Faster Algorithms for the Maximum Common Subtree Isomorphism Problem

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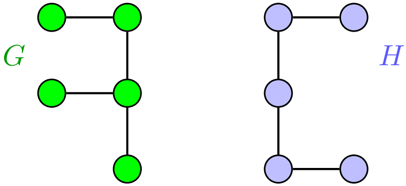
Maximum Common Subtree Isomorphism (MCSI) Problem

Input: Trees G and H



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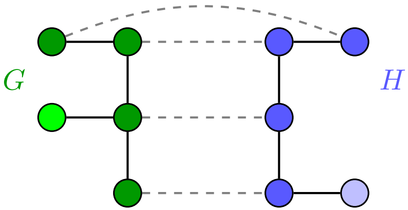
Input: Trees G and H

Output: An isomorphism between subtrees of G and H with the maximum possible number of vertices



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- Trees or graphs are often used as an abstract representation for e.g. molecules, XML, or social networks

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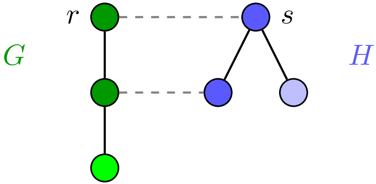
- Application examples:
  - Chemistry, Biology [Ehrlich and Rarey, 2011]
  - Computer Vision [Englert and Kovács, 2015]
  - Binary Programs [Gao et al., 2008]

Problem variants

- Rooted MCSI
  - Map roots of input trees



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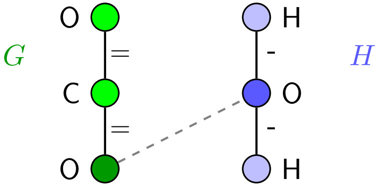
- Labelled Trees
  - Labels on vertices/edges must match



Problem variants

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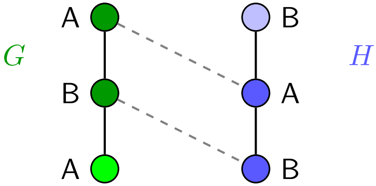
  - Map roots of input trees
- Labelled Trees
  - Labels on vertices/edges must match
- Weight function $w : V_G \times V_H \to \mathbb{R}$ on pairs of vertices
  - Maximize weight
    - Example: $w(\text{A,A}) = w(\text{B,B}) = 2,\ w(\text{A,B}) = w(\text{B,A}) = 1$



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- Subgraph Isomorphism
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- Graph Isomorphism
  - Unknown if NP-hard or in P

Related problems, cont.

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- Subtree Isomorphism, polynomial time solvable
  - $\mathcal{O}(n^{2.5})$, rooted trees [Matula, 1978]
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  - $\mathcal{O}(n^{2.5}\log n)$, integer weights in $\mathcal{O}(n)$
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- MCSI on unrooted trees: $\mathcal{O}(n^{5})$ [Matula, 1978]

Our contribution, main result

MCSI in time $\mathcal{O}(|G||H|\Delta(G,H)) \subseteq \mathcal{O}(n^3)$

- Unrooted trees G and H
- Weight function
- $\Delta(G,H) := \min\{\Delta(G),\Delta(H)\} + \log\max\{\Delta(G),\Delta(H)\}$

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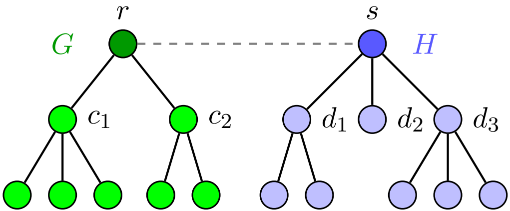
4) Lower bounds

Dynamic Programming Approach between rooted trees

- Rooted trees G and H, $r \mapsto s$



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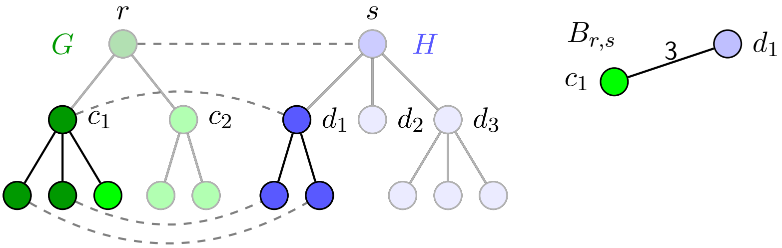

