Trees, Subtrees and Isomorphism: A Revisit

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Definitions

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Graph isomorphism : two graphs (V_1, E_1) and (V_2, E_2), are called isomorphic, if there exists a bijection $\phi : V_1 \to V_2$, such that, for every vertex pair $u, v \in V_1$, $uv \in E_1$ iff $\phi(u)\phi(v) \in E_2$.

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Subtree : a subtree of an unrooted tree T is either T itself, or one of the two components obtained by removing any edge of T.
A subtree rooted at u of a rooted tree T, is the rooted tree containing u all descendants of u.

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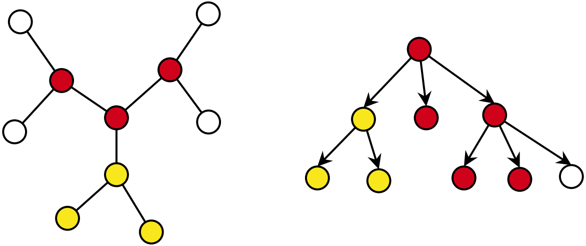

Figure: The yellow part is a subtree of the whole graph; the red part is a g-subtree of the whole tree.

Rooted Tree Isomorphism

Given two rooted trees T_1 and T_2, decide if they are isomorphic.

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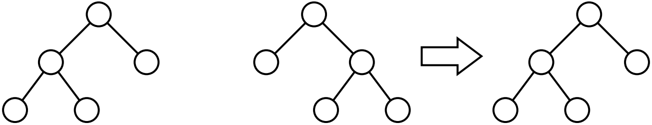

Figure: Canonicalization of trees via sorting.

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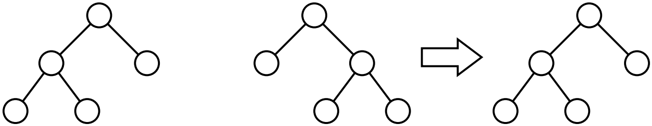

Figure: Canonicalization of trees via sorting.

We can also use tree hashing to avoid sorting.

Unrooted Tree Isomorphism

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Unrooted Tree Isomorphism

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Theorem

We can solve the unrooted tree isomorphism problem based on rooted tree isomorphism algorithm in the same asymptotic time.

Basic idea: root the trees at their centroids. A tree has either one or two centroids. In case that a tree has two centroids, try both possibilities.

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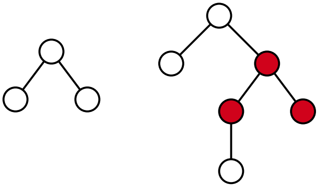
The centroids of a tree can be found in linear time by dynamic programming or running BFS twice.

Subtree Isomorphism, Rooted

Given rooted trees S and T, decide if there exists a **g-subtree** of T isomorphic to S.



There might be exponentially many g-subtrees in a given tree!

Subtree Isomorphism, Rooted

Solution (dynamic programming)

We may use dynamic programming to solve this problem. Let for $u \in S, v \in T$, define $M[u, v] = 1$ if S_u is isomorphic to some g-subtree of T rooted at v; otherwise $M[u, v] = 0$. $M[u, v]$ can be computed from $M[x, y]$ where $x \in C(u), y \in C(v)$.

We may define a bipartite graph $C(u) \cup C(v)$ where $x \in C(u)$ and $y \in C(v)$ are connected by an edge if $M[x, y] = 1$. Note that $M[u, v] = 1$ if and only if the bipartite graph has a $C(u)$-perfect matching.

