Explicit Modular Decomposition

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Faculty of Science
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WU Wien, 2024

Research

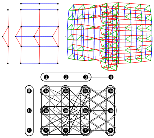
Research

Discrete Mathematics

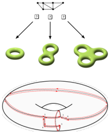
Research

Discrete Mathematics

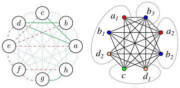
- Graph and Hypergraph Theory
- Discrete Optimization and Matroid Theory
- Combinatorics and Geometric Graph Theory



Products of Graphs and Hypergraphs



Planarity and 1-Face Embeddings (= particular planar drawing on orientable manifolds)



Packings, Edge- and Vertex-Colorings

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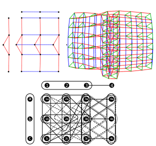
Computer Science



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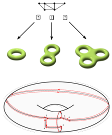

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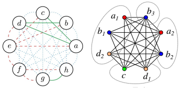

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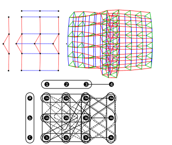
  (Co)NP-completeness, Fixed-Parameter Tractability (FPT)
- Algorithm Design
  Exact algorithms, Heuristics, Integer Linear Programming (ILP), Approximation algorithms



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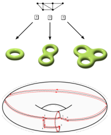

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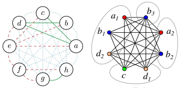

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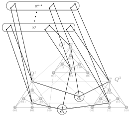

Reductions, NP-hardness,
ILP, FPT, approx. algorithms

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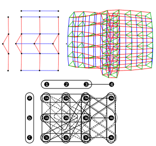
Applied Mathematics & Math. Data Science



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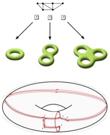

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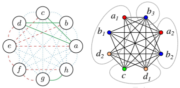

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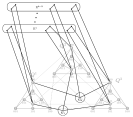

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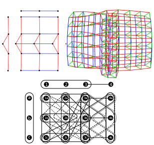
Applied Mathematics & Math. Data Science

- General Focus: mathematical characterization of discrete data and structures that naturally occur in Life Sciences or Engineering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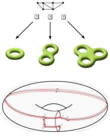
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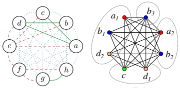

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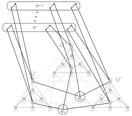
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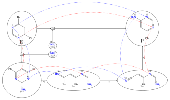
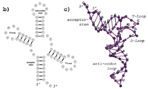
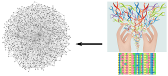

Graph Grammars, Cayley Graphs,
Chemical Reaction Networks

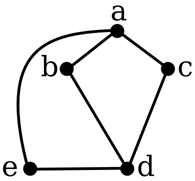


Combinatorics of RNA structures


Genomics and Evolutionary Biology

Basics: Graphs and their Representation

undirected, simple graph G



Aim:

find efficient representation

that provides deep structural insights

and helps to understand complexity of certain problems

Basics: Graphs and their Representation

Representation

$$A(G) = \begin{array}{c} \begin{array}{ccccc} \mathbf{a} & \mathbf{b} & \mathbf{c} & \mathbf{d} & \mathbf{e} \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix} \end{array} \begin{array}{c} \\ \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \\ \mathbf{d} \\ \mathbf{e} \end{array}$$

$$A_{\text{list}}(G) = \begin{array}{c|ccc} a & b & c & e \\ b & a & d & \\ c & a & d & \\ d & b & c & e \\ e & a & d & \end{array}$$

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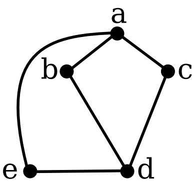

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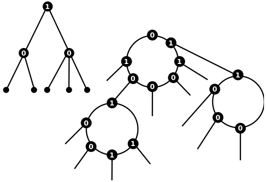
Use other discrete structures as a way to present graphs



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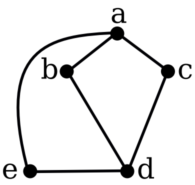

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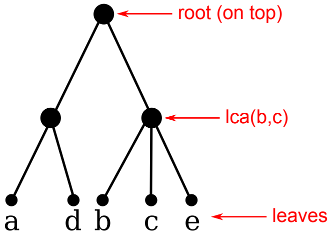
Basics: Graphs and their Representation

Representation via (T, t)



lca = last common ancestor

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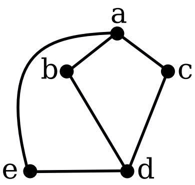

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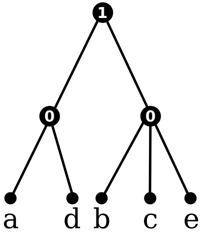
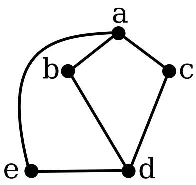


lca = last common ancestor
rooted tree T with 0/1-labeling t

undirected, simple graph G



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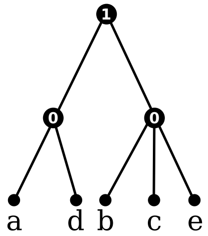

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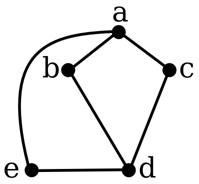

In this example, (T,t) contains all structural information of G and can be used to recover G, i.e.,

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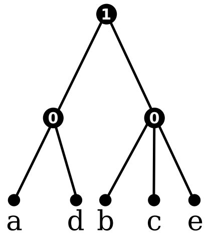

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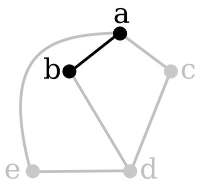

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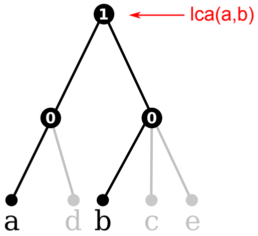

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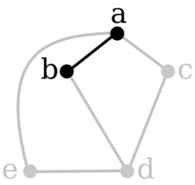

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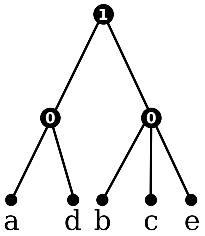

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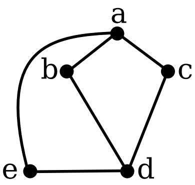

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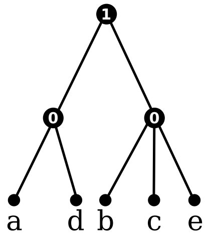

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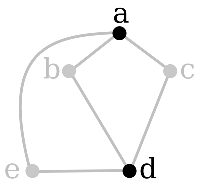

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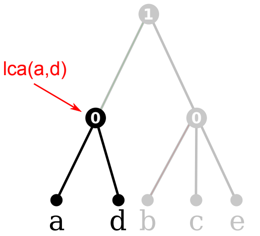

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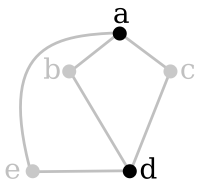

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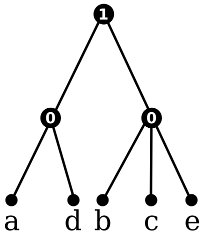

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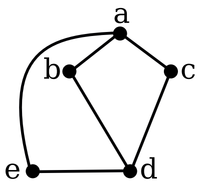

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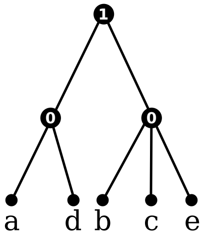

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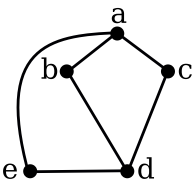

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Cographs ?

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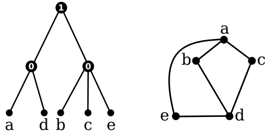

Cotree (T,t) explains cograph G

discovered independently by several authors since the 1970s; Jung (1978), Lerchs (1971), Seinsche (1974), and Sumner (1974).

Cographs

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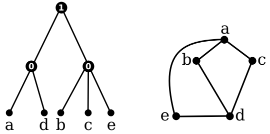

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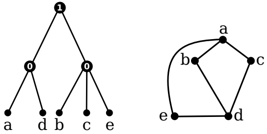

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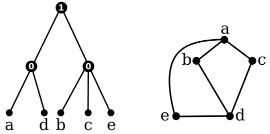

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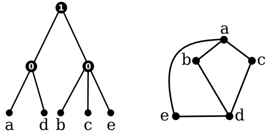

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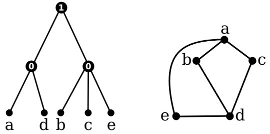

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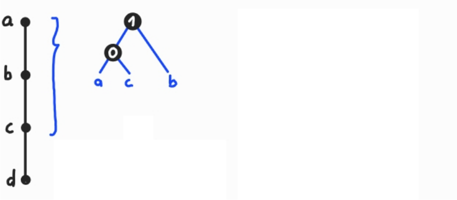

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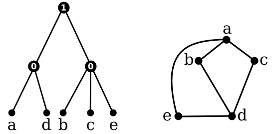

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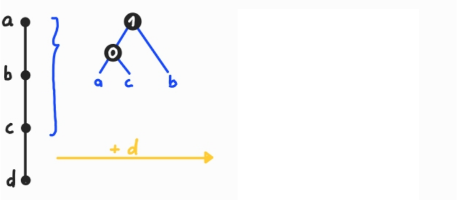

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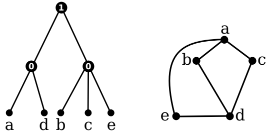

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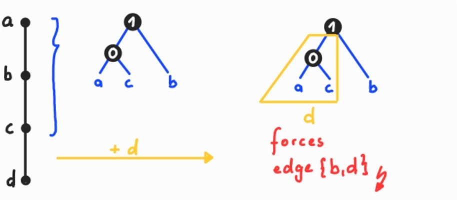

