Algorithm Selection for Maximum Common Subgraph

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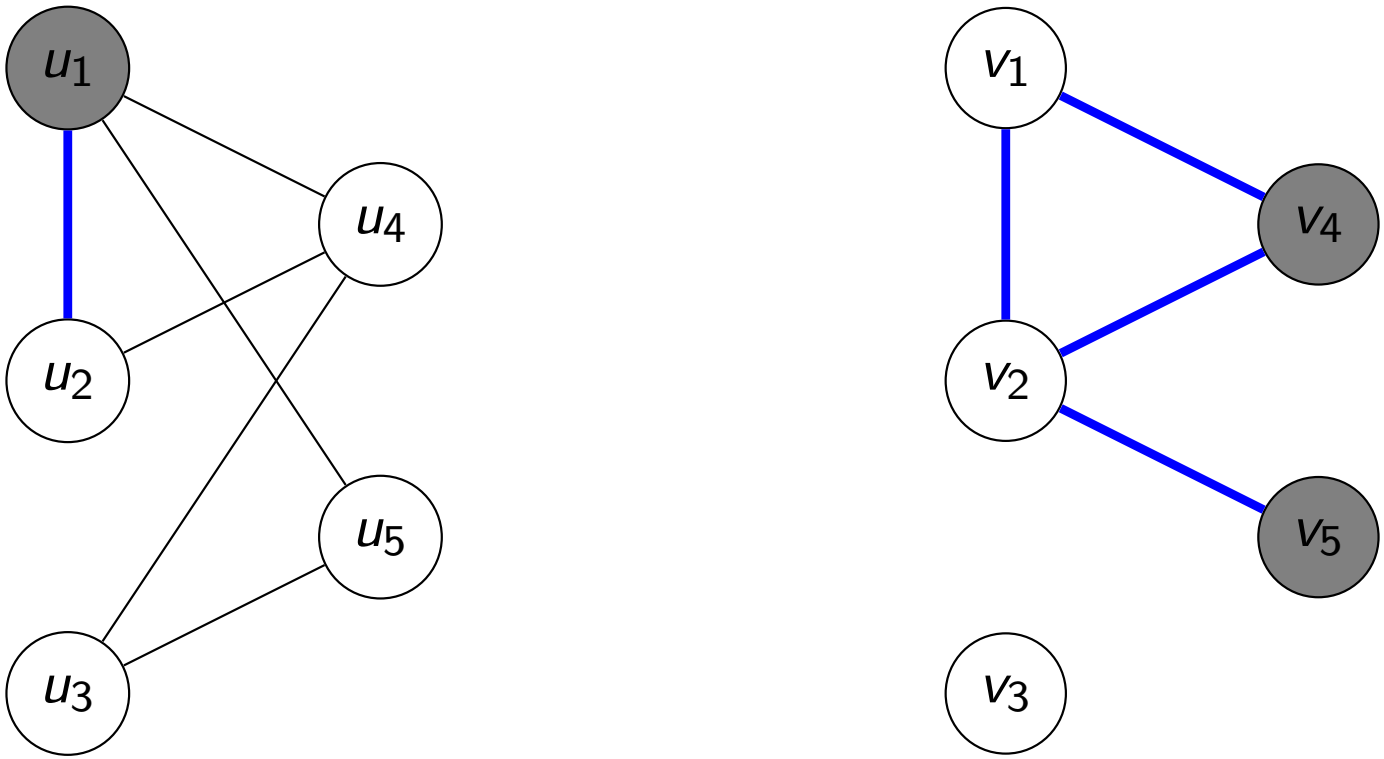
The Problem: Maximum Common Subgraph



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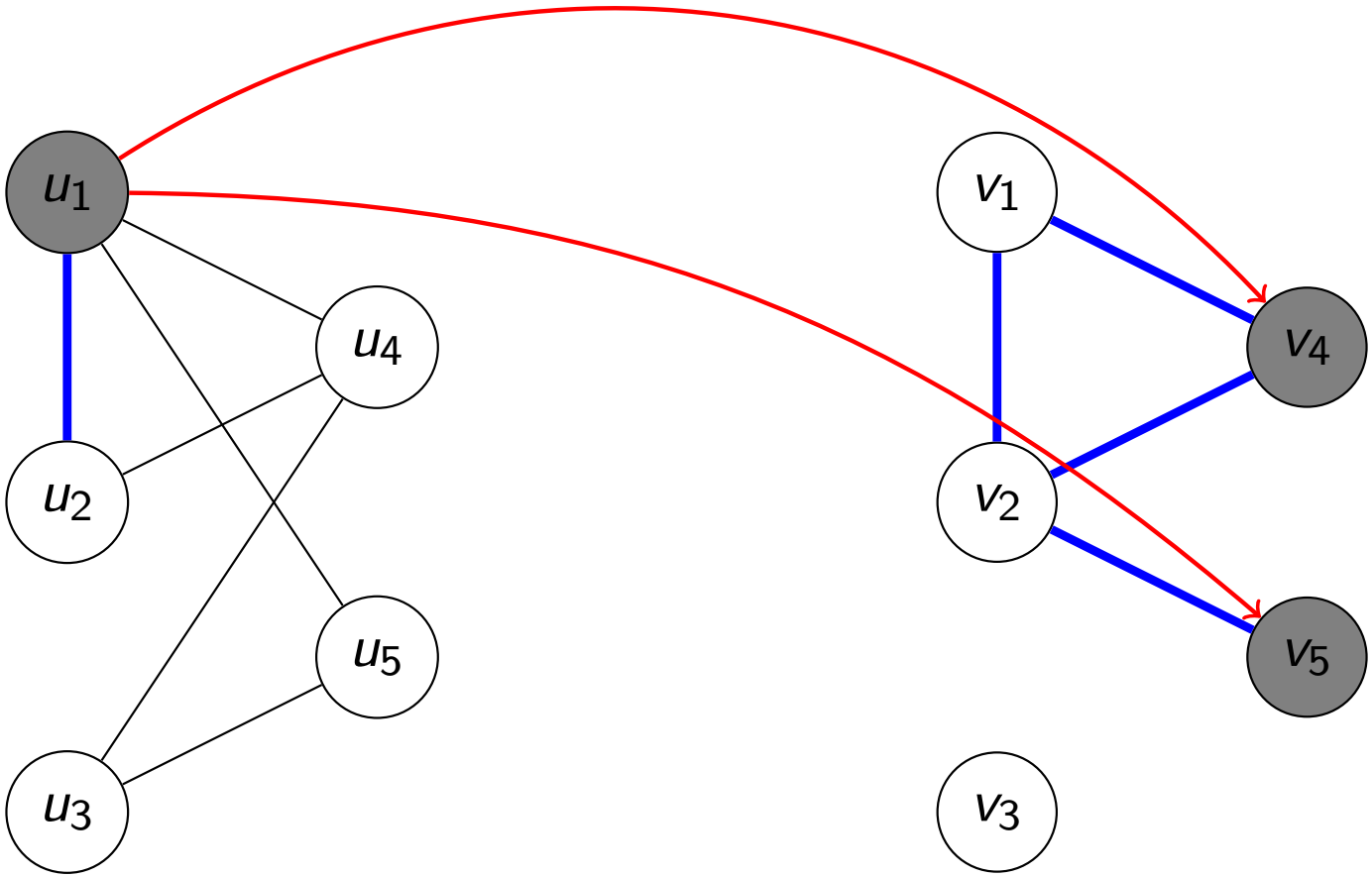