Subtree Isomorphism, Rooted

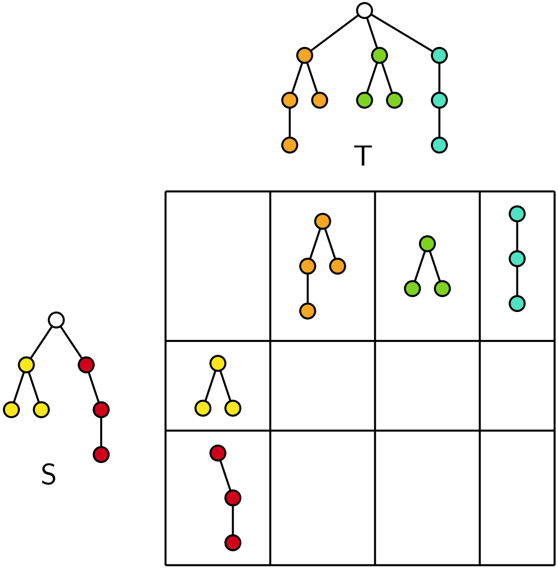
Algorithm 1 Rooted Subtree Isomorphism

Input: two rooted trees S and T

Output: decide if S is isomorphic to some g-subtree of T

```
initialize M[·,·] with 0
for vertex v in post-order traversal of T do
    for each vertex u is S do
        build bipartite graph G = (C(u) ∪ C(v), M[C(u), C(v)])
        set M[u, v] = 1 is G has a C(u)-perfect matching
    end for
end for
return true if M[root(S), v] = 1 for some v ∈ T
```

Subtree Isomorphism, Rooted



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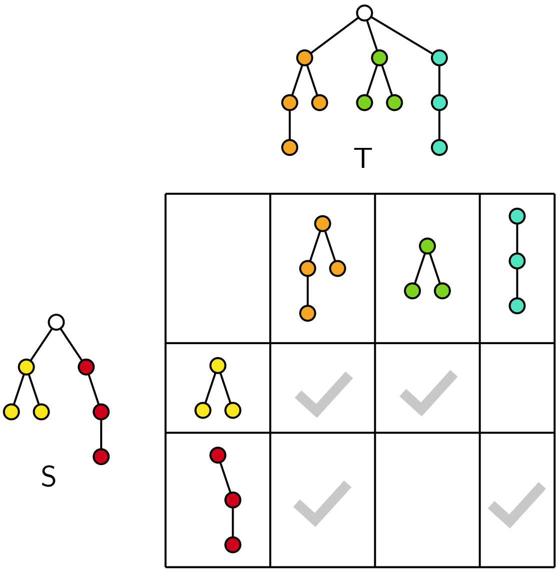

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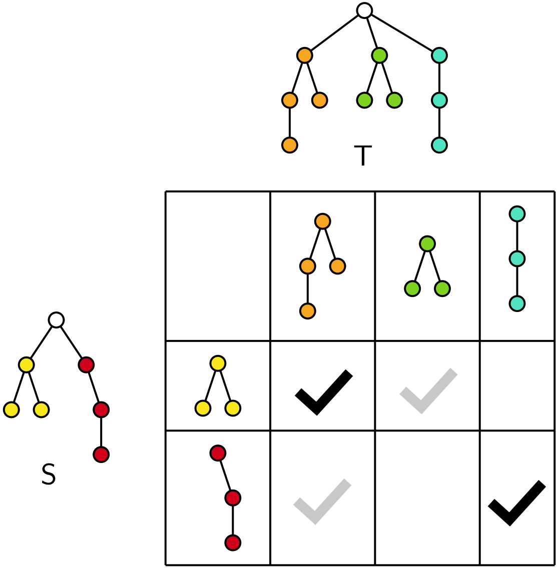

Subtree Isomorphism, Rooted

Assume we use Hopcroft-Karp algorithm (or, equivalently, Dinic's maximum flow) to find a maximum matching in $O(E\sqrt{V})$ time. The total time complexity is

$$\begin{aligned} time &= \sum_{u \in S} \sum_{v \in T} time(u, v) \\ &= \sum_{u \in S} \sum_{v \in T} \deg(u) \deg(v) \sqrt{\deg(u) + \deg(v)} \\ &\leq \sum_{u \in S} \sum_{v \in T} \deg(u) \deg(v) \sqrt{n_s + n_t} \\ &\leq n_s n_t \sqrt{n_s + n_t} \\ &= O(n_s n_t^{3/2}) \end{aligned}$$

