# Bridging the gap between rooted and unrooted networks

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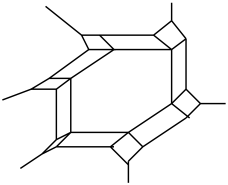
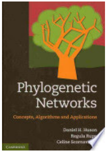
University of East Anglia, UK.

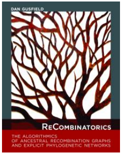
July 27, 2015

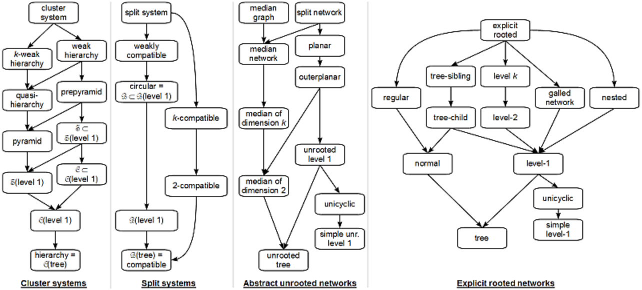
Joint work with Philippe Gambette and Guillaume Scholz



# The world of phylogenetic networks

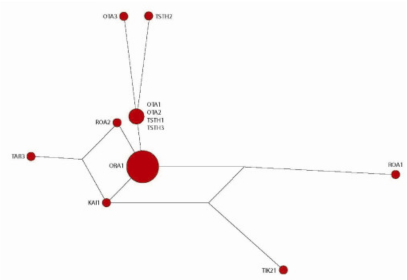


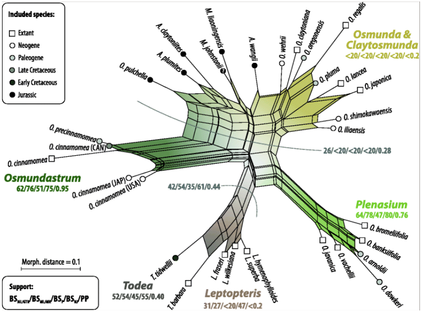




igm.univ-mlv.fr/ gambette/RePhylogeneticNetworks.php

# Unrooted networks

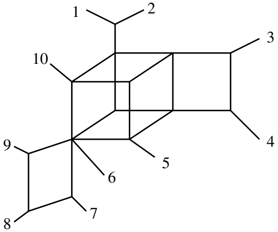



Lambertini et al. BMC Genetics 2010 11:52



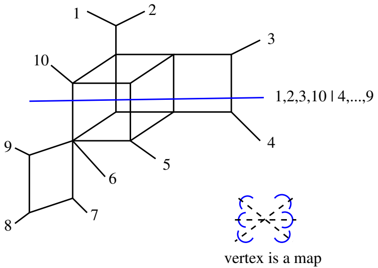

Bomfleur et al. BMC Evol. Biol. 2015 15:126

# How can we reconstruct them?

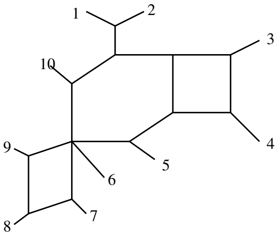



Buneman graph (aka median network)

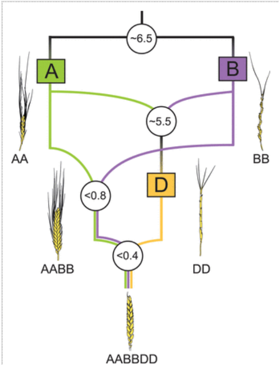
# From a combinatorial point of view, ...

