Visualization of Barrier Tree Sequences Revisited

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Ivo L. Hofacker[2] Peter F. Stadler[3]

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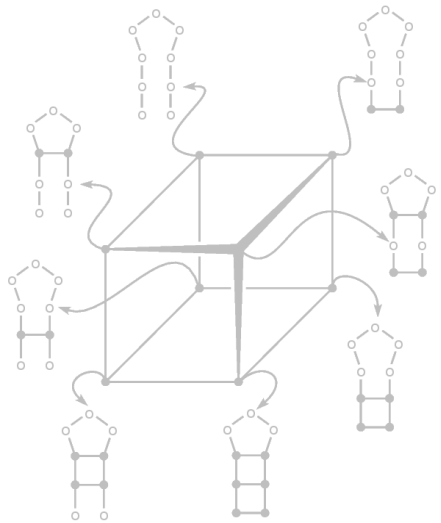
University of Vienna

EMBIO Meeting 2007
2007-05-18, Leipzig, Germany

Outline

Neighborhood of RNA Secondary Structure

- e.g., all secondary structures that differ by one base pair



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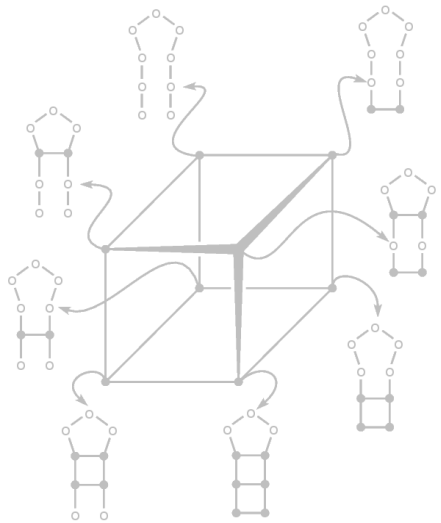

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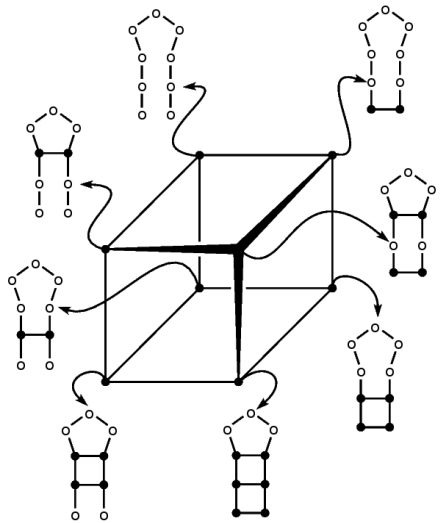

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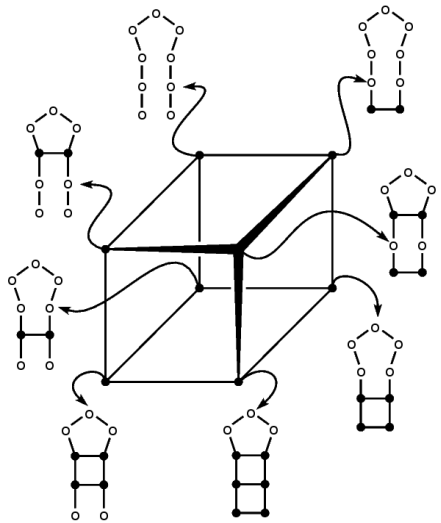

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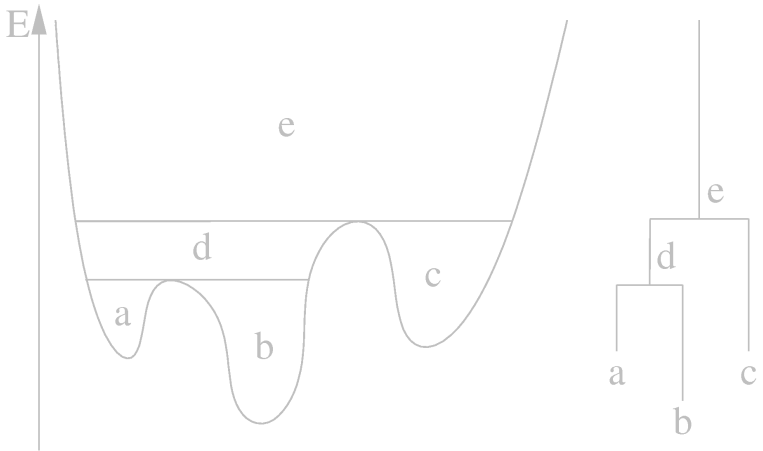
- reduction of the conformational space for kinetic folding simulation



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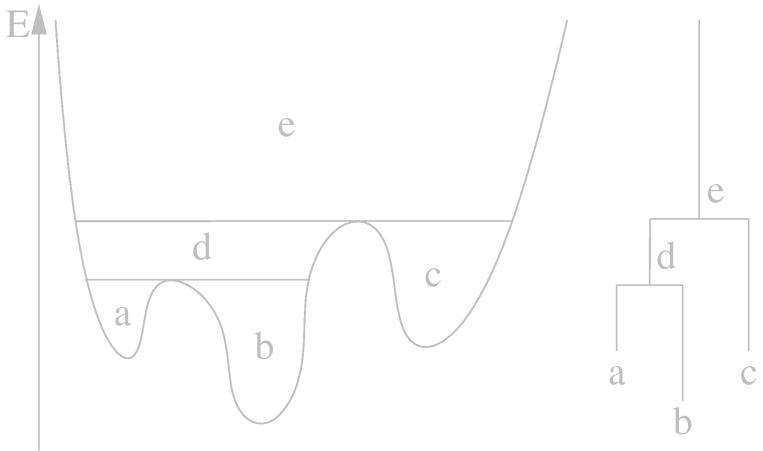

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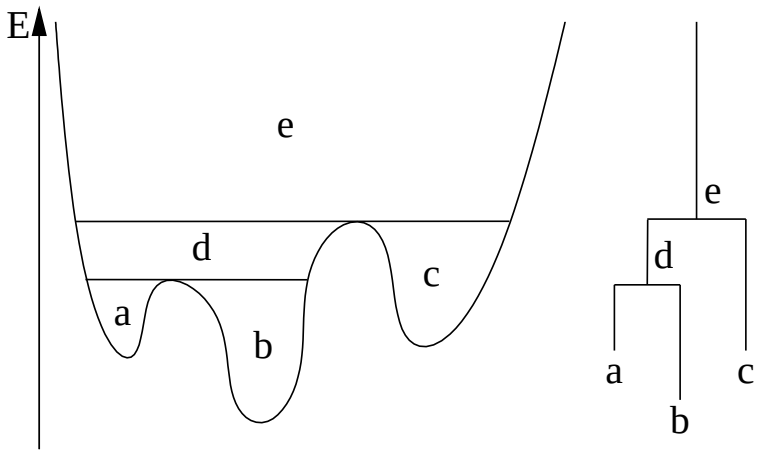

Barrier Tree Sequences

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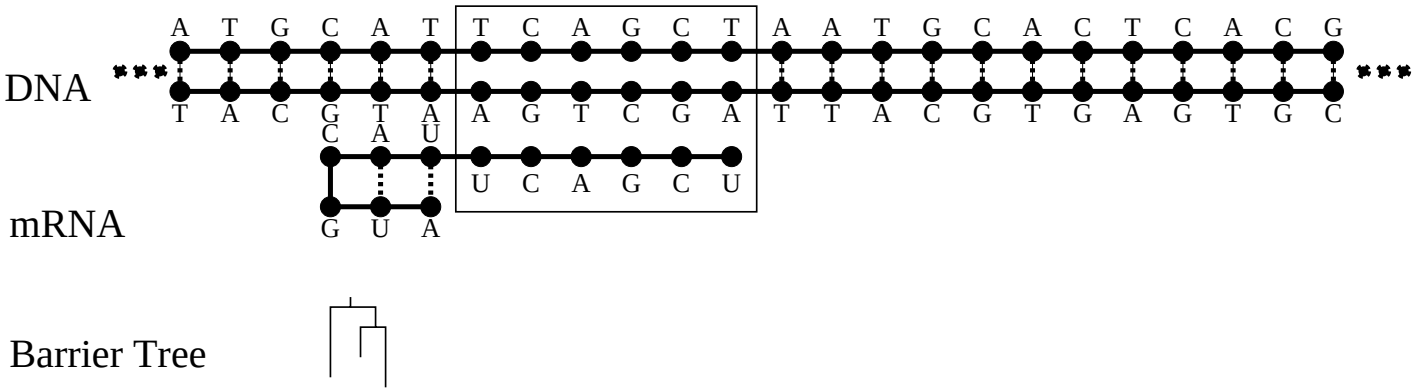