Subtree Isomorphism, Rooted

About Maximum Bipartite Matching

Algorithm 2 Hopcroft-Karp Algorithm, $O(E\sqrt{V})$

Input: a bipartite graph $U \cup V$
Output: a maximum matching $\mathscr{M}$

set $\mathscr{M} = \varnothing$
while there exists augmenting path **do**
    let A be a **maximal** set of vertex-disjoint shortest augmenting paths
    set $\mathscr{M} = \mathscr{M} \oplus A$
end while
return $\mathscr{M}$

Lemma

The length of shortest augmenting path strictly increases after each iteration of Hopcroft-Karp algorithm.

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- Each iteration of Hopcroft-Karp can be done in $O(E)$;
- After the first $\sqrt{V}$ iterations the length of shortest augmenting path is at least $\sqrt{V}$;
- Now the symmetric difference of the current matching and the maximum matching is the disjoint union of several augmenting paths and alternating cycles; Since each augmenting path has length at least $\sqrt{V}$, there are at most $\sqrt{V}$ augmenting paths;
- Conclusion: Hopcroft-Karp terminates after at most $2\sqrt{V}$ iterations.

Subtree Isomorphism, Unrooted

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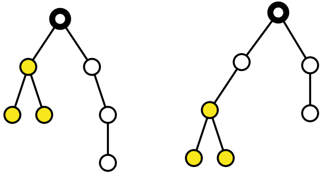
But we can still optimize the algorithm. The basic observation is, there may be common subtrees in different rootings of S.

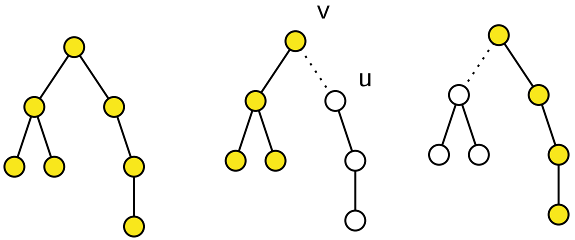


A natural idea is to use hashmap to dedupliate subtrees. However, this helps little in the worst case (consider a star-like graph).

Subtree Isomorphism, Unrooted

Note that all subtrees can be found as follows:

> *Root S at u. The resulting rooted tree S^u itself is a rooted subtree. Also, removing any child subtree of S^u yields a rooted subtree.*



We use $S[u, v]$ to denote the subtree rooted at v after removing child subtree u.

Subtree Isomorphism, Unrooted

We may compute the maximum bipartite matchings for all these trees together. Formally, let U_i denote U removing the i-th element u_i, we want to compute maximum bipartite matching for $U_i \cup V$ for every i. This results in an unrooted subtree isomorphism algorithm in the same time as the rooted case.

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Note that removing u_i decreases the size of maximum matching by at most 1. In case that u_i is unmatched, or reachable from any unmatched vertex via alternating path, in any maximum bipartite matching of $U \cup V$, the removal of u_i won't decrease the size of maximum matching.

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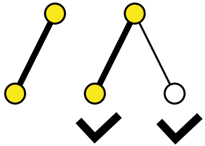


Subtree Isomorphism, Unrooted

Algorithm 3 Unooted Subtree Isomorphism

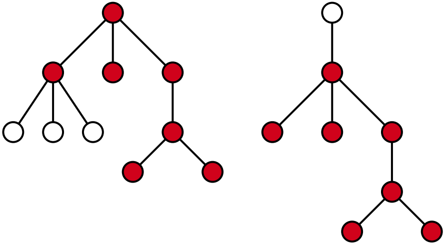
Input: two unrooted trees S and T

Output: decide if S is isomorphic to some g-subtree of T

```
root T arbitrarily
initialize M[·,·] with 0
for vertex v in post-order traversal of T do
    for each vertex u is S do
        compute the maximum bipartite matchings of C(S[w,u]) ∪ C(v) for each w ∈ N(u) ∪ {NIL}
    end for
end for
return true if M[S[NIL,u], root(T)] = 1 for some u ∈ S
```

Maximum Common Subtrees, Rooted

Given two rooted trees S, T, find a maximum size g-subtree of S isomorphic to some g-subtree of T.



