *before* removing empty components.

A `MergeRollbackInfo` object `m` contains the following fields:

`m.component1` = pointer to $\mathtt{C}_1$

`m.component2` = pointer to $\mathtt{C}_2$, or NULL if $\mathtt{C}_2$ is trivial.

`m.component2_first` = pointer to the first element of $\mathtt{C}_2$`.T`, or NULL if $\mathtt{C}_2$ is trivial.

`m.orig_solution` = pointer to the original solution $\mathtt{C}_1$`.S`.

Figure 5: Definitions for the `RollbackInfo` and `MergeRollbackInfo`.

components. We note that implied splits are only ever appended to the end of S.I. Therefore, as an additional optimization we can simply record the original length of S.I, and revert to the original version by truncating the array to that length.

The MergeRollbackInfo record type

When merging two non-trivial components $\mathtt{C}_1$ and $\mathtt{C}_2$, let us assume that $\mathtt{C}_2$ is the smaller component. The modifications that occur to $\mathtt{C}_1$, $\mathtt{C}_2$, and S are the following:

- S.M $[t]$ is set to $\mathtt{C}_1$ for each taxon $t \in \mathtt{C}_2$.T.
- the elements of $\mathtt{C}_2$.T are removed and appended to $\mathtt{C}_1$.T.
- $\mathtt{C}_1$.S is set to Null.

We can restore $\mathtt{C}_1$.S from the saved reference. The pointer to the first element of $\mathtt{C}_2$.T allows us to split the linked list $\mathtt{C}_1$.T in two at the proper place, and return the latter half to $\mathtt{C}_2$.T. We can then walk the restored elements of $\mathtt{C}_2$.T and set S.M$[t]$ $=\mathtt{C}_2$ for each $t \in \mathtt{C}_2$.T.

Sometimes we merge a non-trivial component C with a trivial component containing the taxon t. In such cases, there is no non-trivial component $\mathtt{C}_2$. We indicate such cases in the RollbackInfo object by setting component2 = Null. Such mergers can be rolled back by removing the last element of $\mathtt{C}_1$.T, setting S.M$[t]$ = Null and setting $\mathtt{C}_1$.S = orig_solution.

Optimizations

Recording and replaying rollback info allows us to avoid discarding saved work. However, both recording and replaying rollback info also have a cost. In order to achieve the optimum speedup from rollback info, we must avoid paying this cost when we do not need to.

Optimization #1

We only need to undo changes to a Solution object if it was part of the previous solution data structure. In order to determine if a Solution object S is part of the previous solution data structure, we initialize a counter S.visits to 0 when creating a new Solution object. We then increment the counter each time the Solution object is visited by BuildIncA. We then avoid appending the rollback info for S to the sequence of changes R if S.visits = 0.

Optimization #2

Sometimes an original Solution object contains only trivial components. In such a case, we do not need to walk the list of merge records in reverse, undoing each component merger. We can simply clear the component list, and set all the entries of S.M to Null.

Optimization #3

If the number of original components is 0, then we will either not record the rollback info `r` at all (optimization #1), or we will record `r` but not look at the merge records (optimization #2). In that case, creating the sequence of merge records is a waste of time. We therefore pass a flag to MergeComponentWithTrivial and MergeComponents indicating whether or not to record merge records.

This optimization is essential because it avoids creating merge records for cases where they will not be used. One of those cases is when implementing Build(Σ) by calling BuildIncA($\mathtt{S}, \Sigma$) for a blank `Solution S`. In order for BuildInc not to be slower than Build, we must avoid creating merge records in this case.

Modifications to BuildIncA

In order to record rollback info, we must make a few modifications to BuildIncA. In `RemoveIrrelevantSplits`, we record the original number of implied splits. In `MergeComponents` we record (i) the original number of components, (ii) a merge-record for each component merger, and (iii) a copy of $\mathcal{C}$ after new components are added, but before empty components are removed.

Rollback(S,r)

After running BuildIncA, BuildInc must run RollbackAll(`S`, `R`) in case of failure. This consists of running RollbackOne(`S`, `r`) on individual `RollbackInfo` objects r.