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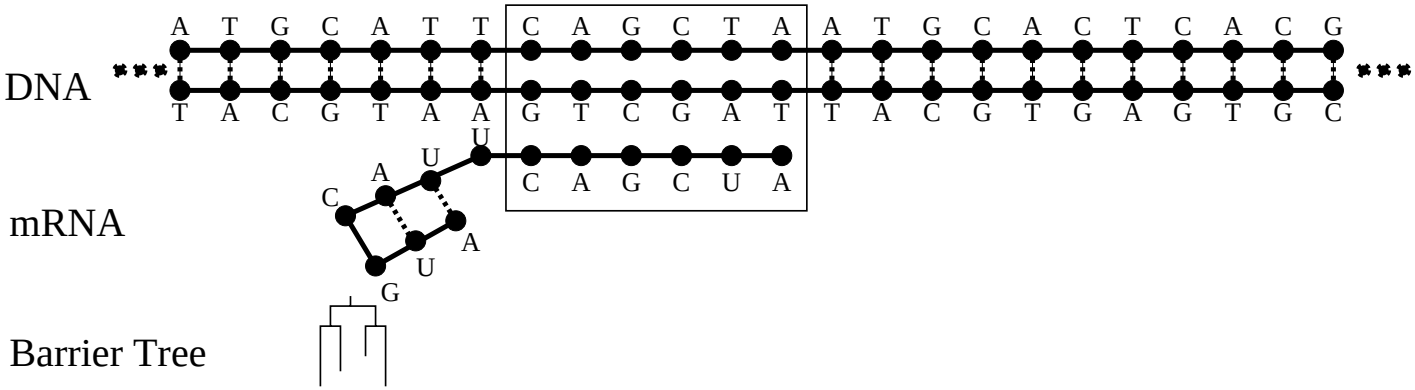

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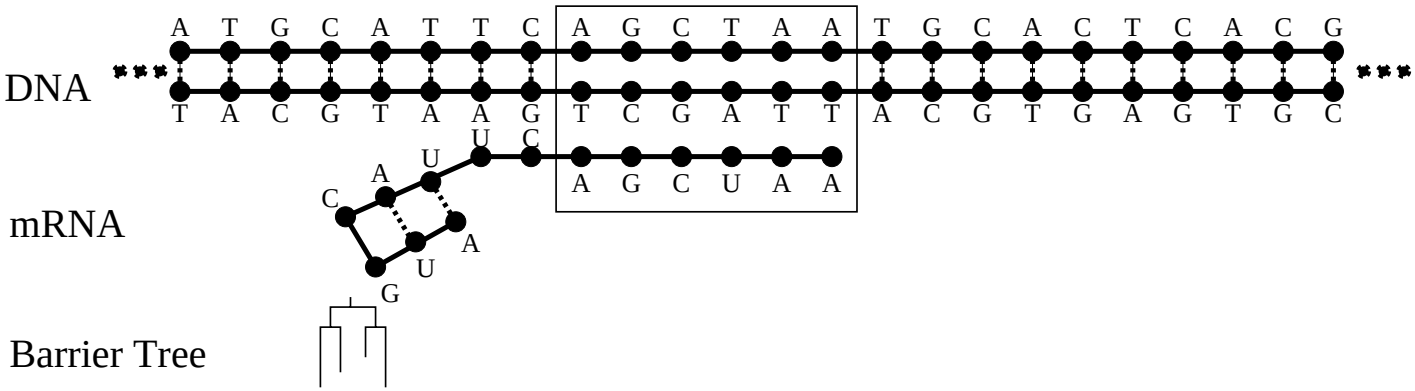

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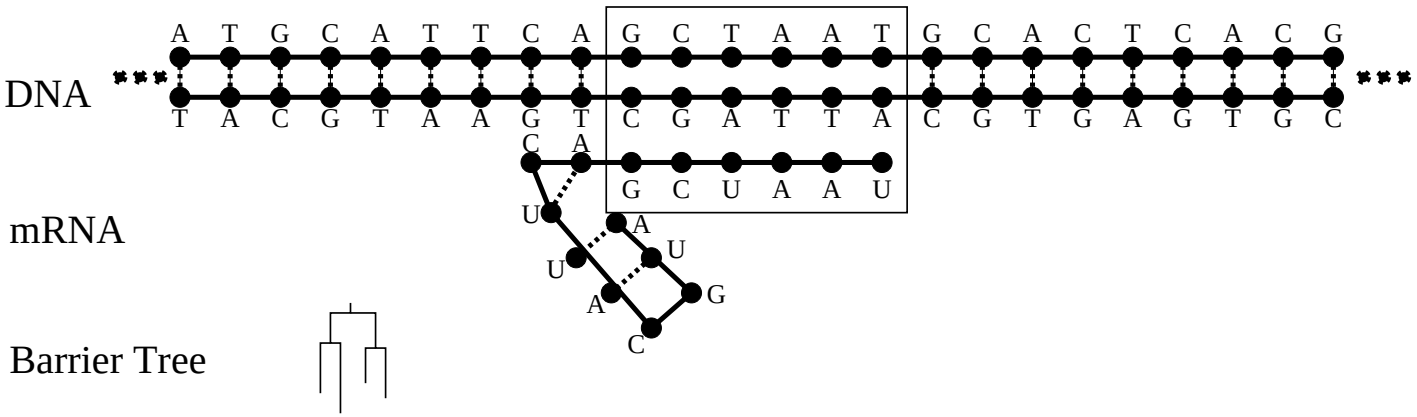

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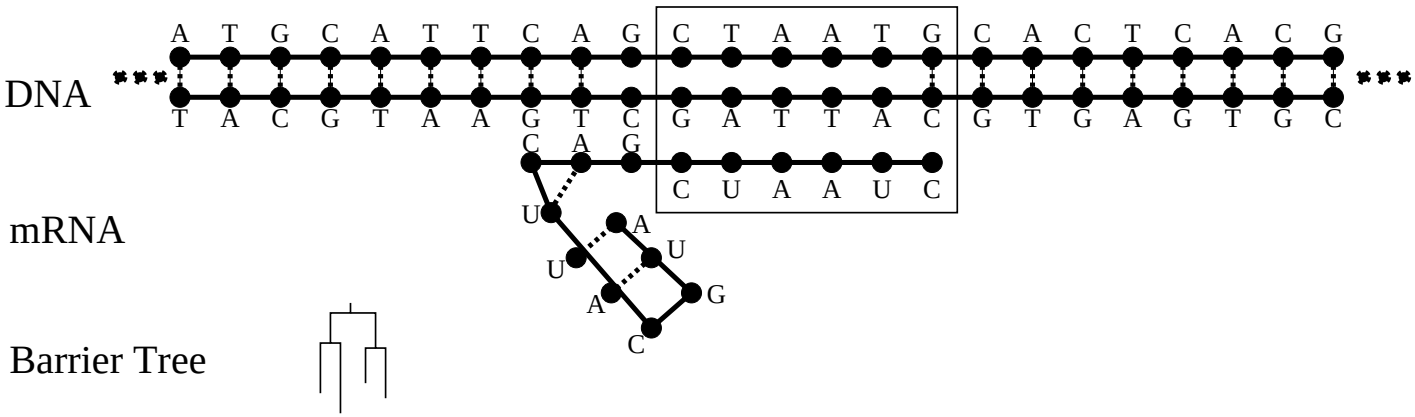