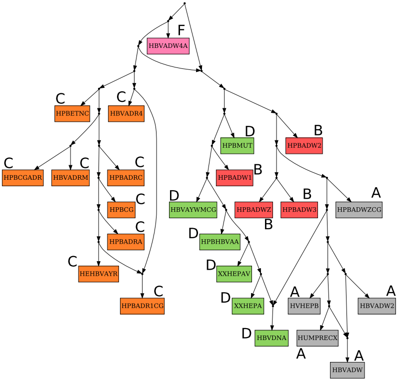


# One tale and two cities!



# Rooted networks

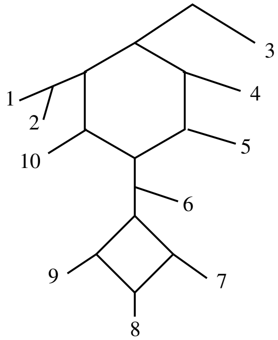



T Marcussen et al., Science 2014: Vol. 345 no. 6194

J Oldman, personal communication

# How can we reconstruct them?




Rooted 1–nested network[1]

Constructions:

- triplets* (e.g. Huber, Iersel, Kelk, Suckecki (Lev1athan); Iersel, Kelk (Marlon, Simplistic).
- rooted trees* (e.g. Iersel, Kelk, Rupp, Huson (Cass); Casens Mardulyn Milinkovitch (CombineTrees); Willson).
- soft/hardwired clusters* (e.g. Huson, Rupp (Cluster networks)).
- sequence alinments (e.g. Oldman, Wu, Iersel, Moulton (Trilonet)).
- multi-labelled trees (e.g. Lott Huber, Moulton, Oxelman (Padre)).
- ultrametric distances (e.g. Chan Jansson, Lam, Yiu (GalledNet); Apostolico, Comin Dress, Parida (Ultranet)).

$\star$: In general, they don't encode! – Gambette & H. 2012

[1] A *1-nested network on some set* $X$ is a rooted DAG with a unique root, leaf set $X$, no vertices of indegree and outdegree 1, and, in its underlying graph, two cycles can share a vertex.

# Unrooting rooted networks

A 2-level cactus model for the system of minimum and minimum+1 edge-cuts in a graph and its incremental maintenance

Yefim Dinitz *
Dept. of Computer Science
Technion, Haifa, Israel

Zeev Nutov †
Dept. of Applied Mathematics
Technion, Haifa, Israel

Abstract. Let λ denote the cardinality of a minimum edge-

Let us consider an undirected connected multi-

STOC'95

IEEE/ACM TRANSACTIONS ON COMPUTATIONAL BIOLOGY AND BIOINFORMATICS, VOL. 3, NO. 1, JANUARY-MARCH 2006

## Unicyclic Networks: Compatibility and Enumeration

Charles Semple and Mike Steel

**Abstract**—Graphs obtained from a binary leaf labeled ("phylogenetic") tree by adding an edge so as to introduce a cycle provide a useful representation of hybrid evolution in molecular evolutionary biology. This class of graphs (which we call "unicyclic networks") also has some attractive combinatorial properties, which we present. We characterize when a set of binary phylogenetic trees is

ELSEVIER
Discrete Applied Mathematics
Volume 157, Issue 10, 28 May 2009, Pages 2361–2369
Networks in Computational Biology

## Phylogenetic graph models beyond trees

Ulrik Brandes, Sabine Cornelsen
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Abstract

A graph model for a set S of splits of a set X
vertices of the graph such that the inclusion-n
Phylogenetic trees are graph models in whic

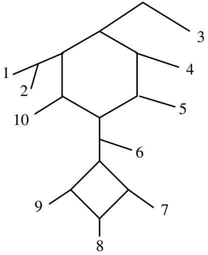
J Bioinform Comput Biol. 2012 Aug;10(4):1250004. doi: 10.1142/S0219720012500047. Epub 2012 Jun 22.

## Quartets and unrooted phylogenetic networks.

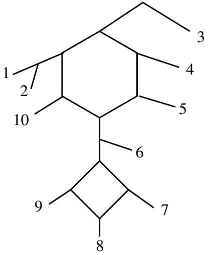
Gambette P[1], Berry V, Paul C.
Author information

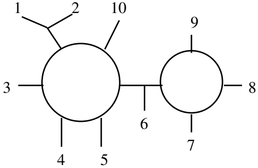
Abstract
Phylogenetic networks were introduced to describe evolution in the presence of exchange

# Unrooting rooted networks



# Unrooting rooted networks

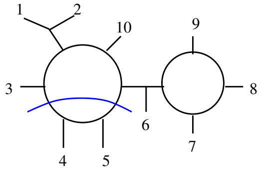



Unrooted 1–nested network[1]

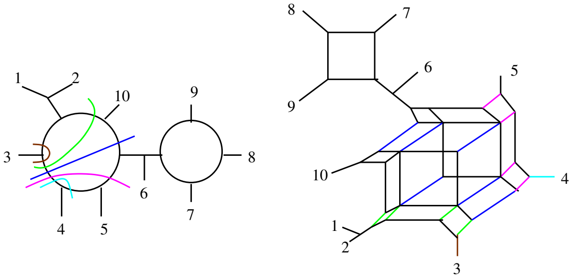
[1] A *unrooted* 1-nested network on $X$ is the underlying graph of a 1-nested network.

