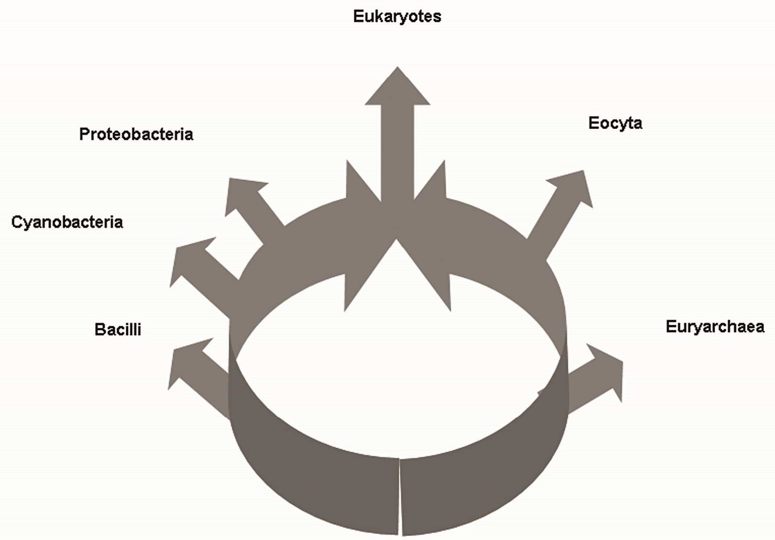
The 'ring of life'

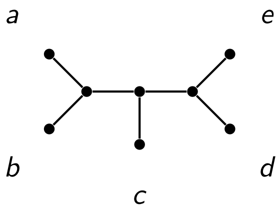
Judith Keijsper and Rudi Pendavingh

Eindhoven

April 24, 2014


Eukaryotes
Proteobacteria
Eocyta
Cyanobacteria
Bacilli
Euryarchaea

Phylogenetic Trees and Quartets



Definition

A phylogenetic tree on X is a tree $G = (V, E)$ such that

- X is the set of leaves of G, and
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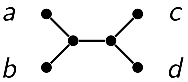
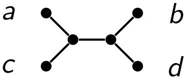
A quartet is a phylogenetic tree on 4 leaves.



$(ab|cd)$



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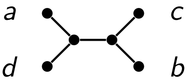

$(ad|bc)$

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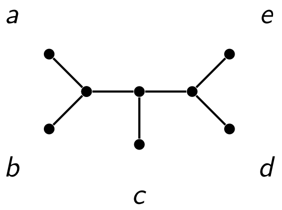

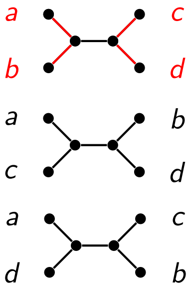

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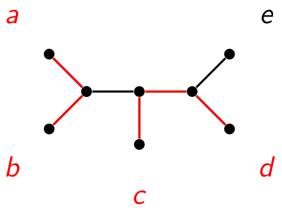

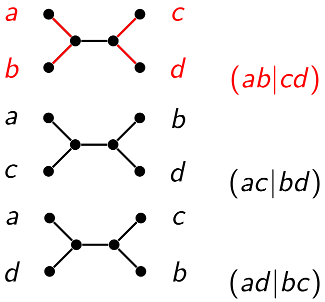

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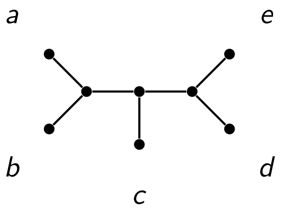

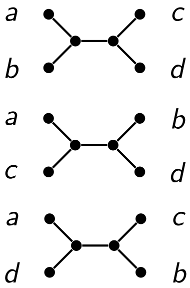

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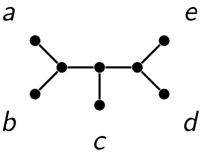
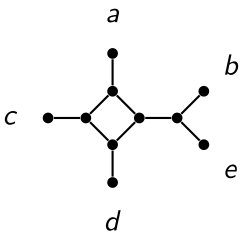
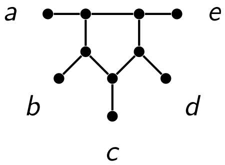
Phylogenetic level-1 Networks







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A level-1 network on X is a connected graph $G = (V, E)$

- in which every two circuits are vertex-disjoint,
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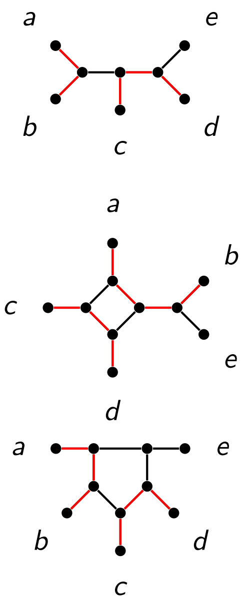

