



UNIVERSITÄT
LEIPZIG

QUASI-BEST MATCH GRAPHS

38th TBI WINTERSEMINAR IN BLED














Annachiara Korchmaros

joint work with David Schaller, Marc Hellmuth, Peter F. Stadler

Bioinformatics Group, University of Leipzig














February 16, 2023

BMG REFERENCES

-  Geiß, Manuela, Edgar Chávez, et al. (2019). “Best match graphs”. In: *Journal of mathematical biology* 78.
-  Geiß, Manuela, Marcos E González Laffitte, et al. (2020). “Best match graphs and reconciliation of gene trees with species trees”. In: *Journal of mathematical biology* 80.5.
-  Hellmuth, Marc, Manuela Geiß, and Peter F Stadler (2020). “Complexity of modification problems for reciprocal best match graphs”. In: *Theoretical Computer Science* 809.
-  Korchmaros, Annachiara (2021). “The structure of 2-colored best match graphs”. In: *Discrete Applied Mathematics* 304.
-  Manuela, Geiß, Peter F Stadler, and Marc Hellmuth (2020). “Reciprocal best match graphs”. In: *Journal of Mathematical Biology* 80.3.
-  Schaller, David, Manuela Geiß, Edgar Chávez, et al. (2021). “Corrigendum to “Best match graphs””. In: *Journal of Mathematical Biology* 82.
-  Schaller, David, Manuela Geiß, Marc Hellmuth, et al. (2021a). “Arc-completion of 2-colored best match graphs to binary-explainable best match graphs”. In: *Algorithms* 14.4.
-  — (2021b). “Heuristic algorithms for best match graph editing”. In: *Algorithms for Molecular Biology* 16.1.
-  — (2021c). “Least resolved trees for two-colored best match graphs”. In: *arXiv preprint arXiv:2101.07000*.
-  Schaller, David, Manuela Geiß, Peter F Stadler, et al. (2021). “Complete characterization of incorrect orthology assignments in best match graphs”. In: *Journal of mathematical biology* 82.3.
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-  Stadler, Peter F et al. (2020). “From pairs of most similar sequences to phylogenetic best matches”. In: *Algorithms for Molecular Biology* 15.1.

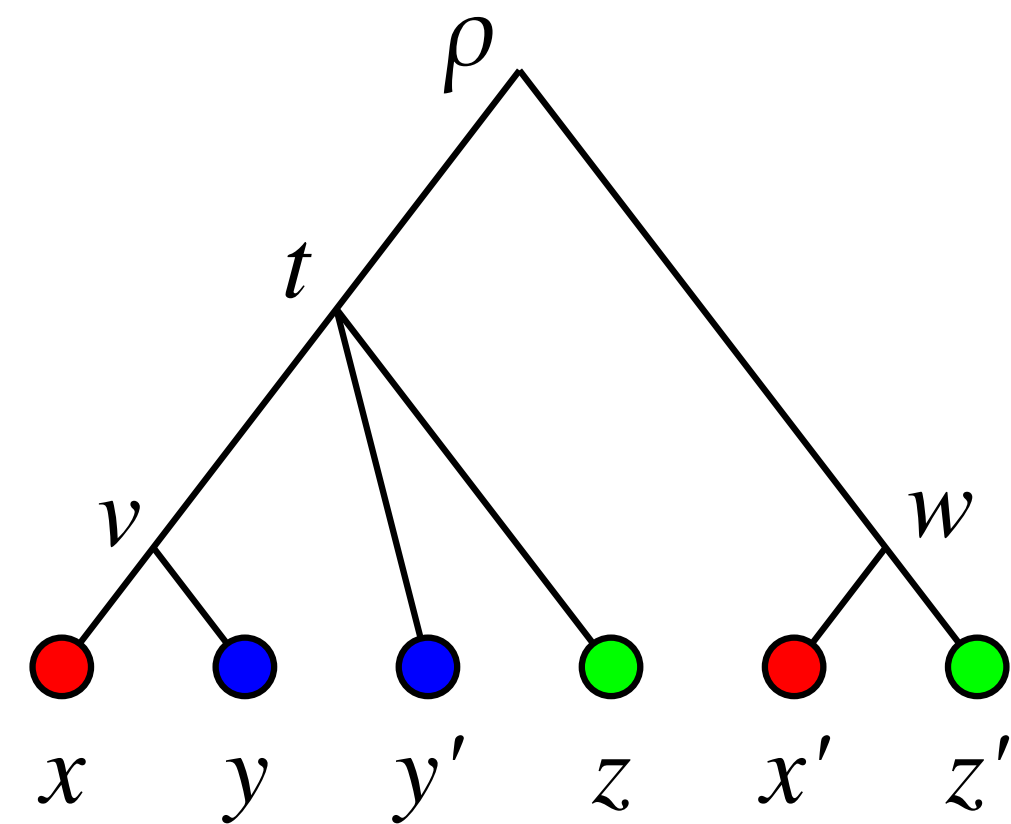
BMG REFERENCES

13 papers
in 3 years

-  Geiß, Manuela, Edgar Chávez, et al. (2019). “Best match graphs”. In: *Journal of mathematical biology* 78.
-  Geiß, Manuela, Marcos E González Laffitte, et al. (2020). “Best match graphs and reconciliation of gene trees with species trees”. In: *Journal of mathematical biology* 80.5.
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BEST MATCH GRAPHS - DEFINITION

- ▶ (T, σ) rooted gene tree, leaf coloring σ on leaf set $L(T)$

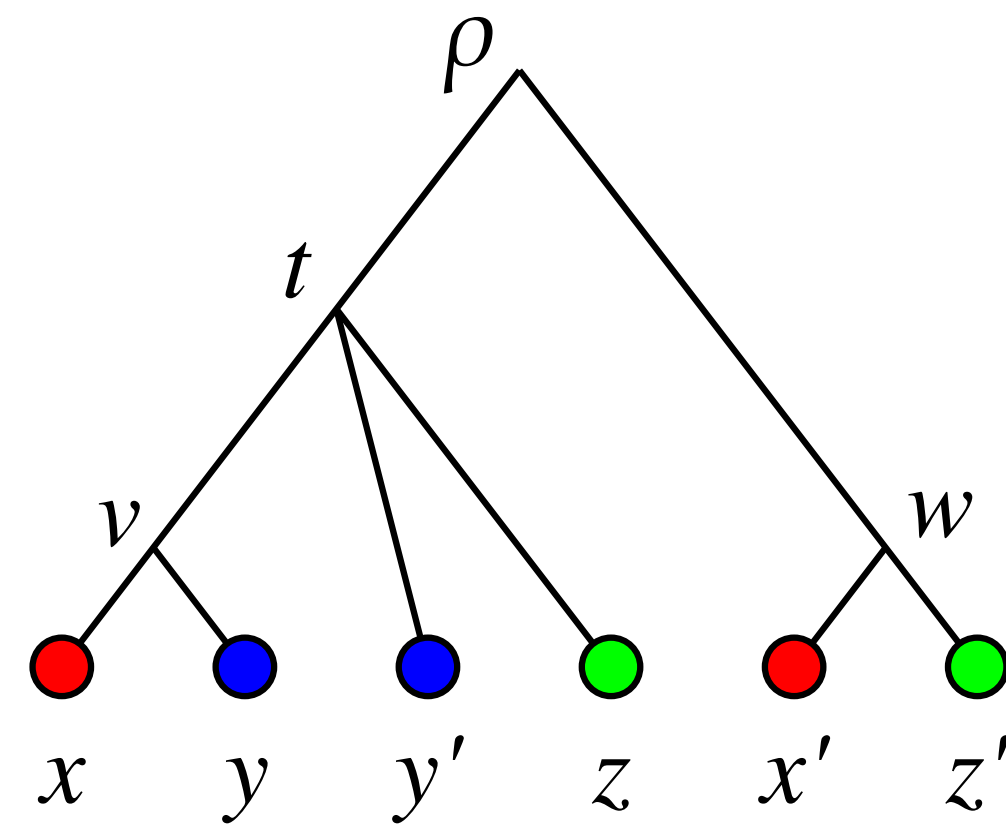


(T, σ)

v, t, w duplications/speciations

BEST MATCH GRAPHS - DEFINITION

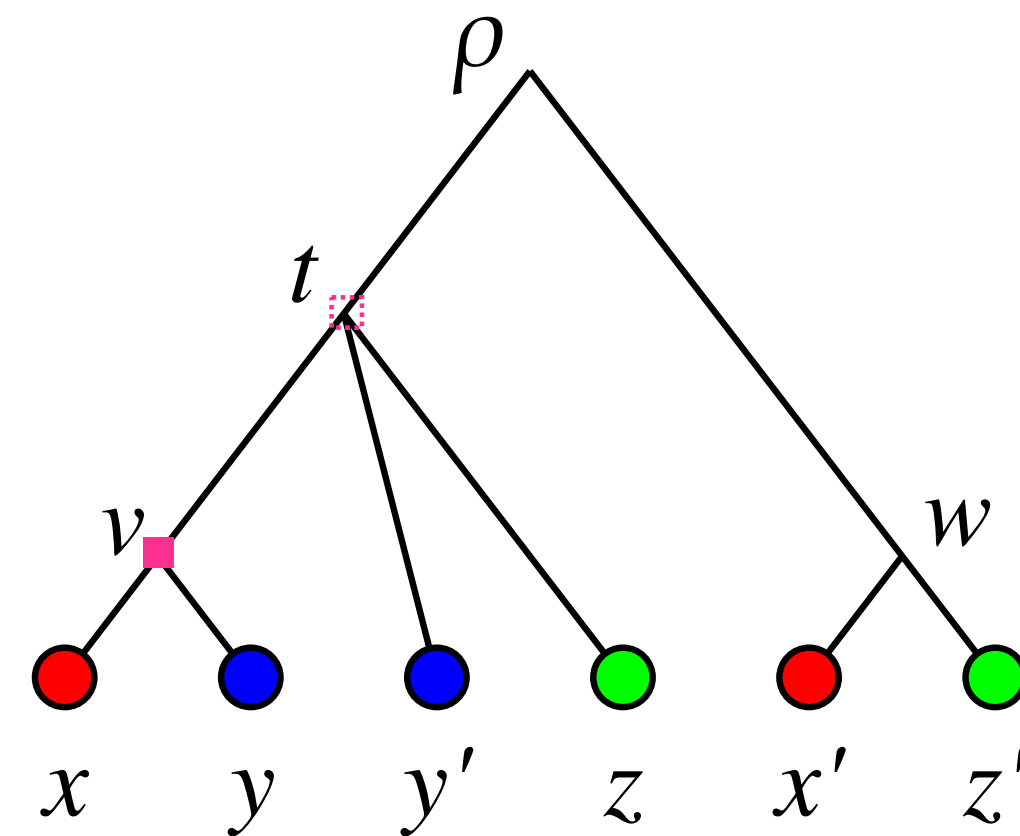
- ▶ (T, σ) rooted gene tree, leaf coloring σ on leaf set $L(T)$
- ▶ $y \in L(T)$ is a **best match** of $x \in L(T)$ if
 1. $\sigma(x) \neq \sigma(y)$ and
 2. $\text{lca}(x, y) \preceq \text{lca}(x, z)$ for all $z \in L(T)$ with $\sigma(z) = \sigma(y)$