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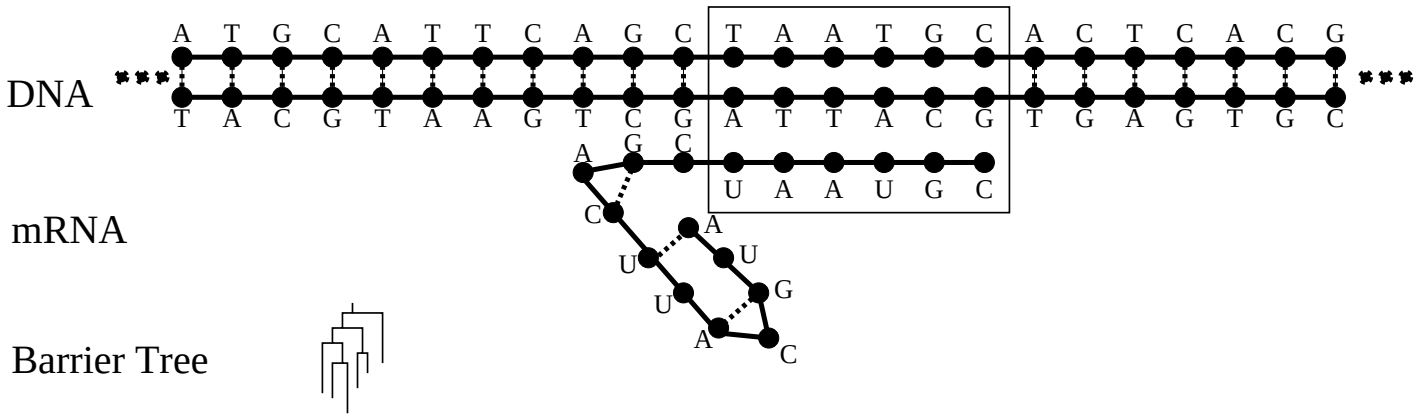

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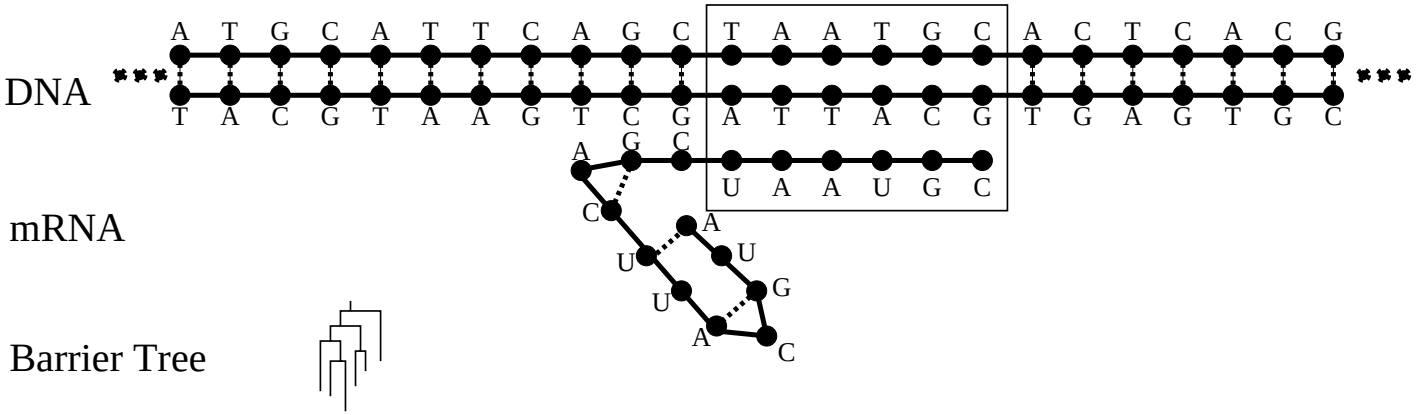

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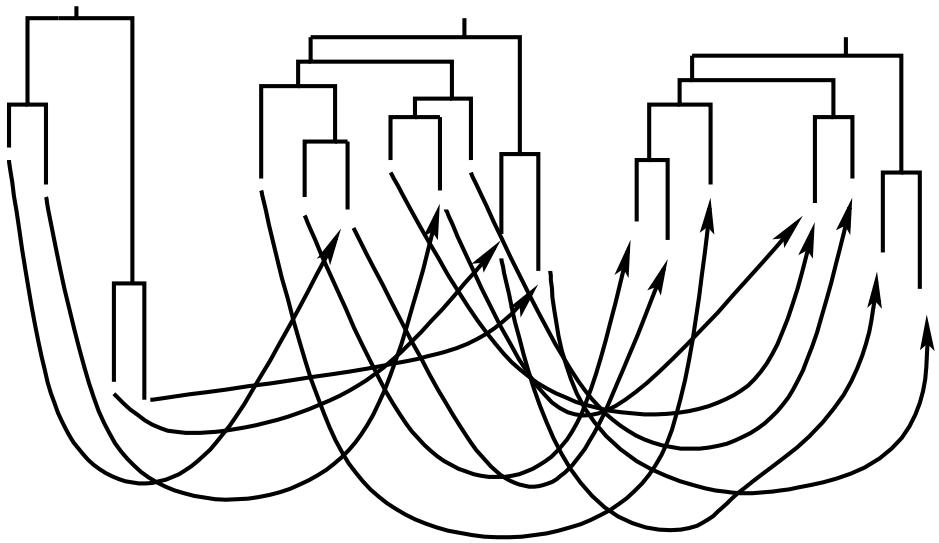

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- it is not sufficient to layout and show each *barrier tree* independently
- in general, static aesthetic criteria fight dynamic aesthetic criteria

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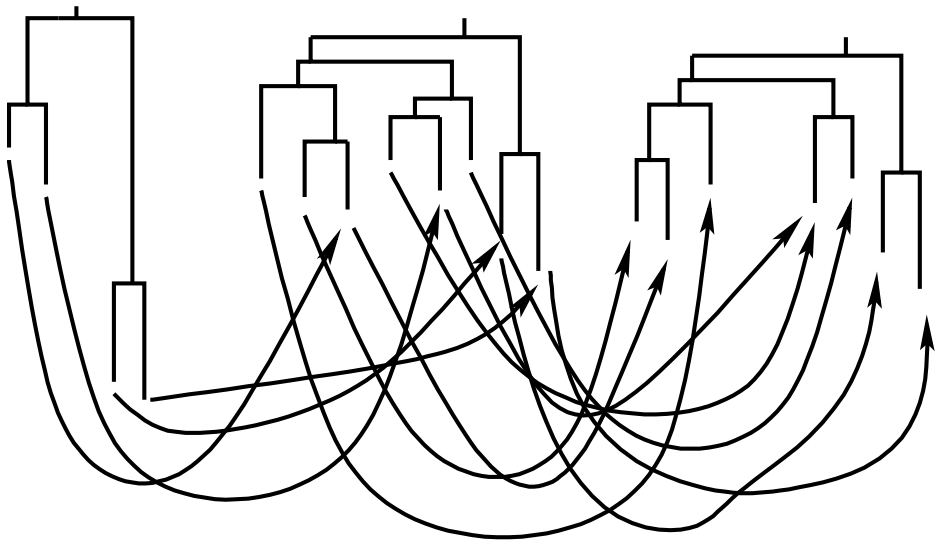

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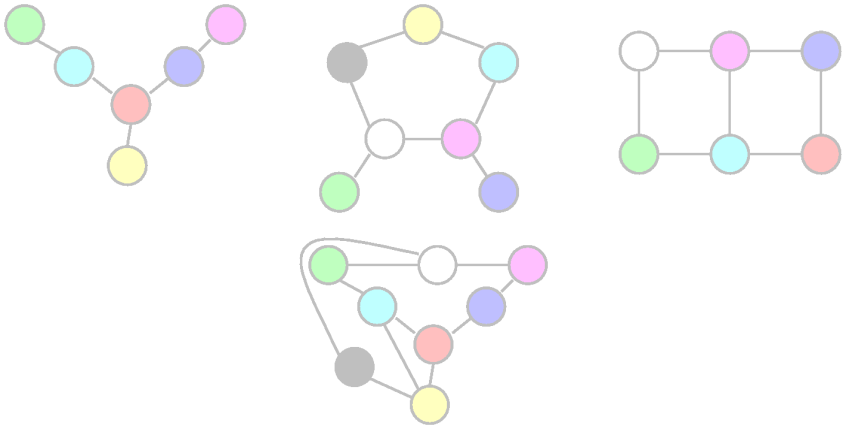
Foresight Layout with Tolerance (Diehl and Görg '02)