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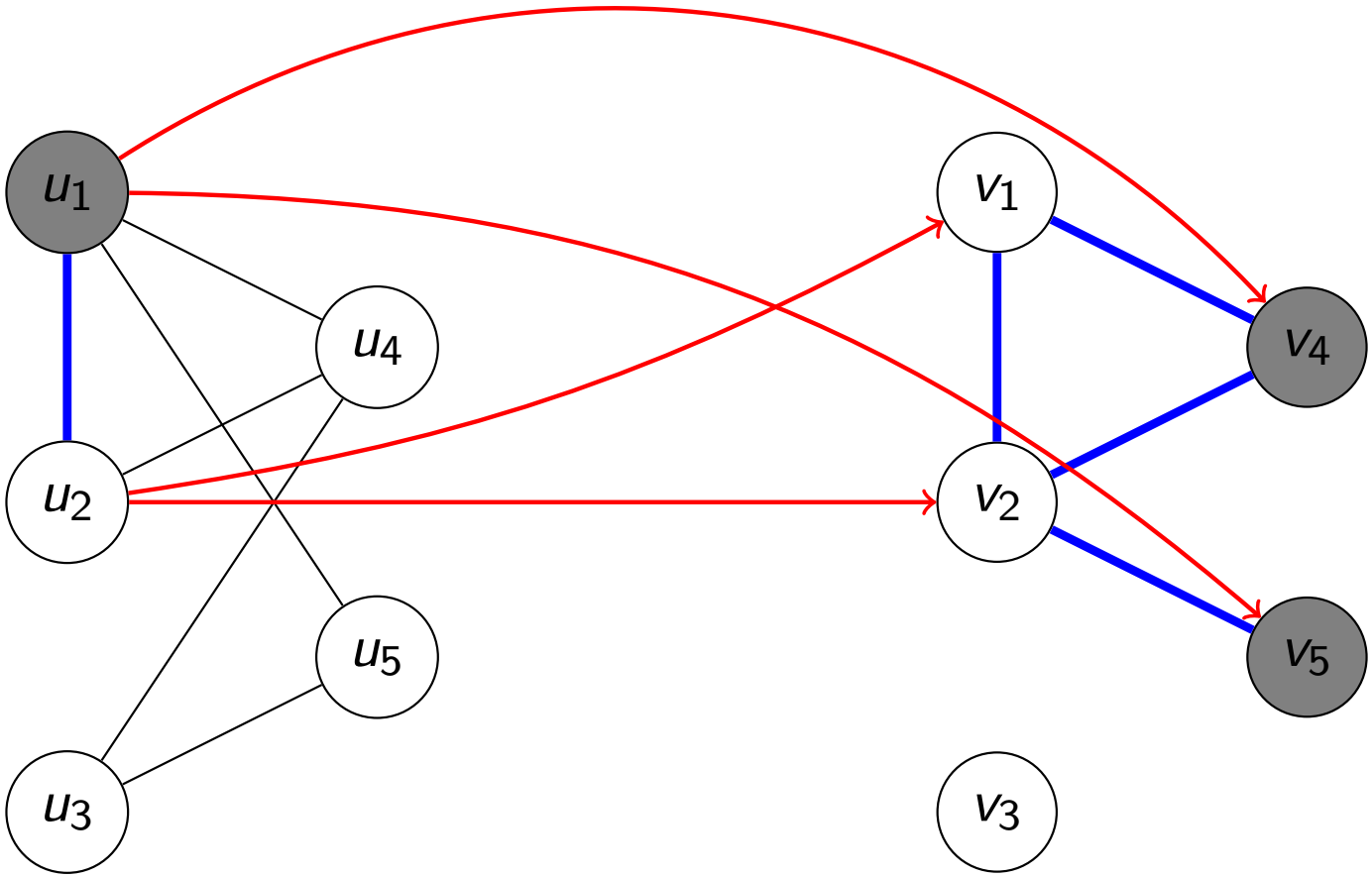

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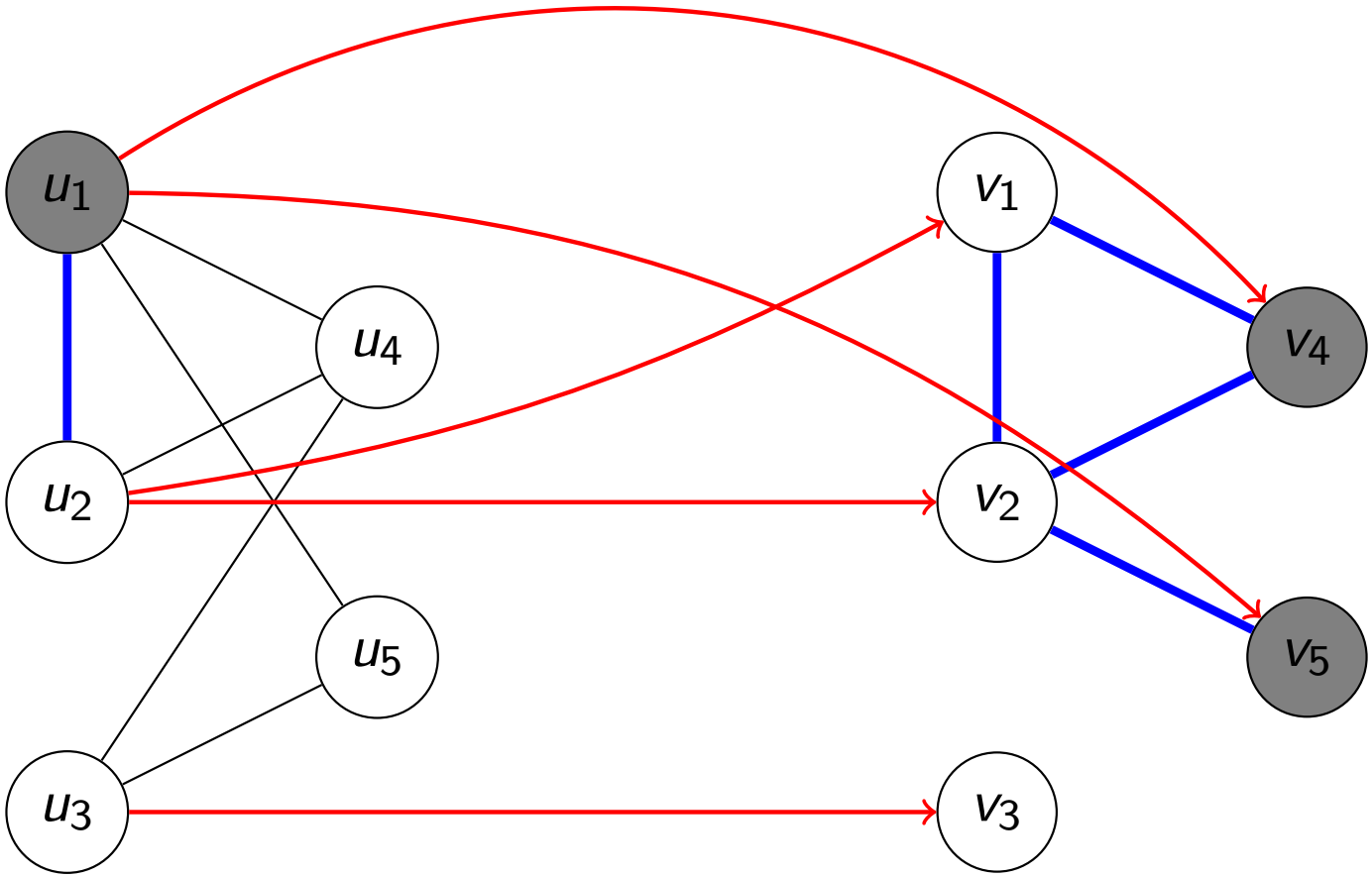