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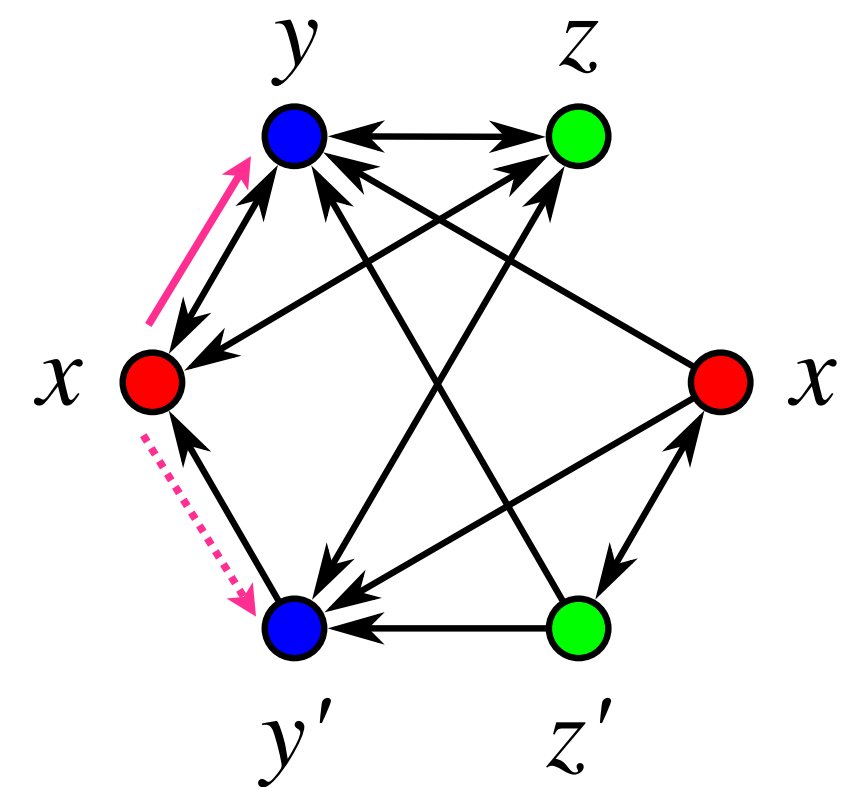
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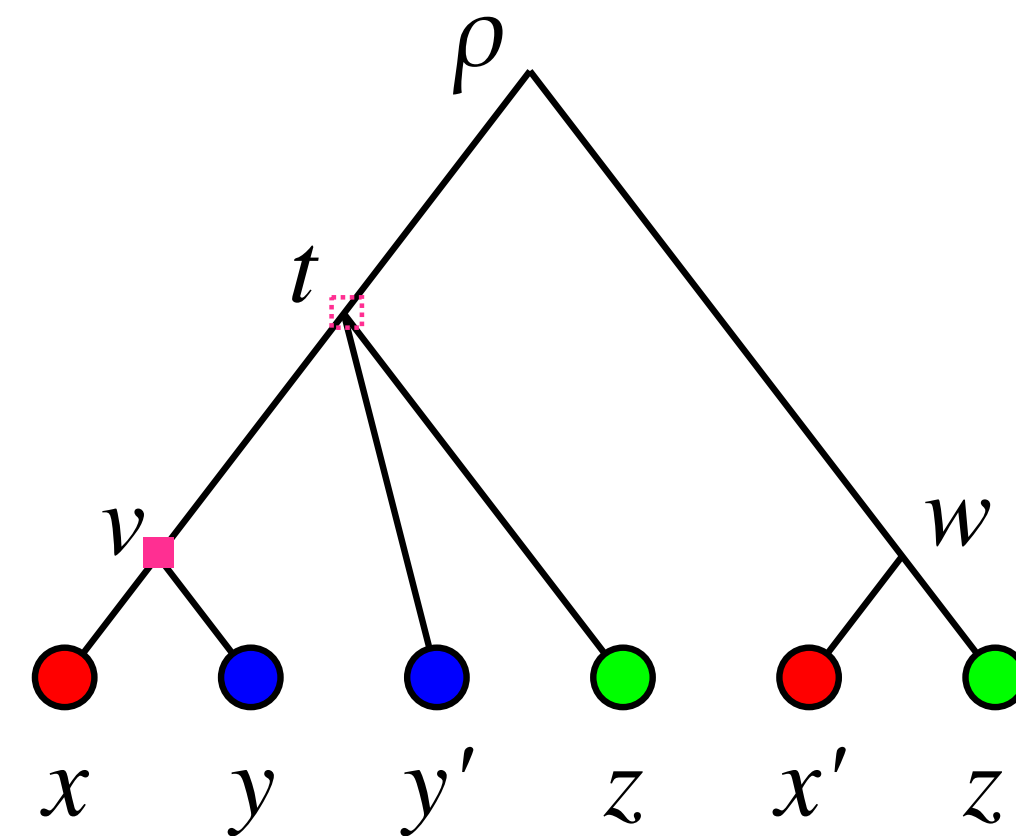
v, t, w duplications/speciations



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

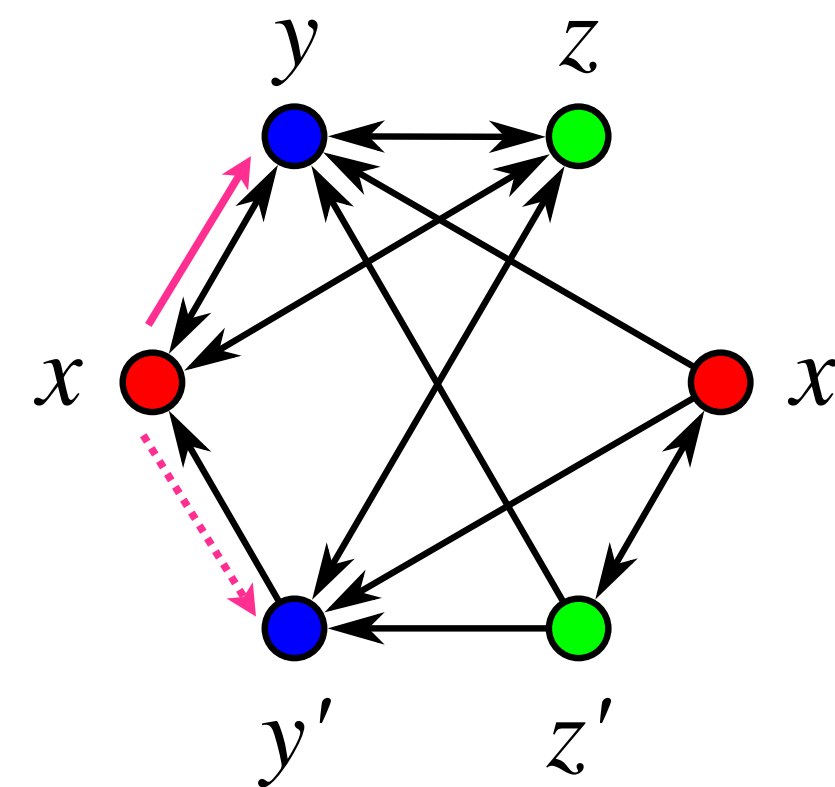
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- ▶ (G, σ) is **BMG** (T, σ) if vertices=leaves colored by σ and $x \rightarrow y$ iff y is a best match of x on (T, σ)



(T, σ)

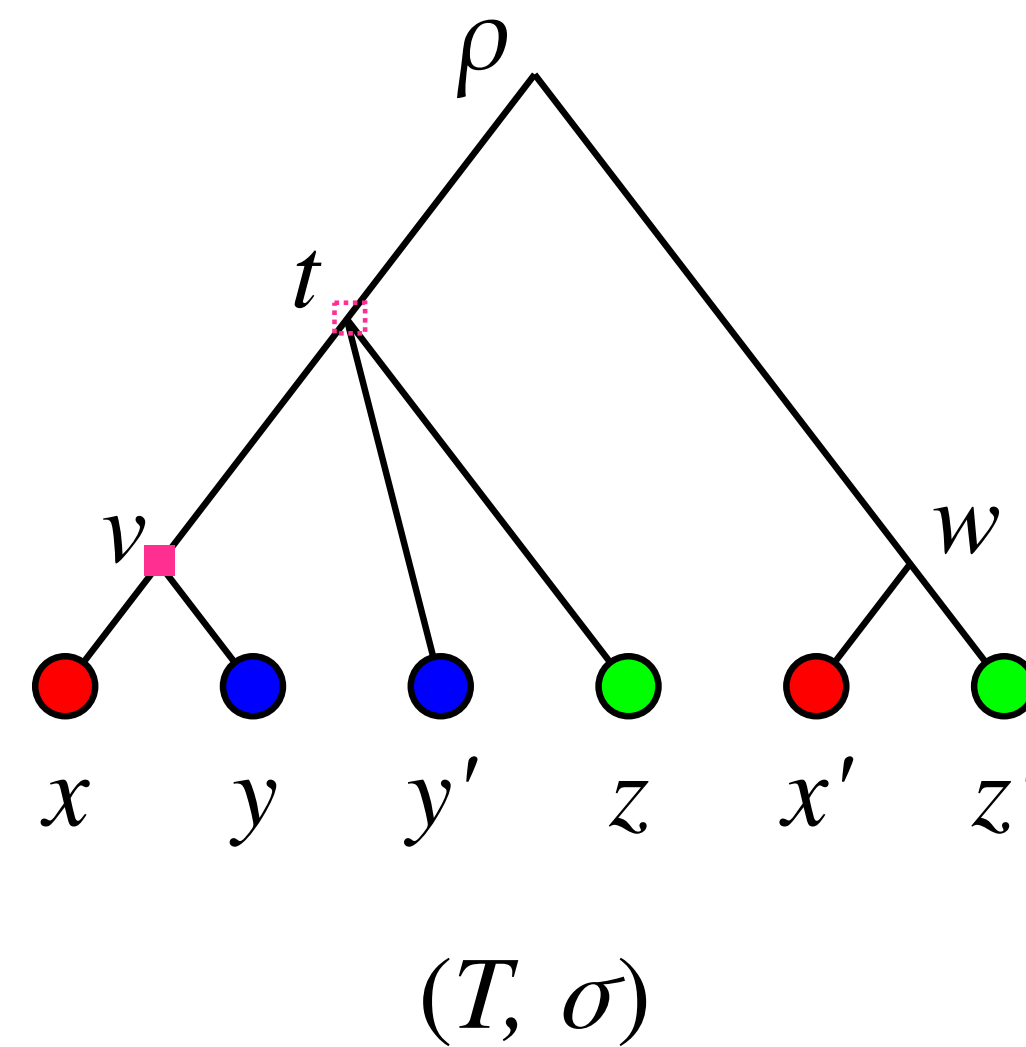
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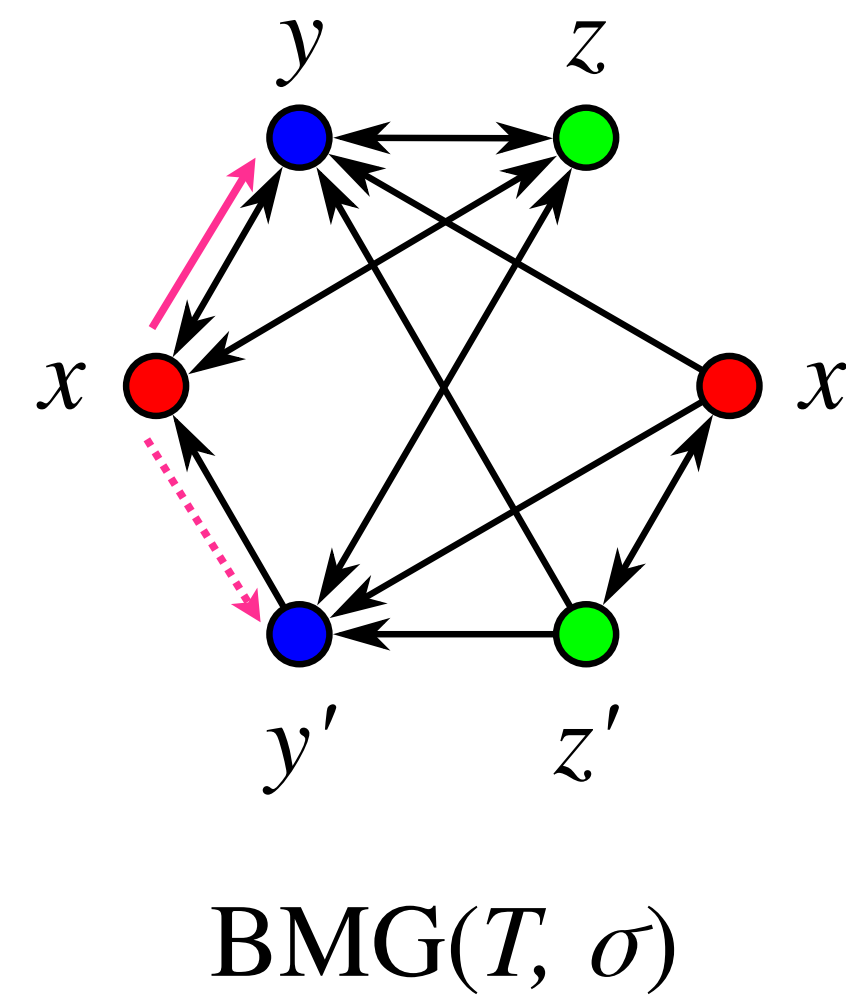
BMG (T, σ)