1. Truncate `S.I` to its previous length `r.n_orig_implied_splits`.
2. If `r.n_orig_components` is equal to 0, then clear $\mathtt{S}.\mathcal{C}$ and set $\mathtt{S.M}[t] =$ Null for each taxon t.
3. If `r.n_orig_components` is more than 0, walk the list of merge records in reverse order, and undo each one.
4. If we recorded the original components vector $\mathtt{S}_0.\mathcal{C}$ then
    (a) swap($\mathtt{S}.\mathcal{C}$, $\mathtt{S}_0.\mathcal{C}$).
    (b) Truncate $\mathtt{S}.\mathcal{C}$ to `r.n_orig_components`.

This process seems simple enough, but one aspect of it that is tricky. Some components are created during merging that (i) are not original components, and also (ii) end up being empty. So they are not final components. We need these components to survive (i.e not be deallocated) so that we can temporarily add elements to them during rollback. We will then move these elements *out* of them into original components.

Batching + Oracle

Batching

Recall that our supertree algorithm works by considering an ordered list of trees. We seek to construct the set of splits from these trees that are jointly compatible.

The batching approach works by batch-adding the splits for the each tree in order. To batch-add a group of splits, we try and add the whole group of splits. If that succeeds, then we keep the whole group. If it fails, and the group has one split then we are done. If it fails, and the group has more than one split, then we batch-add the first half of the group, followed by the second half of the group. This ends up being both simpler and more efficient than trying fixed-size batches because we do not need to figure out the ideal batch size and it has exponential back-off.

Batching improves efficiency when Σ is large because the cost of determining the compatibility of $\Sigma + \Delta\Sigma$ does not increase much as the size of $\Delta\Sigma$ increases. If all the splits in $\Delta\Sigma$ will be accepted, it is thus substantially more efficient to add them in one batch.

Oracle

The oracle first runs conflict analysis on each input phylogeny T to identify branches of T that conflict with the tree of currently accepted splits. We then batch-add splits corresponding to the non-conflicting branches of T. This makes batching more efficient by making it more likely that large batches do not contain any conflicting splits.

Unfortunately, the oracle cannot filter splits for the taxonomy tree if there are any *incertae sedis* taxa. This is because taxonomy branches may correspond to *partial* splits in the presence of *incertae sedis* taxa. Our current conflict analysis does not handle partial splits.

Simulation experiments

The simulations script (`gen_subproblem.py`) can be found in the otcetera repository on GitHub (`https://github.com/OpenTreeOfLife/otcetera`). The user of the script specifies: (a) a number of leaves in the full tree, (b) a number of phylogenetic input trees to simulate, (c) a tip inclusion probability for each phylogenetic input, (d) a number of edge-contract-refine (ECR) moves to conduct on each input tree, and (e) an edge contraction probability for the taxonomy. For each replicate, the script uses DendroPy [Sukumaran and Holder, 2010] to generate a pure birth (Yule) tree with the specified number of leaves as the true (model) full tree for that replicate. The specified number of phylogenetic inputs are created by sub-sampling the full tree (using the tip-inclusion probability to assess whether a tip remains in the sampled input); if all tips are deleted a new phylogenetic input is drawn, rather than emitting an empty tree.

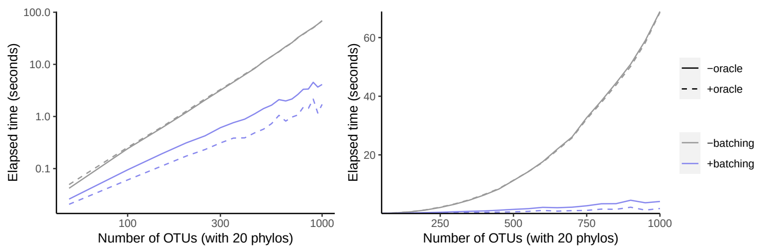


Figure 6: Effect of oracle and batch optimizations on run time. The left panel is log-scaled, whereas the right panel is not. Run time versus number of OTUs where each sample data set has 20 phylogenetic trees as inputs.

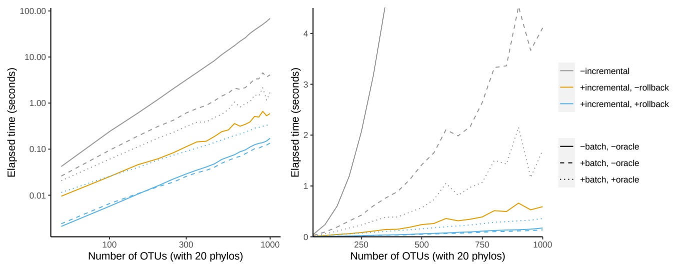


Figure 7: Comparison of incremental BUILD and batch+oracle optimizations. The left panel is log-scaled, whereas the right panel is not. Run time versus number of OTUs where each sample data set has 20 phylogenetic trees as inputs.

