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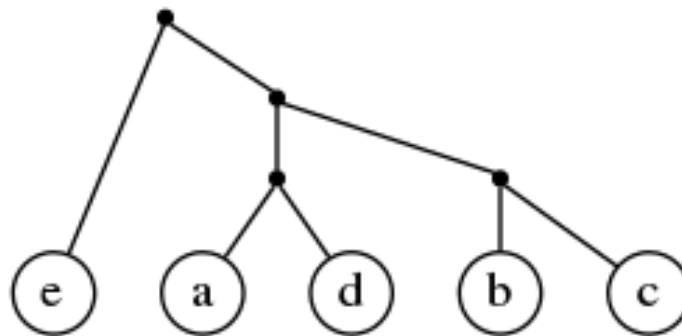
Constructing parsimonious hybridization networks using a SAT-solver

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presented by **Alexey Sergushichev**

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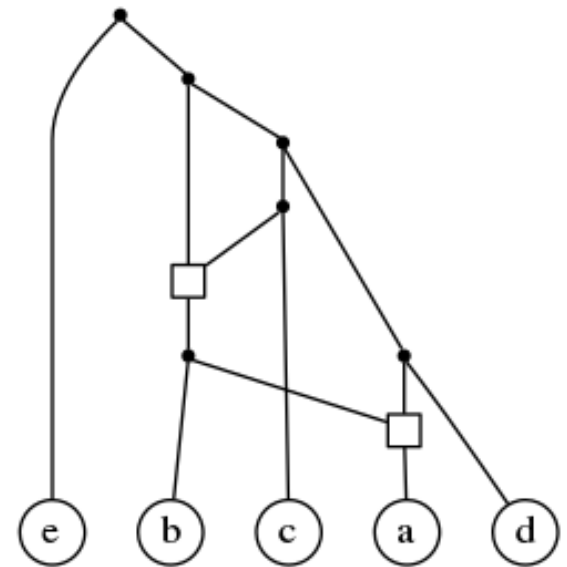
Phylogenetic tree

- Binary tree with set of taxa as leaves
- Can be defined for a particular gene



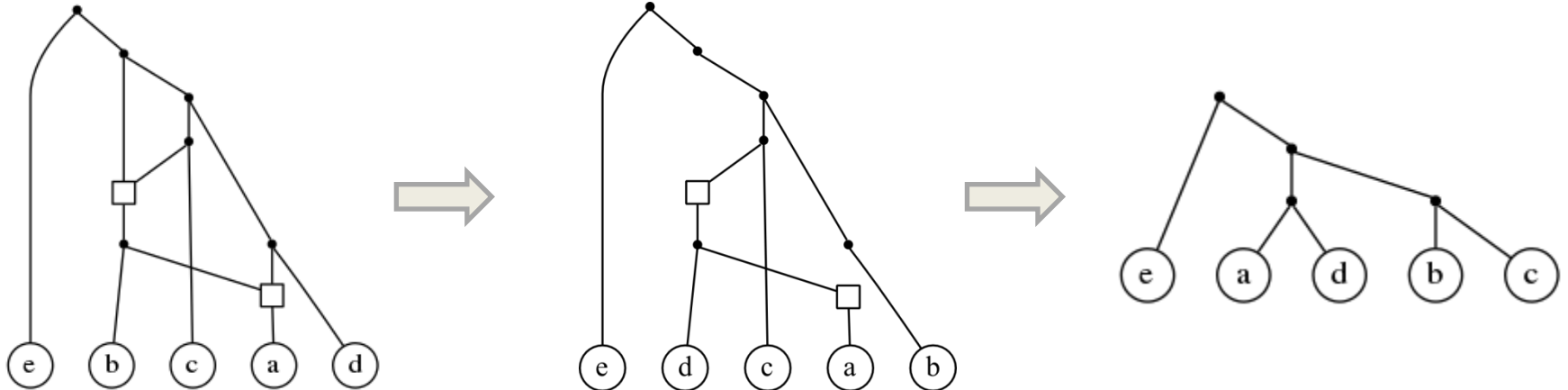
Hybridization network

- Directed acyclic graph with a single root
- Reticulation nodes:
in-degree=2, out-degree=1
- Regular nodes:
in-degree=1, out-degree=2
- Leaves: taxa