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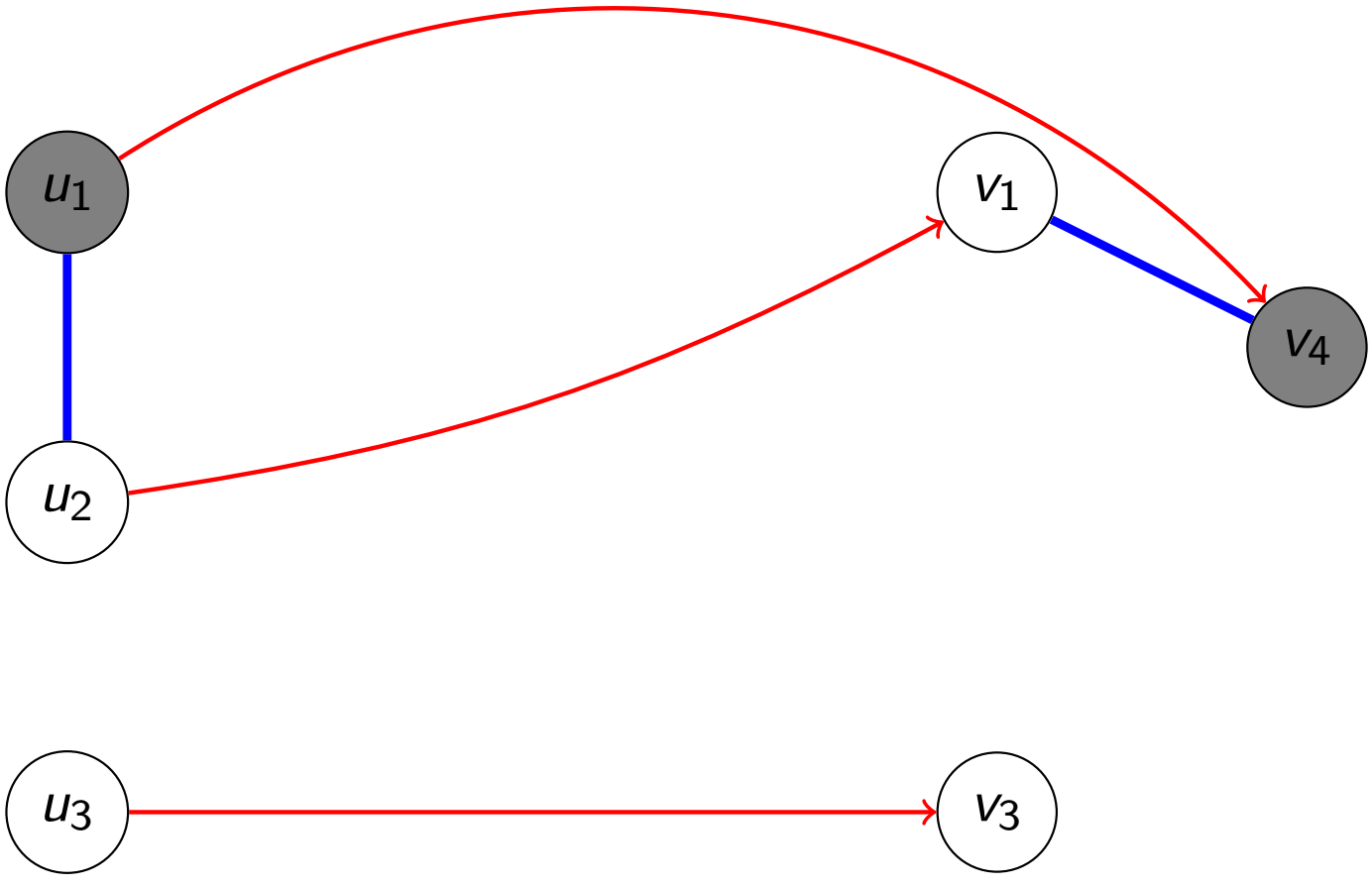

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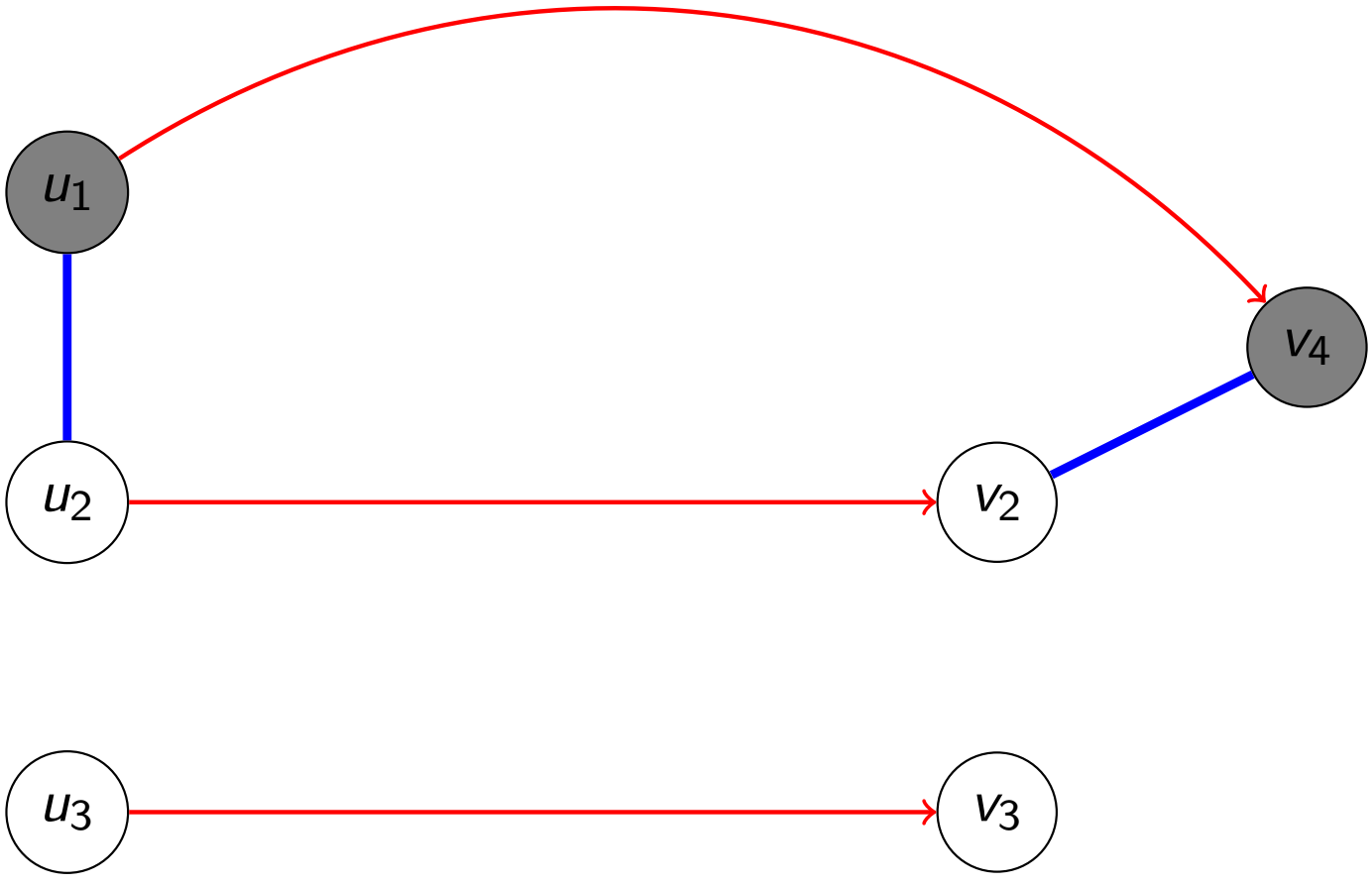

