A short note on exponential-time algorithms for hybridization number

Leo van Iersel, Steven Kelk, Nela Lekić, Leen Stougie

December 5, 2013

Abstract

In this short note we prove that, given two (not necessarily binary) rooted phylogenetic trees $T_1, T_2$ on the same set of taxa $X$, where $|X| = n$, the hybridization number of $T_1$ and $T_2$ can be computed in time $O^*(2^n)$ i.e. $O(2^n \cdot \text{poly}(n))$. The result also means that a Maximum Acyclic Agreement Forest (MAAF) can be computed within the same time bound.

1 Introduction

Let $X$ be a finite set. A rooted phylogenetic $X$-tree, henceforth abbreviated to tree, is a rooted tree with no vertices with indegree 1 and outdegree 1, a root with indegree 0 and outdegree at least 2, and leaves bijectively labelled by the elements of $X$. A rooted phylogenetic network, henceforth abbreviated to network, is a directed acyclic graph with no vertices with indegree 1 and outdegree 1 and leaves bijectively labelled by the elements of $X$.

A tree $T$ is displayed by a network $N$ if $T$ can be obtained from a subgraph of $N$ by contracting edges. Note that, when $T$ is not binary, this means that the image of $T$ inside $N$ can be more “resolved” than $T$ itself. Using $d^-(v)$ to denote the indegree of a vertex $v$, a reticulation is a vertex $v$ with $d^-(v) \geq 2$. The reticulation number of a network $N$ with vertex set $V$ is given by

$$r(N) = \sum_{v \in V : d^-(v) \geq 2} (d^-(v) - 1).$$

Given two (not necessarily binary) trees $T_1$, $T_2$, the hybridization number problem (originally introduced in [2]) asks us to minimize $r(N)$ ranging over all networks that display $T_1$ and $T_2$.

There has been extensive work on fixed-parameter tractable (FPT) algorithms for the hybridization number problem. The fastest such algorithm currently works only on binary trees and has a running time of $O(3.18^n \cdot \text{poly}(n))$ where $r$ is the hybridization number and $n = |X|$ [7]. Given that $n$ is a trivial upper bound on the hybridization number of two trees this immediately yields an exponential-time algorithm with running time $O^*(3.18^n)$ for the binary case. In [5] a $O^*(3^n)$ algorithm was presented (again restricted to the binary case). In [3] a $O^*(2^n)$ algorithm was implied but this relied on the claimed equivalence between the softwired cluster model and the model described in [1], which was not formally proven. Here we describe explicitly a $O^*(2^n)$ algorithm that does not rely on this equivalence. This also means that a Maximum Acyclic Agreement Forest (MAAF) can be computed within the same time bound (see e.g. [6] for related discussions).

For further background and definitions on hybridization number and phylogenetic networks we refer the reader to recent articles such as [4]. For background and definitions on softwired clusters (which the proof below uses heavily) see [3].


2 Results

Theorem 1. Let $T_1$ and $T_2$ be two (not necessarily binary) rooted phylogenetic trees on the same set of taxa $X$, where $|X| = n$. Then the hybridization number $h(T_1, T_2)$ can be computed in time $O^{*}(2^n)$.