$G_i = (V_i, E_i)$



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no layout

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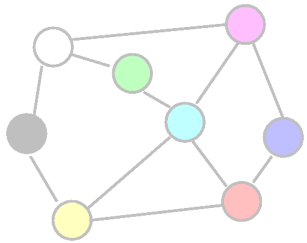
with layout

$L = L(G)$



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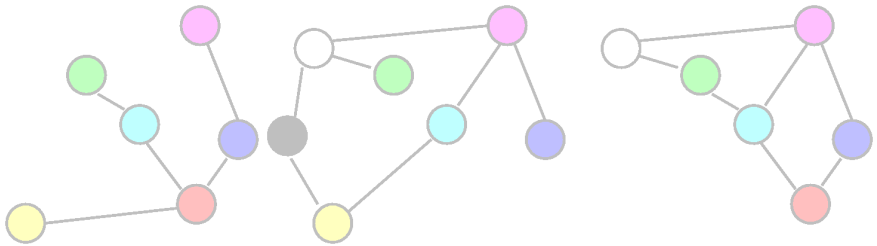

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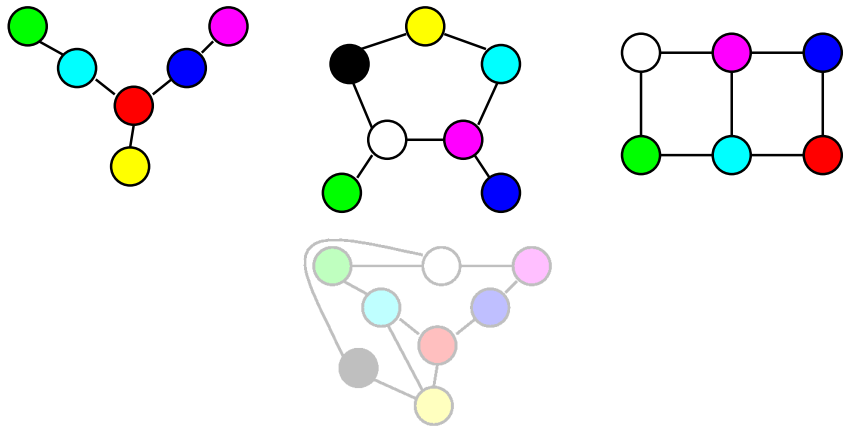

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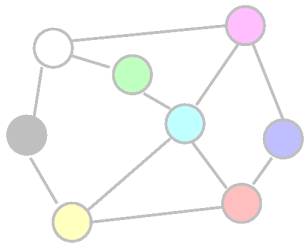

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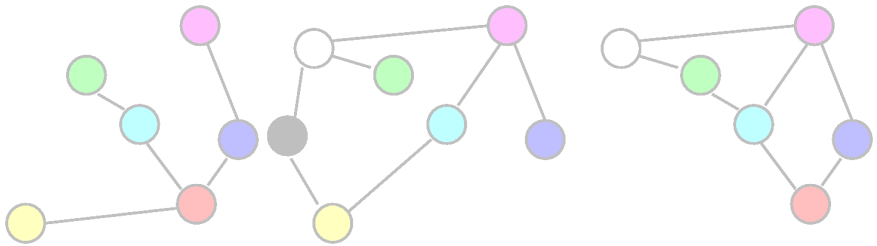

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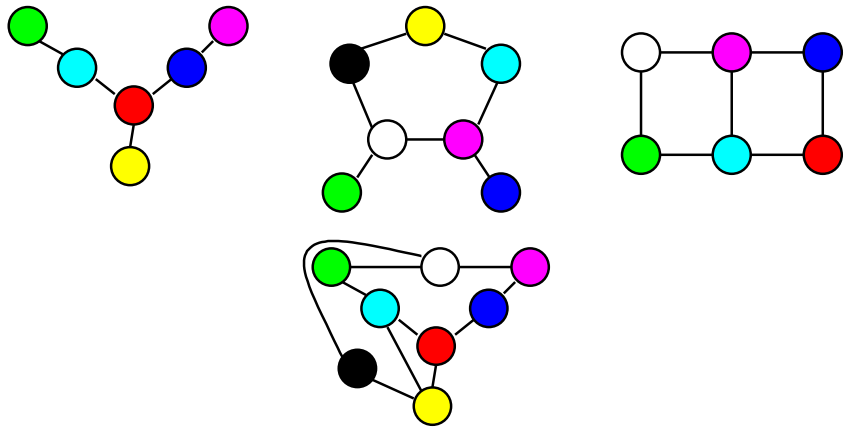

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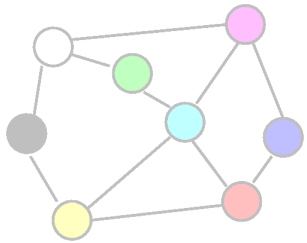

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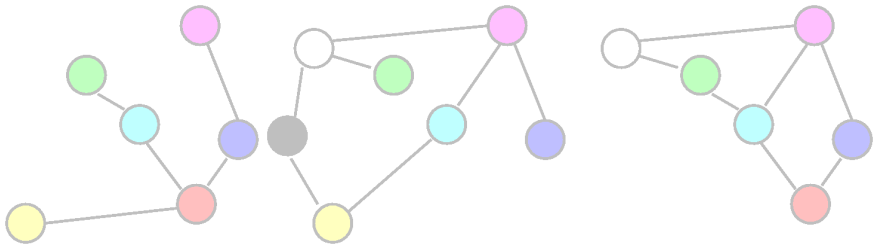

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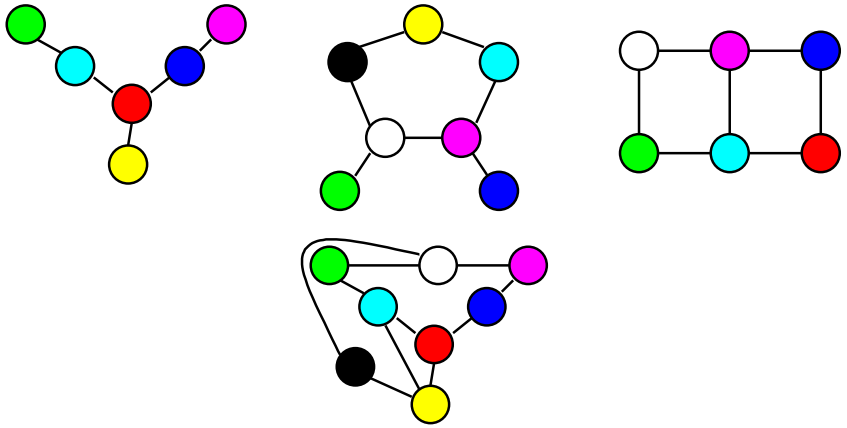

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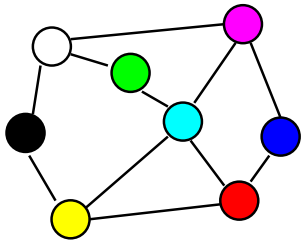

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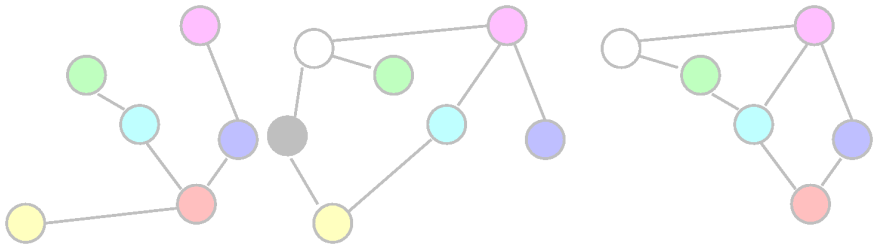