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- ▶ (G, σ) is **BMG** (T, σ) if vertices=leaves colored by σ and $x \rightarrow y$ iff y is a best match of x on (T, σ)
- ▶ Bio connection: orthologs \implies reciprocal best matches (symmetric best matches)

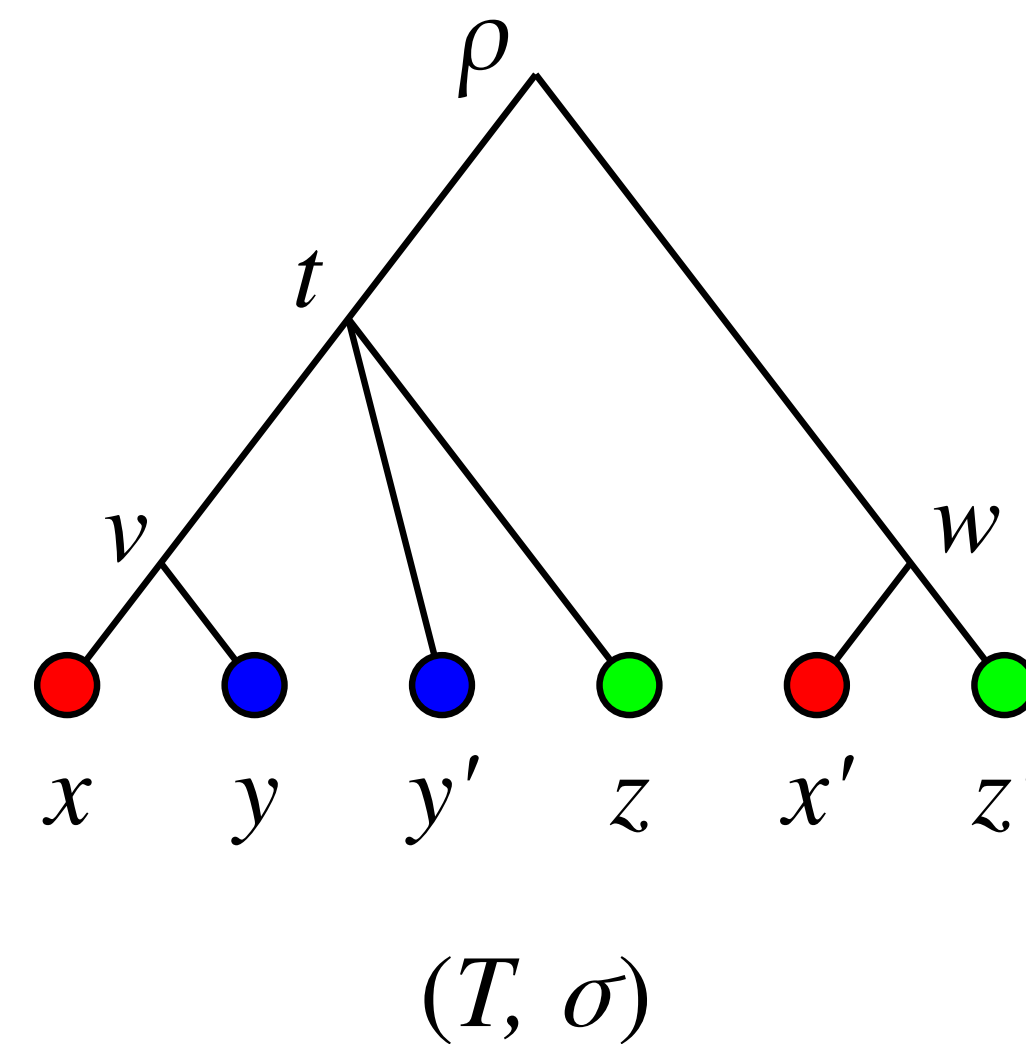


v, t, w duplications/speciations

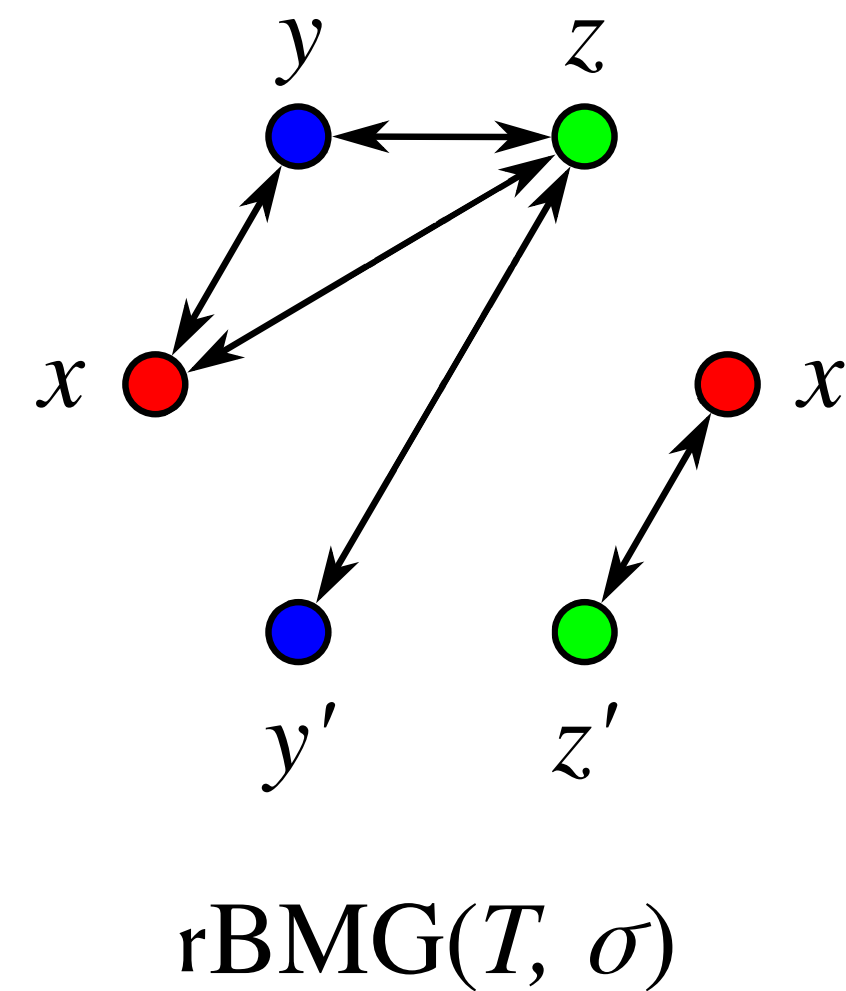


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BEST MATCH GRAPHS - NON-HEREDITARY

BMGs are

- ▶ properly colored, no loops, no multiple edges

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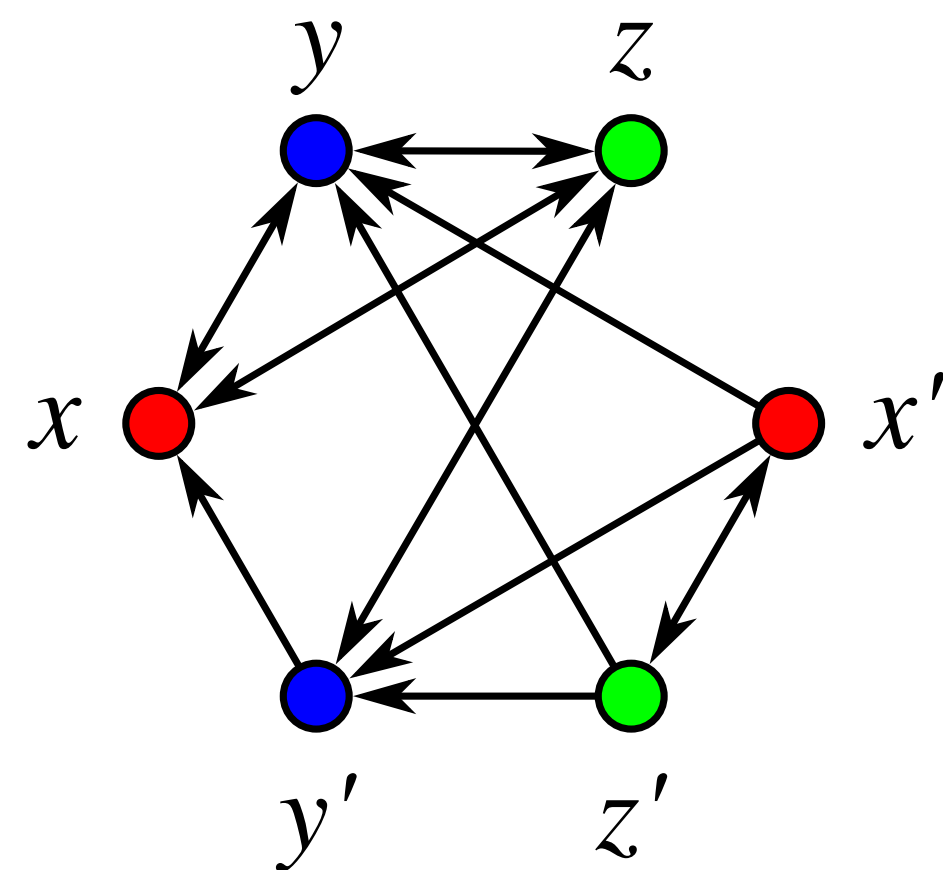
- ▶ properly colored, no loops, no multiple edges
- ▶ **color-sink-free** (every vertex has a best match for every species)
- ▶ not a **hereditary** class (induced subgraphs are not necessary BMGs)