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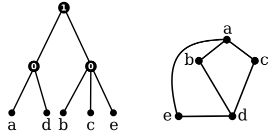

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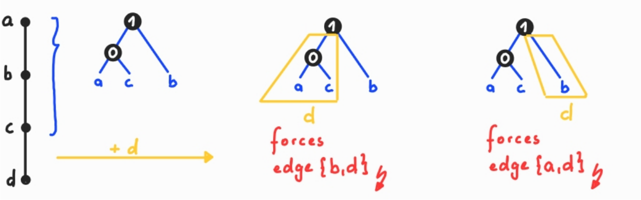

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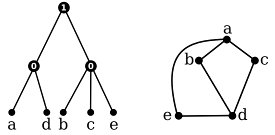

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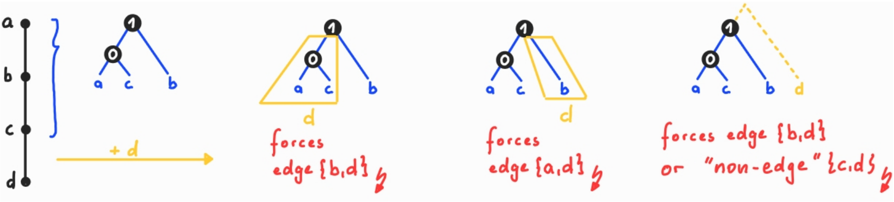

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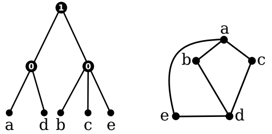

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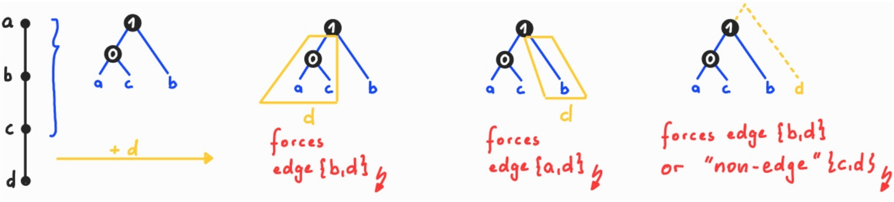

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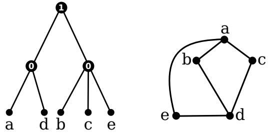

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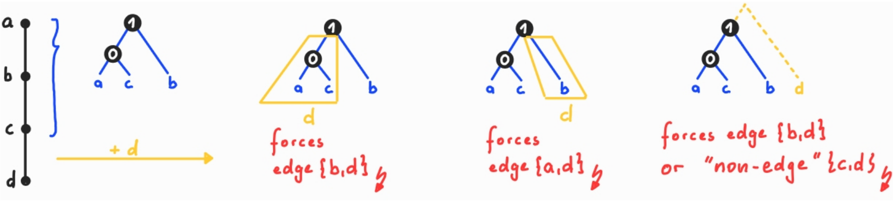

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Basics: Graphs and their Representation

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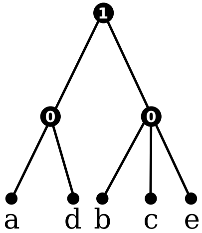
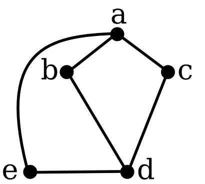


lca = last common ancestor
rooted tree T with 0/1-labeling t

undirected, simple graph G



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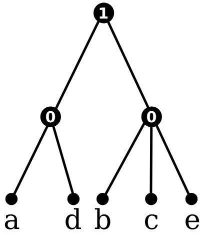

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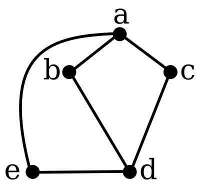

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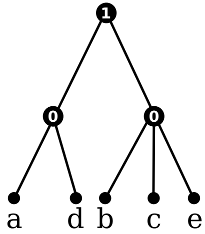

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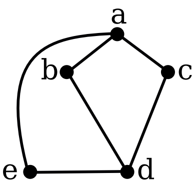

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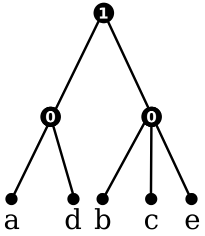

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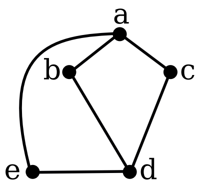

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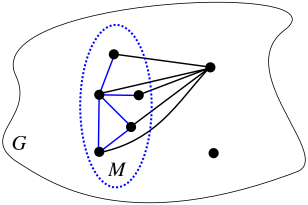
GOOD news: Every graph G has a unique **Modular Decomposition Tree** that at least to some extent provides structural information of G

Basics: Modular Decomposition (MD)*

$M \subseteq V(G)$ is a **module** in G if $N(x) \setminus M = N(y) \setminus M$ for all $x, y \in M$



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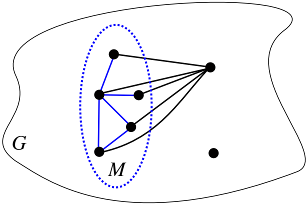

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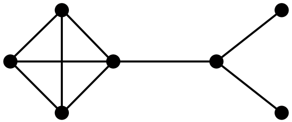

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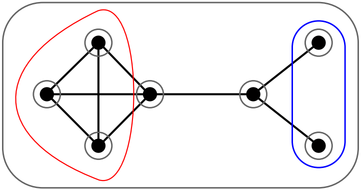

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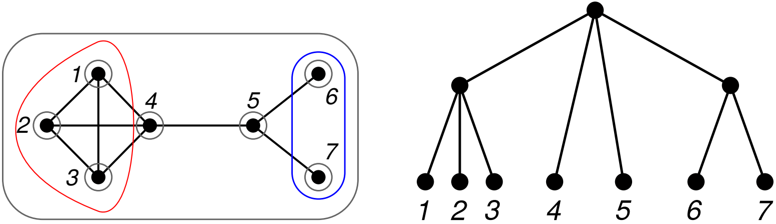

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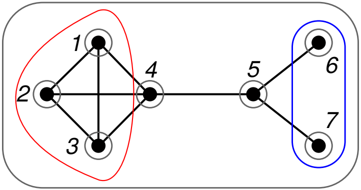

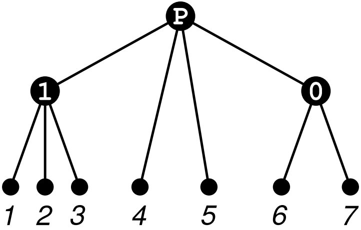

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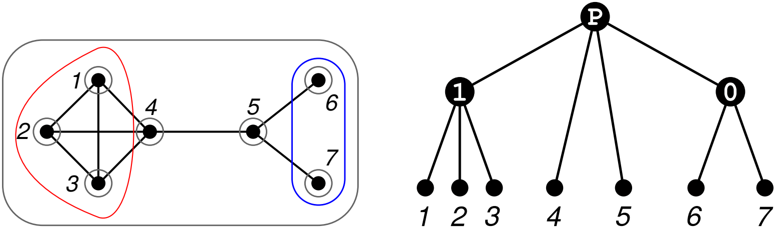

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> 0, 1 and P (Prime) modules
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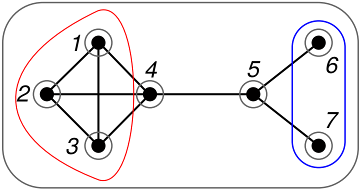

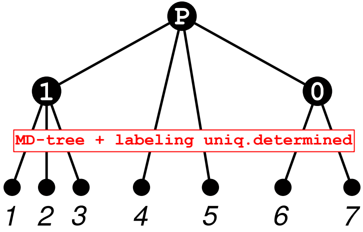

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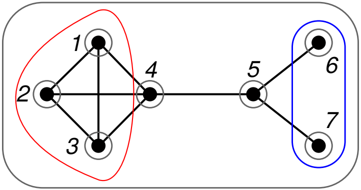

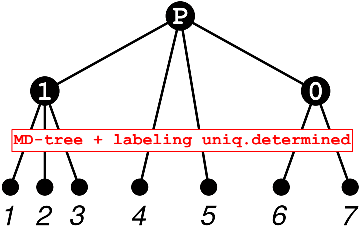

0- and 1-vertices in MD-tree are good:

$$t(\mathrm{lca}(x,y)) = 0 \implies \{x,y\} \notin E(G) \quad \text{and} \quad t(\mathrm{lca}(x,y)) = 1 \implies \{x,y\} \in E(G)$$

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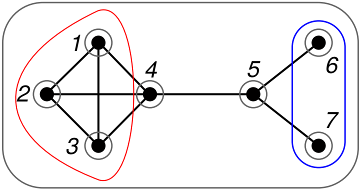

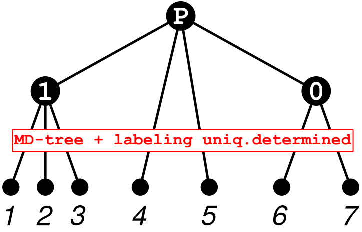

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BUT, not all structural information of G is provided by the MD-tree if it contains P-vertices.