# Splits re-visited




A split $S$ of $X$ is *displayed* by a 1-nested network $N$ if there exists a set-inclusion minimal cut of $N$ that induces $S$.

# Interestingly, ...




Both graphs display the *same* split system!

# Questions

Given a set $\Sigma$ of splits on $X$:

**1:** When does there exist an (unrooted) 1-nested network displaying all splits in $\Sigma$?

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**1:** When does there exist an (unrooted) 1-nested network displaying all splits in $\Sigma$?

**2:** When does there exist an (unrooted) 1-nested network displaying exactly $\Sigma$ and what about uniqueness? (see also Brandes and Cornelsen, 2009).

# Questions

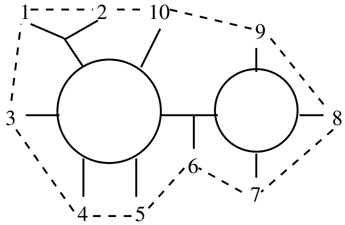
Given a set $\Sigma$ of splits on $X$:

**1:** When does there exist an (unrooted) 1-nested network displaying all splits in $\Sigma$?

**2:** When does there exist an (unrooted) 1-nested network displaying exactly $\Sigma$ and what about uniqueness? (see also Brandes and Cornelsen, 2009).

**3:** Provided that $\Sigma$ can be displayed by an (unrooted) 1-nested network, can we find an optimal one?

# When does there exist an (unrooted) 1-nested network displaying all splits in Σ?



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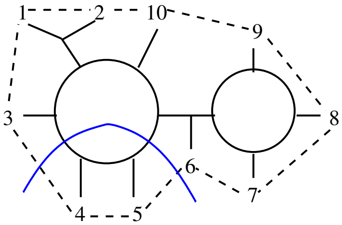
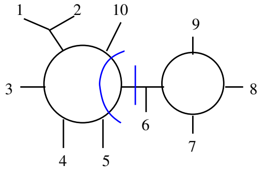



**Theorem 1 (Gambette, H., Scholz)** *There exists a 1-nested network N displaying Σ if and only if Σ is circular.*

# When does there exist an (unrooted) 1-nested network displaying exactly Σ and what about uniqueness?

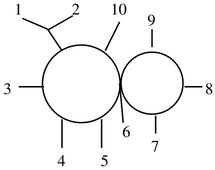
Observation 1:




Both cuts induce the same split!

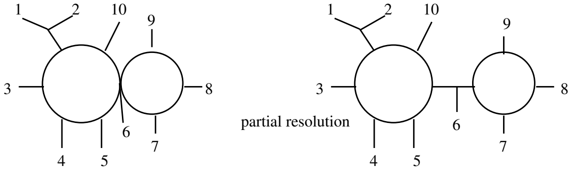
# When does there exist an (unrooted) 1-nested network displaying exactly $\Sigma$ and what about uniqueness?

Observation 1:



# When does there exist an (unrooted) 1-nested network displaying exactly $\Sigma$ and what about uniqueness?

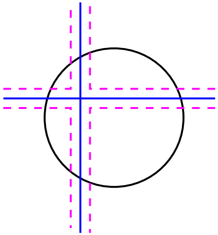
Observation 1:




Same split system but not multiset of splits!

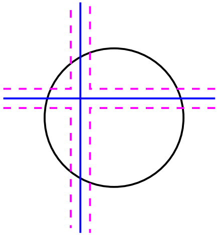
# When does there exist an (unrooted) 1-nested network displaying exactly $\Sigma$?