BEST MATCH GRAPHS - NON-HEREDITARY

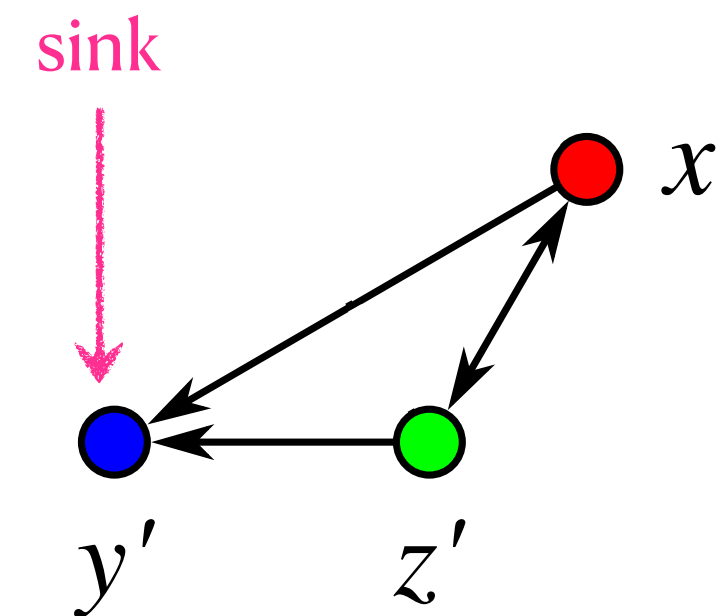
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F is induced subgraph of G if $x, y \in V(F)$ and $(x, y) \in E(G) \Rightarrow (x, y) \in E(F)$



BMG(T, σ)



BMG(T, σ)[$\{x', y', z'\}$]

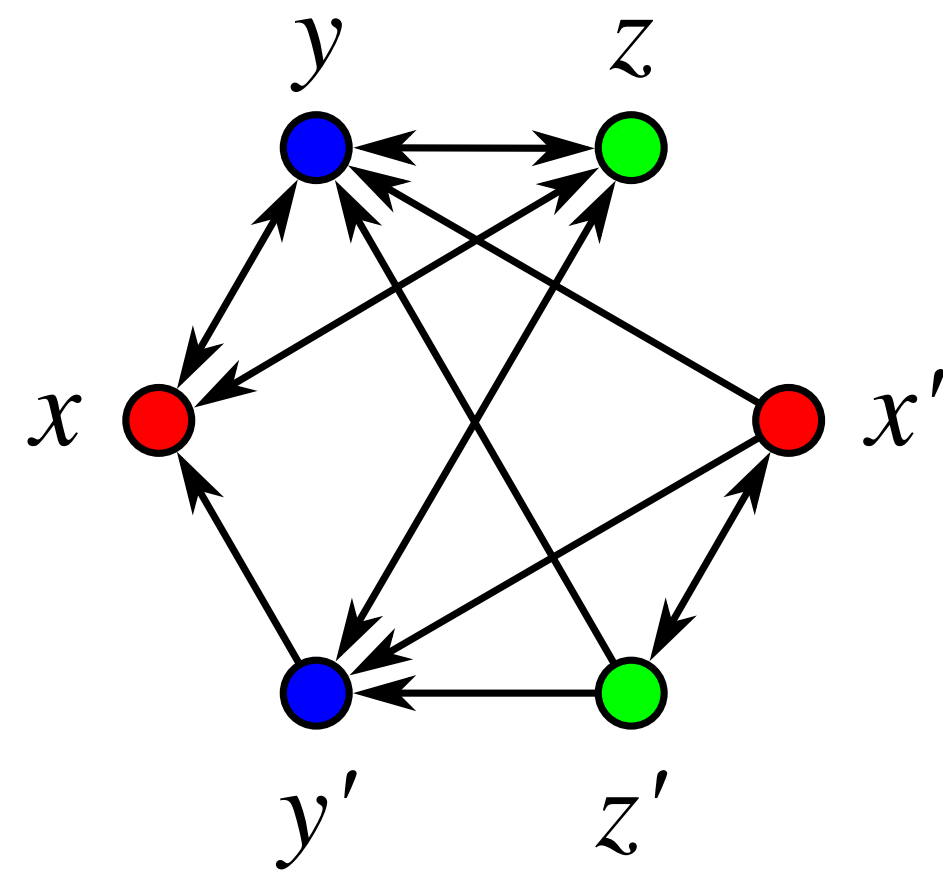
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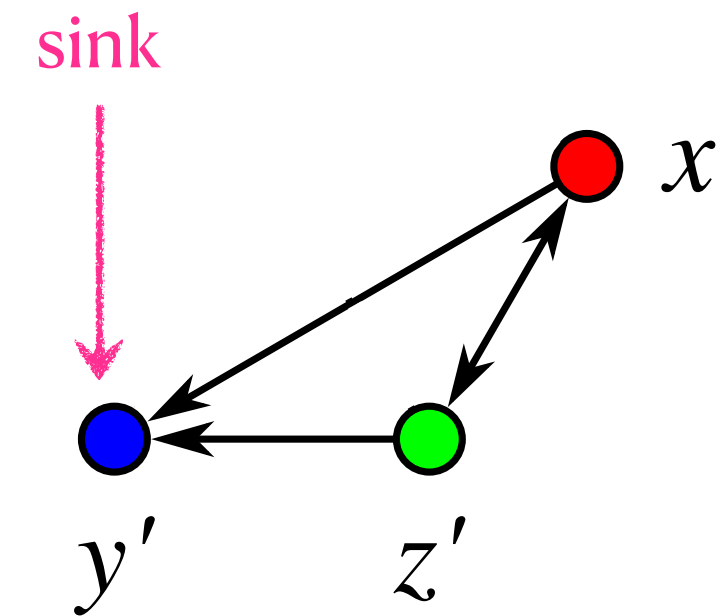
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Bio connection: Can we recognize BMGs?



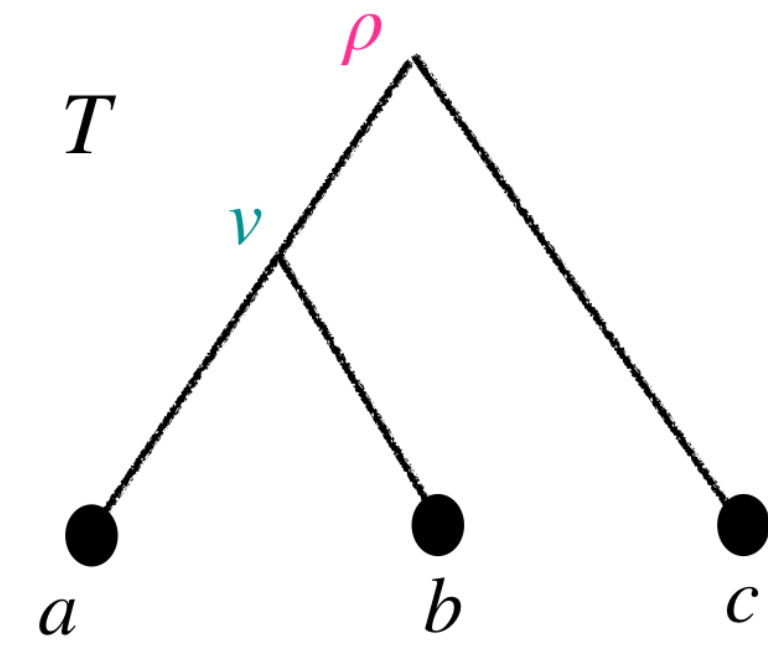
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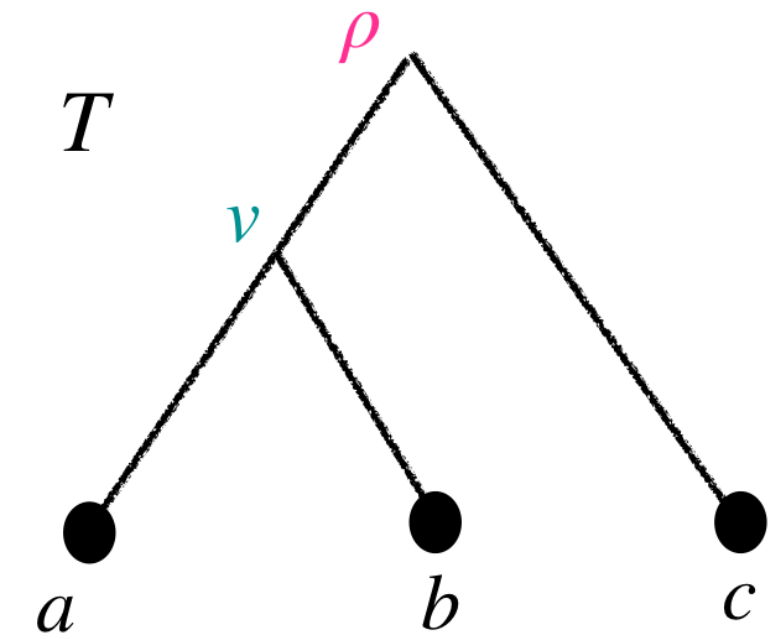
BEST MATCH GRAPHS - TRIPLES

- ▶ $ab|c$ is a (rooted) **triple** if $\text{lca}(a, b)$ is descendent in T of $\text{lca}(a, c) = \text{lca}(b, c)$



BEST MATCH GRAPHS - TRIPLES

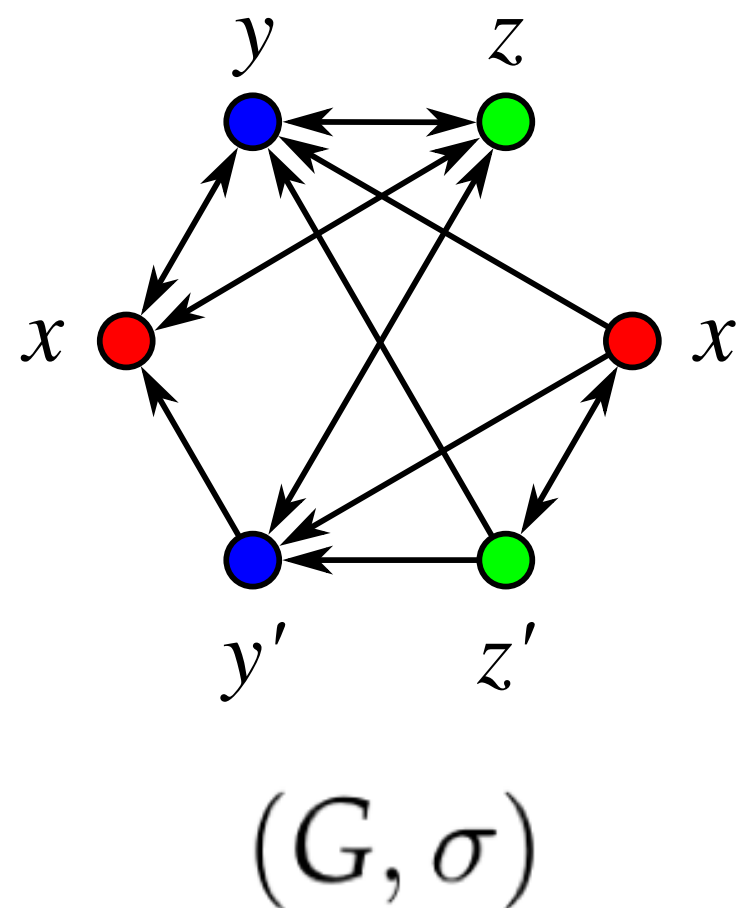
▶ $ab|c$ is a (rooted) **triple** if $\text{lca}(a, b)$ is descendent in T of $\text{lca}(a, c) = \text{lca}(b, c)$