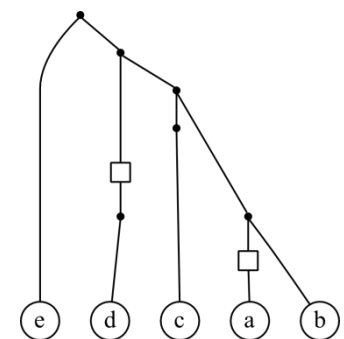
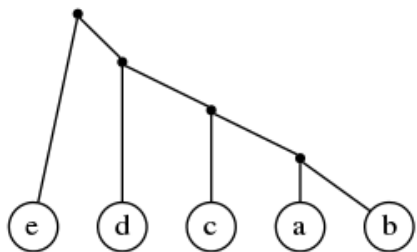
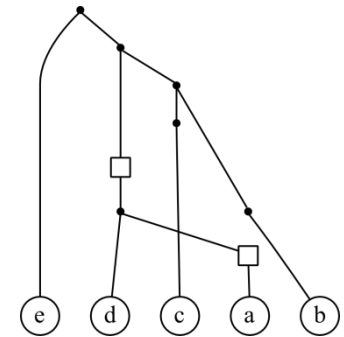
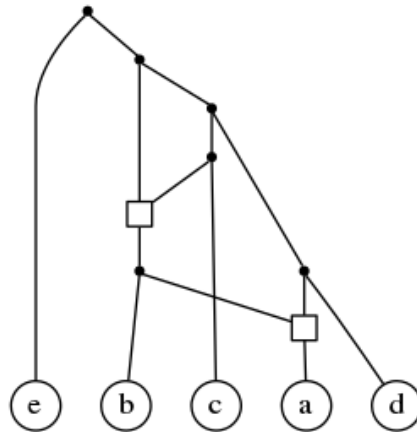
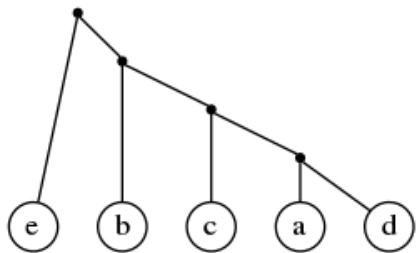
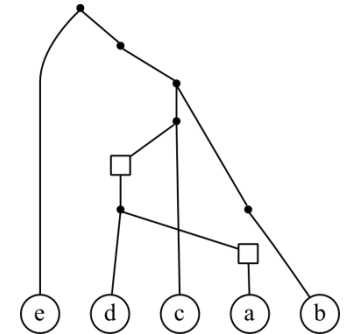
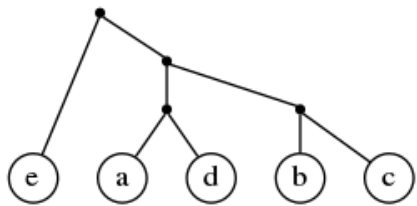


Displaying a tree

- Select direction a reticulation nodes
- Collapse simple paths



Hybridization network problem



Most parsimonious network

- Find a hybridization network for a set of phylogenetic trees T_1, T_2, \dots, T_t with the minimal number of reticulation nodes
- Is NP-complete even for $t=2$

Existing solutions

For two trees:

- CASS (heuristic)
- MURPAR (heuristic)

For multiple trees:

- PIRN_{CH} (heuristic)
- **PIRN_{C} (exact)**

Reduction to SAT

- Fix hybridization number k
- Make Boolean formula f so that $f \in \text{SAT}$ iff there is a hybridization network for k
- Check satisfiability with a SAT-solver
- Find minimal k with satisfiable formula
- Restore the network

SAT

- Boolean formula f in CNF form:
$$f(v_1, v_2, \dots) = (v_1 \vee \neg v_2 \vee \dots) \wedge (\dots) \wedge \dots$$
- Whether values for v_1, v_2, \dots exist that makes f true
- Can be seen as conjunction of multiple constraints
- Constraints can be of the form
$$(v_1 \wedge \neg v_2 \wedge \dots) \rightarrow v_3$$

Network structure

- $2n + 2k - 1$ nodes
 - $[1, n]$ — leaves (L)
 - $[n+1, 2n + k - 1]$ — regular nodes (V)
 - $[2n+k, 2n+2k-1]$ — reticulation nodes (R)

Network structure variables

- $l_{v,u}$ and $r_{v,u}$ — u is a left (right) child of v for v in V
- $p_{v,u}$ — u is parent of v for v in $L+V$
- p^l, p^r and c — parent child relations for reticulation nodes
- $O(n^2)$ variables

Network consistency constraints

- Nodes have only one left child, right child, parent
- u is child of $v \rightarrow v$ is parent of u
- u is parent of $v \rightarrow v$ is left of right child of u
- $O(n^3)$ constraints

Network consistency constraints:

Actual clauses

| | Clause | Range |
|------|--|--|
| 1.1 | $p_{v,u_1} \vee \dots \vee p_{v,u_k}$ | $v \in V; u_1 \dots u_k \in PP(v)$ |
| 1.2 | $p_{v,u} \rightarrow \neg p_{v,w}$ | $v \in V; u, w \in PP(v)$ |
| 2.1 | $l_{v,u_1} \vee \dots \vee l_{v,u_k}$ | $v \in V; u_1 \dots u_k \in PC(v)$ |
| 2.2 | $r_{v,u_1} \vee \dots \vee r_{v,u_k}$ | |
| 2.3 | $l_{v,u} \rightarrow \neg l_{v,w}$ | $v \in V; u, w \in PC(v)$ |
| 2.4 | $r_{v,u} \rightarrow \neg r_{v,w}$ | |
| 3.1 | $c_{v,u_1} \vee \dots \vee c_{v,u_k}$ | $v \in R; u_1 \dots u_k \in PC(v)$ |
| 3.2 | $c_{v,u} \rightarrow \neg c_{v,w}$ | $v \in R; u, w \in PC(v)$ |
| 4.1 | $p_{v,u_1}^l \vee \dots \vee p_{v,u_k}^l$ | $v \in R; u_1 \dots u_k \in PP(v)$ |
| 4.2 | $p_{v,u_1}^r \vee \dots \vee p_{v,u_k}^r$ | |
| 4.3 | $p_{v,u}^l \rightarrow \neg p_{v,w}^l$ | $v \in R; u, w \in PP(v)$ |
| 4.4 | $p_{v,u}^r \rightarrow \neg p_{v,w}^r$ | |
| 5.1 | $l_{v,u} \rightarrow \neg r_{v,w}$ | $v \in V; u, w \in PC(v) : u \geq w$ |
| 5.2 | $p_{v,u}^l \rightarrow \neg p_{v,w}^r$ | $v \in R; u, w \in PP(v) : u \geq w$ |
| 6.1 | $l_{v,u} \rightarrow p_{u,v}$ | |
| 6.2 | $r_{v,u} \rightarrow p_{u,v}$ | $v \in V; u \in V \cap PC(v)$ |
| 6.3 | $p_{u,v} \rightarrow (l_{v,u} \vee r_{v,u})$ | |
| 7.1 | $l_{v,u} \rightarrow (p_{u,v}^l \vee p_{u,v}^r)$ | |
| 7.2 | $r_{v,u} \rightarrow (p_{u,v}^l \vee p_{u,v}^r)$ | $v \in V; u \in R \cap PC(v)$ |
| 7.3 | $p_{u,v}^l \rightarrow (l_{v,u} \vee r_{v,u})$ | |
| 7.4 | $p_{u,v}^r \rightarrow (l_{v,u} \vee r_{v,u})$ | |
| 8.1 | $c_{v,u} \rightarrow p_{u,v}$ | |
| 8.2 | $p_{u,v} \rightarrow c_{v,u}$ | $v \in R; u \in V \cap PC(v)$ |
| 9.1 | $c_{v,u} \rightarrow (p_{u,v}^l \vee p_{u,v}^r)$ | |
| 9.2 | $p_{u,v}^l \rightarrow c_{v,u}$ | $v \in R; u \in R \cap PC(v)$ |
| 9.3 | $p_{u,v}^r \rightarrow c_{v,u}$ | |
| 10.1 | $c_{v,u} \rightarrow \neg p_{v,w}^l$ | $v \in R; u \in PC(v); w \in PP(v) : u \geq w$ |
| 10.2 | $c_{v,u} \rightarrow \neg p_{v,w}^r$ | |

| | Clause |
|-----|---------------------------------------|
| 1.1 | $p_{v,u_1} \vee \dots \vee p_{v,u_k}$ |
| 1.2 | $p_{v,u} \rightarrow \neg p_{v,w}$ |
| 2.1 | $l_{v,u_1} \vee \dots \vee l_{v,u_k}$ |
| 2.2 | $r_{v,u_1} \vee \dots \vee r_{v,u_k}$ |
| 2.3 | $l_{v,u} \rightarrow \neg l_{v,w}$ |
| 2.4 | $r_{v,u} \rightarrow \neg r_{v,w}$ |

Displaying structure

- For a tree T
- Choice of a parent for reticulation nodes
- Variables for correspondence between network and tree nodes
- Collapsing non-branching paths
 - Whether particular nodes were removed or not
 - Parent relations after collapsing
- $O(tn^2)$ variables

Displaying consistency constraints

- All T nodes are uniquely mapped to network nodes
- Parent relations in the tree uniquely correspond to the network structure after selecting directions at reticulation points and collapsing paths
- Parent relations in the network are consistent
- $O(tn^3)$ constraints

Displaying consistency constraints:

Actual clauses (1)

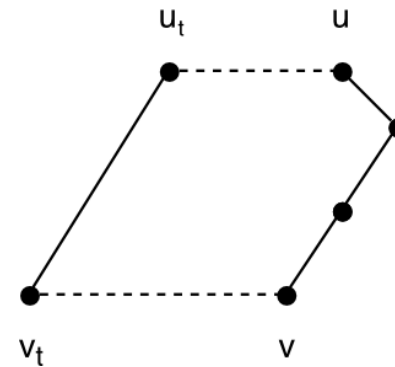
| | Clause | Range |
|-----|--|---|
| 1.1 | $a_{t,v,u_1} \vee \dots \vee a_{t,v,u_k}$ | $t \in T; v \in V \cup L \cup R; u_1 \dots u_k \in PU(v)$ |
| 1.2 | $a_{t,v,u} \rightarrow \neg a_{t,v,w}$ | $t \in T; v \in V \cup L \cup R; u, w \in PU(v)$ |
| 2.1 | $x_{t,v_t,v_1} \vee \dots \vee x_{t,v_t,v_k}$ | $t \in T; v_t \in V(t); v_1 \dots v_k \in V$ |
| 2.2 | $x_{t,v_t,v} \rightarrow \neg x_{t,v_t,w}$ | $t \in T; v_t \in V(t); v, w \in V$ |
| 2.3 | $x_{t,v_t,v} \rightarrow \neg x_{t,u_t,v}$ | $t \in T; v_t, u_t \in V(t); v \in V$ |
| 3.1 | $x_{t,v_t,v} \rightarrow u_{t,v}$ | $t \in T; v \in V; v_t \in V(t)$ |
| 3.2 | $x_{t,\rho_t,\rho}$ | $t \in T; \rho_t = \rho(t)$ |
| 4.1 | $x_{t,u_t,u} \rightarrow a_{t,v,u}$ | $t \in T; v \in L; u \in PP(v); u_t = p(v_t)$ |
| 4.2 | $a_{t,v,u} \rightarrow x_{t,u_t,u}$ | |
| 4.3 | $(x_{t,v_t,v} \wedge x_{t,u_t,u}) \rightarrow a_{t,v,u}$ | $t \in T; v \in V; u \in PP(v); v_t \in V(t); u_t = p(v_t)$ |
| 4.4 | $(x_{t,v_t,v} \wedge a_{t,v,u}) \rightarrow x_{t,u_t,u}$ | |
| 4.5 | $x_{t,v_t,v} \rightarrow \neg x_{t,u_t,u}$ | $t \in T; v \in V; u \in V; v_t \in V(t); u_t = p(v_t) : u < v$ |
| 5.1 | $\neg x_{t,v_t,v}$ | $t \in T; v \in V; v_t \in V(t) : v_t < \text{size}(\text{subtree}(v_t))$ |
| 5.2 | $\neg x_{t,v_t,v}$ | $t \in T; v \in V; v_t \in V(t) : v_t > \text{size}(t) - \text{depth}(v_t)$ |
| 5.3 | $\neg x_{t,v_t,v} \vee \neg x_{t',v_{t'},v}$ | $t, t' \in T; v \in V; v_t \in V(t); v_{t'} \in V(t') :$ subtrees of t and t' have disjoint sets of taxa |

Displaying consistency constraints:

Actual clauses (2)

