

Subgraph isomorphism problems

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Subgraph isomorphism

Problem

For two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, we want to find an induced subgraph of G_2 that is isomorphic to G_1 .

In the weighted case, for a given weight function $w : V_1 \times V_2 \rightarrow \mathbb{R}$, we want to find an embedding of G_1 into G_2 with maximum weight.

Clique problem

Goal: Find a maximum-weight embedding of G_1 into G_2 .

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If $|V_1| = k$, then G is k -partite, and the k -cliques in G correspond to the embeddings of G_1 into G_2 .

Finding a maximum-weight embedding is therefore equivalent to finding a maximum-weight k -clique in the product graph.

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- Proteins can be represented by protein graphs.
- To predict the position of the molecule, we need to find the embeddings of the small protein graph into the bigger protein graph with the best weights.
- We do this by finding the 100 greatest weight k -cliques in the product graph.

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- Dominance relations
- Edge-to-Node transformation

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- Implement a more efficient weighted clique search algorithm to solve protein docking quicker,
- Find a way to avoid infeasible embeddings,
- Apply the kernelization methods directly to the subgraph problem.

Usage of AI tools

Throughout the project, no AI tools were used.