▶ (G, σ) digraph, vertex-colored by σ

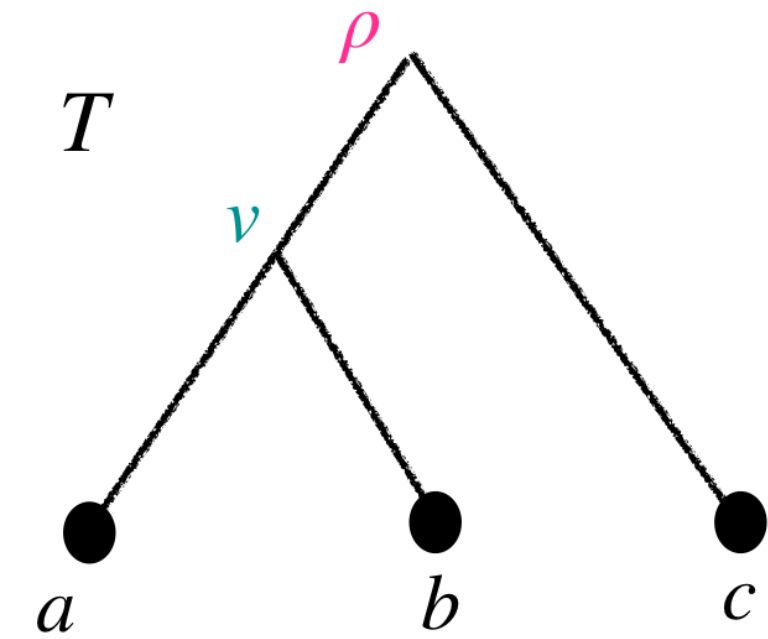
- $\mathcal{R}(G, \sigma) := \{ab|b' : \sigma(a) \neq \sigma(b) = \sigma(b'), ab \in E(G), \text{ and } ab' \notin E(G)\}$ **informative triples**

$xy|y' \in \mathcal{R}(G, \sigma)$



BEST MATCH GRAPHS - TRIPLES

▶ $ab|c$ is a (rooted) **triple** if $\text{lca}(a, b)$ is descendent in T of $\text{lca}(a, c)=\text{lca}(b, c)$

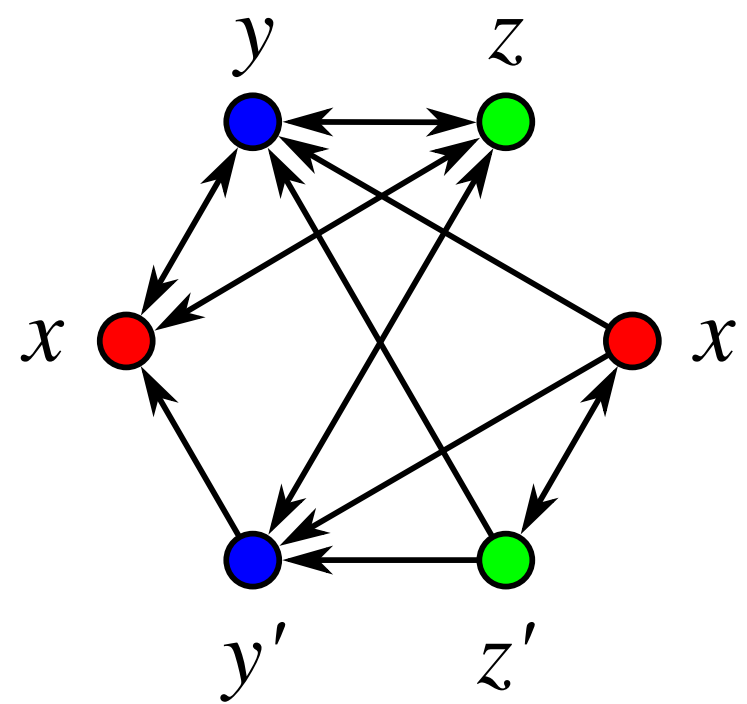


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- $\mathcal{R}(G, \sigma) := \{ab|b' : \sigma(a) \neq \sigma(b) = \sigma(b'), ab \in E(G), \text{ and } ab' \notin E(G)\}$ **informative triples**
- $\mathcal{F}(G, \sigma) := \{ab|b' : \sigma(a) \neq \sigma(b) = \sigma(b'), b \neq b', \text{ and } ab, ab' \in E(G)\}$ **forbidden triples**

$xy|y' \in \mathcal{R}(G, \sigma)$

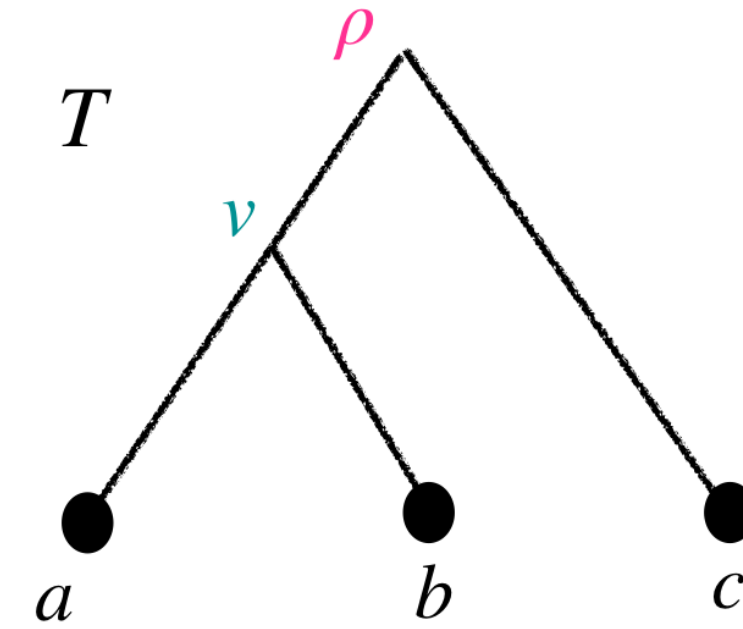
$z'y'|y \in \mathcal{F}(G, \sigma)$



(G, σ)

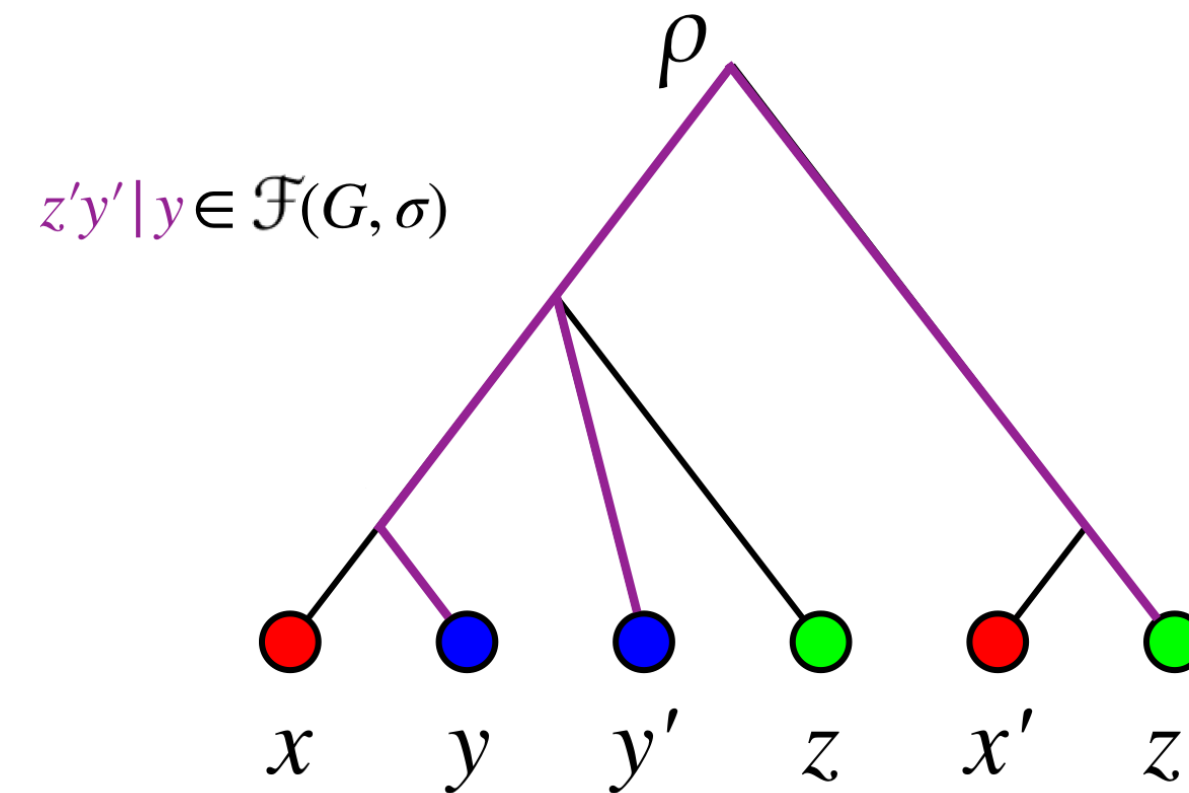
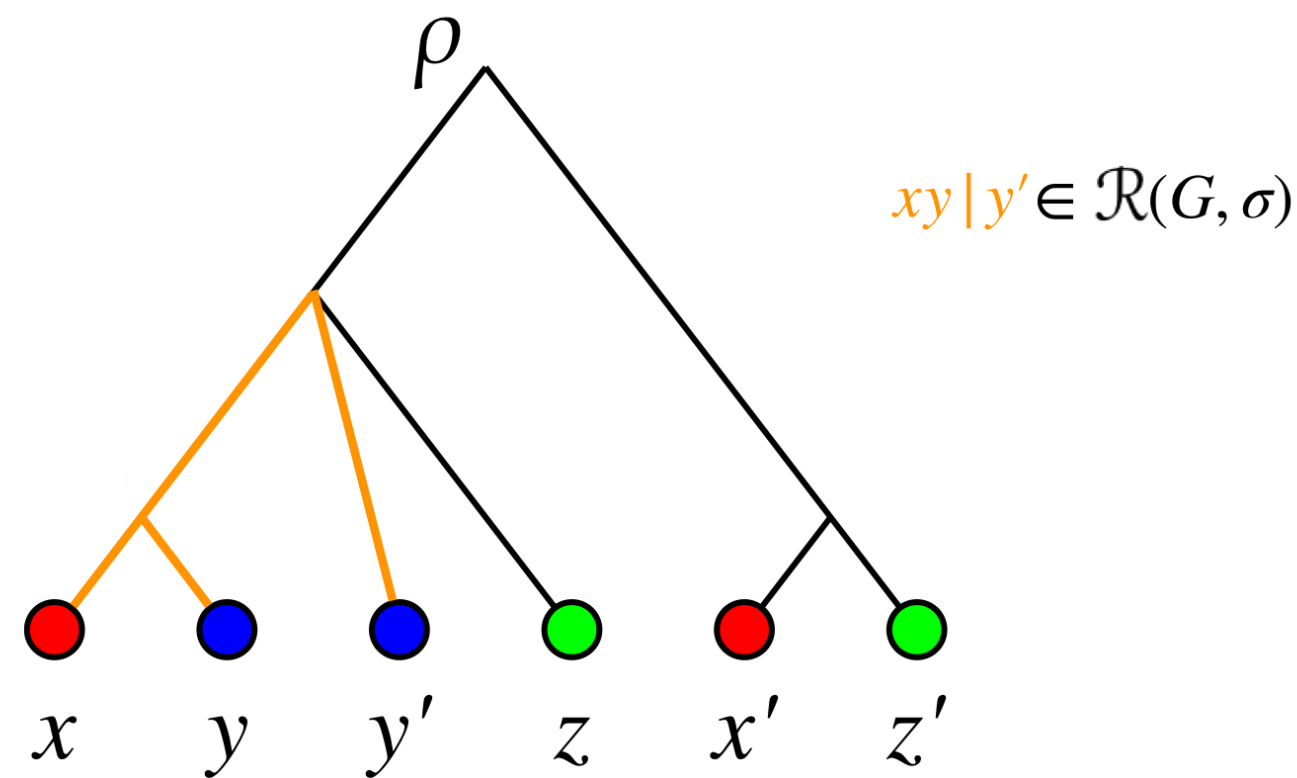
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Theorem