| | Clause | Range |
|------|--|--|
| 1.1 | $(p_{v,u} \wedge u_{t,u}) \rightarrow a_{t,v,u}$ | $t \in T; v \in V \cup L; u \in V \cap PP(v)$ |
| 1.2 | $(p_{v,u} \wedge a_{t,v,u}) \rightarrow u_{t,u}$ | |
| 1.3 | $(p_{v,u} \wedge \neg u_{t,u} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ | |
| 1.4 | $(p_{v,u} \wedge \neg u_{t,u} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ | |
| 2.1 | $(p_{v,u}^l \wedge d_{t,v} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ | $t \in T; v \in R; u \in R \cap PP(v); w \in PU(u)$ |
| 2.2 | $(p_{v,u}^l \wedge d_{t,v} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ | |
| 2.3 | $(p_{v,u}^r \wedge \neg d_{t,v} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ | |
| 2.4 | $(p_{v,u}^r \wedge \neg d_{t,v} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ | |
| 2.5 | $(p_{v,u}^l \wedge d_{t,v} \wedge u_{t,u}) \rightarrow a_{t,v,u}$ | $t \in T; v \in R; u \in V \cap PP(v)$ |
| 2.6 | $(p_{v,u}^l \wedge \neg d_{t,v} \wedge u_{t,u}) \rightarrow a_{t,v,u}$ | |
| 2.7 | $(p_{v,u}^l \wedge d_{t,v} \wedge \neg u_{t,u} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ | |
| 2.8 | $(p_{v,u}^l \wedge d_{t,v} \wedge \neg u_{t,u} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ | |
| 2.9 | $(p_{v,u}^r \wedge \neg d_{t,v} \wedge \neg u_{t,u} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ | $t \in T; v \in R; u \in V \cap PP(v); w \in PU(u)$ |
| 2.10 | $(p_{v,u}^r \wedge \neg d_{t,v} \wedge \neg u_{t,u} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ | |
| 3.1 | $(p_{v,u}^l \wedge \neg d_{t,v}) \rightarrow \neg u_{t,u}^r$ | |
| 3.2 | $(p_{v,u}^r \wedge d_{t,v}) \rightarrow \neg u_{t,u}^l$ | |
| 3.3 | $(p_{v,u}^l \wedge \neg d_{t,v}) \rightarrow \neg u_{t,u}$ | $t \in T; v \in R; u \in V \cap PP(v)$ |
| 3.4 | $(p_{v,u}^r \wedge d_{t,v}) \rightarrow \neg u_{t,u}$ | |
| 4.1 | $(p_{v,u}^l \wedge d_{t,v} \wedge u_{t,v}^r) \rightarrow u_{t,u}^r$ | $t \in T; v \in R; u \in R \cap PP(v)$ |
| 4.2 | $(p_{v,u}^r \wedge \neg d_{t,v} \wedge u_{t,v}^l) \rightarrow u_{t,u}^l$ | |
| 4.3 | $(c_{u,v} \wedge \neg u_{t,v}^r) \rightarrow \neg u_{t,u}^r$ | |
| 4.4 | $(p_{v,u}^l \wedge \neg u_{t,v}^r) \rightarrow \neg u_{t,u}$ | |
| 4.5 | $(p_{v,u}^r \wedge \neg u_{t,v}^l) \rightarrow \neg u_{t,u}$ | $t \in T; v \in R; u \in V \cap PP(v)$ |
| 4.6 | $c_{v,u} \rightarrow u_{t,v}^l$ | |
| 5.1 | $p_{v,u} \rightarrow \neg a_{t,u,w}$ | $t \in T; v \in V \cup L; u \in R \cap PP(v);$ $w \in PU(u) : w \leq v$ |
| 5.2 | $(p_{v,u} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ | $t \in T; v \in V \cup L; u \in R \cap PP(v);$ $w \in PU(u) : w > v$ |
| 5.3 | $(p_{v,u} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ | $t \in T; v \in V \cup L; u \in R \cap PP(v);$ $w \in PU(u) : w > v$ |

| | Clause |
|-----|--|
| 1.1 | $(p_{v,u} \wedge u_{t,u}) \rightarrow a_{t,v,u}$ |
| 1.2 | $(p_{v,u} \wedge a_{t,v,u}) \rightarrow u_{t,u}$ |
| 1.3 | $(p_{v,u} \wedge \neg u_{t,u} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ |
| 1.4 | $(p_{v,u} \wedge \neg u_{t,u} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ |