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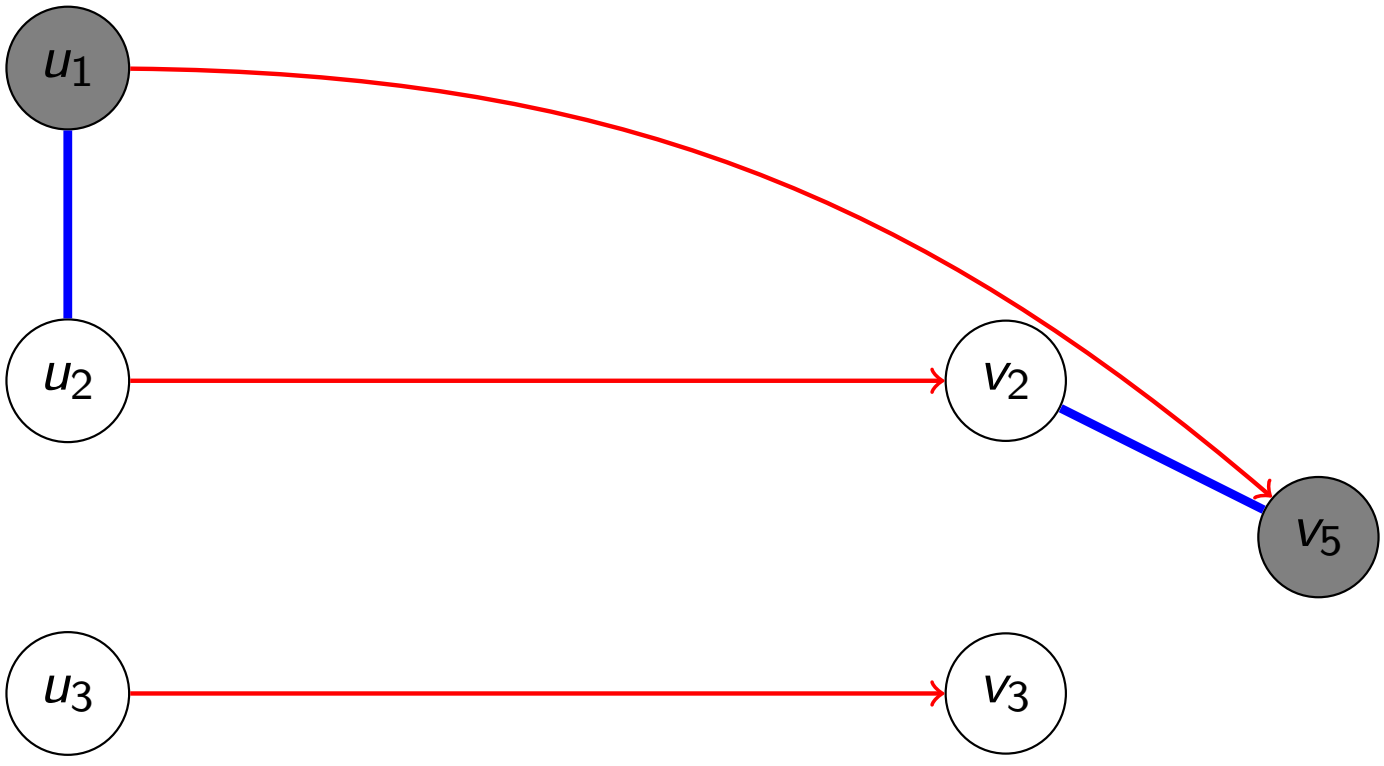
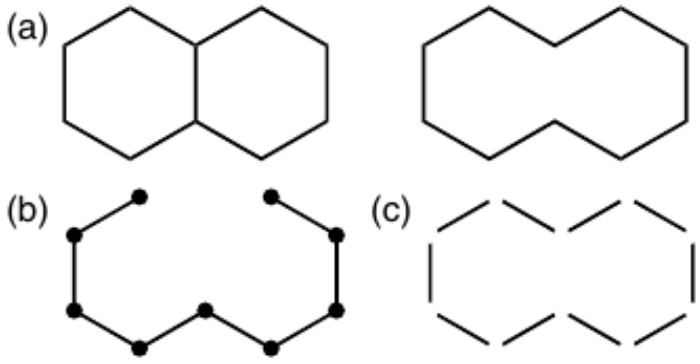
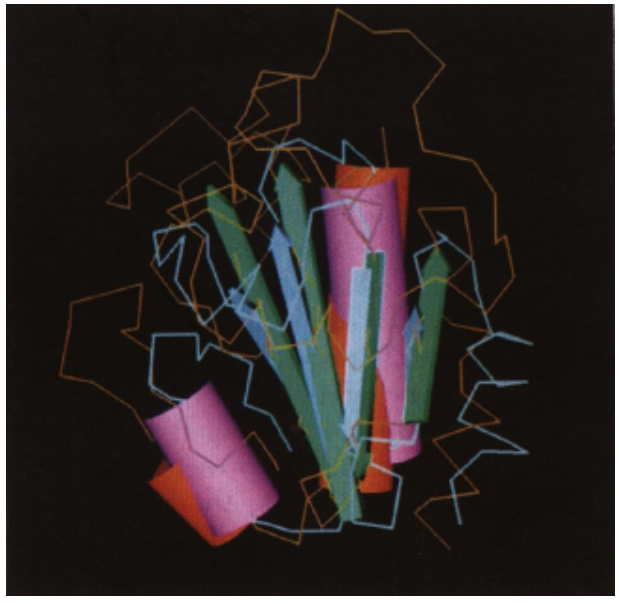


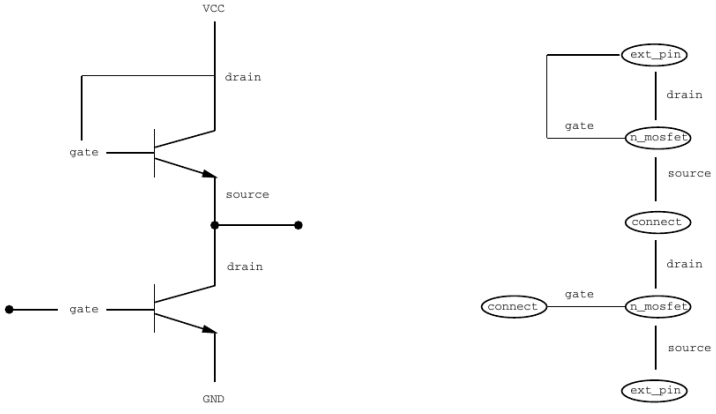
Why Is It Important?



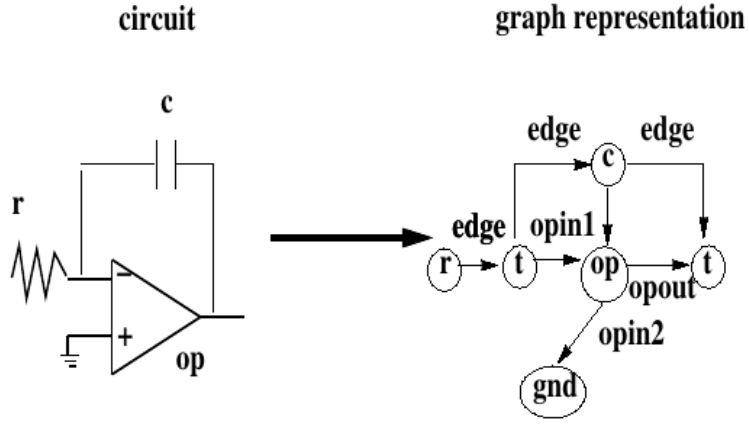
Source: Ehrlich and Rarey 2011



Source: M. Grindley et al. 1993



Source: Cook and Holder 1994



Source: Djoko, Cook and Holder 1997

Existing Ways to Solve It

- McSplit, McSplit↓
  - McCreesh, Prosser and Trimble 2017
- clique encoding
  - McCreesh, Ndiaye et al. 2016
- k↓
  - Hoffmann, McCreesh and Reilly 2017

Solution: Algorithm Selection

(G_1, G_2)

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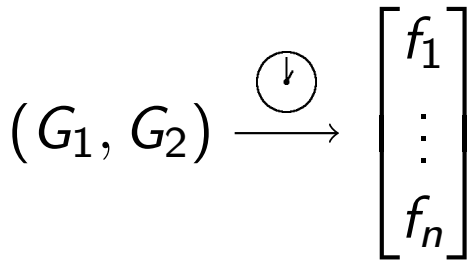

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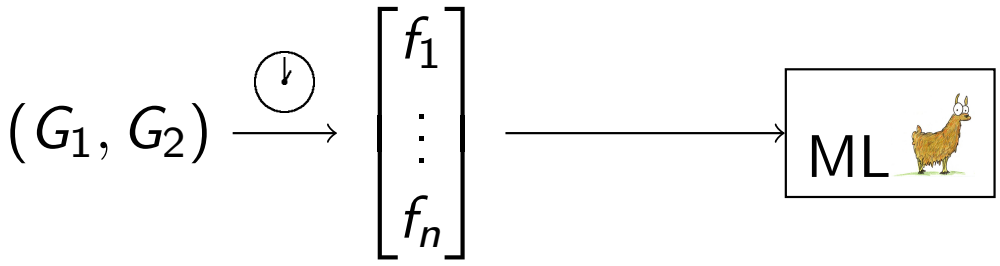