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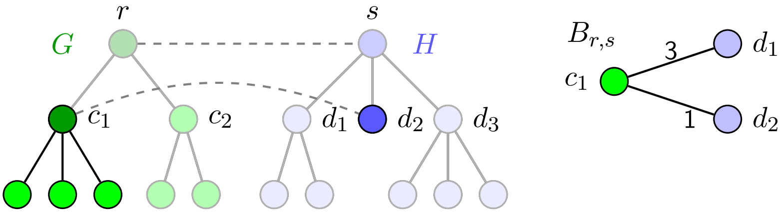

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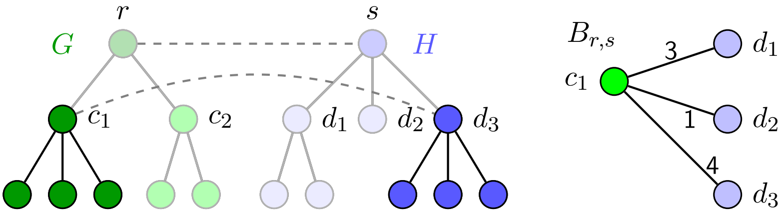

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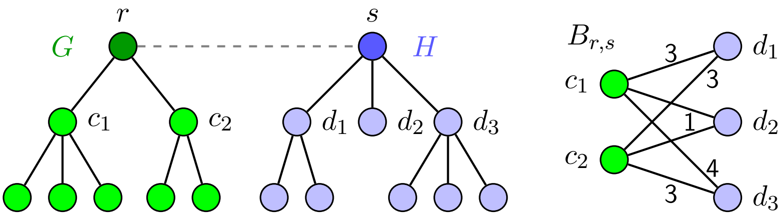

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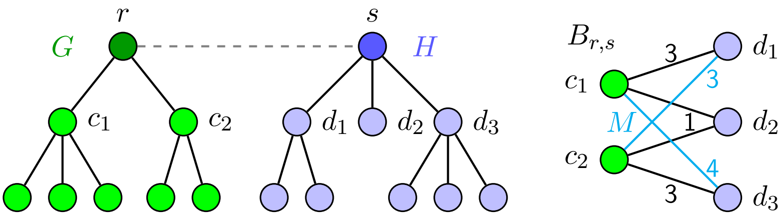

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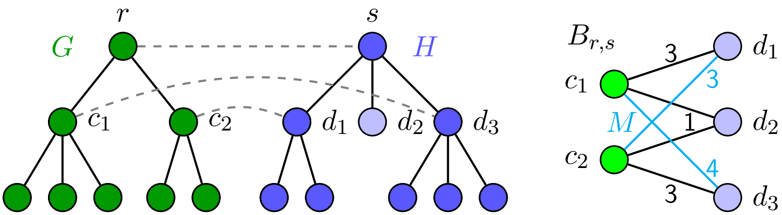
- Edges of M determine MCSI between G and H



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  - If not, returned solution is no MCSI, but...

Reduce the number of subproblems, cont.

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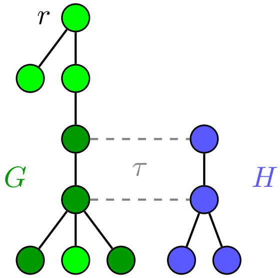

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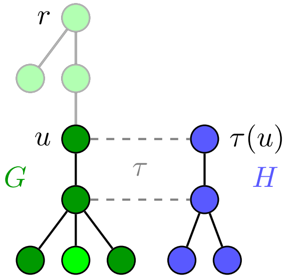

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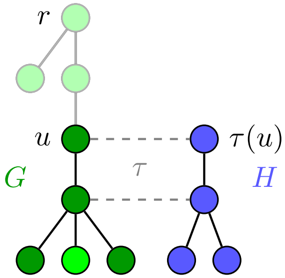