$t(\text{lca}(3,4)) = P$ and $\{3,4\} \in E(G)$

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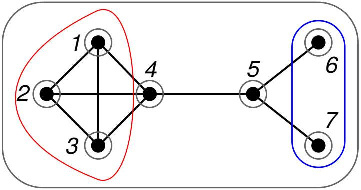

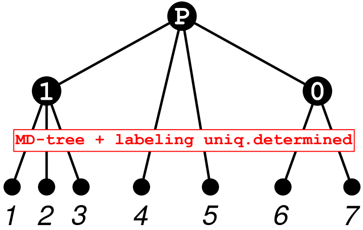

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Full information of G is provided only if MD-tree does not contain P-vertices (**cographs**)

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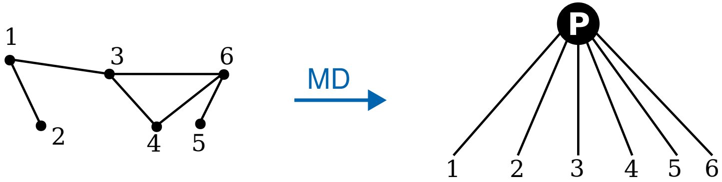

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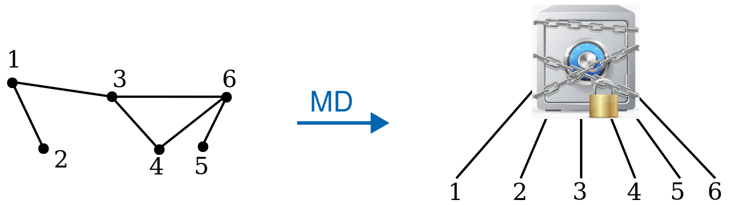

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P-vertices $\widehat{=}$ extremely secured closed box hiding structural information.

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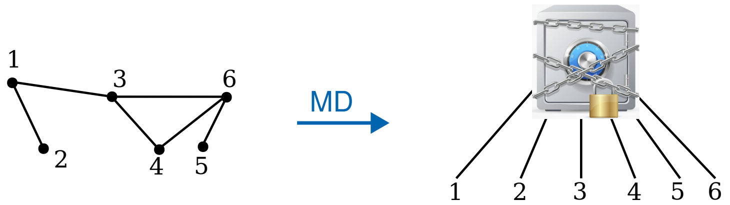

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Can we break and unbox the P-vertices to obtain 0/1-labeled rooted networks that provides the missing structural information of G ?

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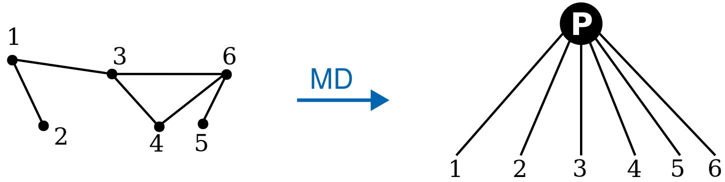

The MD-tree cannot be used to recover G (structural information gets lost on P-vertices)

P-vertices $\widehat{=}$ extremely secured closed box hiding structural information.

Can we break and unbox the P-vertices to obtain 0/1-labeled rooted networks that provides the missing structural information of G ?

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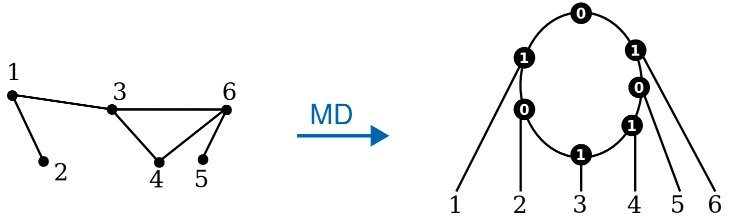

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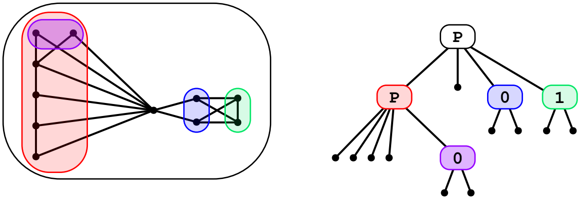
$\Longrightarrow$ **Explicit Modular Decomposition**

Explicit Modular Decomposition



General Aim:

- Preserve the main features of the MD-tree,
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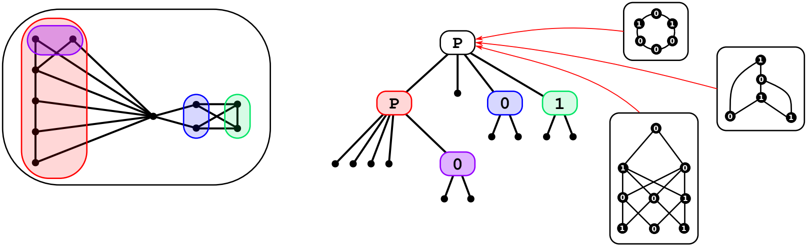

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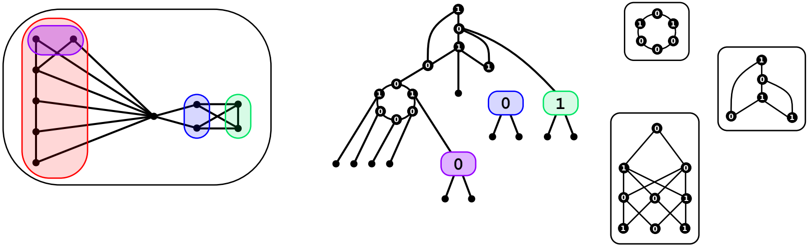

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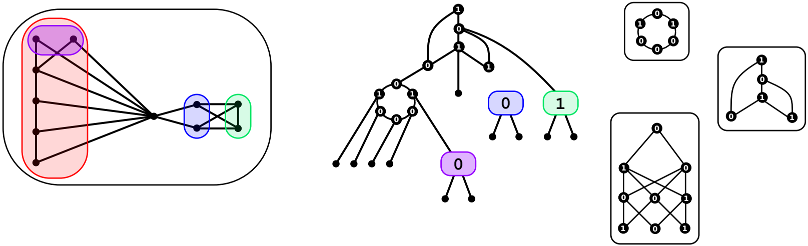

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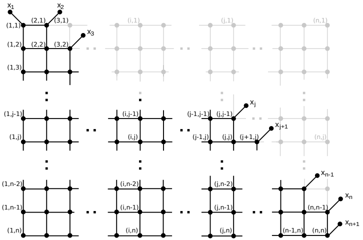
Proof of Concept: Half-grid networks.

Explicit Modular Decomposition: Half-grids



Bruckmann, Stadler, Hellmuth, **From Modular Decomposition Trees to Rooted Median Graphs**, *Discr. Appl. Math*, 2021

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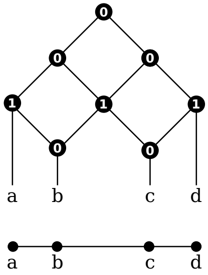

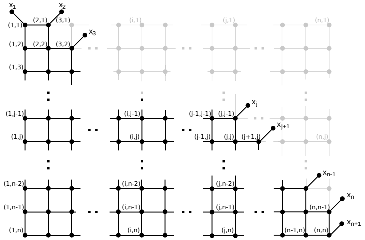

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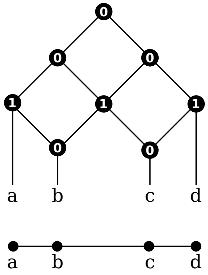

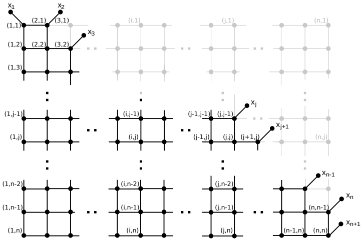

Theorem (2021)

Every graph G can be explained by a 0/1-labeled half-grid and thus, by a network obtained from MDT by locally replacing "P"-vertices by half-grids = median graphs.

Proof: In half-grids we have $\text{lca}(x,y) \neq \text{lca}(x',y')$ for distinct pairs x,y and x',y'.

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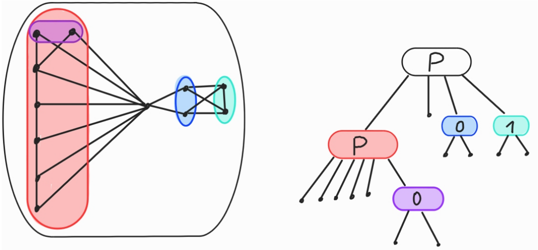

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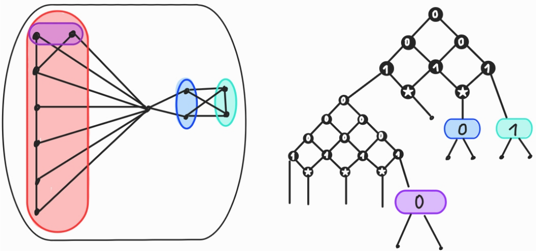

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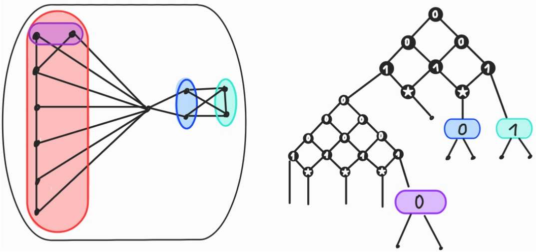

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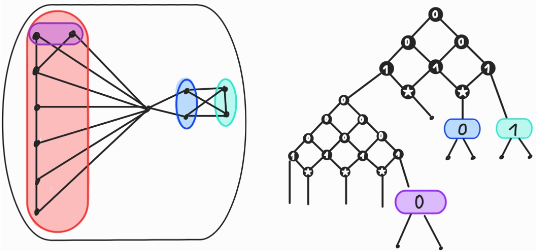

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But half-grids are only as suitable as representing G with its adjacency matrix (no deep structural insights)

