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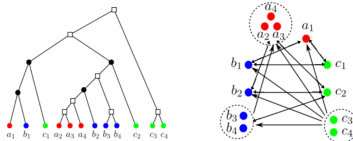
Combinatorics 2022
Mantua, May 30 - June 3

Best match graphs and generalizations

Annachiara Korchmaros
Leipzig Bioinformatics Group

- Gene trees T

- Rooted trees with leaf coloring $\sigma : L \rightarrow S$
- Leaves set L = mutated copies of a gene
- Leaves colors S = species

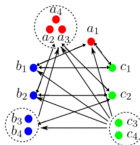
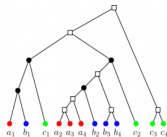


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- Best matches = most closely related leaves

$y \in L$ is a **best match**¹ of $x \in L$ if $\sigma(x) \neq \sigma(y)$ and $\text{lca}(x, y) \preceq \text{lca}(x, z)$ for all $z \in L$ with $\sigma(z) = \sigma(y)$



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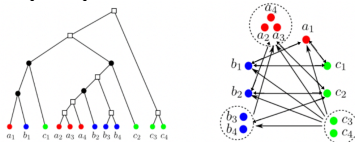
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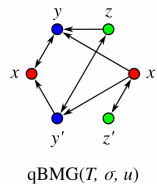
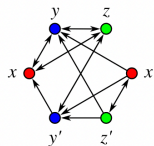
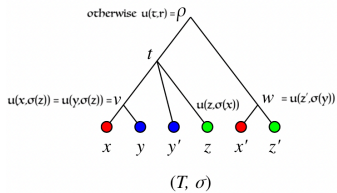
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- $G = (V, E)$ vertex colored digraph is **BMG** of T if

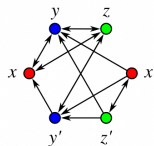
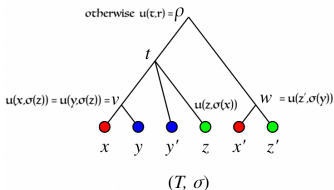
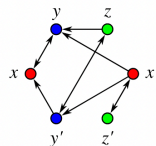
$V = L$ and $x \rightarrow y$ iff y is a best match of x





Truncation map of T is $u : L \times S \rightarrow V$; V (vertex set of T) st

- $u(x, \sigma(x)) = x$
- $u(x, s), s \neq \sigma(x)$ is a node on the path from x to ρ


$$\text{BMG}(T, \sigma)$$

$$\text{qBMG}(T, \sigma, u)$$

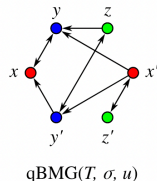
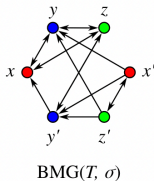
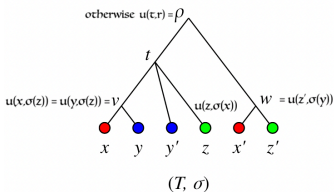
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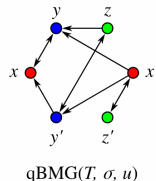
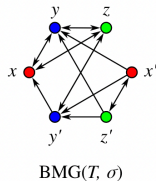
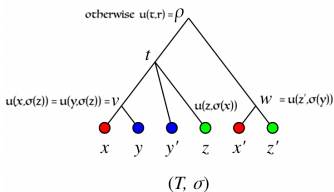
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$V = L$ and $x \rightarrow y$ iff y is a quasi-best match of x in T



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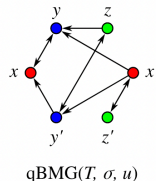
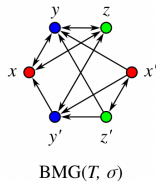
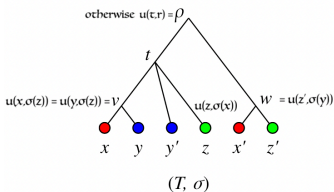
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BMGs are qBMGs !! ($u(x, r) = \rho$)

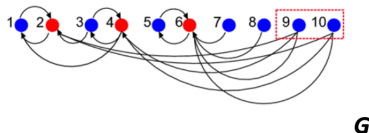
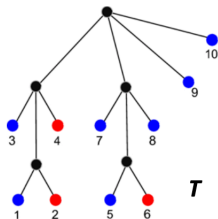


Outline

1. Gene trees
2. 2-BMGs
3. 2-qBMGs

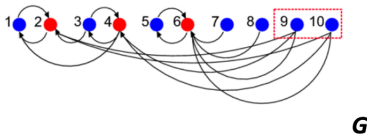
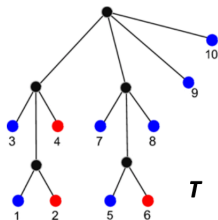
Theorem 1 (Schaller et al. 2021)

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1. Let G be a vertex colored digraph. G is a BMG iff its connected components are BMGs on the same color sets.
2. If a connected vertex colored digraph is a BMG, then all its induced subgraphs on 2 colors are BMGs (**2-BMGs**).