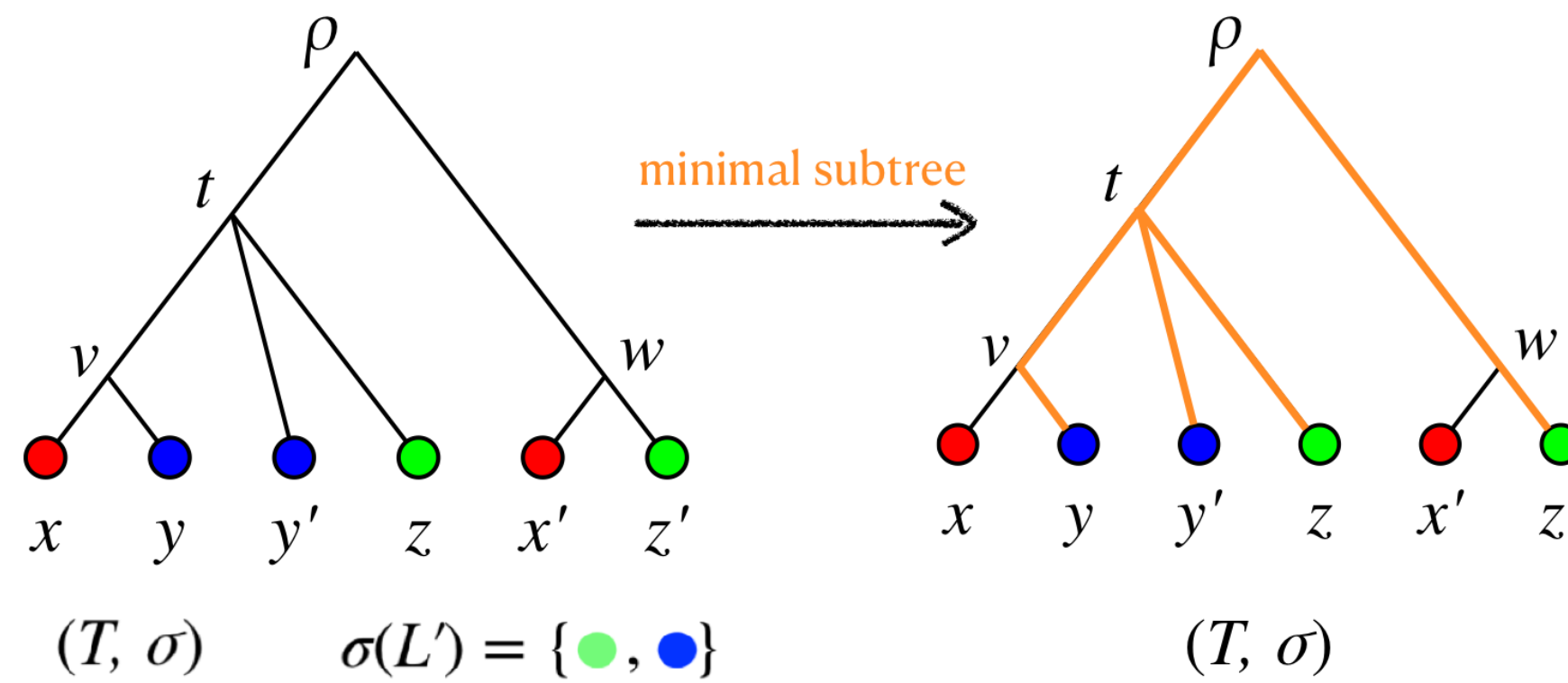
(G, σ) properly colored digraph is a BMG iff (i) (G, σ) is color-sink free, and (ii) there exists (T, σ) displaying all triples in $\mathcal{R}(G, \sigma)$ but none of the triples in $\mathcal{F}(G, \sigma)$

BEST MATCH GRAPHS - UNIQUE LRT

- ▶ Problem: different trees associated to $BMG(G, \sigma)$, how to choose the most parsimonious???

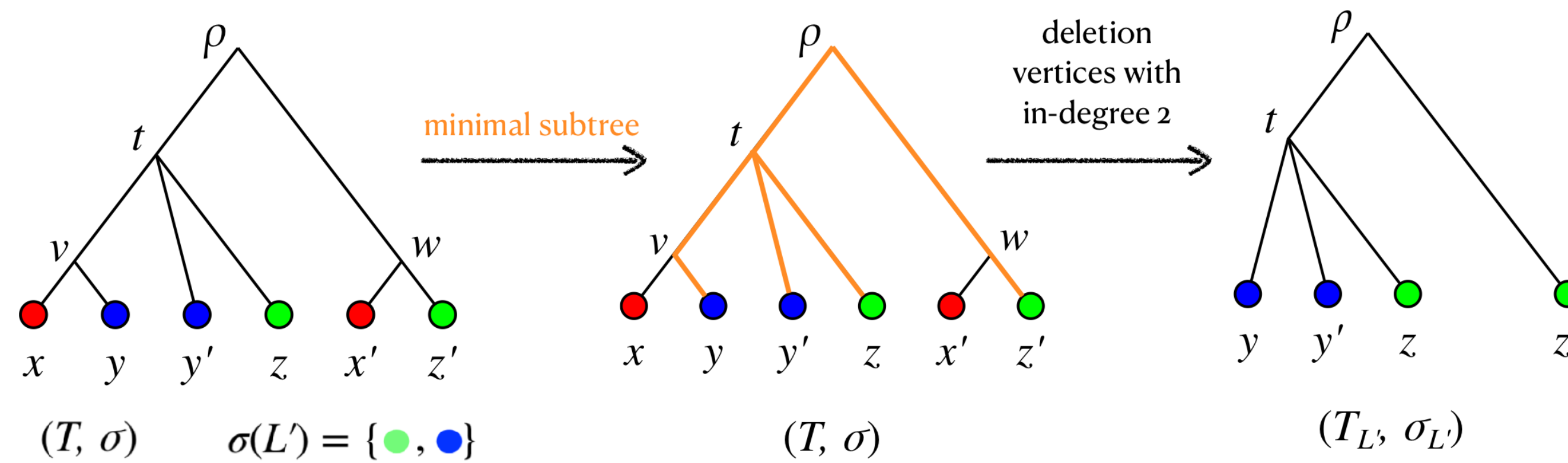
BEST MATCH GRAPHS - UNIQUE LRT

- ▶ Problem: different trees associated to $BMG(G, \sigma)$, how to choose the most parsimonious???
- ▶ $T_{L'}$ is a **restriction** of T to a subset L' of leaves of T



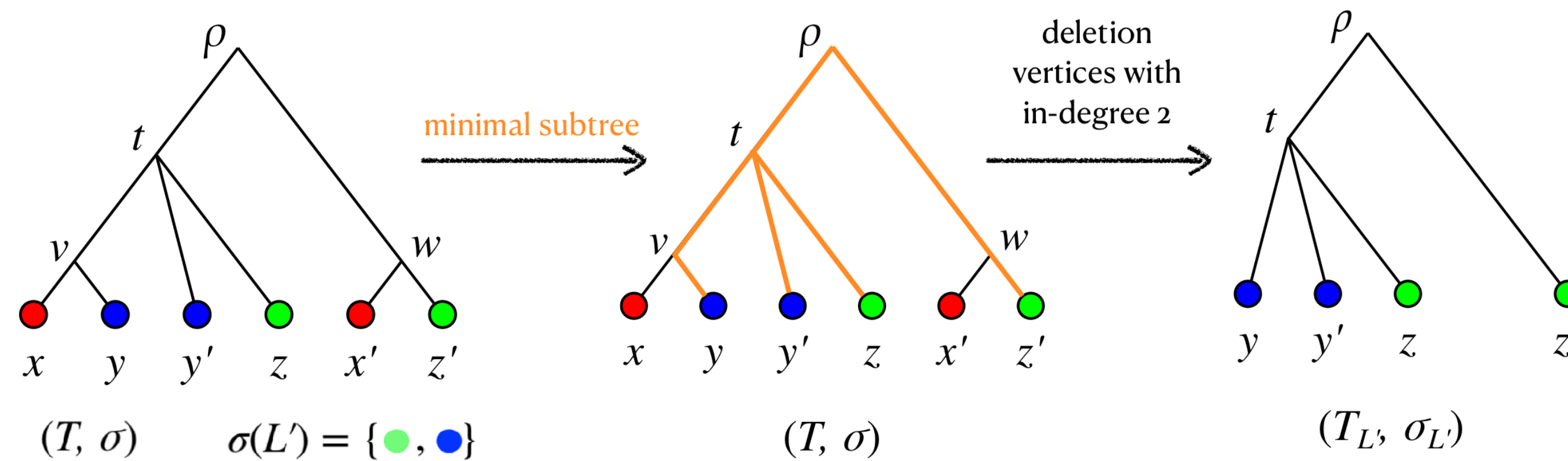
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BEST MATCH GRAPHS - UNIQUE LRT

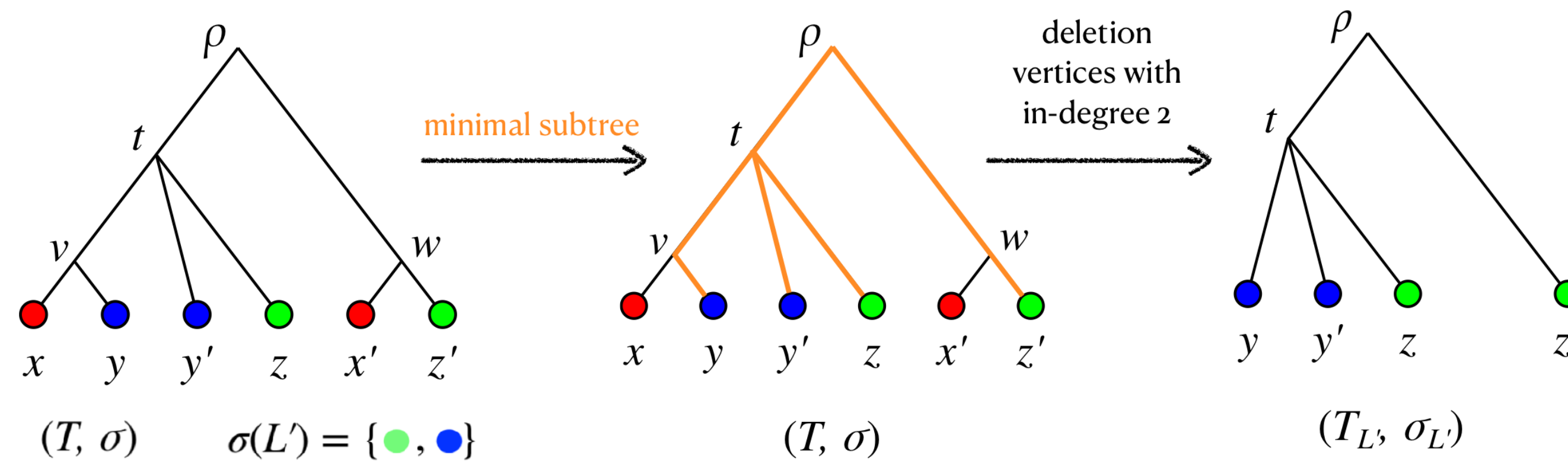
- ▶ Problem: different trees associated to $BMG(G, \sigma)$, how to choose the most parsimonious???
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- ▶ (T, σ) is **LRT** if there is NO $T' = T_{L'} (+ \text{inner edge contractions})$ st $BMG(T, \sigma) = BMG(T', \sigma)$