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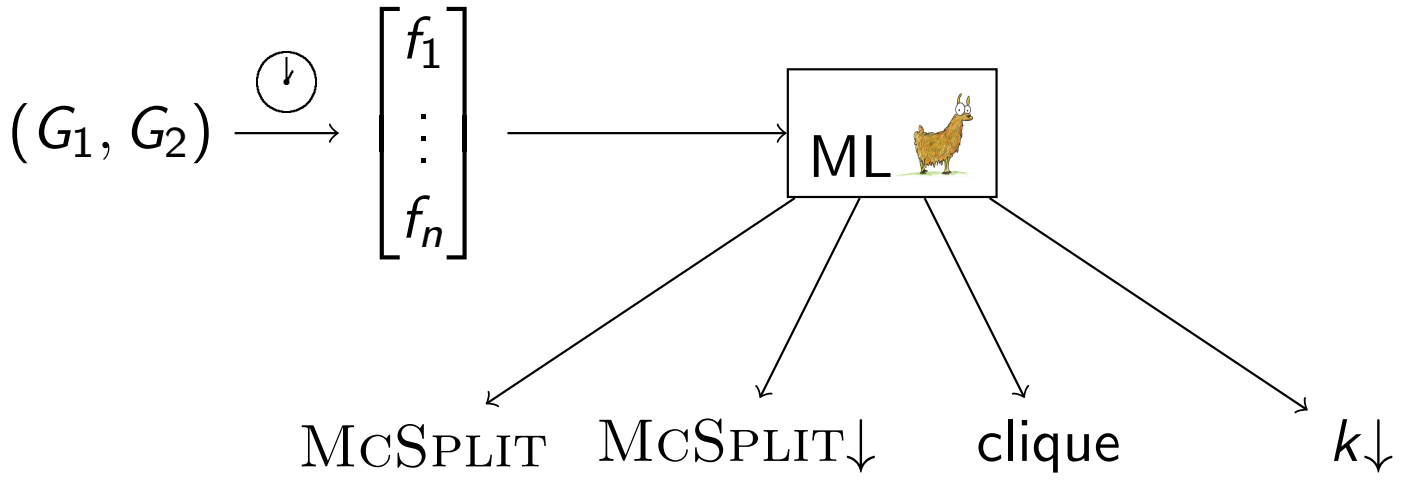

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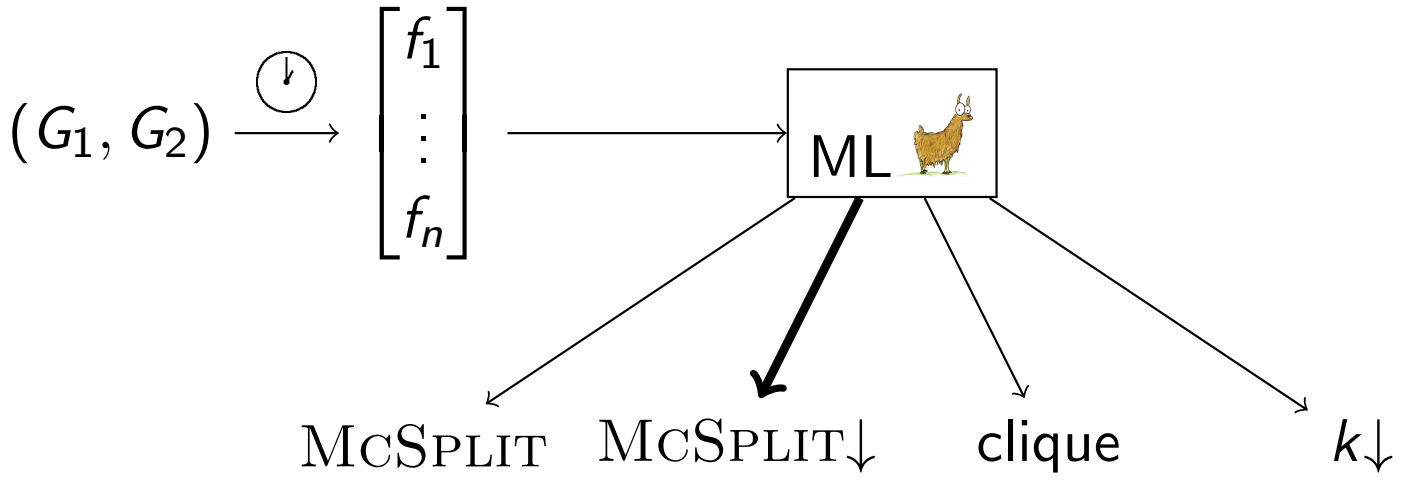

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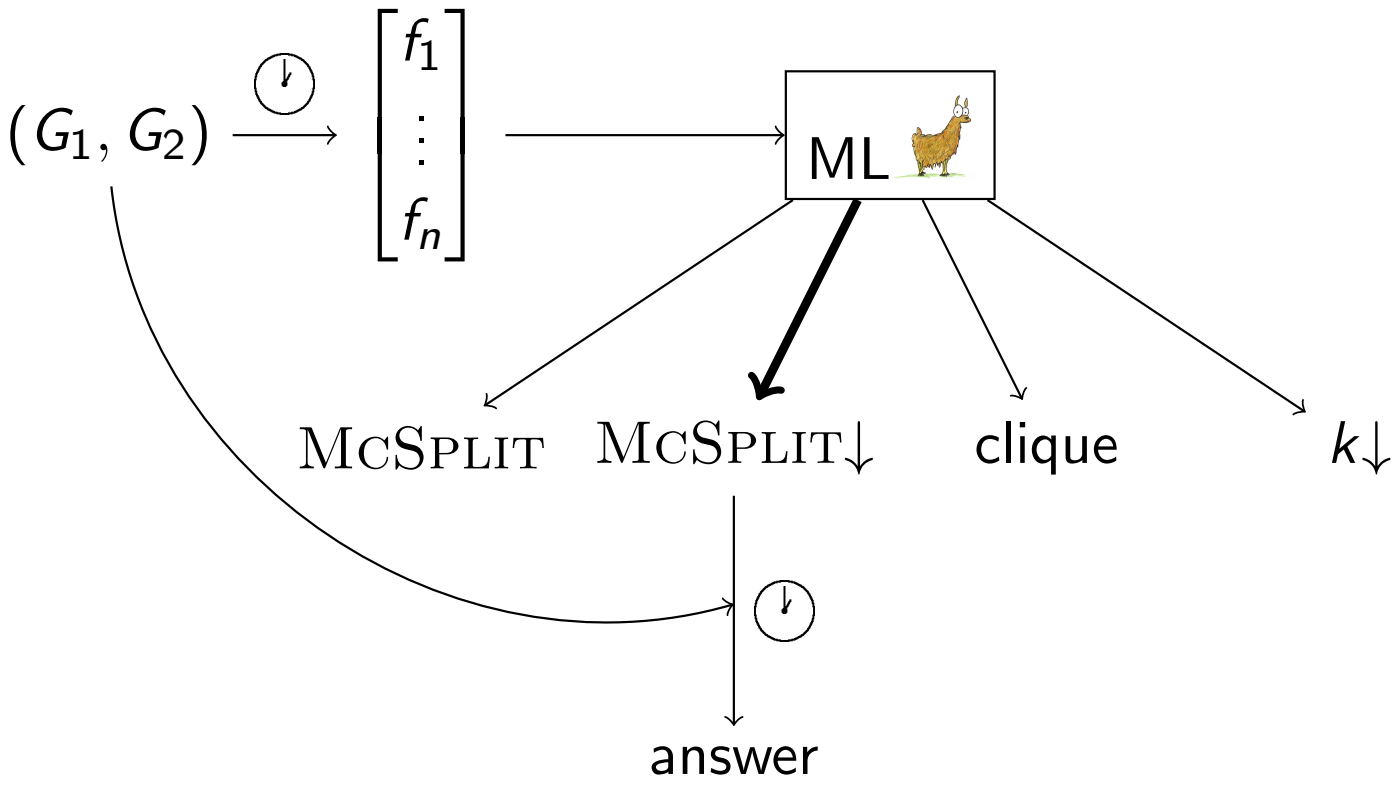