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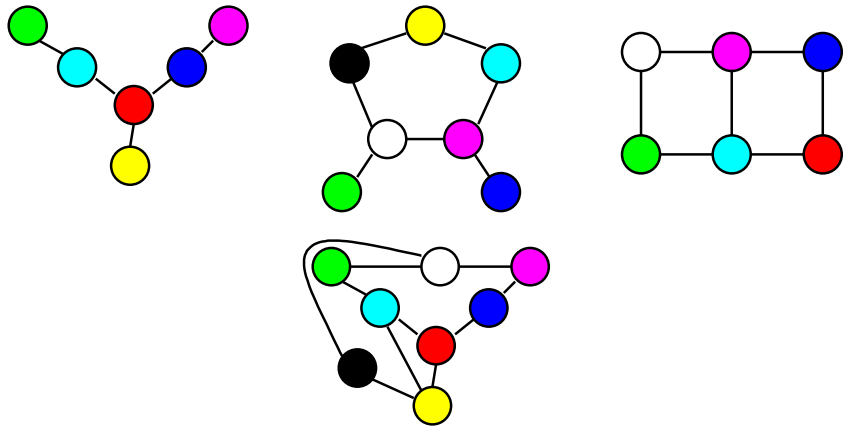

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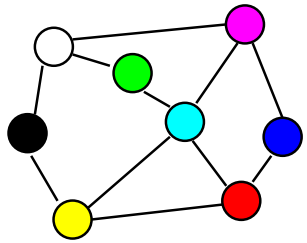

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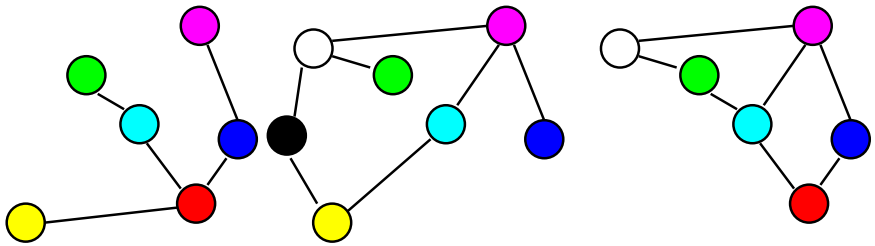
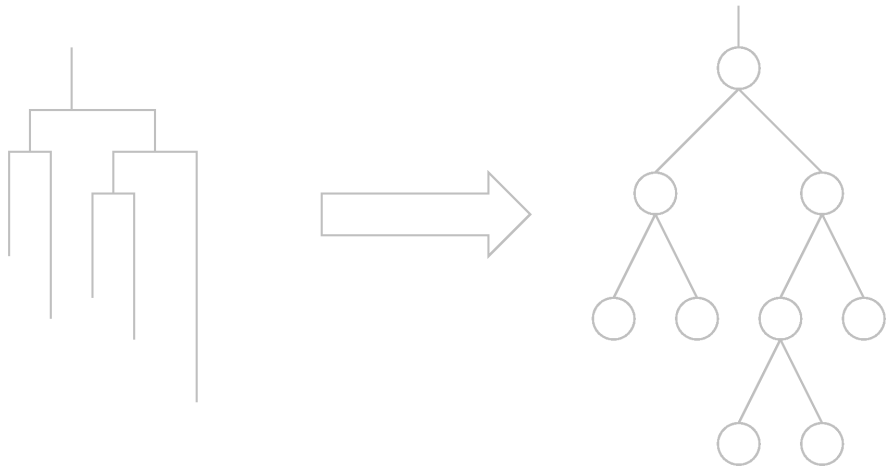


What is wrong with the Supergraph Construction?

algorithm overview:

- preserve only father-son-relations of *barrier trees*



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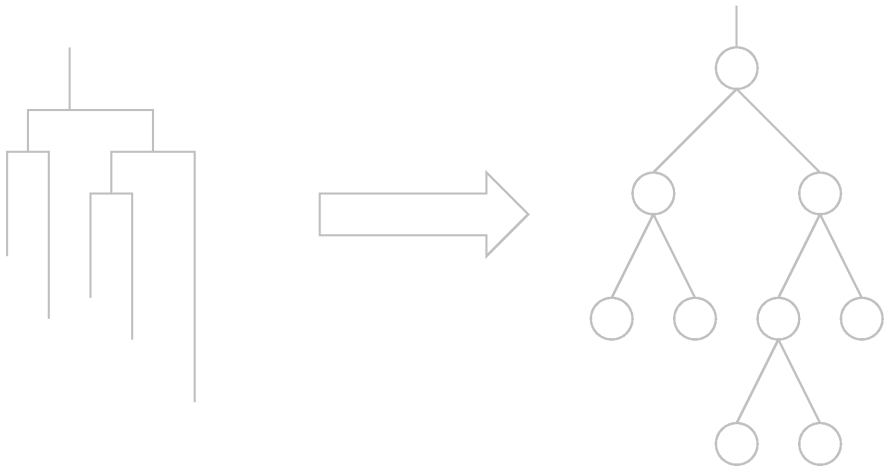

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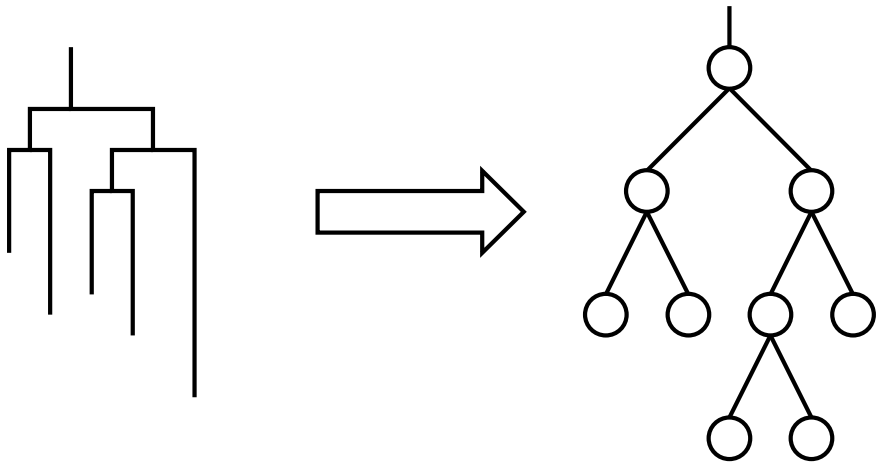
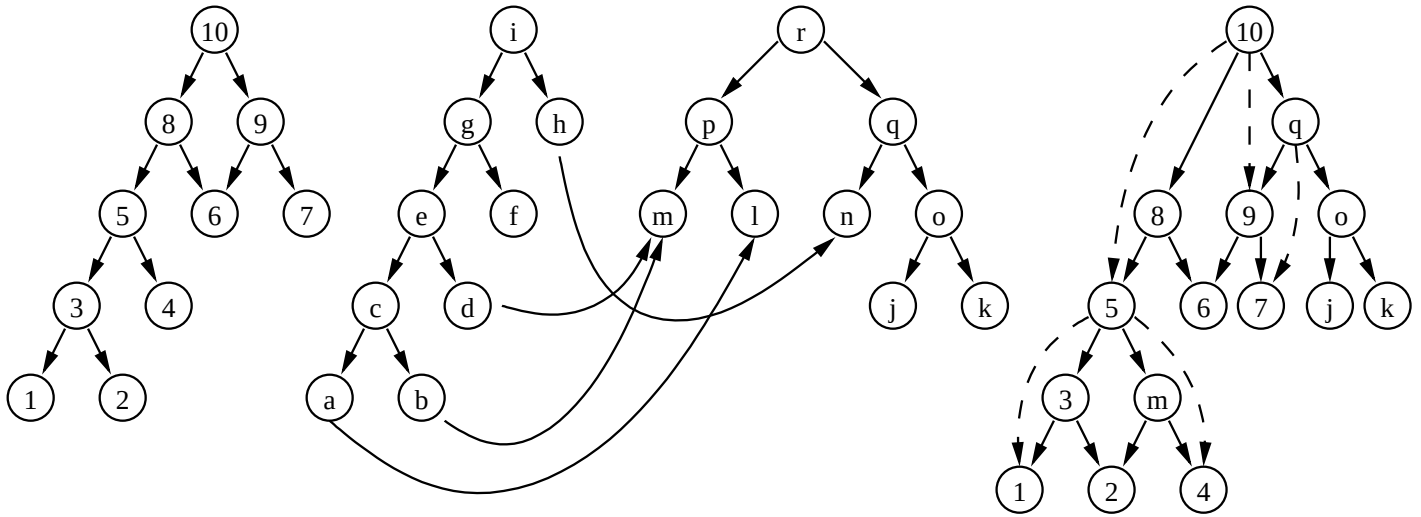