Improvement 2: Efficiently solve similar subproblems

- Let G be rooted at r
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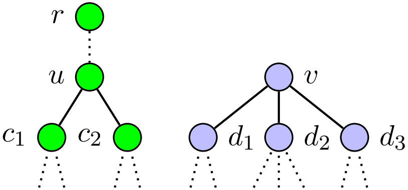

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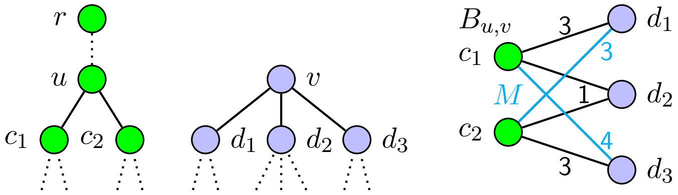

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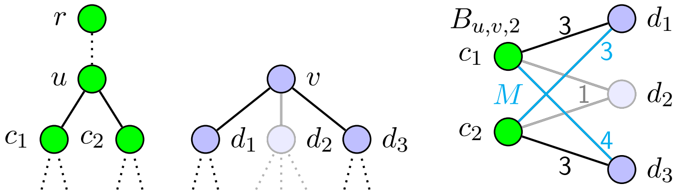

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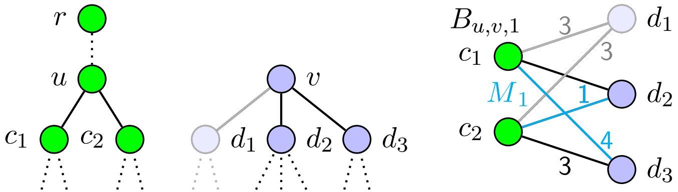
3) Root $d_j \in V_H$, $j \in \{1,3\}$: derive MWMs M_j from M



1) Time $\mathcal{O}(kl(\min\{k,l\} + \log \max\{k,l\}))$, 2) $\mathcal{O}(1)$, 3) as 1) for all M_j

Theorem

An MCSI between two trees G and H can be computed in time $\mathcal{O}(|G||H|\Delta(G,H))$.

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Proposition

For trees of bounded degree we obtain running time $\Theta(|G||H|)$, which is optimal.

Lower bound for unrestricted degree

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- Time $o(n^3)$ for MCSI $\Rightarrow$ Time $o(n^3)$ for the assignment problem.

Conclusion

We developed/showed

- An algorithm for MCSI, time $\mathcal{O}(|G||H|\Delta(G, H))$
- Achieved this improved time bound by:
  - Rooting one tree, but also consider subtrees of this tree
  - Efficiently solving similar subproblems
- Results about optimality

Next up

- Improve time bound for MCSI on unweighted trees
- Adapt our algorithm to other graph classes

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A. Abboud, A. Backurs, T. D. Hansen, V. V. Williams, and O. Zamir. Subtree isomorphism revisited. In *Proceedings of the Twenty-Seventh Annual ACM-SIAM Symposium on Discrete Algorithms*, SODA '16, pages 1256–1271. SIAM, 2016. ISBN 978-1-611974-33-1.

A. Droschinsky, B. Heinemann, N. Kriege, and P. Mutzel. Enumeration of maximum common subtree isomorphisms with polynomial-delay. In H.-K. Ahn and C.-S. Shin, editors, *Algorithms and Computation (ISAAC)*, LNCS, pages 81–93. Springer, 2014. ISBN 978-3-319-13074-3. doi:10.1007/978-3-319-13075-0_7.

H.-C. Ehrlich and M. Rarey. Maximum common subgraph isomorphism algorithms and their applications in molecular science: a review. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 1(1):68–79, 2011. ISSN 1759-0884. doi:10.1002/wcms.5. URL `http://dx.doi.org/10.1002/wcms.5`.

D. W. Matula. Subtree isomorphism in $O(n^{5/2})$. In P. H. B. Alspach and D. Miller, editors, *Algorithmic Aspects of Combinatorics*, volume 2 of *Annals of Discrete Mathematics*, pages 91–106. Elsevier, 1978. doi:10.1016/S0167-5060(08)70324-8.

G. Valiente. *Algorithms on Trees and Graphs*. Springer-Verlag, Berlin, 2002. ISBN 3-540-43550-6.