The Process

- Three cases:
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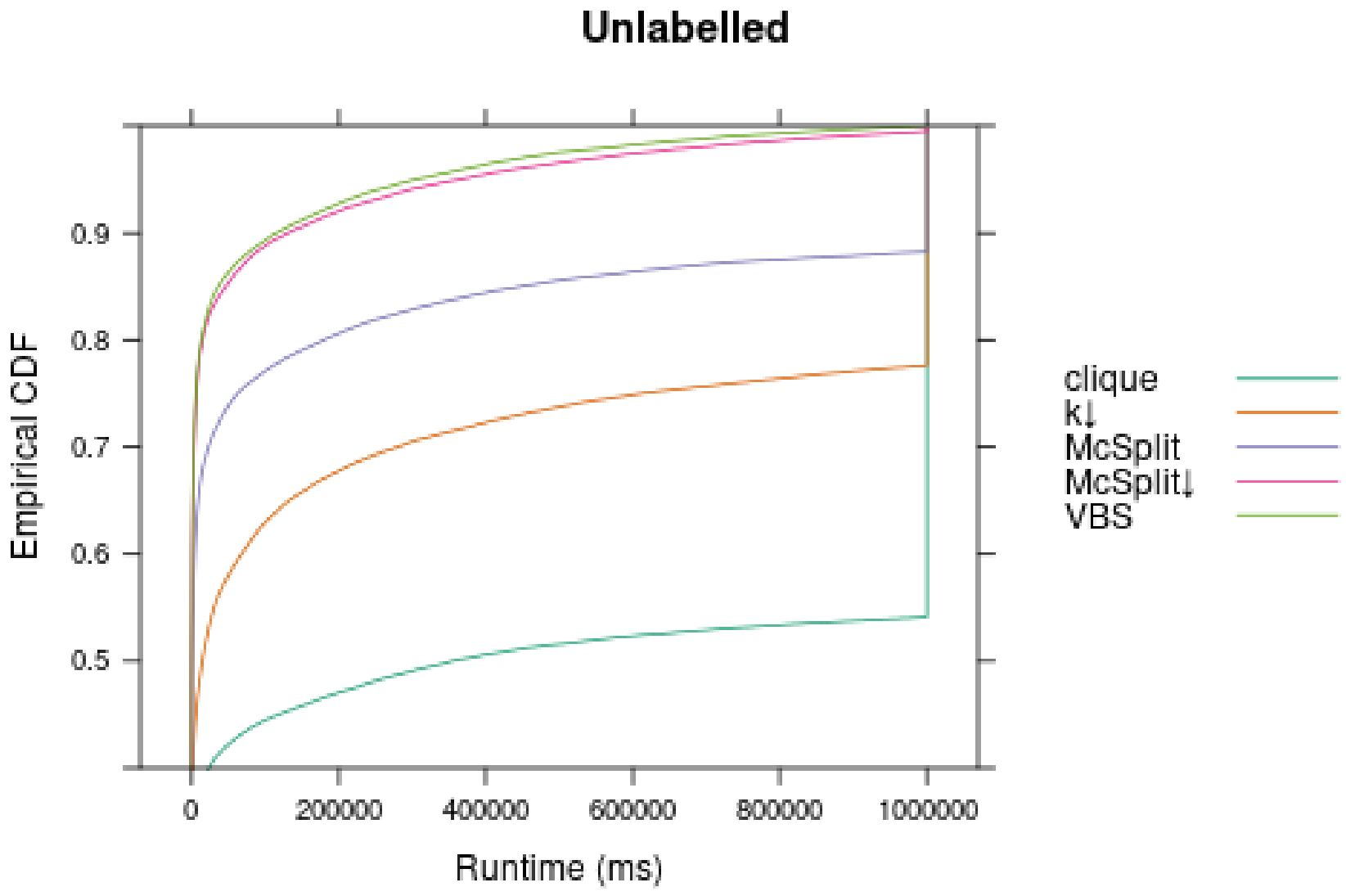
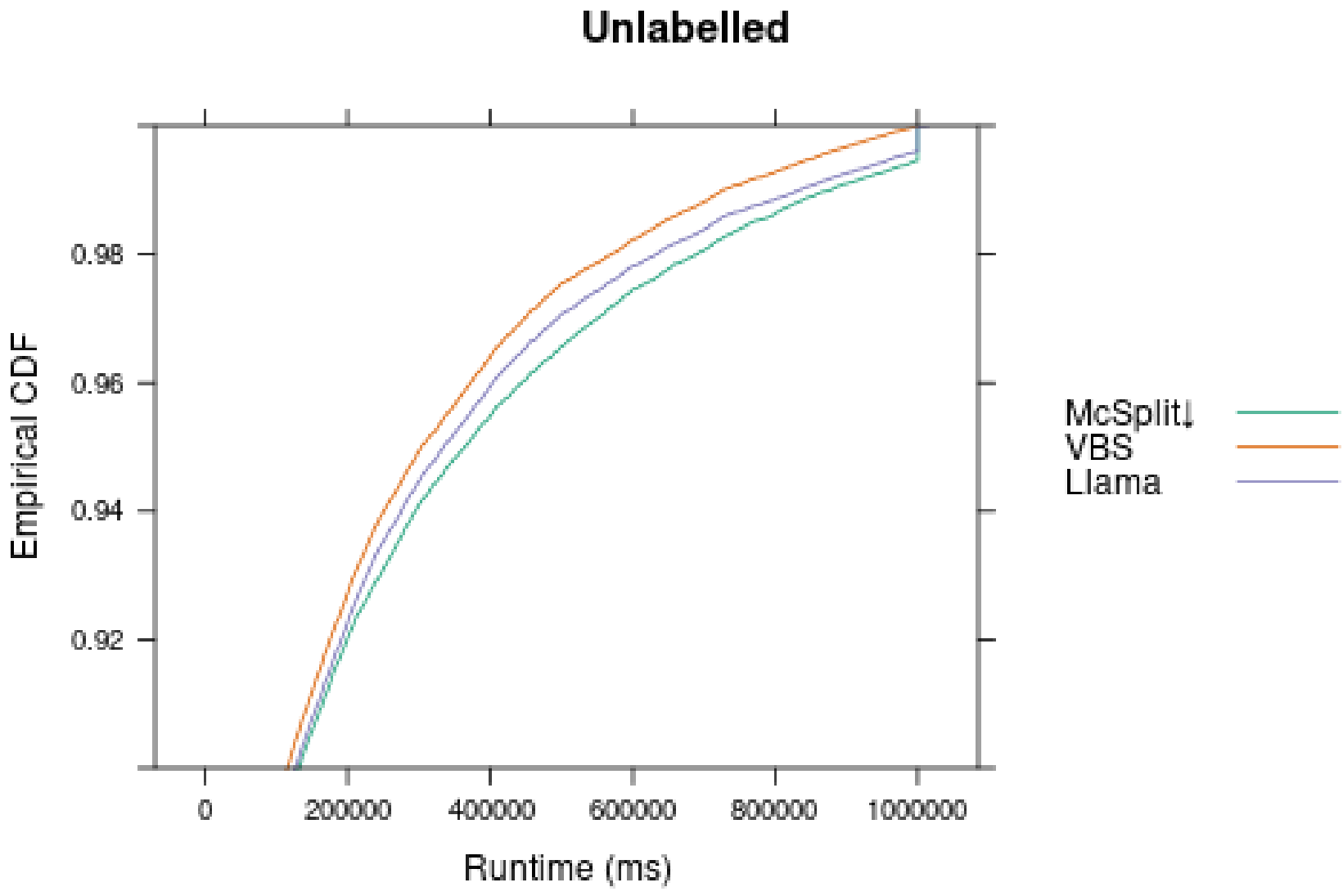
- Train machine learning models
- Evaluate their performance and usefulness