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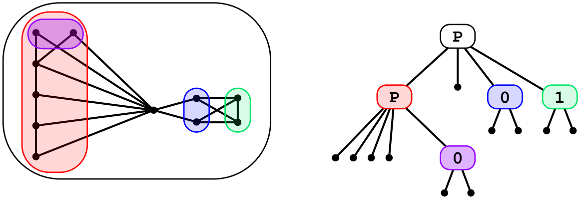

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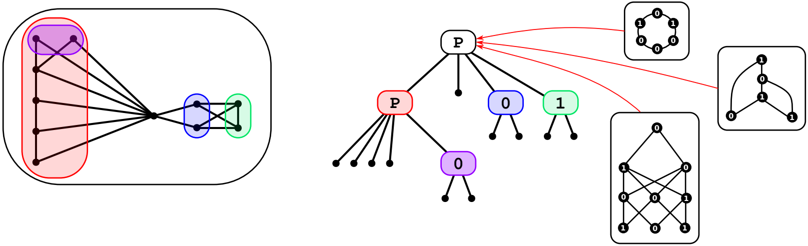

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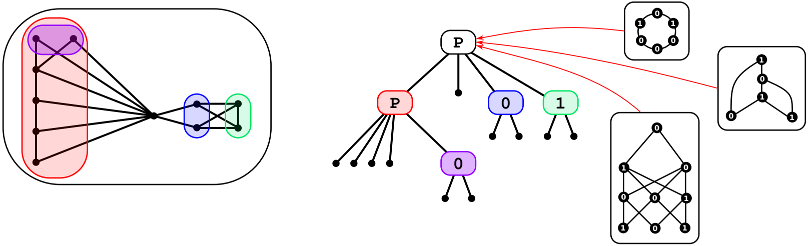

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Use the most-simplest non-tree structure to replace P-vertices.

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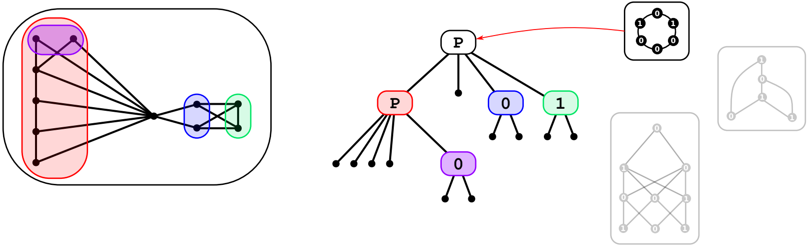

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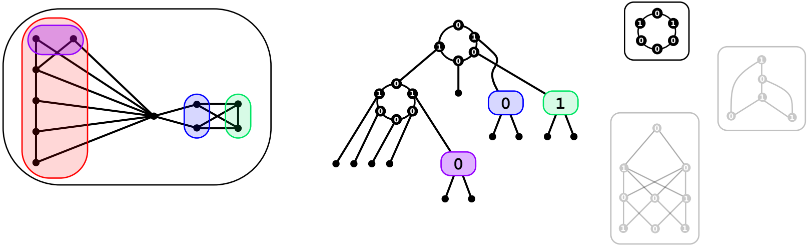

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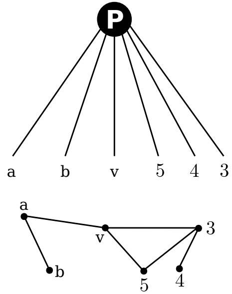
Question: Which type of graphs can be explained by such networks (N, t)?

Simple case: Single P-vertex

Consider graphs G whose MD-tree is a star-tree with single P-vertex



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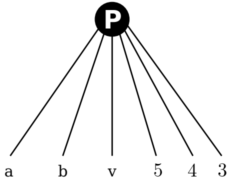

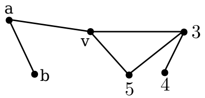

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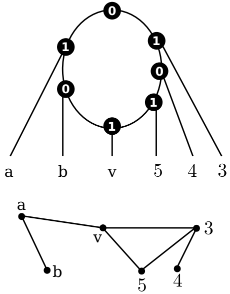

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Simple case: Single P-vertex and Pseudo-cographs

Scholz & Hellmuth, **From Modular Decomposition Trees to Level-1 networks: Pseudo-Cographs, Polar-Cats and Prime Polar-Cats**, *Discr. Appl. Math*, 2022

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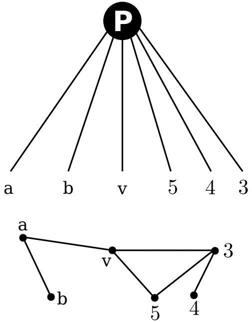

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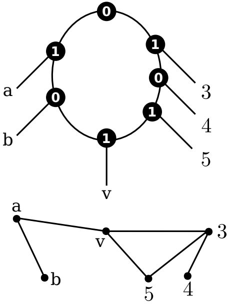

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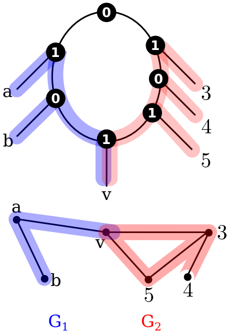

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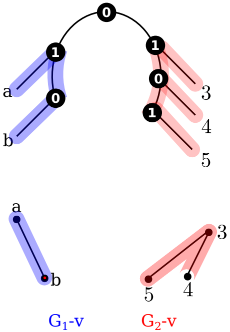

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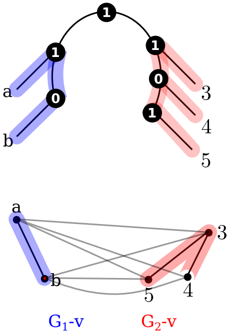

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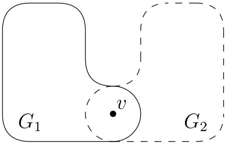

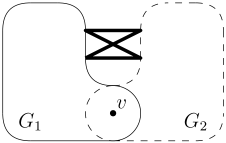

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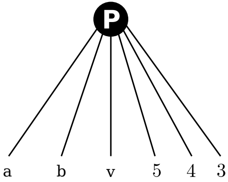

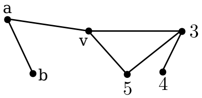

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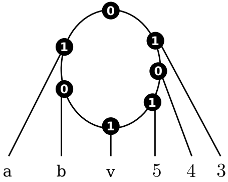

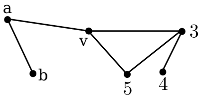

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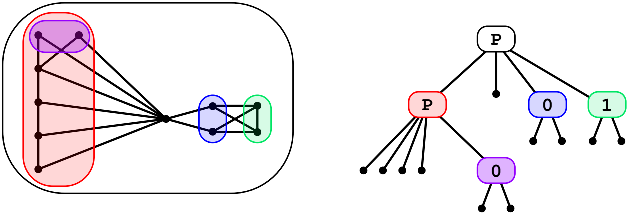
The general case: GaTEx graphs



General Aim: Characterize graphs G where

- MD-tree is *any tree* with *several* P-vertices and
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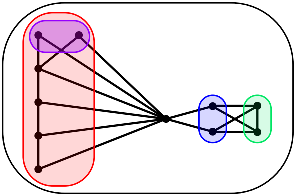
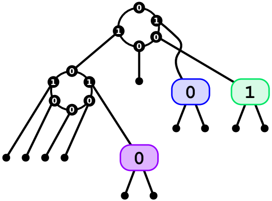
The general case: GaTEx graphs





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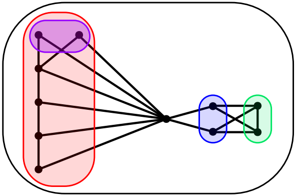

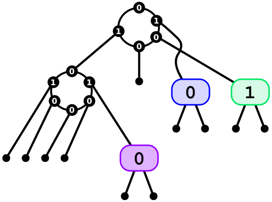

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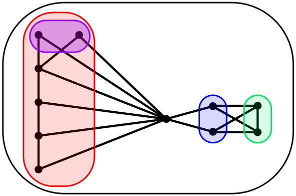

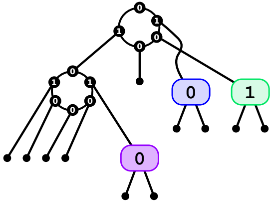

Galled-tree := 0/1-labeled rooted network where all cycles are edge-disjoint

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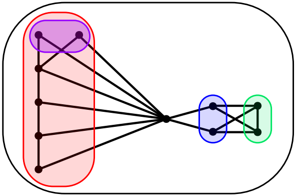

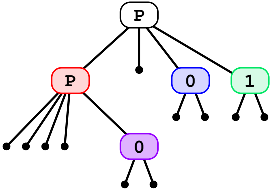

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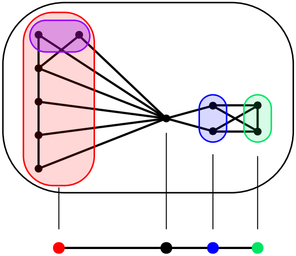

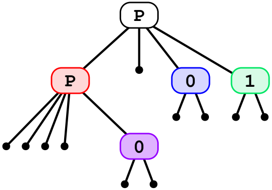

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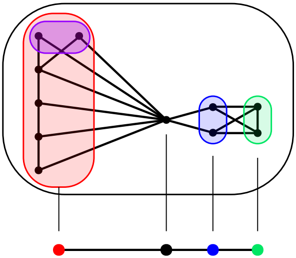

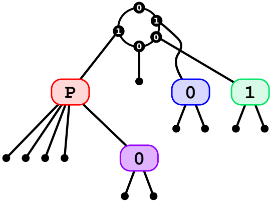

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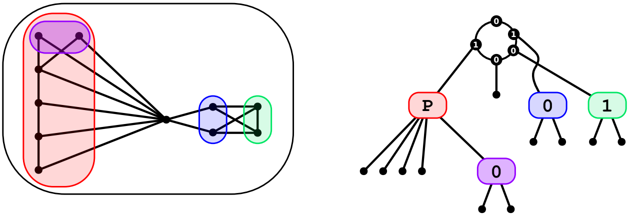

