Constructing the simplest possible phylogenetic network from triplets

(Two efficient algorithms for combining multiple smaller evolutionary hypotheses into one overall hypothesis)

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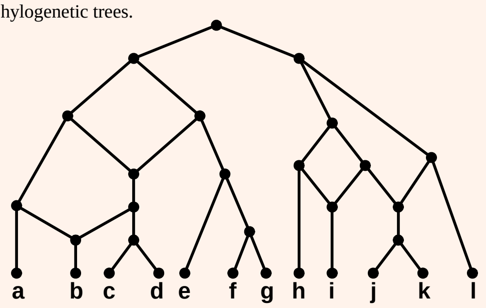
1) Phylogenetic networks generalise phylogenetic (evolutionary) trees

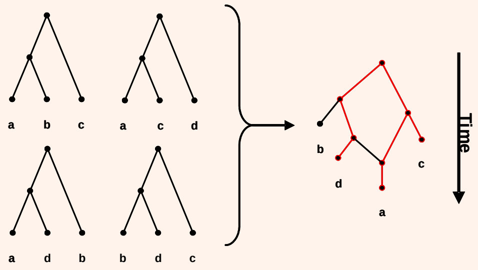
A phylogenetic network is a directed acyclic graph that visualises a rooted evolutionary history containing so-called reticulations such as recombinations, hybridisations or lateral gene transfers. Phylogenetic networks are thus **powerful generalisations** of phylogenetic trees.



An example of a (level-2) phylogenetic network. Arcs are assumed to be directed downwards, away from the root.

Here we consider the construction of a **simplest possible** phylogenetic network consistent with an input set T, where T contains at least one phylogenetic tree on three leaves (a triplet) for each combination of three taxa. Each triplet represents a hypothesis about the evolutionary history of those three taxa. In essence, we thus wish to find a single phylogenetic network containing all the taxa and **which does not contradict any of the hypotheses represented by the input triplets**.

To quantify the complexity of a network we consider both the total number of reticulations (i.e. vertices with indegree 2) and the number of reticulations per biconnected component, called the **level** of the network. The lower the level of a network, the more 'tree-like' it is, with level-0 networks being phylogenetic trees.

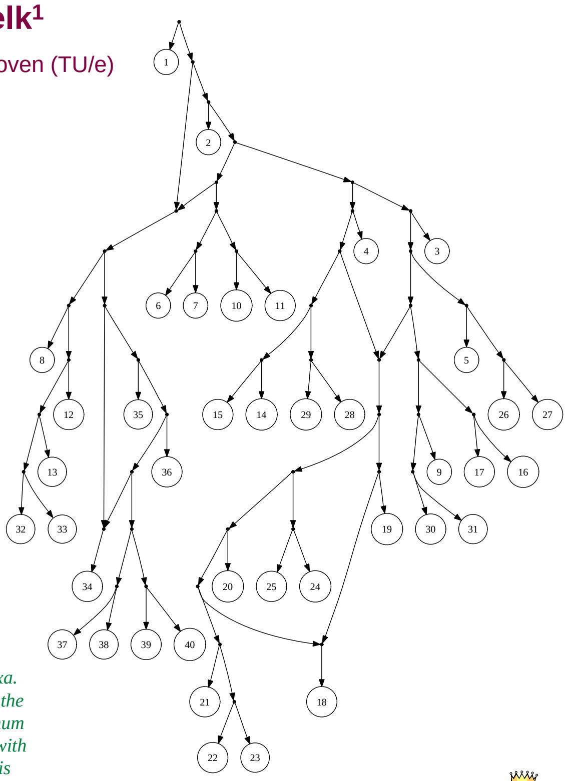


*In this example we are given as input the triplets ab|c, ac|d, ad|b and bd|c. We say a network is consistent with a triplet if there is a subdivision of the triplet embedded in the network. There is no rooted binary tree with leaf set {a,b,c,d} that is consistent with all four triplets. But, as shown here, there does exist a rooted **network** consistent with all four of them. By way of illustration an embedding of ac|d within the network is shown in red. The network is level-1.*

3) From theory to practice: MARLON (Minimum Amount of Reticulation Level One Network)

We have implemented the level-1 algorithm in Java and, using the Maximum Likelihood (ML) package PHYML to generate the input triplets, have tested it on simulated data with promising results. The resulting package **MARLON** has been made publicly available alongside the accompanying test data.

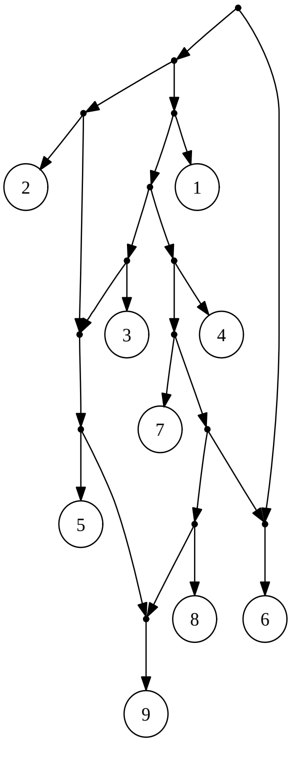
The figure on the right shows the output of MARLON on simulated triplet data for 40 taxa. Amongst all level-1 networks consistent with the triplet set, this is guaranteed to have a minimum number of reticulation vertices (i.e. vertices with indegree 2). Simulations in which MARLON is compared to the package T-REX suggest MARLON is competitive in terms of its capacity to recreate the original network.



4) From theory to practice: SIMPLISTIC (SIMPLe network heurISTIC)

Our theoretical results also form the basis for a second package, **SIMPLISTIC**, that we have also made publicly available. The chief advantage of SIMPLISTIC is that it **always** returns some phylogenetic network consistent with all the input triplets as a solution (whilst striving to minimise the level of that network) even if there are many errors in the input triplets and/or the underlying evolution is of a high level.

Tests of SIMPLISTIC on yeast data of Fraser et al. (Same-sex mating and the origin of the Vancouver Island Cryptococcus gattii outbreak, Fraser et al, Nature 437:7063, 1360-1364 (2005)) have produced interesting insights into the possible location of reticulate evolutionary events within that group of yeasts.



The figure on the left shows a simple example of the type of networks that SIMPLISTIC can produce. (This is a level-3 network: there are three reticulation vertices nested together.) Existing algorithms such as MARLON (and the related algorithm LEVEL2 [1]) perform well if the input data is consistent with level-1 or level-2 networks. SIMPLISTIC complements this approach by always returning a network even if the input data is more complex than level-2.

2) Theoretical results

We give polynomial-time (i.e. efficient) algorithms for constructing a level-1 respectively a level-2 network that contains a minimum number of reticulations and is consistent with T (if such a network exists) [2]. These algorithms extend the results given in [3] and [1]. In addition, we show that if T is precisely equal to the set of triplets consistent with some network, then we can construct such a network with smallest possible level in polynomial time, if k is a fixed upper bound on the level of the network [2].

5) Next steps

MARLON and SIMPLISTIC are freely available on-line [4]. A basic, but important step is to add a graphical user interface to SIMPLISTIC. A crucial extension to SIMPLISTIC which will further extend its relevance to real-world data is to relax the constraint that it only returns networks consistent with 100% of the input triplets. This is important because, although SIMPLISTIC is theoretically efficient, it can take a long time to terminate if the input data is heavily 'knotted' i.e. is only consistent with networks of very high level. This is work in progress!

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Literature

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[4] http://homepages.cwi.nl/~kelk