All clauses

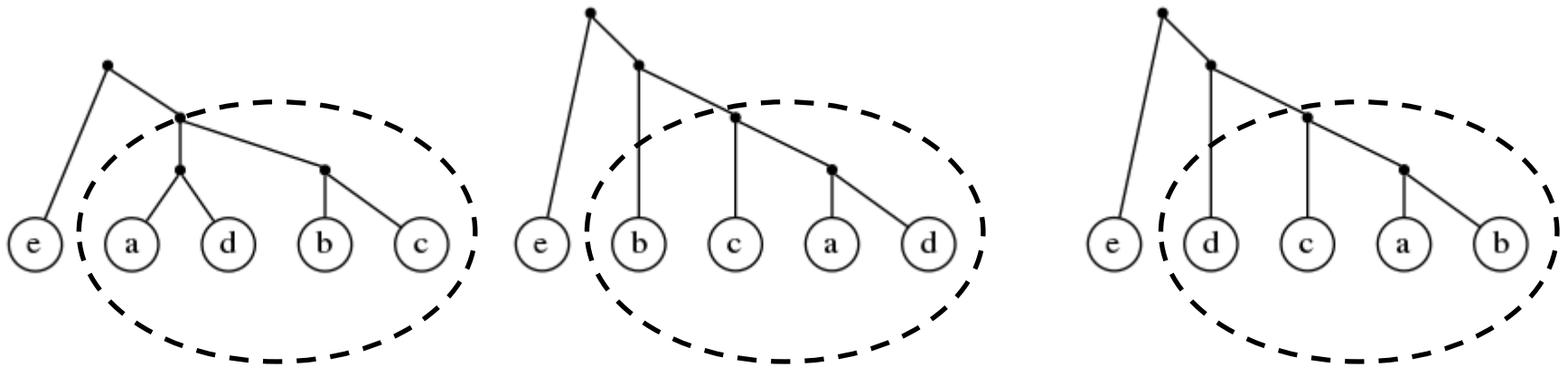
| Clause | Range |
|---|---|
| 1.1 $(p_{v,u} \wedge u_{t,u}) \rightarrow a_{t,v,u}$ | $t \in T; v \in V \cup L; u \in V \cap PP(v)$ |
| 1.2 $(p_{v,u} \wedge a_{t,v,u}) \rightarrow u_{t,u}$ | |
| 1.3 $(p_{v,u} \wedge \neg u_{t,u} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ | $t \in T; v \in V \cup L; u \in V \cap PP(v); w \in PP(u)$ |
| 1.4 $(p_{v,u} \wedge \neg u_{t,u} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ | |
| 2.1 $(p_{v,u}^l \wedge d_{t,v} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ | |
| 2.2 $(p_{v,u}^l \wedge d_{t,v} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ | $t \in T; v \in R; u \in R \cap PP(v); w \in PU(u)$ |
| 2.3 $(p_{v,u}^r \wedge \neg d_{t,v} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ | |
| 2.4 $(p_{v,u}^r \wedge \neg d_{t,v} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ | |
| 2.5 $(p_{v,u}^l \wedge d_{t,v} \wedge u_{t,u}) \rightarrow a_{t,v,u}$ | $t \in T; v \in R; u \in V \cap PP(v)$ |
| 2.6 $(p_{v,u}^l \wedge \neg d_{t,v} \wedge u_{t,u}) \rightarrow a_{t,v,u}$ | |
| 2.7 $(p_{v,u}^l \wedge d_{t,v} \wedge \neg u_{t,u} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ | |
| 2.8 $(p_{v,u}^l \wedge d_{t,v} \wedge \neg u_{t,u} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ | $t \in T; v \in R; u \in V \cap PP(v); w \in PU(u)$ |
| 2.9 $(p_{v,u}^r \wedge \neg d_{t,v} \wedge \neg u_{t,u} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ | |
| 2.10 $(p_{v,u}^r \wedge \neg d_{t,v} \wedge \neg u_{t,u} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ | |
| 3.1 $(p_{v,u} \wedge \neg d_{t,v}) \rightarrow \neg u_{t,u}^r$ | $t \in T; v \in R; u \in R \cap PP(v)$ |
| 3.2 $(p_{v,u}^l \wedge d_{t,v}) \rightarrow \neg u_{t,u}^l$ | |
| 3.3 $(p_{v,u}^l \wedge \neg d_{t,v}) \rightarrow \neg u_{t,u}$ | $t \in T; v \in R; u \in V \cap PP(v)$ |
| 3.4 $(p_{v,u}^r \wedge d_{t,v}) \rightarrow \neg u_{t,u}$ | |
| 4.1 $(p_{v,u}^l \wedge d_{t,v} \wedge u_{t,u}^r) \rightarrow u_{t,u}^r$ | |
| 4.2 $(p_{v,u}^l \wedge \neg d_{t,v} \wedge u_{t,u}^r) \rightarrow u_{t,u}^r$ | $t \in T; v \in R; u \in R \cap PP(v)$ |
| 4.3 $(c_{u,v} \wedge \neg u_{t,v}^r) \rightarrow \neg u_{t,u}^r$ | |
| 4.4 $(p_{v,u} \wedge \neg u_{t,u}^l) \rightarrow \neg u_{t,u}$ | $t \in T; v \in R; u \in V \cap PP(v)$ |
| 4.5 $(p_{v,u}^r \wedge \neg u_{t,u}^r) \rightarrow \neg u_{t,u}$ | |
| 4.6 $c_{v,u} \rightarrow u_{t,v}^r$ | $t \in T; v \in R; u \in (V \cup L) \cap PC(v)$ |
| 5.1 $p_{v,u} \rightarrow \neg a_{t,u,w}$ | $t \in T; v \in V \cup L; u \in R \cap PP(v); w \in PU(u) : w \leq v$ |
| 5.2 $(p_{v,u} \wedge a_{t,u,w}) \rightarrow a_{t,v,w}$ | $t \in T; v \in V \cup L; u \in R \cap PP(v); w \in PU(u) : w > v$ |
| 5.3 $(p_{v,u} \wedge a_{t,v,w}) \rightarrow a_{t,u,w}$ | $t \in T; v \in V \cup L; u \in R \cap PP(v); w \in PU(u) : w > v$ |