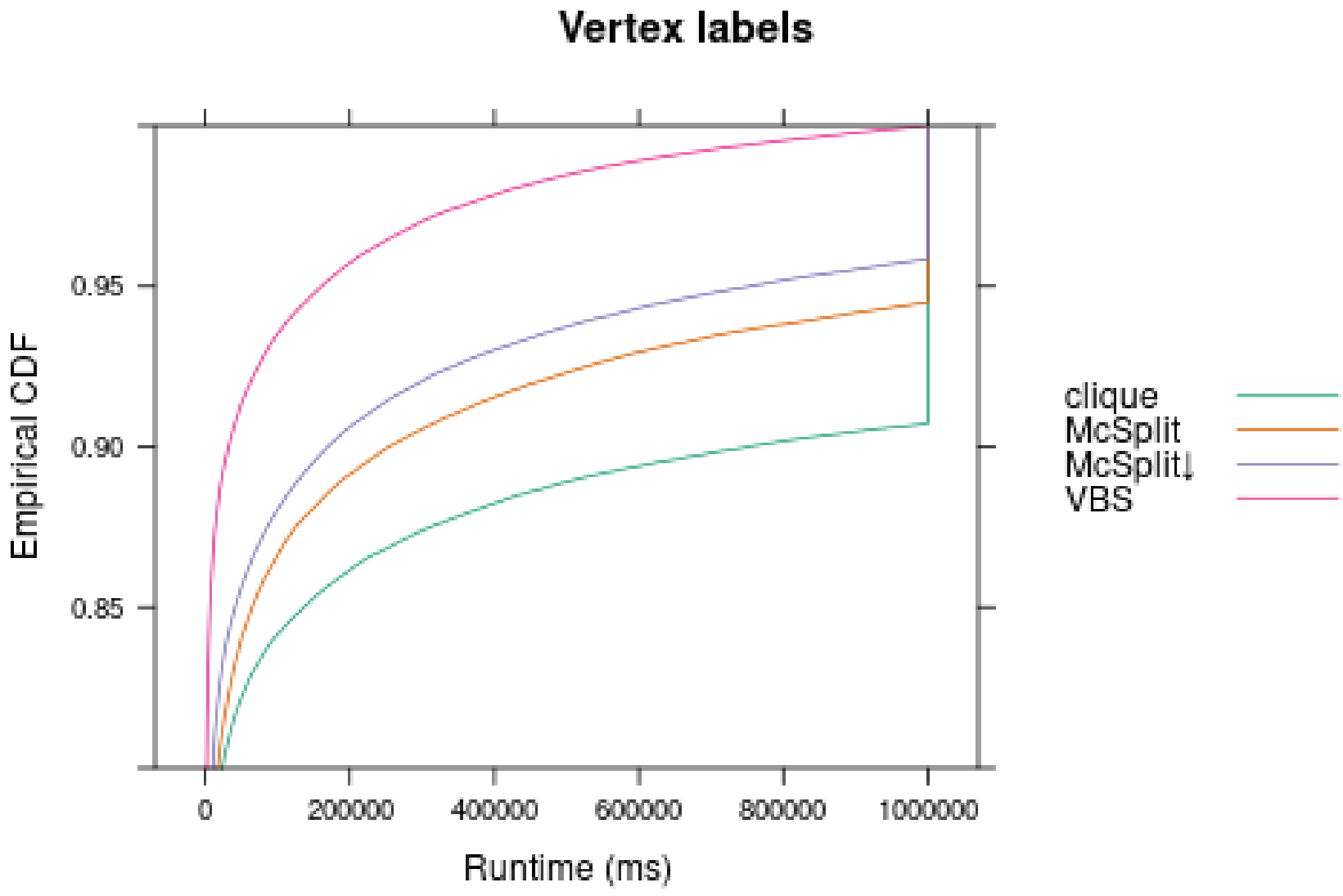
Results


Unlabelled
Empirical CDF
0.9
0.8
0.7
0.6
0.5
0
200000
400000
600000
800000
1000000
Runtime (ms)
clique
k↓
McSplit
McSplit↓
VBS

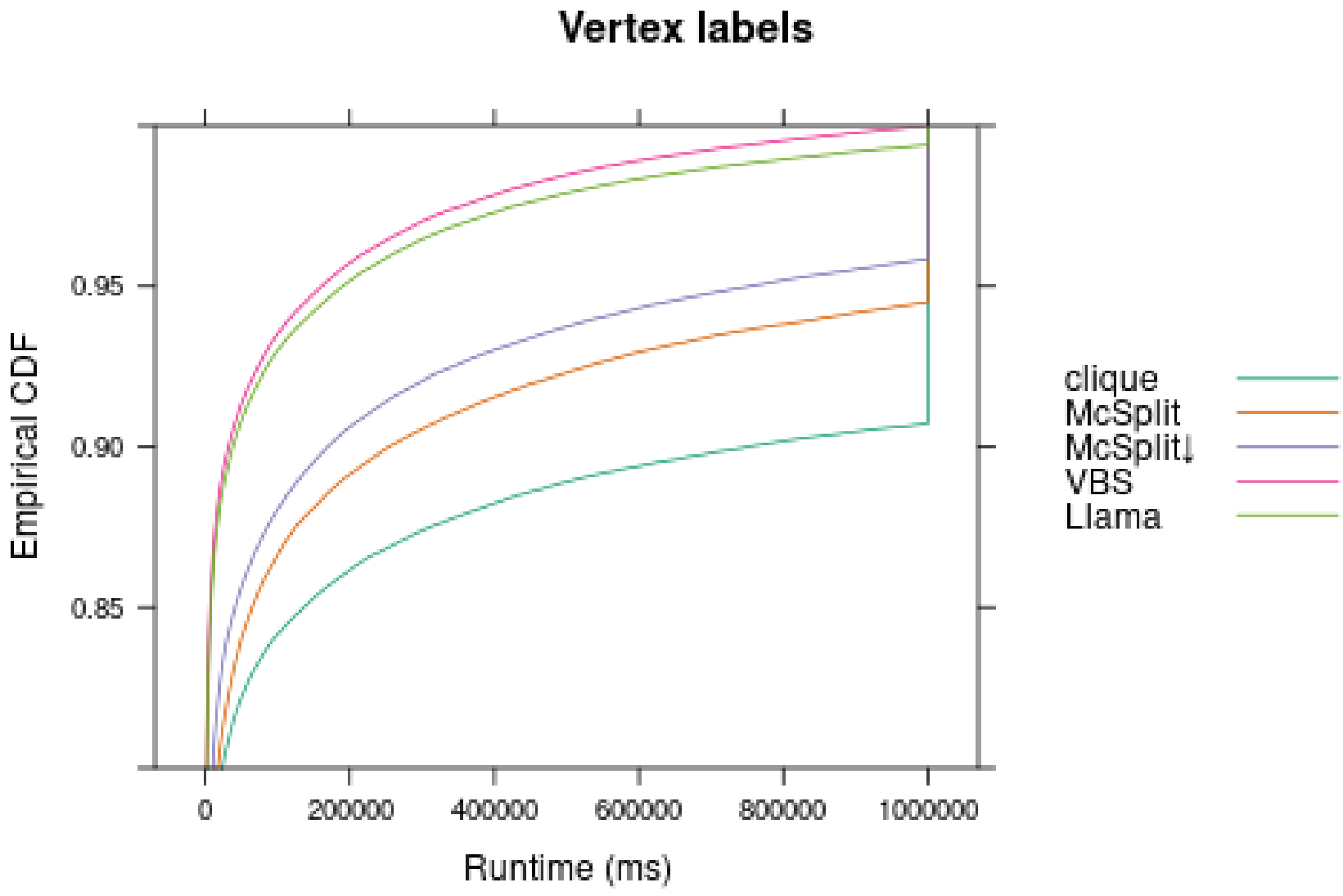
Results (27%)


Unlabelled
Empirical CDF
0.98
0.96
0.94
0.92
0
200000
400000
600000
800000
1000000
Runtime (ms)
McSplit↓
VBS
Llama