Consider the rooted case first.

Algorithm 4 Rooted Maximum Common Subtrees

Input: two rooted trees S and T

Output: the size of maximum common g-subtrees of S and T

1: **for** vertex v in post-order traversal of T **do**

2: **for** each vertex u is S **do**

3: build a weighted bipartite graph

$$G = (C(u) \cup C(v), M[C(u), C(v)])$$

4: let $M[u, v]$ be the maximum weight matching of G, plus 1

5: **end for**

6: **end for**

7: **return** $\max_{u \in S, v \in T} M[u, v]$

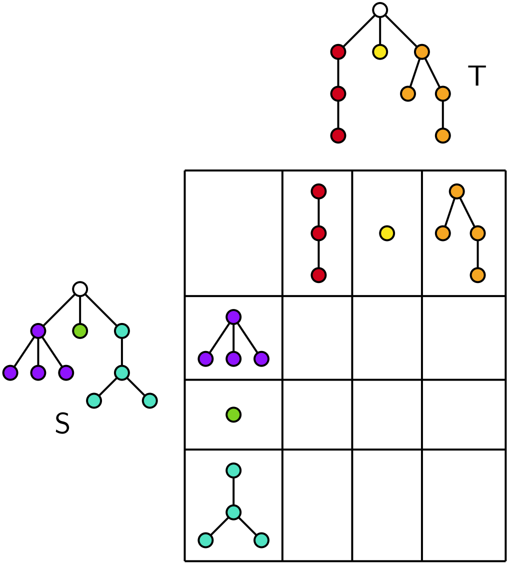
Maximum Common Subtrees, Rooted

Solution (dynamic programming)

We may again use dynamic programming to solve this problem. Let for $u \in S, v \in T$, define $M[u, v]$ as the size of maximum common subtrees rooted at u and v. The value of $M(u, v)$ can be computed from $M[x, y]$ $(x \in C(u), y \in C(v))$.

We may similarly construct a bipartite graph. The value $M[u, v]$ is computed from maximum weight bipartite matching (instead of maximum cardinality bipartite matching).

Maximum Common Subtrees, Rooted



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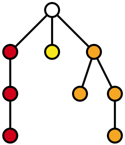

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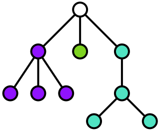

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			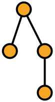
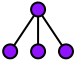	2	1	3
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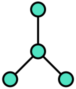
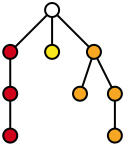
	3	1	3

Maximum Common Subtrees, Rooted



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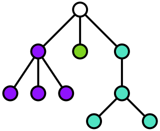

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			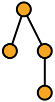
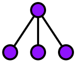	2	1	3
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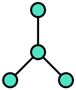	3	1	3

Maximum Common Subtrees, Rooted

By using a careful implementation of Kuhn-Munkres algorithm, the maximum weight bipartite matching of $U \cup V$ ($|U| < |V|$) can be solved in $O(|U||V|^2)$ time.

Applying an analysis similar to the subtree isomorphism problem, the total time complexity is $O(n^3)$.

Maximum Common Subtrees, Unrooted

What about unrooted case?

Maximum Common Subtrees, Unrooted

What about unrooted case?

It is easy to obtain an $O(n^4)$ algorithm by trying all possible roots of one tree.

The same technique in subtree isomorphism may apply here to obtain a cubic time algorithm, by not taking maximum weight bipartite matching as black box.