| Clause | Range |
|--|---|
| 1.1 $a_{t,v,u_1} \vee \dots \vee a_{t,v,u_k}$ | $t \in T; v \in V \cup L \cup R; u_1 \dots u_k \in PU(v)$ |
| 1.2 $a_{t,v,u} \rightarrow \neg a_{t,v,w}$ | $t \in T; v \in V \cup L \cup R; u, w \in PU(v)$ |
| 2.1 $x_{t,v_t,v_1} \vee \dots \vee x_{t,v_t,v_k}$ | $t \in T; v_t \in V(t); v_1 \dots v_k \in V$ |
| 2.2 $x_{t,v_t,v} \rightarrow \neg x_{t,v_t,w}$ | $t \in T; v_t \in V(t); v, w \in V$ |
| 2.3 $x_{t,v_t,v} \rightarrow \neg x_{t,u_t,v}$ | $t \in T; v_t, u_t \in V(t); v \in V$ |
| 3.1 $x_{t,v_t,v} \rightarrow u_{t,v}$ | $t \in T; v \in V; v_t \in V(t)$ |
| 3.2 $x_{t,\rho_t,\rho}$ | $t \in T; \rho_t = \rho(t)$ |
| 4.1 $x_{t,u_t,u} \rightarrow a_{t,v,u}$ | $t \in T; v \in L; u \in PP(v); u_t = p(v_t)$ |
| 4.2 $a_{t,v,u} \rightarrow x_{t,u_t,u}$ | |
| 4.3 $(x_{t,v_t,v} \wedge x_{t,u_t,u}) \rightarrow a_{t,v,u}$ | $t \in T; v \in V; u \in PP(v); v_t \in V(t); u_t = p(v_t)$ |
| 4.4 $(x_{t,v_t,v} \wedge a_{t,v,u}) \rightarrow x_{t,u_t,u}$ | |
| 4.5 $x_{t,v_t,v} \rightarrow \neg x_{t,u_t,u}$ | $t \in T; v \in V; u \in V; v_t \in V(t); u_t = p(v_t) : u < v$ |
| 5.1 $\neg x_{t,v_t,v}$ | $t \in T; v \in V; v_t \in V(t) : v_t < \text{size}(\text{subtree}(v_t))$ |
| 5.2 $\neg x_{t,v_t,v}$ | $t \in T; v \in V; v_t \in V(t) : v_t > \text{size}(t) - \text{depth}(v_t)$ |
| 5.3 $\neg x_{t,v_t,v} \vee \neg x_{t',v_{t'},v}$ | $t, t' \in T; v \in V; v_t \in V(t); v_{t'} \in V(t') : \text{subtrees of } t \text{ and } t' \text{ have disjoint sets of taxa}$ |