Theorem 2 (Schaller et al. 2021)

Let $G = (V, E)$ be a connected bipartite vertex colored digraph and $N(x)$ the set of outneighbours of x . G is a 2-BMG iff

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N0 G is sink free.

N1 If u and v are independent vertices, then there exist no vertices w and t st $ut, vw, tw \in E$.



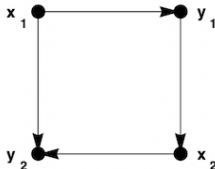
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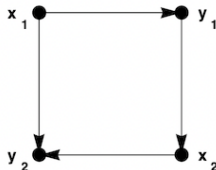
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N3 If $N(u) \cap N(v) \neq \emptyset \Rightarrow N(u) \subseteq N(v)$ or $N(v) \subseteq N(u)$.



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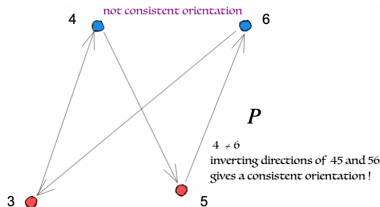
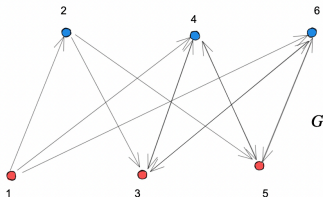
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- **Consistent orientation**³ of G if it preserves \sim

Not all orientations are consistent !!



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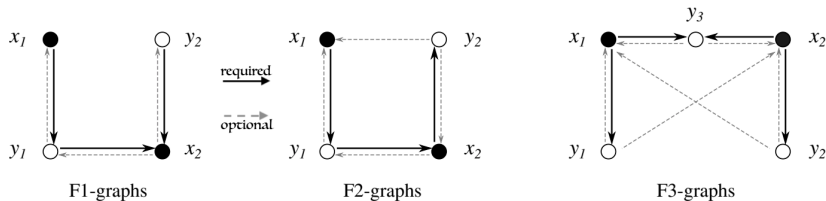
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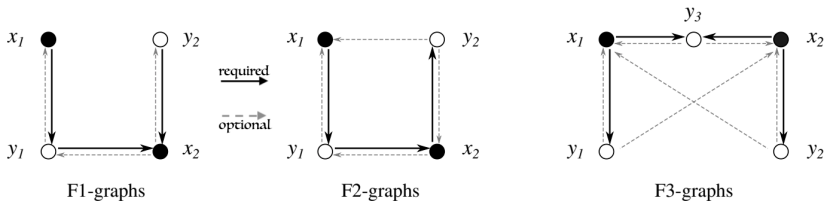
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There are 17 non-isomorphic forbidden induced subgraphs⁴

2-qBMGs

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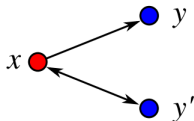
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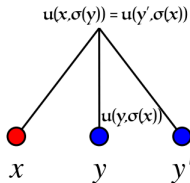
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(G, σ)



(T, σ, u)

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2-BMGs do not form an hereditary digraph class
(sink-freeness is not hereditary) !!

Theorem 6 (A.K., Schaller, Stadler, Hellmuth 2021)

Let G be a bipartite (non necessary connected) vertex colored digraph. If G does not contain an induced F_1 -, F_2 -, or F_3 -graph, then G is a 2-qBMG.

Theorem 6 (A.K., Schaller, Stadler, Hellmuth 2021)

Let G be a bipartite (non necessary connected) vertex colored digraph. If G does not contain an induced F_1 -, F_2 -, or F_3 -graph, then G is a 2-qBMG.

Proposition 2 (A.K., Schaller, Stadler, Hellmuth 2021)

Let G be digraph satisfying N_1 and N_2 , then G is bipartite.

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Case $L = |V|$: Rooted start tree

$u(x, \sigma(y)) = \rho$ if $xy \in E$; $u(x, \sigma(y)) = x$ if $xy \notin E$.

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(b) What is the qBMG-chromatic number of (G, σ) ?
(minimum number of colors for which G is a qBMG).

If a L -coloring exists this can be transformed in an $L + 1$ -coloring (by arbitrarily splitting a color class)⁶.

Thank you

- Peter Stadler
- David Schaller
- Marc Hellmut



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Is every orientation of G acyclic? No, P has a 4-cycle.