Proof. Let $C = Cl(T_1) \cup Cl(T_2)$ be the union of the sets of clusters induced by the edges of the trees $T_1$ and $T_2$. It has been shown that $r(C)$, the minimum reticulation number of a phylogenetic network representing all the clusters in $C$, is exactly equal to $h(T_1, T_2)$ [3] Lemma 12 and that optimal solutions for one problem can be transformed in polynomial time into optimal solutions for the other [4]. We hence focus on computation of $r(C)$. Recall that an ST-set $S$ of a set of clusters is a subset of $X$ such that $S$ is compatible with every cluster in $C$, and such that all clusters in $C|S$ are pairwise compatible, where $C|S = \{C \cap S : C \in C\}$. (The non-empty ST-sets are in one-to-one correspondence with common pendant subtrees of $T_1$ and $T_2$ [4].) For $X' \subseteq X$, we write $C \setminus X'$ to denote $\{C \setminus X' : C \in C\}$. An ST-set sequence of length $k$ is a sequence $S_1, S_2, \ldots, S_k$ such that each $S_i$ is an ST-set of $C_{i-1}$, where $C_0 = C$ and for $1 \leq i \leq k$, $C_i = C_{i-1} \setminus S_i$. Such a sequence is a tree sequence if $C_k$ is compatible. Note that if $C$ is compatible then this is characterized by the empty tree sequence and we say that $k = 0$. The value $r(C)$ is equivalent to the minimum possible length ranging over all ST-set tree sequences [3] Corollary 9. Without loss of generality we can assume that $S_k$ is a maximal ST-set sequence i.e. where each $S_i$ is a maximal ST-set of $C_{i-1}$. For a given set of clusters on $n$ taxa there are at most $n$ maximal ST-sets, they partition the set of taxa and they can be computed in polynomial time [3]. Clearly, $r(C) = 0$ if $C$ is compatible which can be checked in polynomial time. Otherwise the above observations yield the following expression, where $ST(C)$ is the set of maximal ST-sets of $C$:

$$r(C) = \min_{S \in ST(C)} \left( 1 + r(C \setminus S) \right)$$

(1)

This can be computed in time $O^{*}(2^n)$ by standard exponential time dynamic programming. That is, compute $r(C)$ by computing $r(C|X')$ for all possible $\emptyset \subset X' \subset X$, increasing the cardinality of $X'$ from small to large. Each $r(C|X')$ can then be computed by consulting at most $n$ smaller subproblems. This yields an overall running time of $O(2^n \cdot \text{poly}(n))$. \hfill \square

3 Discussion

A consequence of the above analysis is that, when solving hybridization number, there are at most $2^n$ relevant subproblems and each such subproblem can be characterized by a subset of $X$. Any algorithm that attempts to compute the hybridization number by iteratively pruning maximal common pendant subtrees (equivalently, maximal ST-sets) until the input trees are compatible, can thus easily attain a $O^{*}(2^n)$ upper bound on its running time, at the expense of potentially consuming exponential space. That is, by storing the solutions to subproblems in a look-up table (i.e. hashtable), indexed by the subset of $X$ that characterises the subproblem.

Finally, an obvious open question that remains is whether the hybridization number of two trees can be computed in time $O^{*}(c^n)$ for any constant $c < 2$.

References

[1] V. Bafna and V. Bansal. Inference about recombination from haplotype data: lower bounds and recombination hotspots. Journal of Computational Biology, 13:501–21, 2006.

[2] M. Baroni, S. Grünewald, V. Moulton, and C. Semple. Bounding the number of hybridisation events for a consistent evolutionary history. Mathematical Biology, 51:171–182, 2005.

[3] S.M. Kelk, C. Scornavacca, and L.J.J. van Iersel. On the elusiveness of clusters. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 9(2):517–534, 2012.
[4] T. Piovesan and S.M. Kelk. A simple fixed parameter tractable algorithm for computing the hybridization number of two (not necessarily binary) trees. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, 10(1):18–25, January 2013.

[5] C. Scornavacca, S. Linz, and B. Albrecht. A first step toward computing all hybridization networks for two rooted binary phylogenetic trees. *Journal of Computational Biology*, 19(11):1227–1242, 2012.

[6] L.J.J. van Iersel, S.M. Kelk, N. Lekić, and L. Stougie. Approximation algorithms for nonbinary agreement forests. To appear in *SIAM Journal on Discrete Mathematics* (2014), ArXiv e-print available at [http://arxiv.org/abs/1210.3211](http://arxiv.org/abs/1210.3211).

[7] C. Whidden, R.G. Beiko, and N. Zeh. Fixed-parameter algorithms for maximum agreement forests. *SIAM Journal on Computing*, 42(4):1431–1466, 2013.