Observation 2: $\mathcal{I}$*(ncompatibility)-intersection*



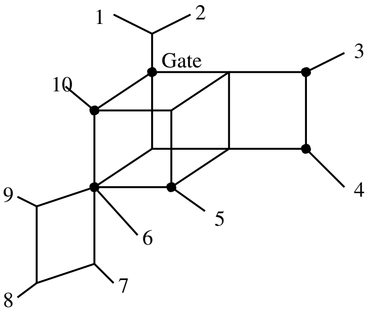
# When does there exist an (unrooted) 1-nested network displaying exactly $\Sigma$?

Observation 2: $\mathcal{I}$*(ncompatibility)-intersection*



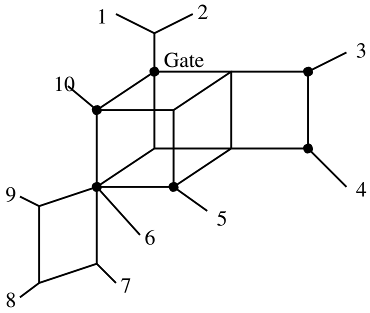
**Theorem 2 (Gambette, H., Scholz)** *Suppose $\Sigma$ is a split system on $X$ that contains all trivial splits on $X$. Then, there exists a (unrooted) 1-nested network on $X$ that displays precisely $\Sigma$ if and only if $\Sigma$ is circular and $\mathcal{I}$-intersection closed.*

# Provided that Σ can be displayed by a unrooted 1-nested network, can we find an optimal one?




- Σ induces a metric on $X$ given by $D(x, y) = \sum_{S \in \Sigma} \delta_S(x, y)$ where $\delta_S$ is a split metric.
- A *gated* subset $Y$ of a metric space $(Z, d)$ if there exists for every $y \in Y$ an element $y_z \in Y$, called the *gate* for $z$, such that $d(y, z) = d(y, y_z) + d(y_z, z)$.

# Provided that Σ can be displayed by a unrooted 1-nested network, can we find an optimal one?

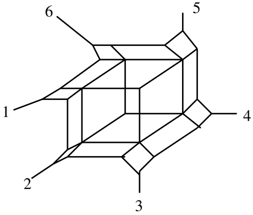



*Blocks* (i.e. maximal 2-connected components) of Buneman graph for Σ are in 1-1 correspondence with connected components of Incompatibility graph for Σ. (Dress, H., Koolen, Moulton, 2011)

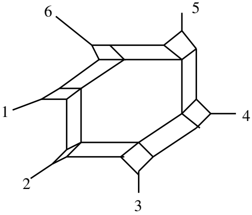
# Provided that Σ can be displayed by a unrooted 1-nested network, can we find an optimal one?

Optimal: Minimize number of additional splits.

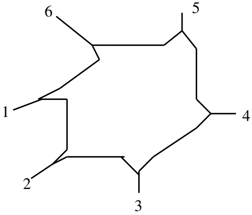
Note: $BunemanGraph(\Sigma) = \Sigma$.




Buneman graph




Marguerite




Simplified Marguerite

# Provided that $\Sigma$ can be displayed by a unrooted 1-nested network, can we find an optimal one?

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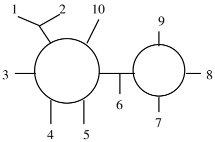


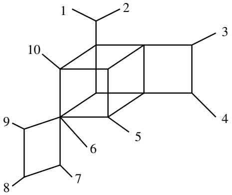


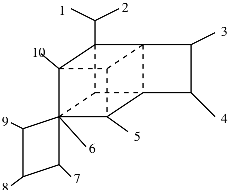


(Simplified) Marguerite graph

# Provided that Σ can be displayed by a unrooted 1-nested network, can we find an optimal one?

Optimal: Minimize number of additional splits.

**Theorem 2 (Gambette, H., Scholz)** *Suppose Σ is a circular split system on $X$ that contains all trivial splits on $X$. Then, the simplified Marguerite graph for Σ*

- *displays Σ,*
- *is optimal (up to isomorphism[1] and partial-resolution), and*
- *can be reconstructed in $O(|X|^2 + |\Sigma|^2)$ time.*

[1]in the usual sense