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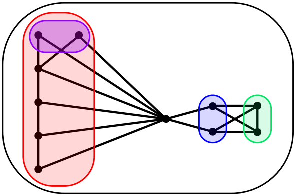

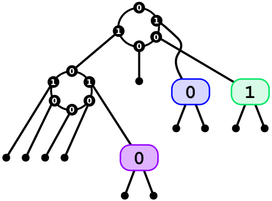

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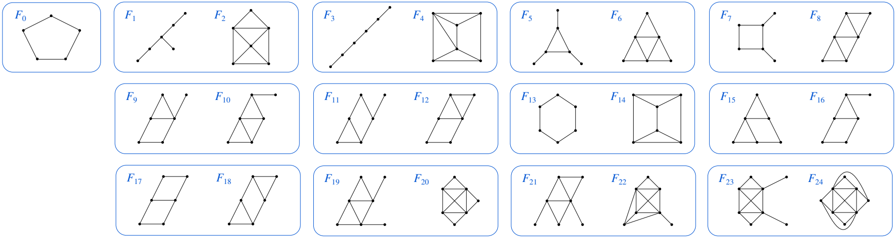

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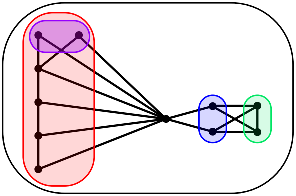

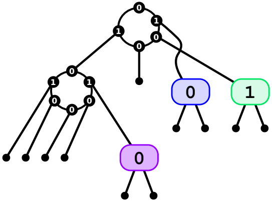

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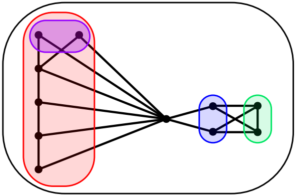

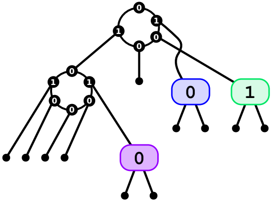

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GaTEx *graphs can have* $O(|n|^2)$ *edges, but can be stored using only* ***linear space****.*

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Consequences

GATEX graphs form a novel and interesting class of graphs that is closely related to many other well-known and famous graph classes.

Among other results, GATEX graphs are:

- perfect graphs

  Chromatic number of every induced subgraph = size of the largest clique of that subgraph

- comparability (=transitive orientable) graphs

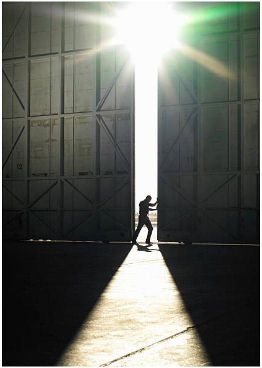
  There exists a transitive orientation on this graphs = represents partial orders in where two elements are connected by an edge if they are comparable to each other in the partial order.

- permutation graphs

  used to represent permutations

- perfectly orderable

  there is an ordering of the vertices of G such that a greedy coloring algorithm with that ordering optimally colors every induced subgraph of the given graph



Every cograph and every graph whose vertices are contained in at one most induced P_4 are GATEX

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NP-hard Problems that become easy . . .

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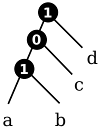

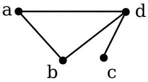

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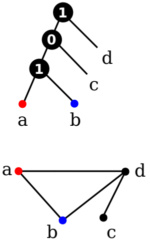

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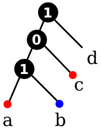

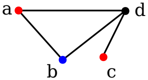

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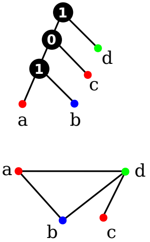

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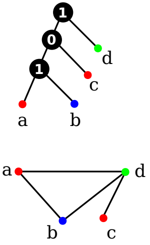

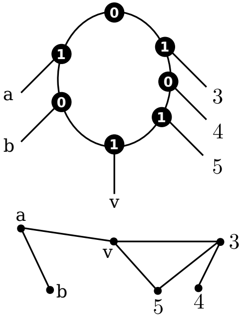

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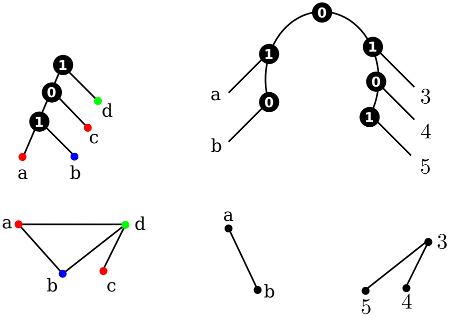

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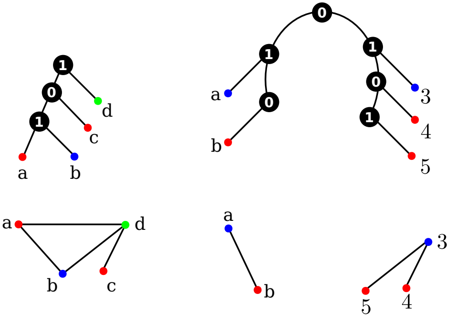

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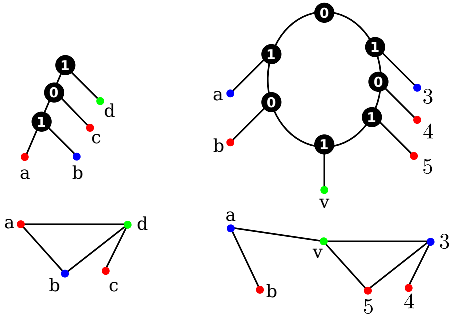

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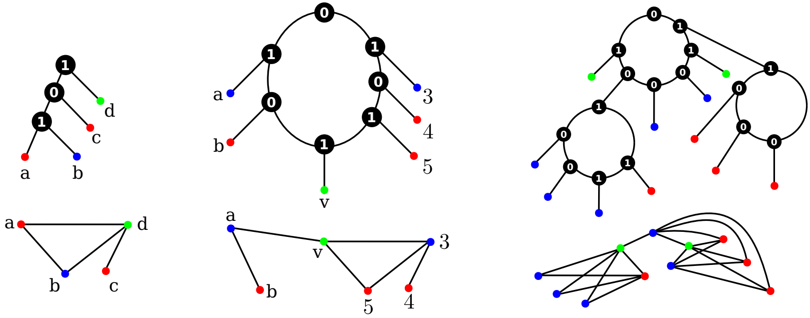

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The following NP-hard problems can be solved in linear-time on GaTEx *graphs.*

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Explicit modular decomposition provides an essential tool-box for solving discrete optimization problems!

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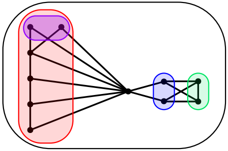

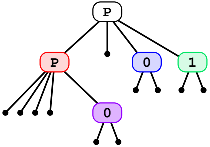

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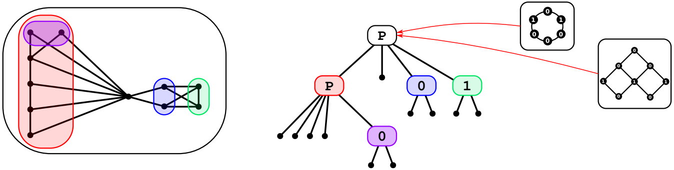

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- **Here:** replace "P" vertices in MD tree by simple cycles or half-grids
  This is only a snapshot of what is possible!

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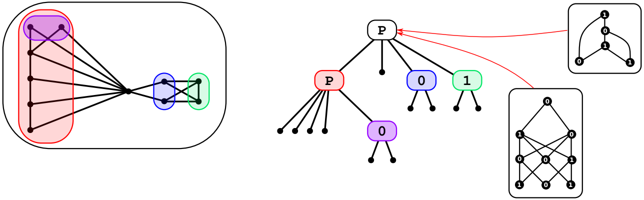

General Aim:

- Preserve the main features of the MD-tree,
  try to modify only the P-vertices
  to obtain 0/1-labeled rooted networks to explain graphs

- **Here:** replace "P" vertices in MD tree by simple cycles or half-grids
  This is only a snapshot of what is possible!

- we are not restricted to resolving P-vertices in the MD-tree by simple cycles or half-grids only
  For generalizations, we can draw on nearly unlimited resources from phylogenetic networks.

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  GATEX graphs are closely related to other famous graph classes
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- Explicit Modular Decomposition is a very novel concept and a great playground (generalizations e.g. edge-colored di-graphs or matroids are coming)!