Then the specified number of ECR moves are applied to the tree to mimic phylogenetic estimation noise. The last tree emitted for each replicate is designed to mimic the taxonomic input in the problems used by the Open Tree of Life project. The taxonomic input is complete (lacks any sub-sampling based on taxon inclusion probabilities). In addition to having errors introduced by ECR moves, the taxonomic input undergoes branch collapsing (using the user-supplied edge-contraction probability on each internal edge independently) to mimic the unresolved character of most taxonomies.

We simulated a collection of supertree problems containing 50-1000 taxa, all with 20 phylo-inputs.

Each OTU was included in the phylogeny inputs with probability 0.5. Each edge in the taxonomy was collapsed with probability 0.75. We introduced two ECR errors per tree. For each simulation condition, we determined the run time by averaging across 15 simulated data sets.

batch	oracle	incremental	rollback	time
0	0	0	0	3323m
1	1	0	0	345m
0	0	1	0	527m
1	1	1	0	271m
0	0	1	1	5m 44s
1	1	1	1	2m 56s

Table 1: Run times for handling the OToL 13.4 data set without subproblem decomposition.

Results

We examined the effect of different optimizations by looking at their run time on simulated data sets and one real data set. Run times are for an Intel i7-5820K CPU with 32 Gb RAM running Linux.

Simulated data

We first examined the effect of the Batching and Oracle optimizations on simulated data sets as the number of taxa increased (Figure 6). Batching yields a speedup that increases from 1.6-fold at 50 taxa to 17-fold at 1000 taxa. Using the oracle to eliminate inconsistent splits shows no speedup when not paired with batching.

However, when combined with batching, the oracle yields an additional speedup that increases from 1.3-fold at 50 taxa to 2.4-fold at 1000 taxa. This indicates that the oracle allows larger batch sizes to succeed.

Given that our simulation protocol performs two ECR edits to each phylogeny, we expect about four splits to be inconsistent with the underlying tree per phylo-input. Therefore larger trees have a smaller fraction of inconsistent splits. That may explain why larger trees recieve a bigger speedup from batching.

Incrementalizing BUILD yields a larger speedup than the Oracle+Batch optimization (Figure 7). The speedup increases from 20-fold at 50 taxa to 398-fold at 1000 taxa. This represents an additional 9.9-fold speedup over Batching + Oracle at 1000 taxa. Much of this speedup relies on the abilty to save work via rollback: the incremental algorithm achieves only a 116-fold speedup at 1000 taxa. Rollback ability thus provides a speedup of 3.4-fold for BUILDINC over BUILDINC$''$.

It is possible to combine the Batching and Oracle optimizations with BUILDINC. This is because BUILDINC allows $\Delta\Sigma$ to include a batch of splits instead of just adding one split at a time. Adding Batching to BUILDINC yields a slight speedup of 27% over BUILDINC alone at 1000 taxa. However adding Batching + Oracle yields a 2.1-fold slowdown.