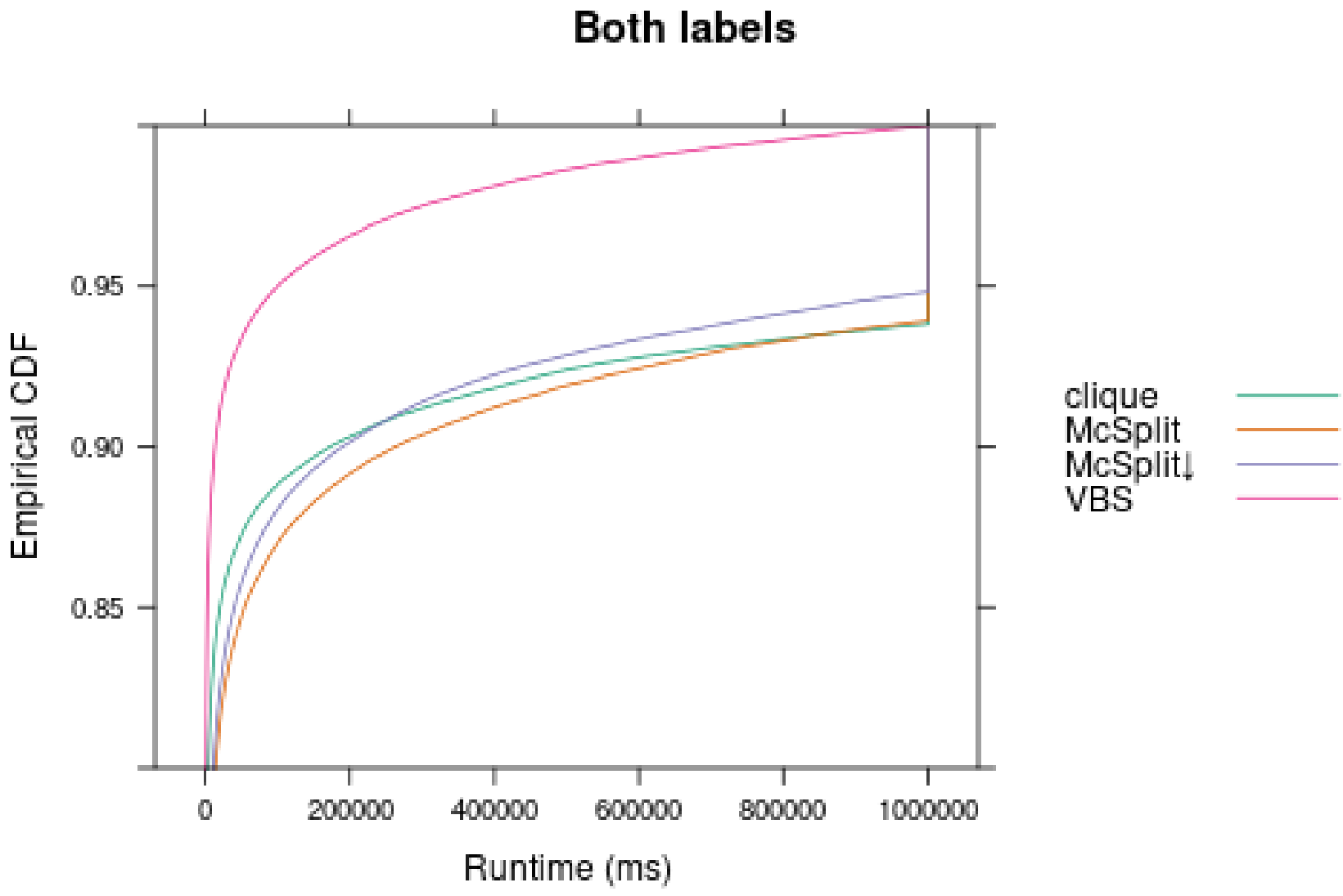
Results


Vertex labels
Empirical CDF
0.95
0.90
0.85
0
200000
400000
600000
800000
1000000
Runtime (ms)
clique
McSplit
McSplit↓
VBS

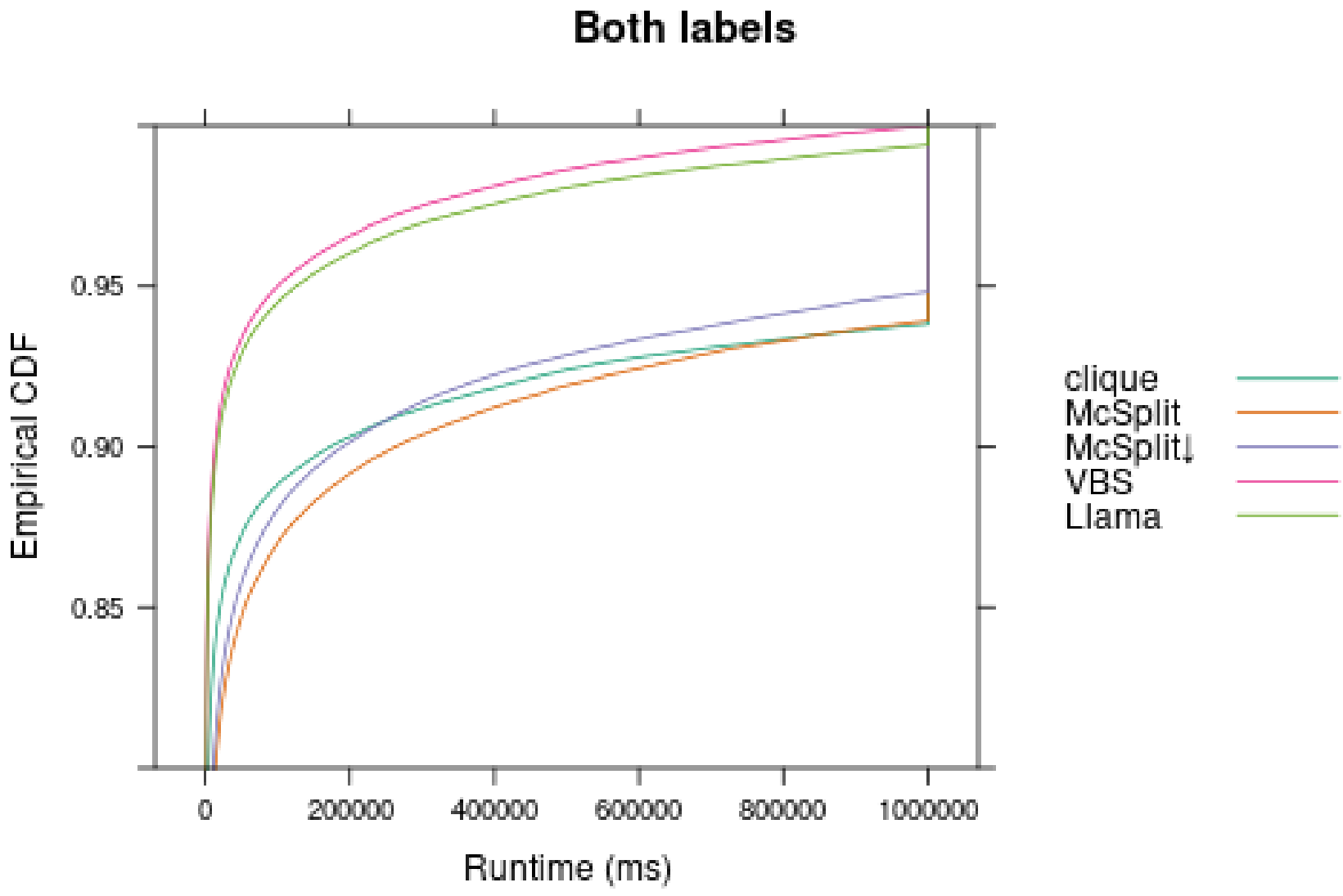
Results (86%)


Vertex labels
Empirical CDF
0.95
0.90
0.85
0
200000
400000
600000
800000
1000000
Runtime (ms)
clique
McSplit
McSplit↓
VBS
Llama

Results


Both labels
Empirical CDF
0.95
0.90
0.85
0
200000
400000
600000
800000
1000000
Runtime (ms)
clique
McSplit
McSplit↓
VBS

Results (88%)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clique
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Other Accomplishments

- Identified important features:
  - labelling percentage, standard deviation of degrees
- Discovered how algorithms' performance changes with fewer labels
- Extended $k\downarrow$ to support vertex labels
  - using neighbourhood degree sequences
- Defined and developed new algorithms capable of switching between McSplit and the clique encoding