Applications

The initial motivation to investigate ”explicit modular decomposition” is based on the fact that we want understand in more detail pairwise relationships between genes (e.g horizontal gene transfer and orthology)

Hellmuth & Wieseke et al., **Phylogenomics with Paralogs**, *Proceedings of the National Academy of Sciences (PNAS)*, 2015

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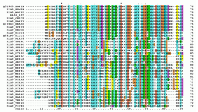
genomic sequence data + similarity information



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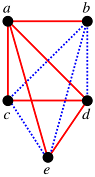

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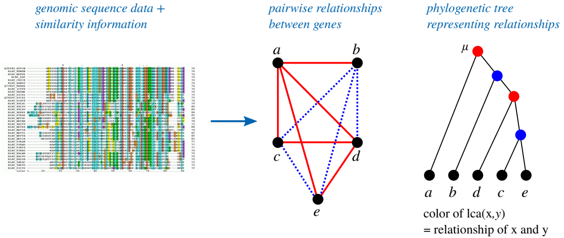

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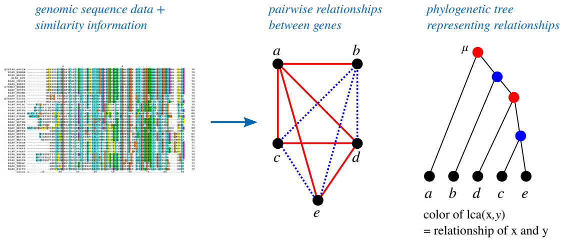

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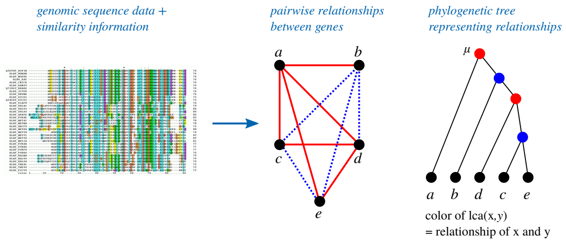

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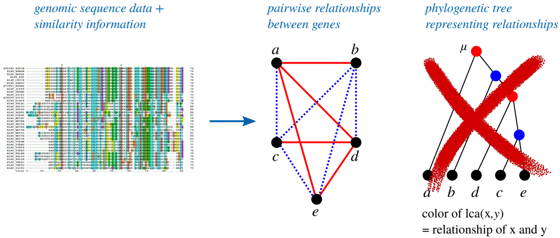

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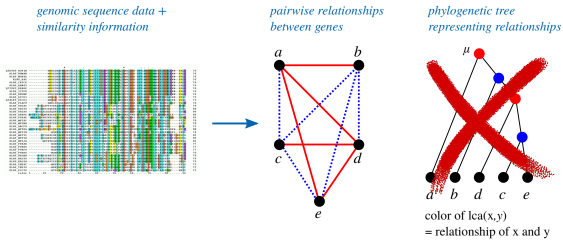

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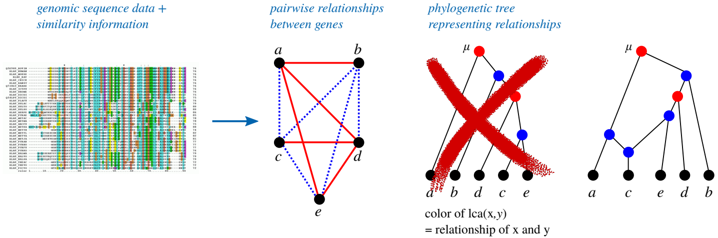

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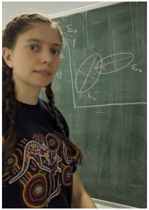
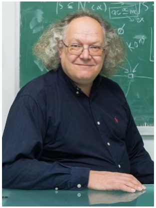


Carmen Bruckmann



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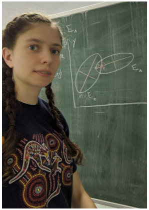

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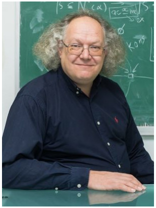

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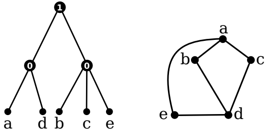
THANK YOU!

Appendix

Cographs : Graphs without prime modules

Cographs . . .



Cotree (T, t) explains cograph G

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Cographs : Graphs without prime modules

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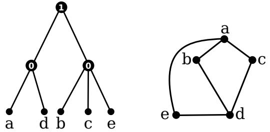
$$\{x,y\} \in E \iff t(\mathsf{lca}(x,y)) = 1$$



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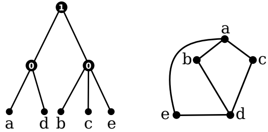

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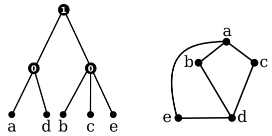

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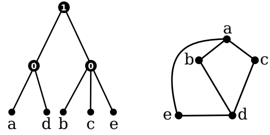

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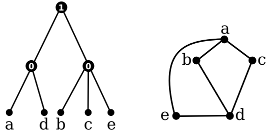

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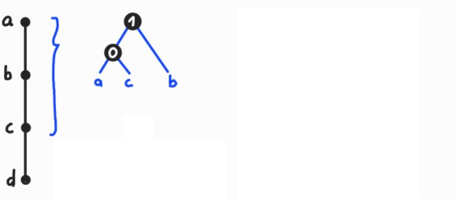

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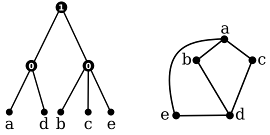

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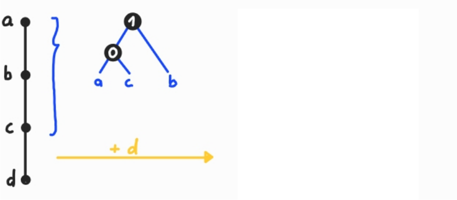

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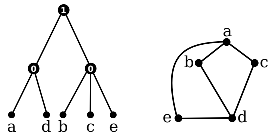

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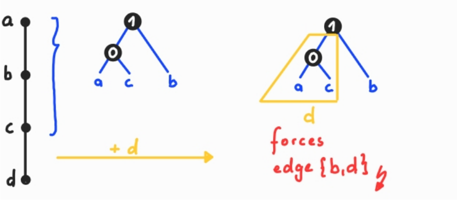

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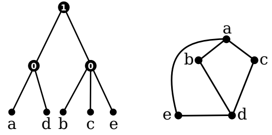

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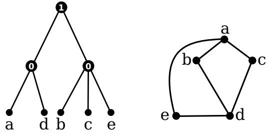

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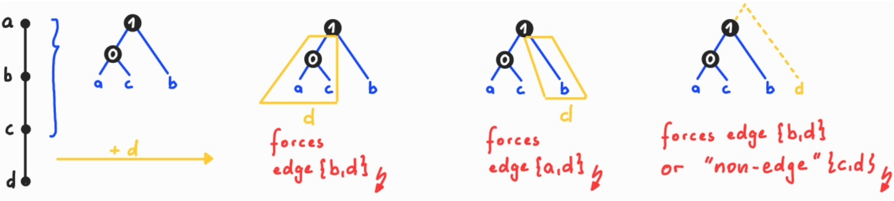

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Pseudo-cographs: Algorithms

Recognition - The Basic Idea

If G cograph - done

Scholz & Hellmuth, **From Modular Decomposition Trees to Level-1 networks: Pseudo-Cographs, Polar-Cats and Prime Polar-Cats**, *Discr. Appl. Math*, 2022

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  For all $v \in P_4$
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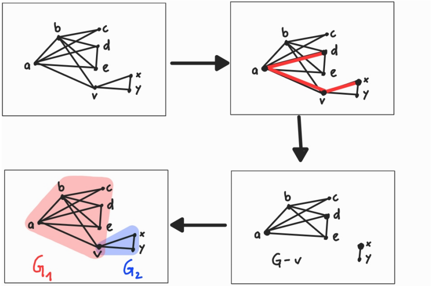

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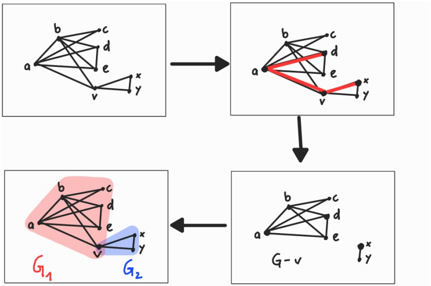

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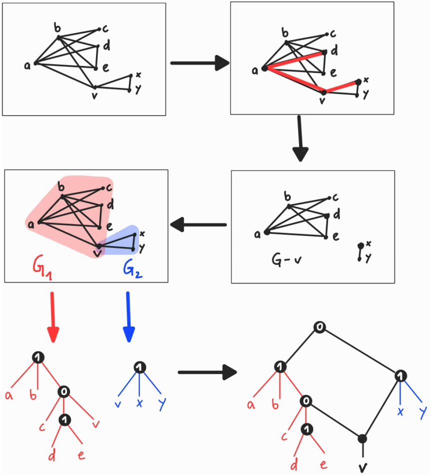

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Pseudo-cographs and galled-tree explainable graphs

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This looks like a very interesting, novel graph class !!

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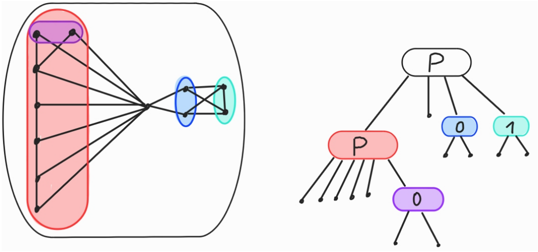

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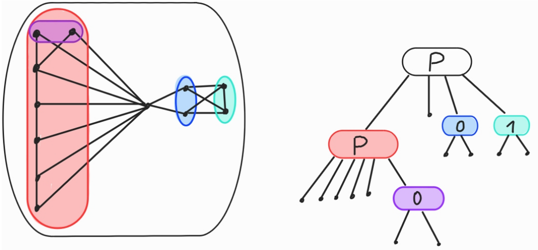

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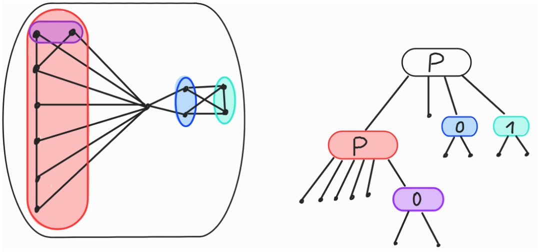

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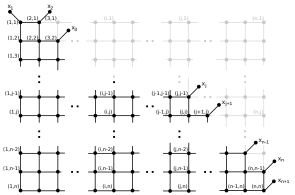
As a first attempt we may ask:

Is there a 0/1-labeled network that can explain EVERY given graph?