Supergraph Construction

- "set of leaves" heuristic (see Heine, Scheuermann, Flamm, Hofacker, and Stadler, *Visualization of Barrier Tree Sequences*, IEEE Transactions on Visualization and Computer Graphics, 12(5), 2006, 781-788.



supergraph n tree n tree $n+1$ supergraph $n+1$

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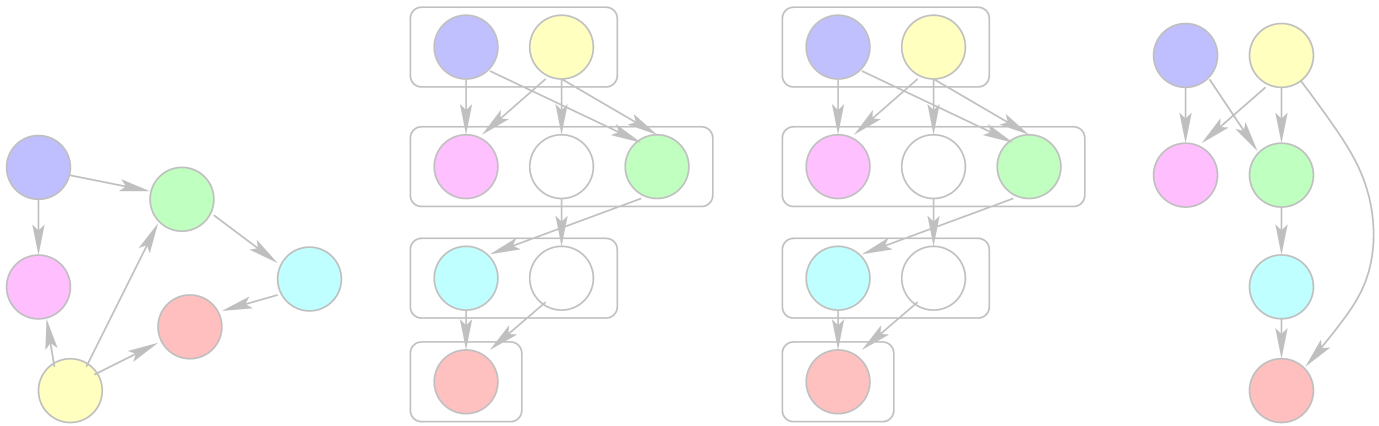
Supergraph layout uses the DOT algorithm (Gansner et al. ’93)
Sugiyama type DAG Layout



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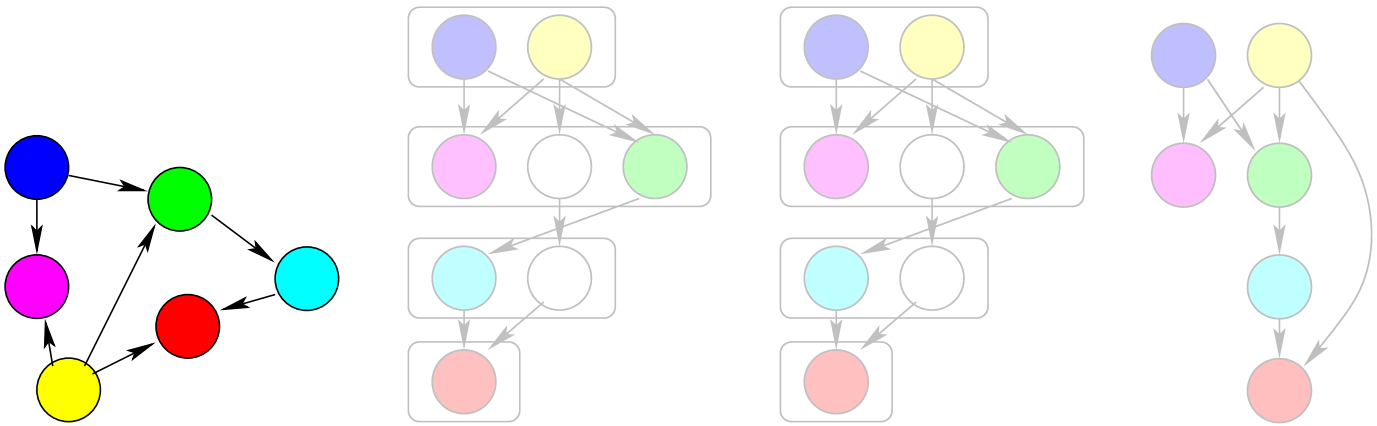

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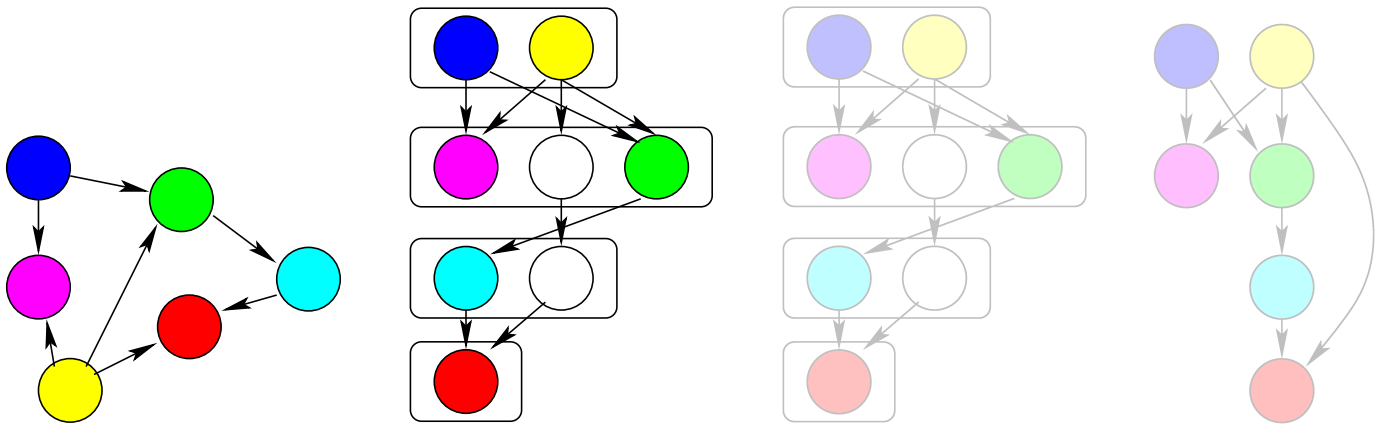