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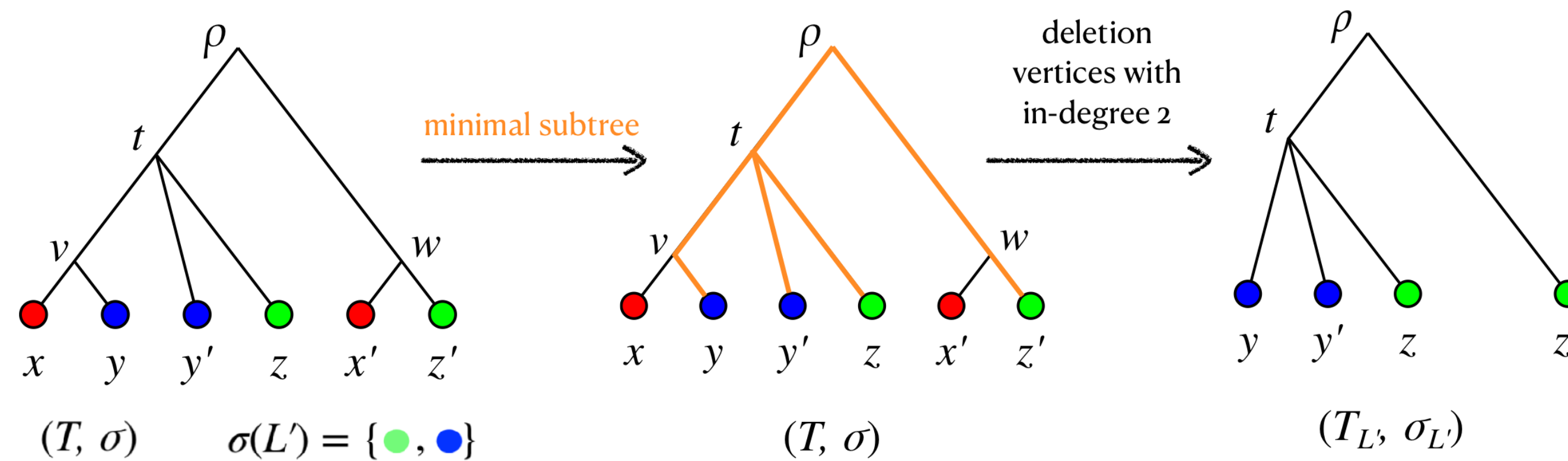
- ▶ (T, σ) is **LRT** if there is NO $T' = T_L$ (+ inner edge contractions) st $BMG(T, \sigma) = BMG(T', \sigma)$

Theorem

- ▶ Every BMG has a unique LRT¹

BEST MATCH GRAPHS - UNIQUE LRT

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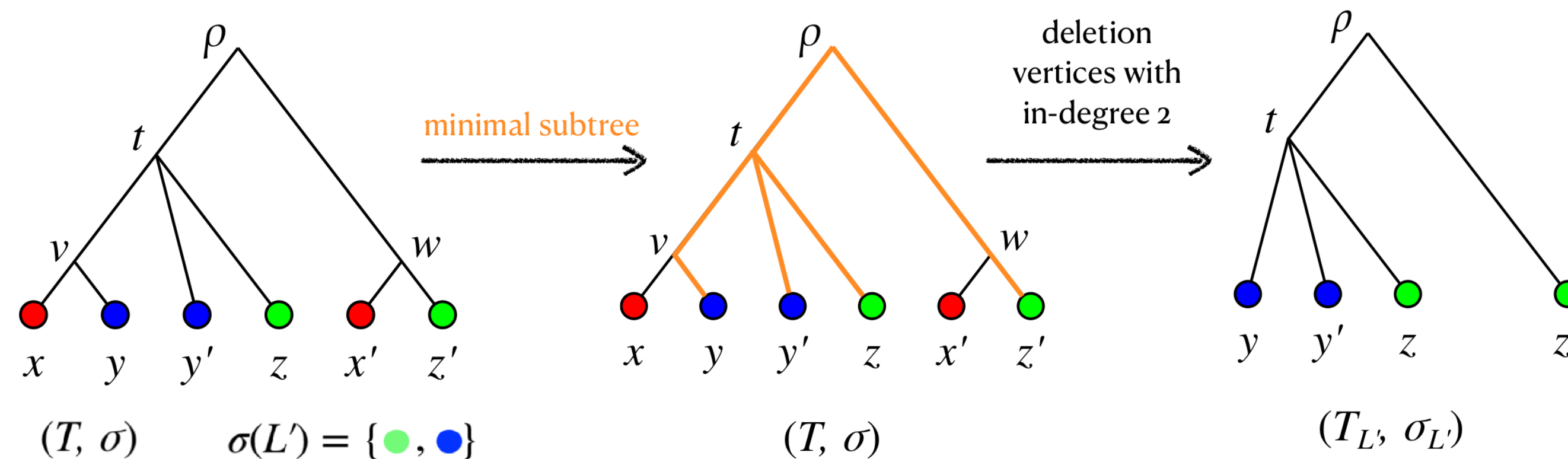
- ▶ Every BMG has a unique LRT¹
- ▶ Build the LRT in polynomial time with MTT algorithm²

¹Manuela Geiß, Edgar Chávez, et al. (2019). "Best match graphs". In: *Journal of mathematical biology* 78.

²Annachiara Korchmaros et al. (2023). "Quasi-best match graphs". In: *Discrete Applied Mathematics* 331, pp. 104–125.

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- ▶ Every BMG has a unique LRT¹
- ▶ Build the LRT in polynomial time with MTT algorithm² \Rightarrow recognize a BMG in polynomial time

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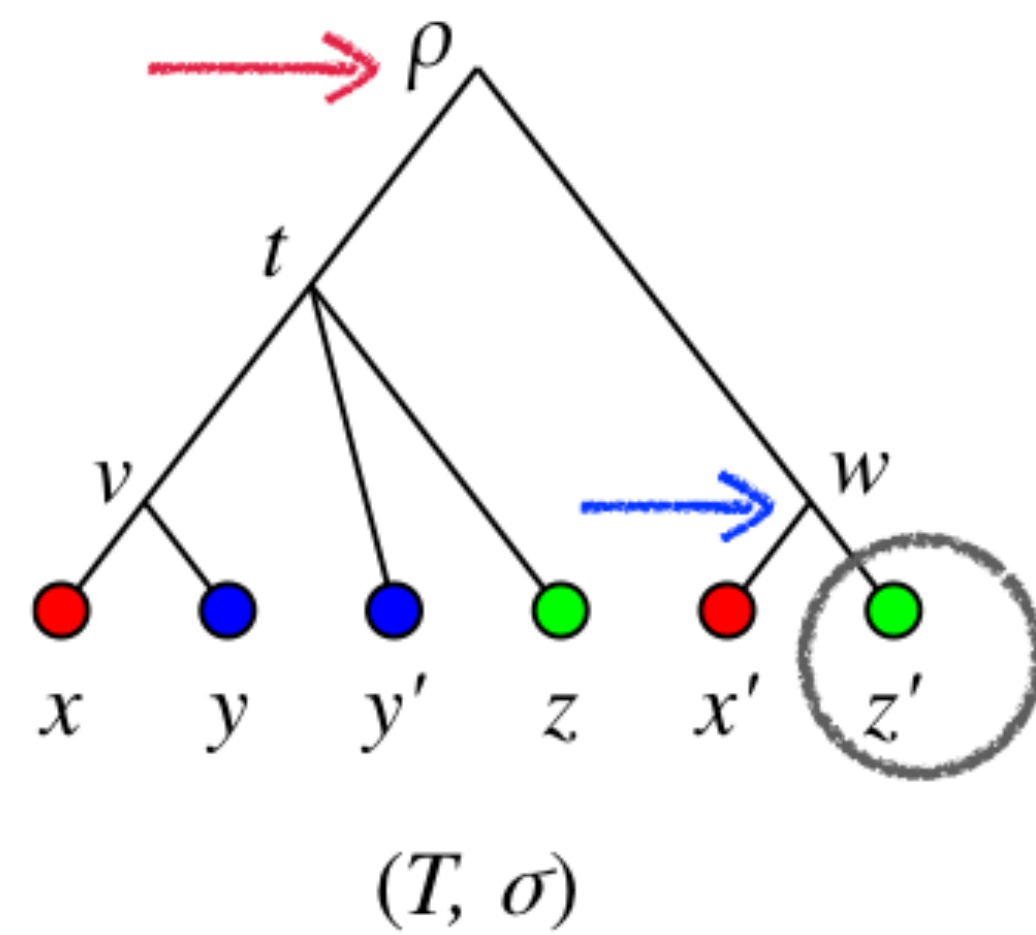
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QUASI-BEST MATCH GRAPHS - DEFINITION

- ▶ How do we relate far-away genes?