Explicit Modular Decomposition: Half-grids

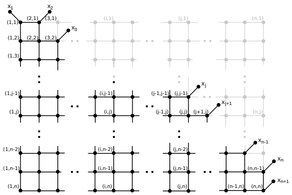


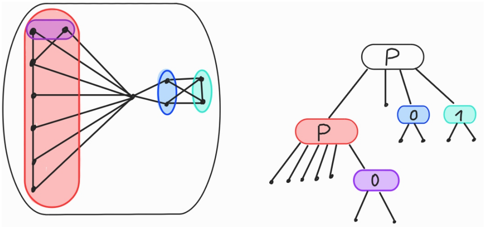
Theorem (2021)

Every graph G can be explained by a 0/1-labeled half-grid and thus, by a network obtained from the MD-tree by locally replacing "P"-vertices by half-grids = median graphs.

Bruckmann, Stadler, Hellmuth, **From Modular Decomposition Trees to Rooted Median Graphs**, *Discr. Appl. Math*, 2021

Explicit Modular Decomposition: Half-grids





Theorem (2021)

Every graph G can be explained by a 0/1-labeled half-grid and thus, by a network obtained from the MD-tree by locally replacing "P"-vertices by half-grids = median graphs.

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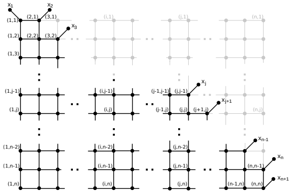

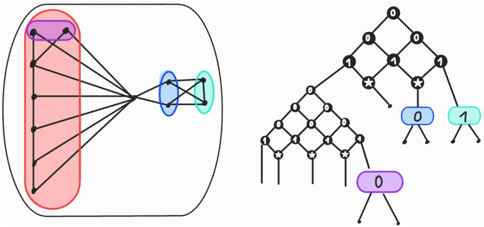

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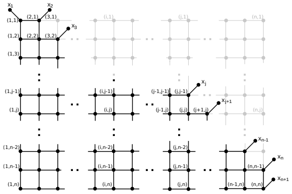

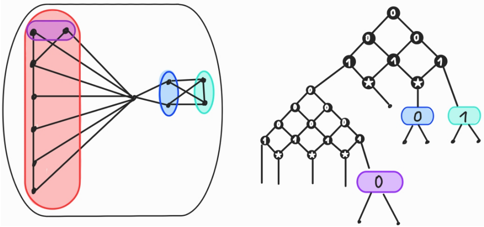

Theorem (2021)

Every graph G can be explained by a 0/1-labeled half-grid and thus, by a network obtained from the MD-tree by locally replacing "P"-vertices by half-grids = median graphs.

Half-grids are rather "heavy" ($O(|V(G)|^2)$ edges and vertices) and of less interest from the structural point and biological point of view.

$\Longrightarrow$ Can we go simpler?

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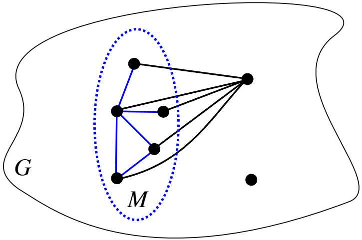
Basics: Modular Decomposition (MD)

$M \subseteq V(G)$ is a **module** in G if $N(x) \setminus M = N(y) \setminus M$ for all $x, y \in M$



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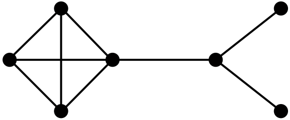

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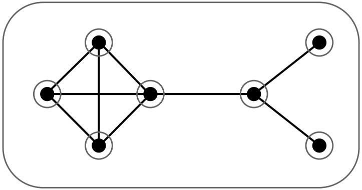

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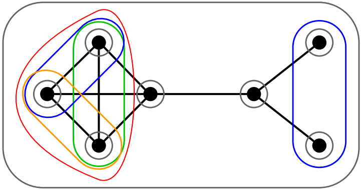

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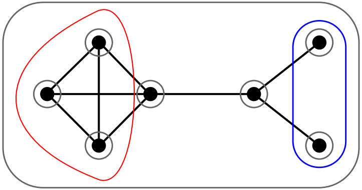

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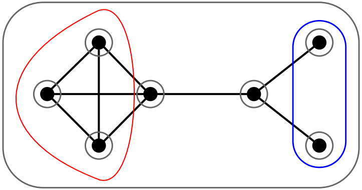

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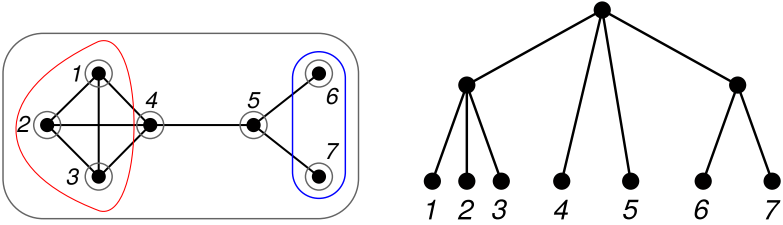

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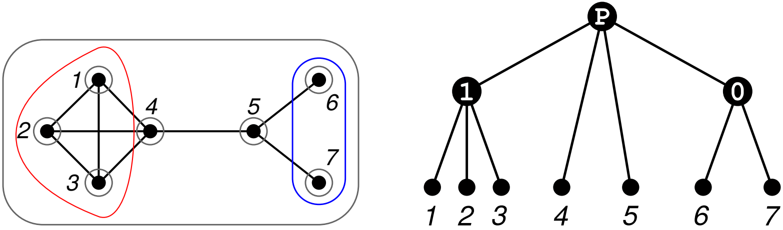

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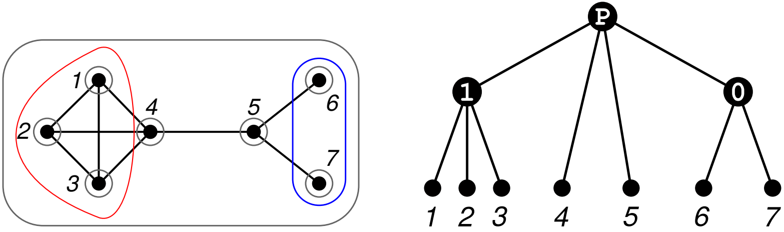

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There are different type of modules:

- Parallel (0), Series (1) and Prime (P) modules
  defined in terms of connectedness conditions (omitted).

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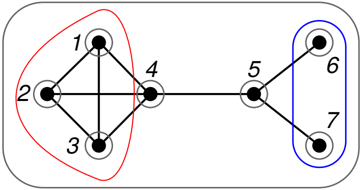

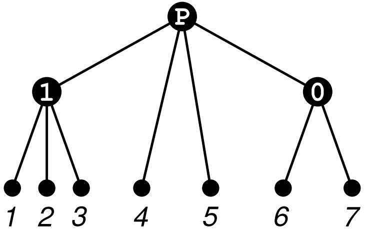

BUT, full information of G is provided only if G does not contain prime modules.

- $t(\text{lca}(3,4)) = \mathtt{P}$ and $\{3,4\} \in E(G)$
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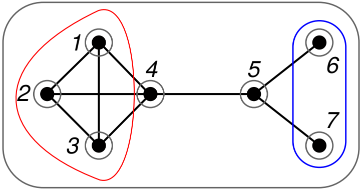

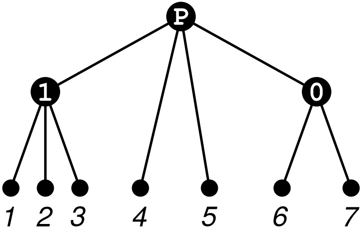

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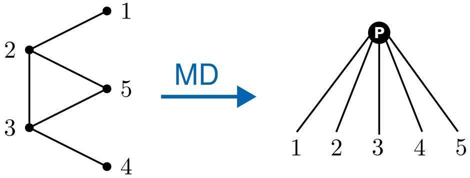

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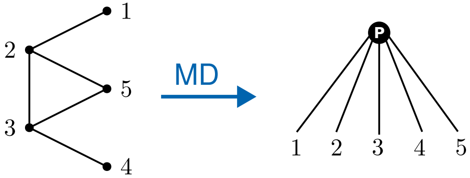

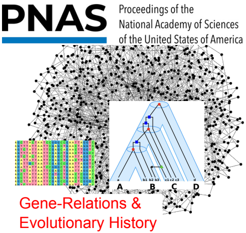

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We used MD and cographs for studies in the context of evolutionary biology

Milestone: How to use “noise” in the data as an additional source of information!

Hellmuth & Wiesecke et al., **Phylogenomics with Paralogs**, *PNAS*, 2015

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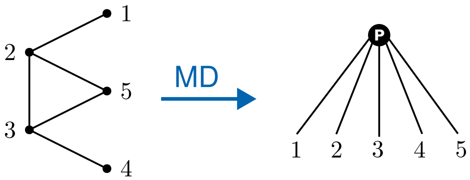

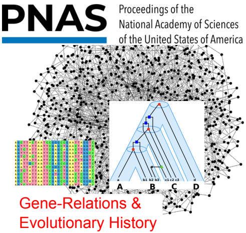

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We observed:

- It is crucial to understand the structure of subgraphs induced by prime modules!
- Evolution is not always tree-like and often better explained by networks!