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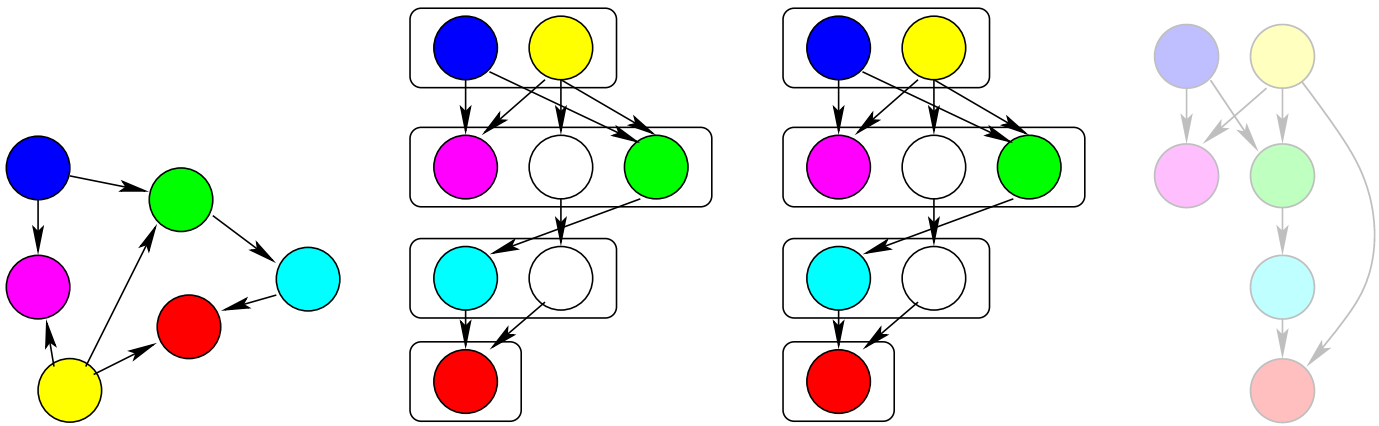

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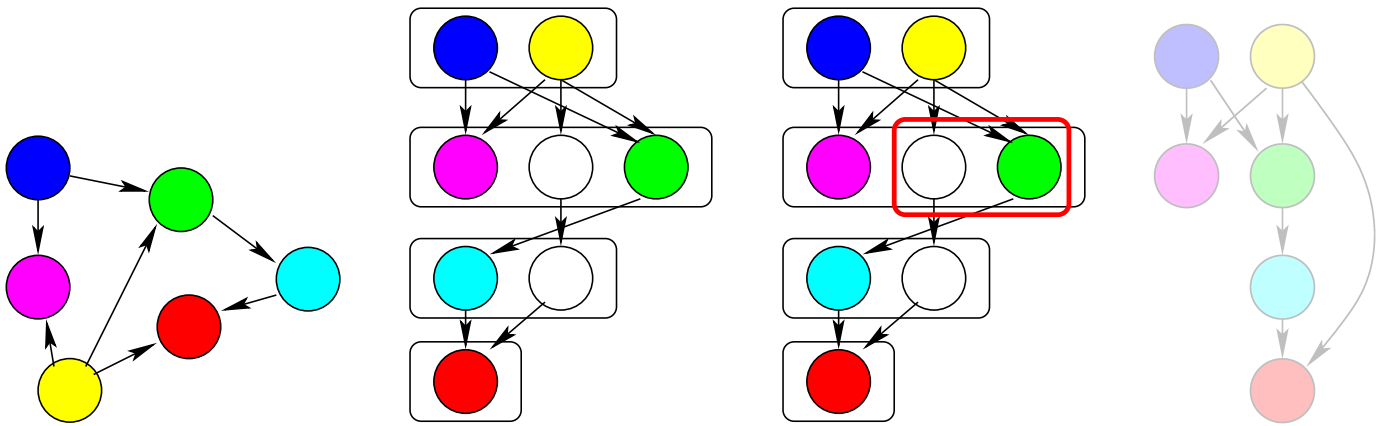

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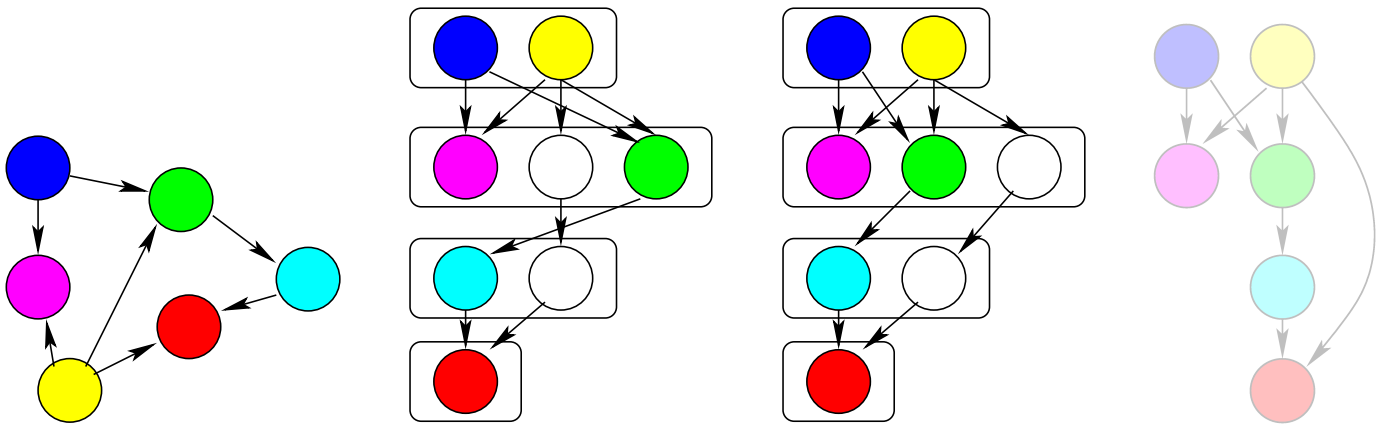

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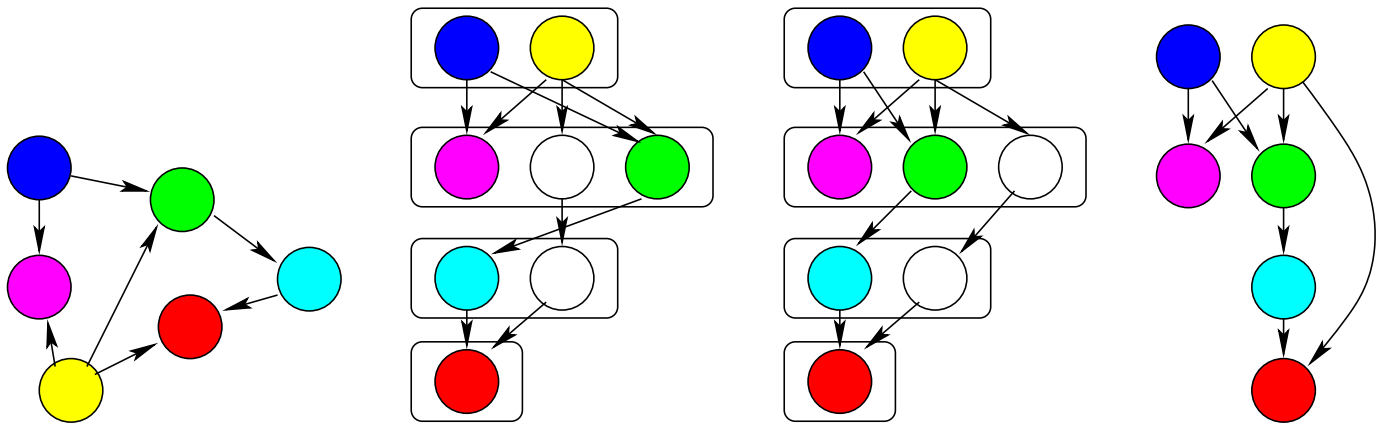