| Clause | Range |
|--|--|
| 1.1 $p_{v,u_1} \vee \dots \vee p_{v,u_k}$ | $v \in V; u_1 \dots u_k \in PP(v)$ |
| 1.2 $p_{v,u} \rightarrow \neg p_{v,w}$ | $v \in V; u, w \in PP(v)$ |
| 2.1 $l_{v,u_1} \vee \dots \vee l_{v,u_k}$ | $v \in V; u_1 \dots u_k \in PC(v)$ |
| 2.2 $r_{v,u_1} \vee \dots \vee r_{v,u_k}$ | |
| 2.3 $l_{v,u} \rightarrow \neg l_{v,w}$ | $v \in V; u, w \in PC(v)$ |
| 2.4 $r_{v,u} \rightarrow \neg r_{v,w}$ | |
| 3.1 $c_{v,u_1} \vee \dots \vee c_{v,u_k}$ | $v \in R; u_1 \dots u_k \in PC(v)$ |
| 3.2 $c_{v,u} \rightarrow \neg c_{v,w}$ | $v \in R; u, w \in PC(v)$ |
| 4.1 $p_{v,u_1}^l \vee \dots \vee p_{v,u_k}^l$ | $v \in R; u_1 \dots u_k \in PP(v)$ |
| 4.2 $p_{v,u_1}^r \vee \dots \vee p_{v,u_k}^r$ | |
| 4.3 $p_{v,u}^l \rightarrow \neg p_{v,w}^l$ | $v \in R; u, w \in PP(v)$ |
| 4.4 $p_{v,u}^r \rightarrow \neg p_{v,w}^r$ | |
| 5.1 $l_{v,u} \rightarrow \neg r_{v,w}$ | $v \in V; u, w \in PC(v) : u \geq w$ |
| 5.2 $p_{v,u}^l \rightarrow \neg p_{v,w}^r$ | $v \in R; u, w \in PP(v) : u \geq w$ |
| 6.1 $l_{v,u} \rightarrow p_{u,v}$ | |
| 6.2 $r_{v,u} \rightarrow p_{u,v}$ | $v \in V; u \in V \cap PC(v)$ |
| 6.3 $p_{u,v} \rightarrow (l_{v,u} \vee r_{v,u})$ | |
| 7.1 $l_{v,u} \rightarrow (p_{u,v}^l \vee p_{u,v}^r)$ | |
| 7.2 $r_{v,u} \rightarrow (p_{u,v}^l \vee p_{u,v}^r)$ | $v \in V; u \in R \cap PC(v)$ |
| 7.3 $p_{u,v} \rightarrow (l_{v,u} \vee r_{v,u})$ | |
| 7.4 $p_{u,v}^r \rightarrow (l_{v,u} \vee r_{v,u})$ | |
| 8.1 $c_{v,u} \rightarrow p_{u,v}$ | $v \in R; u \in V \cap PC(v)$ |
| 8.2 $p_{u,v} \rightarrow c_{v,u}$ | |
| 9.1 $c_{v,u} \rightarrow (p_{u,v}^l \vee p_{u,v}^r)$ | |
| 9.2 $p_{u,v}^l \rightarrow c_{v,u}$ | $v \in R; u \in R \cap PC(v)$ |
| 9.3 $p_{u,v}^r \rightarrow c_{v,u}$ | |
| 10.1 $c_{v,u} \rightarrow \neg p_{v,w}^l$ | $v \in R; u \in PC(v); w \in PP(v) : u \geq w$ |
| 10.2 $c_{v,u} \rightarrow \neg p_{v,w}^r$ | |

Additional optimizations

- Splitting into independent problems



- Symmetry breaking

Experiments

- 57 grasses dataset by Group G.P.W. et al
- CryptoMiniSAT solver
- 1000 s time limit
- Comparison with PIRNs

Experiments

- 57 grasses datasets by ~~Group G.P.W. et al~~
Grass Phylogeny Working Group
- CryptoMiniSAT solver
- 1000s time limit
- Comparison with PIRNs

Results

- Exact solution (out of 57)
 - PhyloSAT: 36
 - PIRN_C : 29
- Non-exact
 - PhyloSAT: 48 (40 optimal)
 - PIRN_{CH} : 43 (36 optimal)

Results for $k \geq 6$

| Test instance | PhyloSAT | PIRN _{CH} | Optimal solution |
|-------------------|-----------|--------------------|------------------|
| 2NdhfPhyt | 6 (9) | 6 (6) | 6 |
| 3NdhfPhytRpoc | 8 (1000) | 8 (28) | 6 |
| 3PhytRbclRpoc | 6 (11) | 6 (3) | 6 |
| 3RbclWaxyIts | 6 (1000) | 7 (4) | 6 |
| 4NdhfRbclWaxyIts | 7 (1000) | 7 (35) | ≥ 6 |
| 4PhytRbclRpocIts | 9 (1000) | 8 (377) | ≥ 6 |
| 2RbclRpoc | 7 (1000) | 7 (42) | 7 |
| 3NdhfWaxyIts | 8 (1000) | 8 (90) | ≥ 7 |
| 3PhytRbclIts | 11 (1000) | 8 (120) | ≥ 7 |
| 3PhytRpocIts | 7 (1000) | 7 (59) | 7 |
| 4NdhfPhytRbclRpoc | 10 (1000) | 10 (287) | ≥ 7 |
| 4NdhfPhytRpocIts | 10 (1000) | - | ≥ 7 |
| 2NdhfPhyt | 8 (12) | - | 8 |
| 2NdhfRbcl | 8 (1) | 8 (851) | 8 |
| 2PhytIts | 8 (41) | 8 (372) | 8 |
| 3NdhfPhytRbcl | 9 (123) | - | 9 |
| 2NdhfRpoc | 9 (954) | 9 (484) | 9 |
| 3NdhfRbclRpoc | 13 (1000) | - | ≥ 10 |
| 3NdhfPhytIts | 13 (1000) | - | ≥ 11 |

hybridization number (time in seconds)

Future work

- Different SAT-solvers
- Improving reduction
- Using upper and lower bounds on k
- Searching for all minimal solutions

Conclusions

- Constructing parsimonious hybridization networks can be approached with reducing to SAT
- This approach outperforms known exact solver and compares well with heuristic solver
- Solving bigger instances is still challenging

The End

<https://github.com/ctlab/PhyloSAT>

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