The maximum weight perfect matching can be written as a linear program:

The primal program:

$$
\begin{aligned}
\max_{x_{uv}} \quad & \sum_{u,v} w_{uv} x_{uv} \\
\text{s.t.} \quad & \sum_{u} x_{uv} = 1 \quad \forall v \\
& \sum_{v} x_{uv} = 1 \quad \forall u \\
& x_{uv} \geq 0
\end{aligned}
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$$

The dual program:

$$
\begin{aligned}
\min_{y_u, y_v} \quad & \sum_{u} y_u + \sum_{v} y_v \\
\text{s.t.} \quad & y_u + y_v \geq w_{uv} \quad \forall u, v
\end{aligned}
$$

Let $\bar{x}_{uv}$ be optimal solution to primal program, $\bar{y}_u, \bar{y}_v$ be optimal solution to dual program.

Theorem (Strong duality theorem)

$$w_{uv}\bar{x}_{uv} = \sum_u \bar{y}_u + \sum_v \bar{y}_v \quad \forall u, v$$

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Theorem (Strong duality theorem)

$$w_{uv}\bar{x}_{uv} = \sum_u \bar{y}_u + \sum_v \bar{y}_v \quad \forall u, v$$

Theorem (Complementary slackness theorem)

$$\sum_{uv} \bar{x}_{uv}(\bar{y}_u + \bar{y}_v - w_{uv}) = 0$$

This means only saturated edges can be in maximum matching.

Maximum Common Subtrees, Unrooted

About Maximum Weight Perfect Bipartite Matching

$$\begin{array}{c|ccc} & 0 & 4 & 3 \\ \hline 0 & 0 & 3 & 0 \\ 0 & 0 & 4 & 2 \\ 0 & 0 & 0 & 3 \end{array} \rightarrow$$

Maximum Common Subtrees, Unrooted

About Maximum Weight Perfect Bipartite Matching

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After removing a vertex:

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\begin{array}{c|ccc} & 0 & 4 & 3 \\ \hline 0 & \mathbf{0} & 3 & 0 \\ 0 & \mathbf{0} & \mathbf{4} & 2 \\ 0 & \mathbf{0} & 0 & 0 \end{array}
\to
\begin{array}{c|ccc} & 0 & 4 & \underline{2} \\ \hline 0 & \mathbf{0} & 3 & 0 \\ 0 & \mathbf{0} & \mathbf{4} & \mathbf{2} \\ 0 & \mathbf{0} & 0 & 0 \end{array}
\to
$$

$$\begin{array}{c|ccc} & 0 & 4 & 3 \\ \hline 0 & 0 & 3 & 0 \\ 0 & 0 & 4 & 2 \\ 0 & 0 & 0 & 3 \end{array} \to \begin{array}{c|ccc} & 0 & 4 & 3 \\ \hline 0 & \mathbf{0} & 3 & 0 \\ 0 & \mathbf{0} & \mathbf{4} & 2 \\ 0 & \mathbf{0} & 0 & \mathbf{3} \end{array} \to \begin{array}{c|ccc} & 0 & 4 & 3 \\ \hline 0 & \boxed{\mathbf{0}} & 3 & 0 \\ 0 & \mathbf{0} & \boxed{\mathbf{4}} & 2 \\ 0 & \mathbf{0} & 0 & \boxed{\mathbf{3}} \end{array}$$