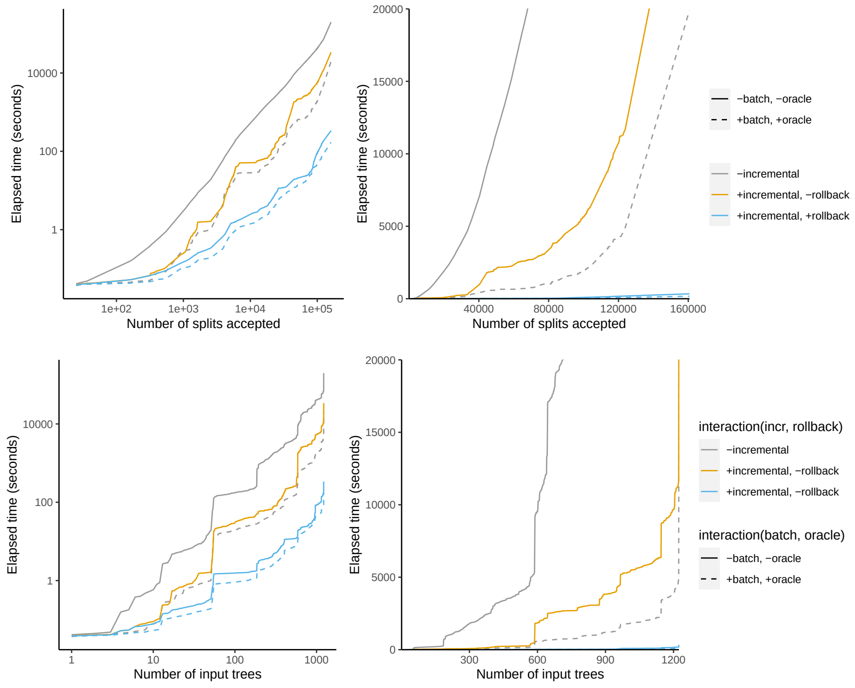


Figure 8: Time taken versus number of input splits accepted (top) or input trees processed (bottom). The left panel is log-scaled, whereas the right panel is not.

OpenTree data

We also examined a data set taken from the OToL synthesis release 13.4. As mentioned above, the OToL project normally divides the full supertree problem into subproblems after taxonomy-only taxa are removed [Redelings and Holder, 2017]. Here we consider the effect of optimizations on running the full supertree problem without dividing it. This is a much larger scale than the simulated data sets, which are designed to be similar to a single subproblem.

The data set includes 1223 non-empty trees in addition to the taxonomy. The taxonomy tree has 94,028 leaves. To give an idea of the size of the input trees, the three largest input trees contain 11217, 8369, and 7160 leaves respectively. All but 80 trees contain fewer than 331 leaves.

The total run time without optimization is 3323 minutes = 55 hours 23 minutes (Table 1). Batching + Oracle decreases the runtime to 345 minutes, which is a 9.6-fold decrease. BuildInc decreases the runtime further to 5 minutes 44s. This is a 60-fold speedup over Batching + Oracle, and a 579-fold speedup overall. Surprisingly, if we disable rollback, the runtime is 527 minutes, which is even slower than Batching + Oracle. This indicates that the OToL supertree problem contains more conflicting splits than the simulated data set above. Additionally, BuildInc + Batching + Oracle achieves an additional 1.95-fold speedup over BuildInc. This is different than in the simulations above, where BuildInc + Batching + Oracle was slower than BuildInc.

When using the naive Build algorithm, our supertree algorithm considers a total of 183850 splits and calls Build 183850 times. Of these splits, 160682 are accepted. So, 87.4% of splits are accepted and 12.6% are rejected.

When the oracle is enabled, 162517 splits are considered. This lowers the fraction of rejected splits to 1.1%. When using the Oracle + Batch optimizations, Build is called only 14481 times.

Figure 8 shows that some phylo-inputs take a lot more time than others. Processing splits from the taxonomy tree takes a large fraction of the total time. However, when graphed against the number of accepted splits, the relationship is more linear, indicating that the effect of large trees is at least partly driven by the fact that large trees have a large number of splits.

Discussion

We set out to improve the speed of our supertree algorithm that calls Build many times in a row. By using an incremental algorithm that re-uses work from previous calls to Build we were able to achieve a speedup of up to 579-fold in practice.

Incrementalizing faster version of Build

Our current approach uses a naive approach to Build that achieves $\mathcal{O}(M^3)$ time. Future research should consider whether it is possible to modify our incremental algorithm to incorporate recent improvements to Build that decrease the order, such as Deng and Fernández-Baca [2018]. In fact, their algorithm relies on another incremental algorithm – incremental graph connectivity – which identifies new connected components that appear as edges are deleted or added [Holm et al., 2001]. One approach might therefore be to replace our map of taxa to `Component` objects at each level with a graph that supports incremental connectivity queries. This would involve incrementally adding any required edges at each recursive level and identifying connected components that are merged.

One difficulty with this strategy is that we assume the data structures used to find connected components on each recursive level are separate. In constrast, Deng and Fernández-Baca [2018] construct a single graph at the beginning of the algorithm, and then remove additional edges from the single, shared graph at each recursive level. It might be possible to adapt this approach by saving a copy of the relevant portion of the graph at each recursive level to preserve a snapshot of previous work that is unmodified by work at deeper levels. However, even if this is feasible, it is not yet clear how much this would change the running time of the algorithm.