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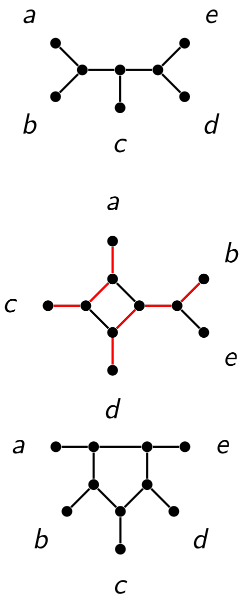

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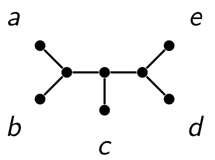

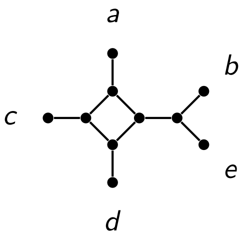

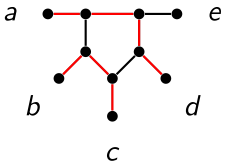

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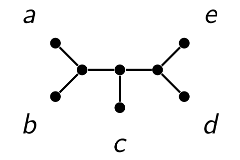

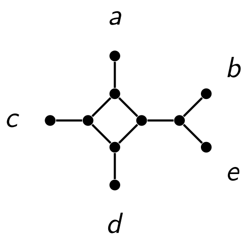

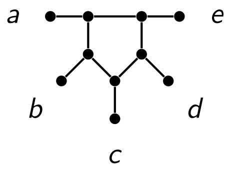

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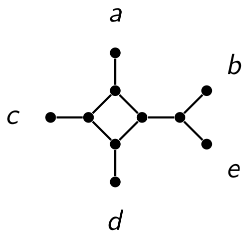
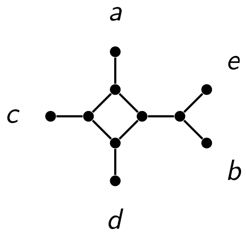
Problem

Given $Q(G)$, reconstruct G in polynomial time.

Level-1 Networks and Cyclic orderings



Any level-1 network G on X can be embedded without crossings in a disk with X on the boundary.



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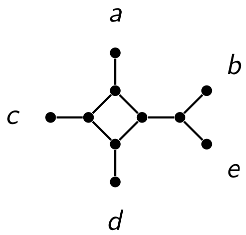

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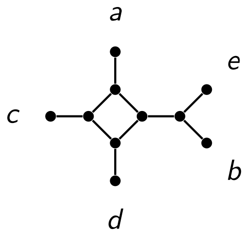
A cyclic ordering C of X is consistent with G if there is an embedding of G that realizes C (clockwise) on the boundary.



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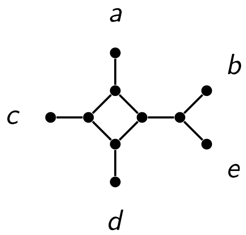

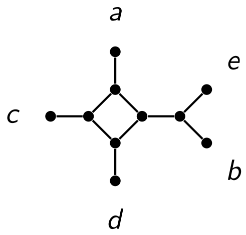

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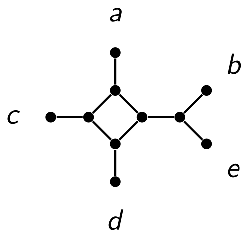

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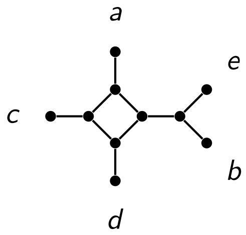

In the picture, $C(G) = \{[abedc], [cdeba], [aebdc], [cdbea]\}$.

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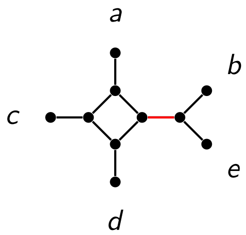

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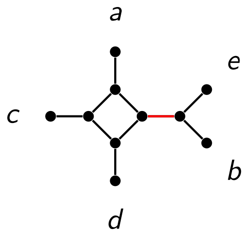
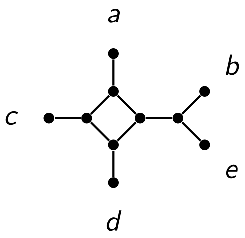


In the picture, $C(G) = \{[abedc], [cdeba], [aebdc], [cdbea]\}$.

Observation

$|C(G)| = 2^{t+1}$, where t is the number of cut-edges not incident with X.