After removing a vertex:

$$\begin{array}{c|ccc} & 0 & 4 & 3 \\ \hline 0 & 0 & 3 & 0 \\ 0 & 0 & 4 & 2 \\ 0 & 0 & 0 & \underline{0} \end{array} \to \begin{array}{c|ccc} & 0 & 4 & 3 \\ \hline 0 & \mathbf{0} & 3 & 0 \\ 0 & \mathbf{0} & \mathbf{4} & 2 \\ 0 & \mathbf{0} & 0 & 0 \end{array} \to \begin{array}{c|ccc} & 0 & 4 & \underline{2} \\ \hline 0 & \mathbf{0} & 3 & 0 \\ 0 & \mathbf{0} & \mathbf{4} & \mathbf{2} \\ 0 & \mathbf{0} & 0 & 0 \end{array} \to$$

$$\begin{array}{c|ccc} & 0 & \underline{3} & \underline{1} \\ \hline 0 & \mathbf{0} & \mathbf{3} & 0 \\ \underline{1} & 0 & \mathbf{4} & \mathbf{2} \\ 0 & \mathbf{0} & 0 & 0 \end{array} \to$$

Maximum Common Subtrees, Unrooted

About Maximum Weight Perfect Bipartite Matching

$$
\begin{array}{c|ccc} & 0 & 4 & 3 \\ \hline 0 & 0 & 3 & 0 \\ 0 & 0 & 4 & 2 \\ 0 & 0 & 0 & 3 \end{array}
\rightarrow
\begin{array}{c|ccc} & 0 & 4 & 3 \\ \hline 0 & \mathbf{0} & 3 & 0 \\ 0 & \mathbf{0} & \mathbf{4} & 2 \\ 0 & \mathbf{0} & 0 & \mathbf{3} \end{array}
\rightarrow
\begin{array}{c|ccc} & 0 & 4 & 3 \\ \hline 0 & \boxed{\mathbf{0}} & 3 & 0 \\ 0 & \mathbf{0} & \boxed{\mathbf{4}} & 2 \\ 0 & \mathbf{0} & 0 & \boxed{\mathbf{3}} \end{array}
$$

After removing a vertex:

$$
\begin{array}{c|ccc} & 0 & 4 & 3 \\ \hline 0 & 0 & 3 & 0 \\ 0 & 0 & 4 & 2 \\ 0 & 0 & 0 & \underline{0} \end{array}
\rightarrow
\begin{array}{c|ccc} & 0 & 4 & 3 \\ \hline 0 & \mathbf{0} & 3 & 0 \\ 0 & \mathbf{0} & \mathbf{4} & 2 \\ 0 & \mathbf{0} & 0 & 0 \end{array}
\rightarrow
\begin{array}{c|ccc} & 0 & 4 & \underline{2} \\ \hline 0 & \mathbf{0} & 3 & 0 \\ 0 & \mathbf{0} & \mathbf{4} & \mathbf{2} \\ 0 & \mathbf{0} & 0 & 0 \end{array}
\rightarrow
$$

$$
\begin{array}{c|ccc} & 0 & \underline{3} & \underline{1} \\ \hline 0 & \mathbf{0} & \mathbf{3} & 0 \\ \underline{1} & 0 & \mathbf{4} & \mathbf{2} \\ 0 & \mathbf{0} & 0 & 0 \end{array}
\rightarrow
\begin{array}{c|ccc} & 0 & 3 & 1 \\ \hline 0 & \mathbf{0} & \boxed{\mathbf{3}} & 0 \\ 1 & 0 & \mathbf{4} & \boxed{\mathbf{2}} \\ 0 & \boxed{\mathbf{0}} & 0 & 0 \end{array}
$$

Overview

- Three fundamental graph theory problems:

	Trees	General Graphs
Graph Isomorphism	$O(n)$	$O(n^{\text{ploy} \log n})$
Subgraph Isomorphism	P	NP-Complete
Maximum Common Subgraphs	P	NP-Hard

- One problem solving framework: turns the original problem into several instances of matching problem.
- Two auxiliary algorithms:
  - Edmonds-Karp algorithm: solves maximum cardinality bipartite matching in $O(E\sqrt{V})$ time;
  - Kuhn-Munkres algorithm: solves maximum weight bipartite matching in $O(V^3)$ time.

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  (this paper gives a slightly faster subtree isomorphism algorithm, but is of less practical significance)
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  (this paper describes a cubic algorithm for unrooted maximum common subtrees in detail)