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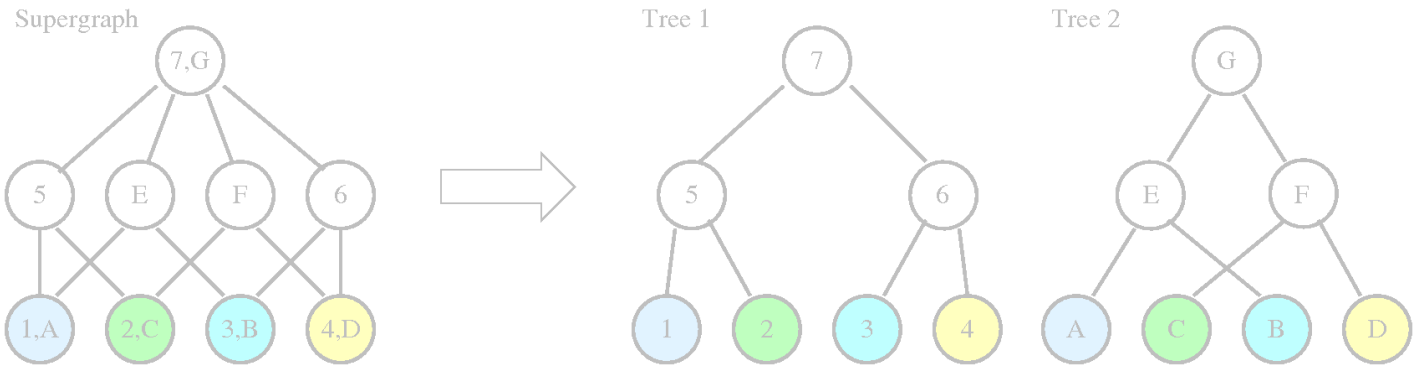

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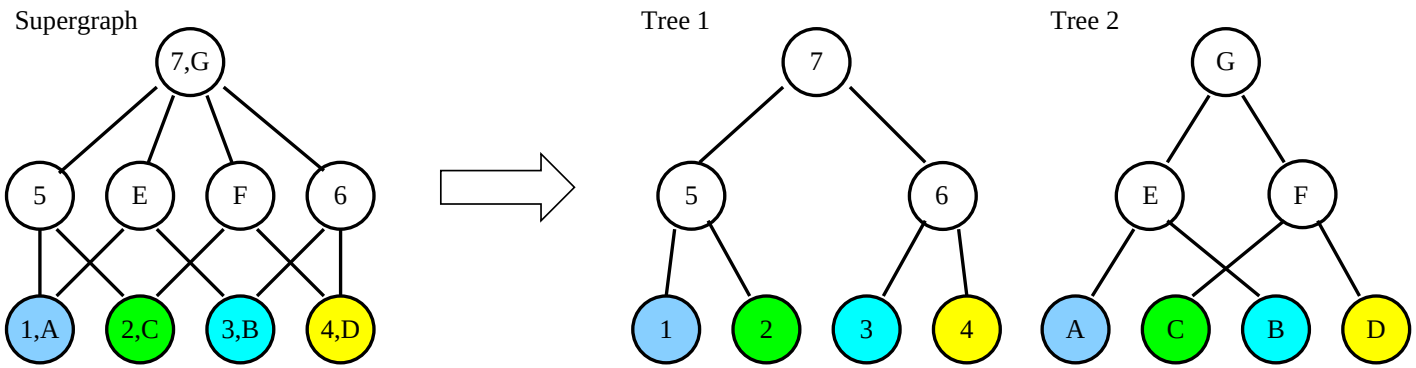

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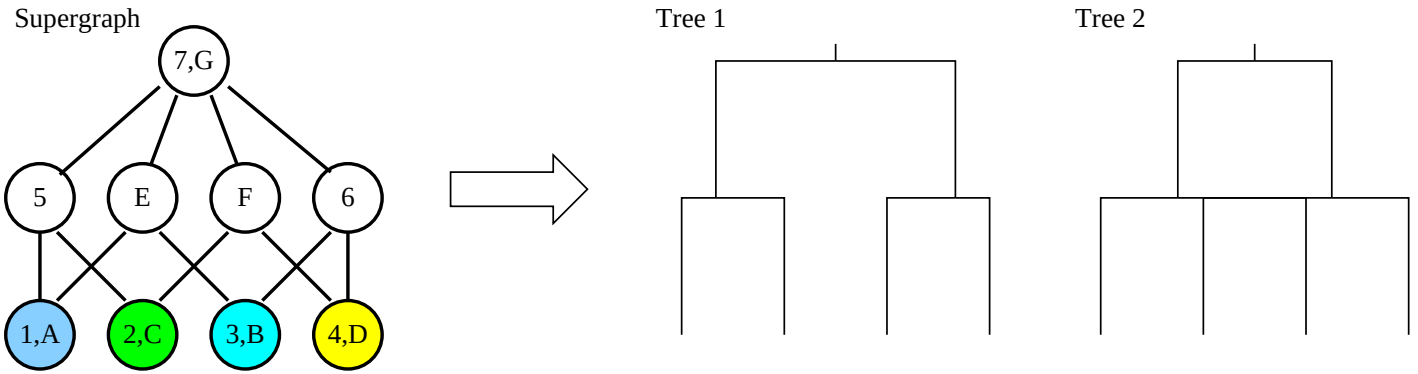

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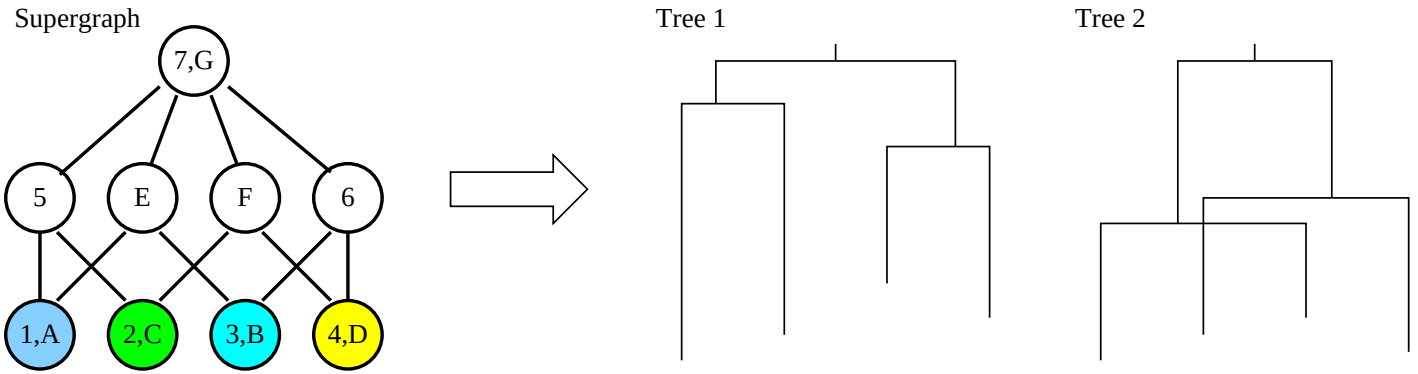

New Layout Algorithm

- identification of equivalent vertices using “set of leaves” approach
- find a permutation of the equivalence classes that makes all trees of the sequence “nice”, formally:

$$\sigma = \underset{O}{\mathit{argmin}} \sum_{i=1}^{N} \left(\alpha \cdot \mathit{crossings}(T_i, O_{V_i}) + \beta \cdot \mathit{localorder}(T_i, O_{V_i}) \right)$$

New Layout Algorithm

- find the solution by repetition of the following:
  - randomly switching two vertices in the permutation,
  - reevaluation cost function $C(\sigma)$
  - keep new permutation with

$$p = \begin{cases} 1 & \Delta C < 0 \\ \frac{1}{1+exp(\Delta C\, T_t^{-1})} & \Delta C \geq 0 \end{cases} \qquad T_t = \frac{n_t - t}{t}$$

- just reducing crossings is not enough
- nice side effect: distribute vertices more uniformly on the screen

Results

- runtime and quality improved greatly for HOK and LEPTO datasets

	equivalence classes	runtime old (1000 iterations)	runtime new (100000 iteration)
ATT	381	37s	27s
LEPTO	1531	3462s	79s
HOK	3793	16790s	182s

Conclusions and Future Work

Conclusion

- strong improvement quality- and runtime-wise over old method

Future Work

- determine optimal number of iterations automatically

more Information:

Christian Heine, Gerik Scheuermann, Christoph Flamm, Ivo L. Hofacker, and Peter F. Stadler, *Visualization of Barrier Tree Sequences Revisited*, to appear in Proceedings of Visualization in Medicine and Life Sciences (VLMS), 2007

Thank You!