Level-1 Networks, Cyclic orderings and Quartets



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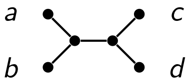

quartet $(ab|cd) \in Q(G)$

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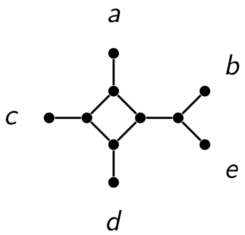

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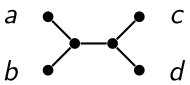

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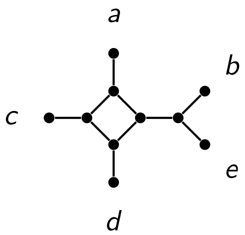

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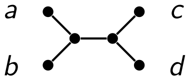

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Theorem

A cyclic ordering is in $C(G)$ if and only if it is consistent with each quartet in $Q(G)$.

Reconstructing a Level-1 Network from Quartets

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Given Q, reconstruct a level-1 network G such that $Q(G) \supseteq Q$.

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Theorem (Gambette, Berry, Paul 2012)

The following problems are NP-complete:

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Theorem (GBP 2012)

Given a quartet set Q, it can be decided in polynomial time whether a level-1 network G exists such that

$$Q(G) = Q.$$

If yes, such a network can be constructed in polynomial time.

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So, we use an efficient encoding of $C(G)$ to do all this in polynomial time.

Encoding cyclic orderings

A cyclic ordering C of X is uniquely encoded as follows

$$u^C(a,b,c) := \begin{cases} 1 & \text{if } a,b,c \in X \text{ distinct, and clockwise in } C \\ 0 & \text{otherwise} \end{cases}$$

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Theorem (Huntington)

Let $u : X^3 \to GF(2)$. Then u is cyclic, i.e. $u = u^C$ for some cyclic ordering C if and only if

(1) $u(a,a,b) = 0$ *for all* $a, b \in X$ *(distinctness)*

(2) $u(a,b,c) + u(b,c,a) = 0$ *for all* $a,b,c \in X$ *(cyclicity)*

(3) $u(a,b,c) + u(c,b,a) = 1$ *for all* $a,b,c \in X$ *(asymmetry)*

(4) $u(a,b,c)u(a,c,d) = u(a,b,d)u(b,c,d)$ *for all* $a,b,c,d \in X$ *(transitivity)*

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$$\mathcal{U}^X := \{u \in GF(2)^{X^3} : u \text{ satisfies (1),(2),(3), and (5) } \}$$

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A cyclic ordering C is consistent with a quartet $(ab|cd)$ if and only if $u^C(a, b, c) = u^C(a, b, d)$

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So in particular, $U(G)$ is an affine subspace of $GF(2)^{X^3}$.

Our algorithm

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Given a quartet set Q, reconstruct a level-1 network G such that $Q(G) = Q$, in polynomial time.

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Theorem

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Proof: The linear algebra over $GF(2)$ involves $|Q| = O(|X|^4)$ sparse equations in $\dim(\mathcal{U}^X) = \binom{|X|-1}{2}$ variables.

The dense case

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Given a dense quartet set Q, reconstruct a level-1 network G such that $Q(G) \supseteq Q$.

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Theorem

These problems can be solved in polynomial time.

Recovering the most tree-like G from $U(G)$

If G is a level-1 network on X, then $S \subseteq X$ is a split of G if

$$S = X \cap U$$

where $|\delta_G(U)| = 1$. We write $\Sigma(G)$ for the set of splits of G.
For a set $S \subseteq X$, we define the vector $v : X^3 \to GF(2)$ by

$$v^S(x,y,z) := \begin{cases} 1 & x,y,z \text{ distinct, and } |\{x,y,z\} \cap S| \geq 2 \\ 0 & \text{otherwise} \end{cases}$$

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Computing $U(G)$ from fewer quartets

Lemma

Let G be a level-1 network on X where $|X| = 5$. For an $x \in X$, let

$$Q_x := \{(ab|cd) \in Q(G) : x \in \{a, b, c, d\}\}$$

Then $U(G) = U(Q_x)$.

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A variant of our algorithm solves the following problem

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Given: *A (general) quartet set* Q *on* X, *and some* $x \in X$.
Find: *a level-1 network* G *with the maximum number of splits such that* $Q(G) \supseteq Q$
or *a certificate of inconsistency* $Q' \subseteq Q$, *where* $|Q'| \leq \binom{|X|-1}{2}$
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Interactive use:

Keep adding new quartets on the 4-tuples Z returned by the algorithm until either a level-1 network G or an inconsistent subset of quartets Q' is obtained.