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A Proof of Invariants

A.1 At least one of `S` or `O` is empty

When BuildIncA$''$ is first called, `O` has no splits, so the invariant holds.

The RemoveIrrelevantSplits step can alter `S` and `O` in two ways. First, if `O` contains a solution `S`$'$ with the same taxon set as `S`, then we can replace `S` with `S`$'$ and clear `O`. Second, if one of the sub-solutions in `O` is punctured, we remove it from `O` and add its child solutions to `O`, but `S` remains empty. In both of these cases, the invariant is preserved. Further steps inside BuildIncA$''$ do not modify `S` or `O`.

When BuildIncA$''$ is recursively called on an unmodified component, `O` will be empty. When BuildIncA$''$ is called on a modified component or a new component, `S` will be empty. So, this invariant is preserved in recursive calls to BuildIncA$''$.

Therefore, since the invariant is initially true, and is preserved within BuildIncA$''$ and at recursive calls, it holds by induction.

A.2 Original solutions in `O` have a taxon set inside `S.T`

`O` is empty when BuildIncA$''$ is first called. When `C.O` is initially filled by merging two components, all the original solutions in `C.O` are for original components that are subsets of the new component. Therefore, when calling BuildIncA$''$(`C.S`, `C.`$\Delta\Sigma$, `C.O`), all the solutions in `O`=`C.O` will have a taxon set inside `S.T`.

When RemoveIrrelevantSplits replaces a punctured solution with its child solutions, the child solutions remain inside the taxon set of the current problem, since they are contained within their parent taxon set, which was inside the taxon set of the current problem. QED.

A.3 Original solutions in `O` have non-overlapping taxon sets

`O` is empty when BuildIncA$''$ is first called. When `O` is initially filled by merging a component, all the solutions in `O` must have non-overlapping taxon sets, since they are solutions for different equivalence classes on the same level.

When RemoveIrrelevantSplits replaces a punctured solution by its child solutions, it preserves this property, since the taxon sets of the child solutions are non-overlapping, and are contained within the taxon set of their removed parent. Thus the solutions in `O` will always have non-overlapping taxon sets.

B Properties of `Solution` s

B.1 Extracting the tree from a Solution

If the full Build algorithm succeeds, a tree can be extracted from the `Solution` object. A `Solution` object `S` maps to a node n in the tree. The node's children consist of either (i) internal nodes (one for each component in `S.`$\mathcal{C}$) or (ii) leaves (one for each trivial component; *i.e.* taxon identifier for which `S.M` is a Null reference). The original `Solution` object created in Build corresponds to the root of the tree.

B.2 Extracting the splits Σ from a Solution

Each `Solution` object `S` is created by performing BUILDA on a set of splits Σ. If BUILDA($\mathtt{S}, \Sigma$) succeeds, then after it is complete `S` will contain the splits Σ. However, only the splits `S.I` are *directly* contained in `S`. The remaining splits of Σ that are not stored in `S.I` are contained in the child solutions of `S` (and their descendants).

We can recover the set of splits in `S` as follows:

$$\Sigma(S) = \mathtt{S.I} \cup \left(\bigcup_{C \in S.\mathcal{C}} \Sigma(C.S) \right). \tag{1}$$

A solution is considered "empty" if it contains no splits. This can only happen if both `S.I` and $\mathtt{S.}\mathcal{C}$ are empty. It is possible for $\mathtt{S.}\mathcal{C}$ to be empty while `S.I` is non-empty, so both fields must be used.

B.3 The relationship between `S.T` and $\Sigma(S)$

Additionally, if `S` is a solution to some component `C`, then the taxon set `S.T` is determined by the splits $\Sigma(\mathtt{S})$:

$$\mathtt{S.T} = \bigcup_{\sigma \in \Sigma(S)} \sigma_1 \tag{2}$$

Addionally the taxa in `S.T` form a connected component that is connected *only* through edges corresponding to splits in $\Sigma(\mathtt{S})$.

The only exception to equation (2) is the top level `Solution`. The top level taxon set is directly initialized by the user and does not correspond to a component that was identified by running BUILDA, so there may be taxa in T that are not mentioned in Σ. These taxa will connect directly to the root since they are not in the include group of any split. However, for `Solution` objects below the top level, equation (2) holds.