

# Algorithm Selection for Maximum Common Subgraph

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## 1 The Problem

Labeled and unlabeled (undirected) maximum common induced subgraph.

## 2 Algorithms

Clique encoding [7]  $k \downarrow$  [3] MCSPLIT [6]

(Somewhere) 1000 s limit, 512 GB limit (clique becomes impossible for some instances), insert CPU specs.

## 3 Problem Instances

### 3.1 ARG database

MCS data is from [1][2].

### 3.2 Benchmarks for the Subgraph Isomorphism Problem

SIP instances are taken from [8] (with the biochemical reaction dataset excluded since we are not dealing with directed graphs).

## 4 Features

Features are based on the algorithm selection paper for the subgraph isomorphism problem [5]. Simple features:

- number of vertices,
- number of edges,
- density,
- number of loops,

- mean degree,
- maximum degree,
- standard deviation of degrees,
- whether the graph is connected,
- mean distance between all pairs of vertices,
- maximum distance between all pairs of vertices,
- proportion of vertex pairs that are at least 2, 3 and 4 apart (?),
- number of labels,
- number of distinct labels.

Features that could be computed if we end up using a presolver:

- uniformity of the distribution of edges,
- how many candidate pairs were removed,
- proportion of candidate pairs removed over all pairs,
- min values removed per variable,
- max values removed per variable,
- CPU time taken to compute all this.

## 5 Selection Model

We’re using LLAMA [4]. Describe k-folding.

## References

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