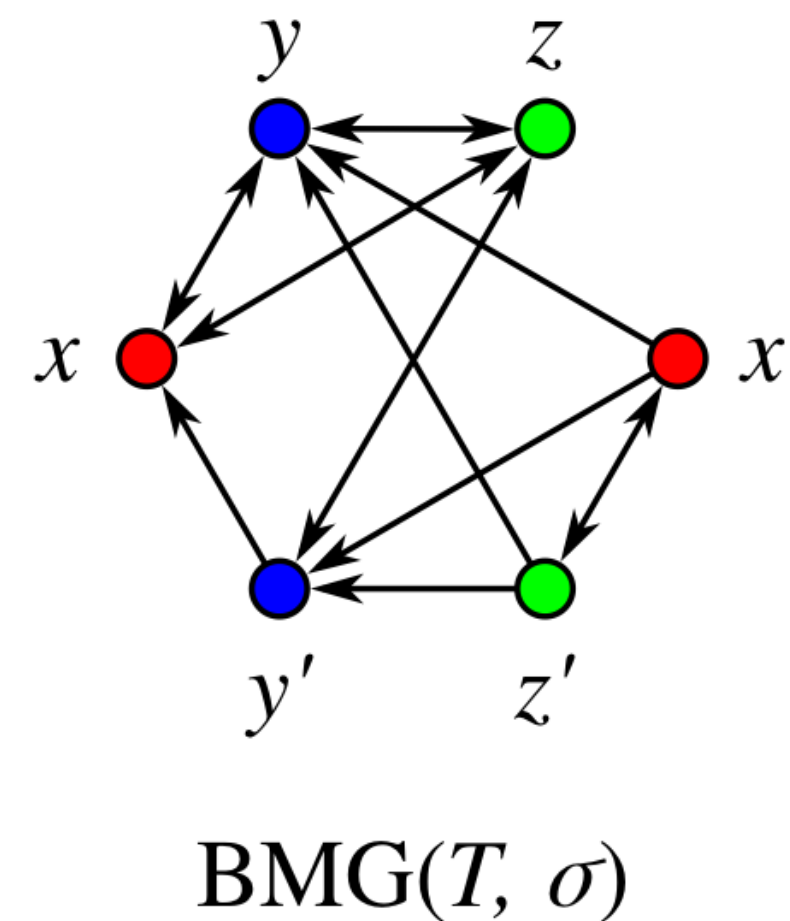
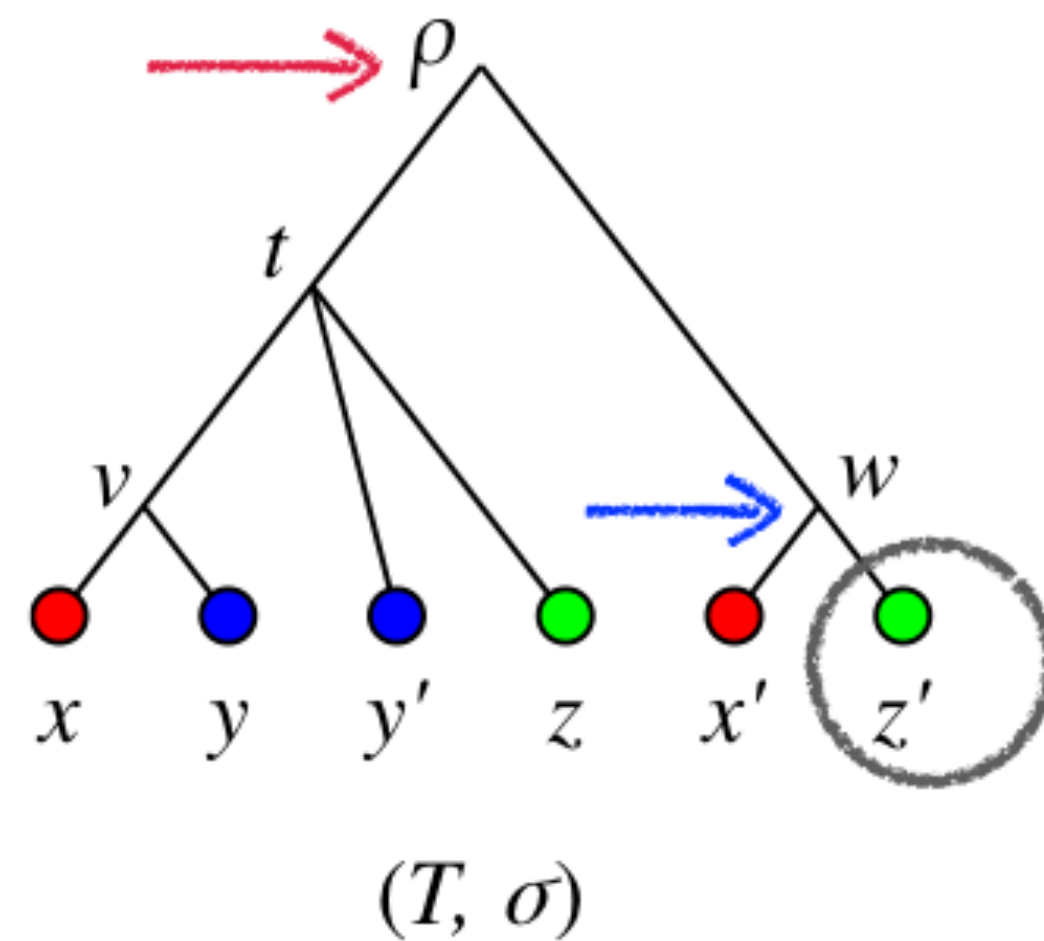
QUASI-BEST MATCH GRAPHS - DEFINITION

- ▶ How do we relate far-away genes? Limit detection of best matches in (T, σ)



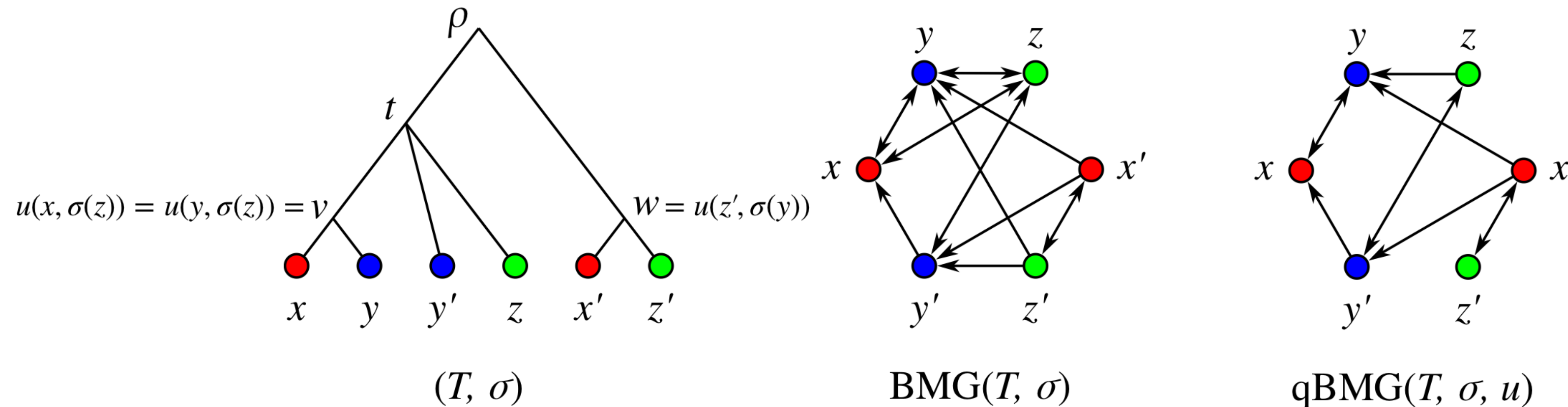
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- ▶ (G, σ) is **qBMG** (T, σ, u) if vertices=leaves colored by σ and $x \rightarrow y$ iff y is **quasi**-best match of x



$$u(z, \sigma(x)) = z, u(q, \sigma(q)) = q, u(q, s) = \rho \text{ and } s \neq \sigma(q)$$

BMGs vs. qBMGs

BMGs vs. qBMGs - LIKENESS

- ▶ Is $BMG(T, \sigma)$ a $qBMG(T, \sigma, u)$?

BMGs vs. qBMGs - LIKENESS

► Is $BMG(T, \sigma)$ a $qBMG(T, \sigma, u^\rho)$? Yes, $u^\rho(x, s) := \begin{cases} x & s = \sigma(x) \\ \rho & \text{otherwise} \end{cases}$

BMGs vs. qBMGs - LIKENESS

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- ▶ When $qBMG(T, \sigma, u)$ is a $BMG(T, \sigma)$?

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- ▶ Is $BMG(T, \sigma)$ a $qBMG(T, \sigma, u^\rho)$? Yes, $u^\rho(x, s) := \begin{cases} x & s = \sigma(x) \\ \rho & \text{otherwise} \end{cases}$
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Theorem

- (G, σ) is a BMG iff (G, σ) is a **color-sink-free** qBMG.

BMGs vs. qBMGs - LIKENESS

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- ▶ When $qBMG(T, \sigma, u)$ is a $BMG(T, \sigma)$?

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BMGs vs. QBMGs - UNLIKENESS

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hereditary class	no, color-sink free	yes
disjoint union	yes, if partition sets ² have same colours	yes
unique LRT	yes ²	no
binary explainable iff finite sets of forbidden graphs	hourglass-free ³	no

¹Annachiara Korchmaros et al. (2023). "Quasi-best match graphs". In: *Discrete Applied Mathematics* 331, pp. 104–125.

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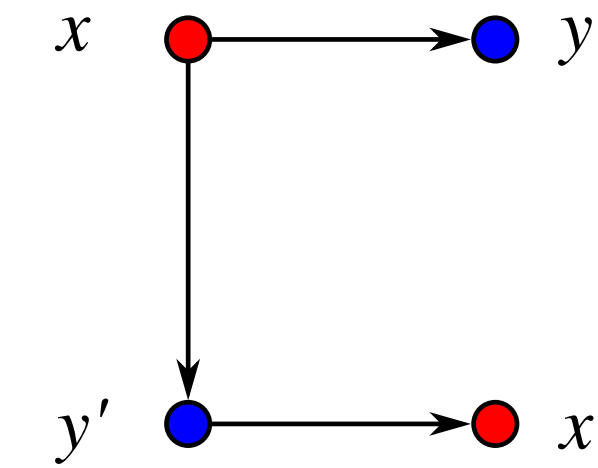
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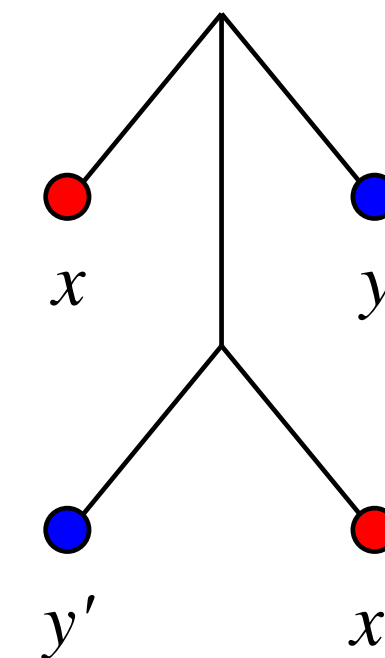
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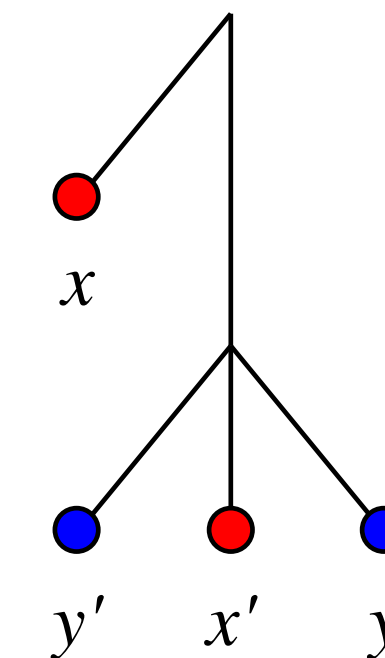
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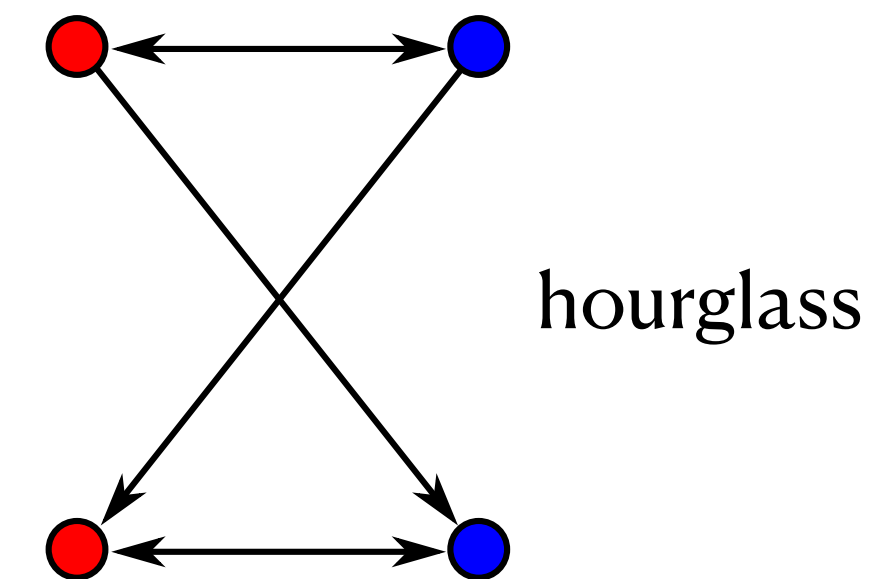
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THANK YOU!