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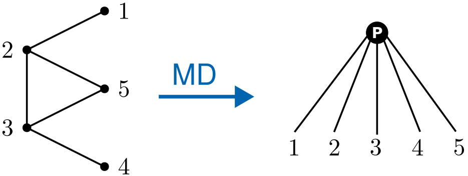

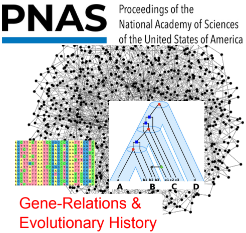

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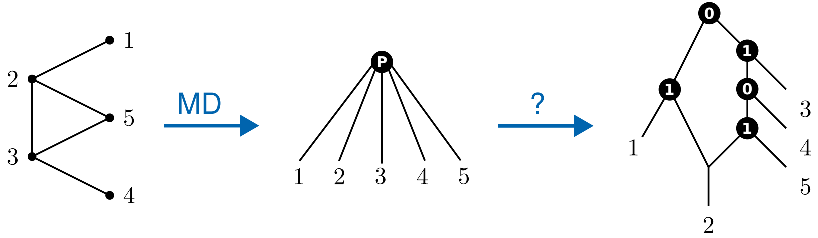

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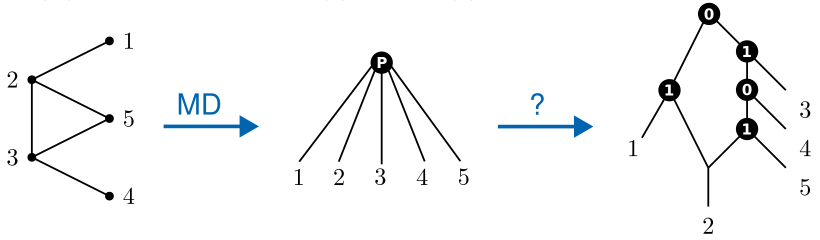

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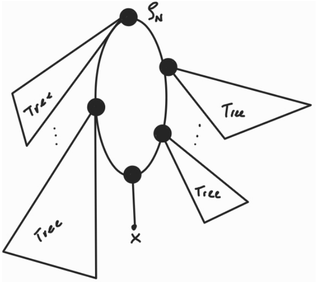
Aim: Understand graph classes that can be explained by 0/1-labeled networks.

Pseudo-cographs: Characterization



Theorem (2022)

G is a pseudo-cograph $\iff$ $|V(G)| \leq 2$ or G can be explained by a galled-tree (N,t) that contains precisely one cycle C such that $\rho_C = \rho_N$ and the (unique) hybrid has precisely one child.

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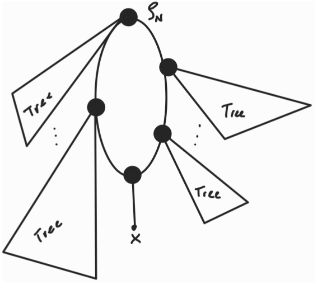

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Pseudo-cographs can be recognized in linear time and a corresponding 0/1-labeled network can be constructed within the same time complexity.

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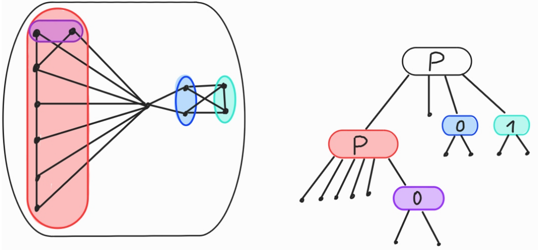

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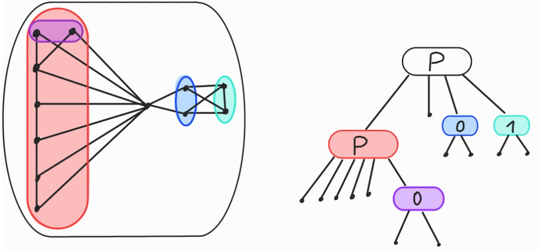
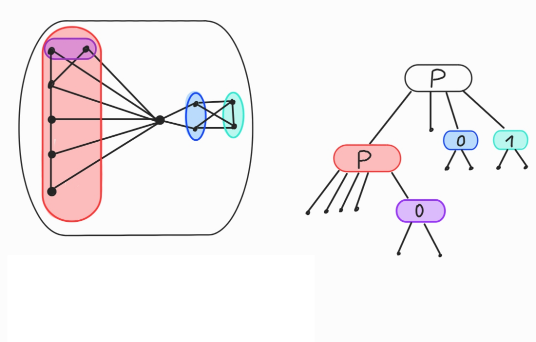


General Aim:

- Preserve the main features of the MD-tree,
  try to modify only the prime-vertices ”P”
  to obtain 0/1-labeled rooted networks to explain graphs
- “unbox” the structure of prime modules

MD and simple cycles



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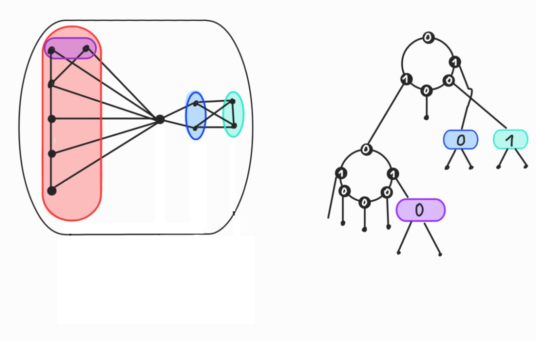

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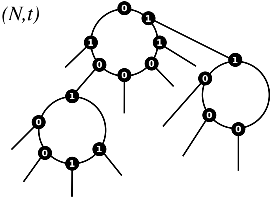

Galled-tree: = 0/1-labeled network “consisting” of edges and simple cycles

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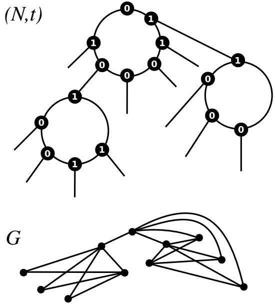

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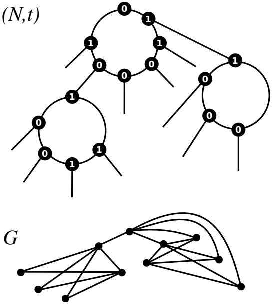

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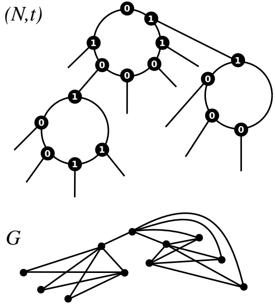

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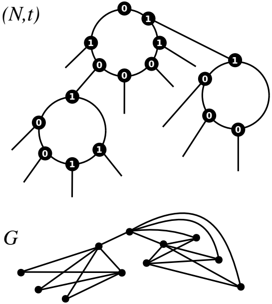

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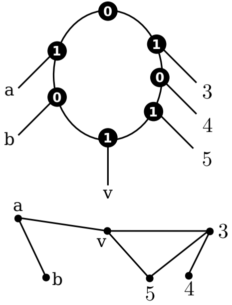

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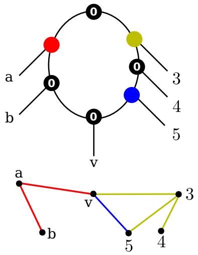
Open Questions:

- 0/1/.../n-labeled networks to explain edge-colored graphs.

$$t(\mathsf{lca}_T(x,y)) = i \iff \{x,y\} \in E \text{ has color } i$$



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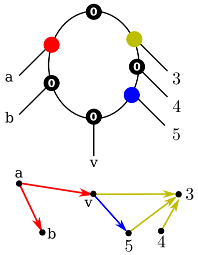

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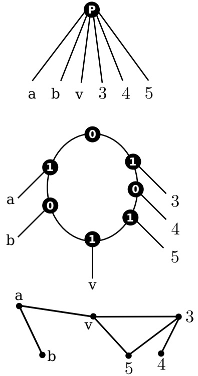
- In the MD-tree (T,t) clusters = modules

  In (N,t), the modules of G form a subset of the clusters in (N,t)

  $\Longrightarrow$ generalization of modules!



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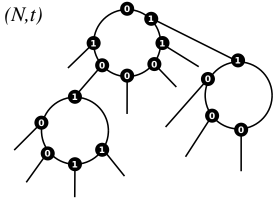

Galled-tree: = 0/1-labeled rooted network “consisting” of edges and simple cycles

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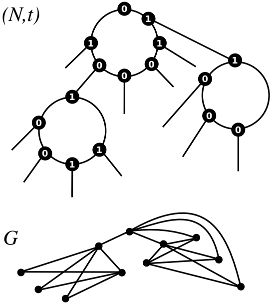

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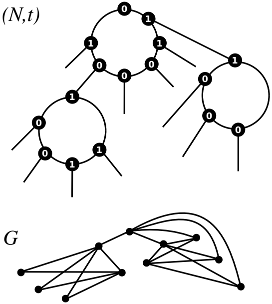

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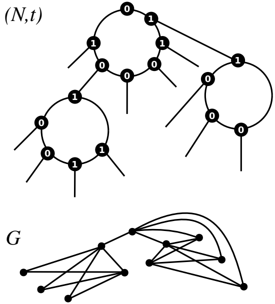

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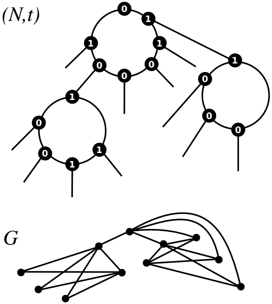

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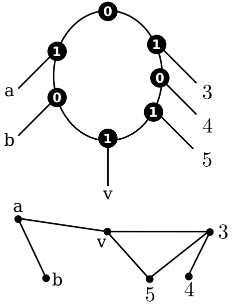

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  0/1/.../n-labeled networks to explain edge-colored graphs.
  $$t(\mathsf{lca}_T(x,y)) = i \iff \{x,y\} \in E \text{ has color } i$$

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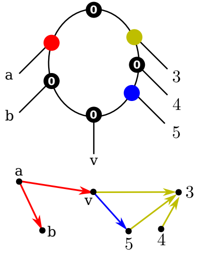

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