Maximum Common Subgraph

Algorithms and Algorithm Portfolios

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Outline

Maximum Common Subgraph

Definition

A *maximum common (induced) subgraph* between graphs G_1 and G_2 is a graph G_3 such that $G_3 = (V_3, E_3)$ is isomorphic to induced subgraphs of both G_1 and G_2 with $|V_3|$ maximised.

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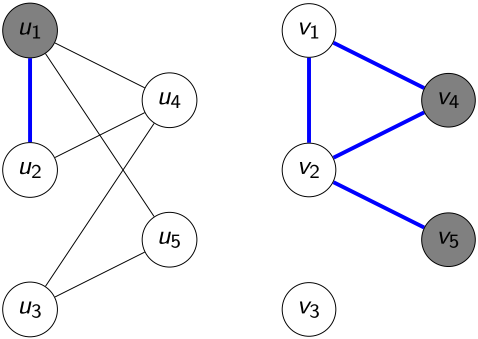

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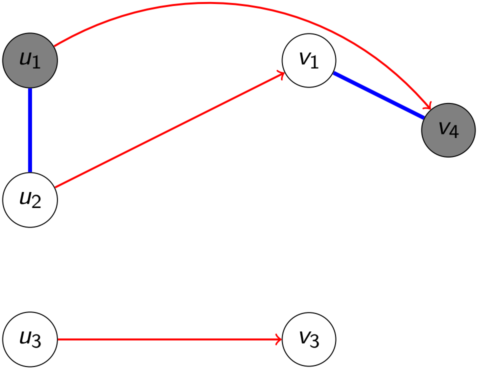
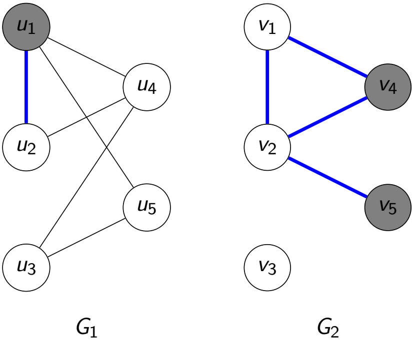


Algorithms

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

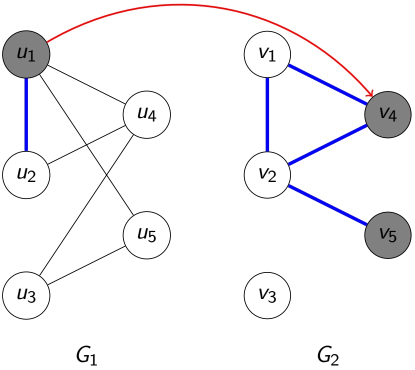
McSplit: a Branch and Bound Algorithm



Partial solution:
Upper bound: 4

Label	G_1	G_2
0	u_2, u_3, u_4, u_5	v_1, v_2, v_3
1	u_1	v_4, v_5

McSplit: a Branch and Bound Algorithm



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Decision: $u_1 \mapsto v_4$

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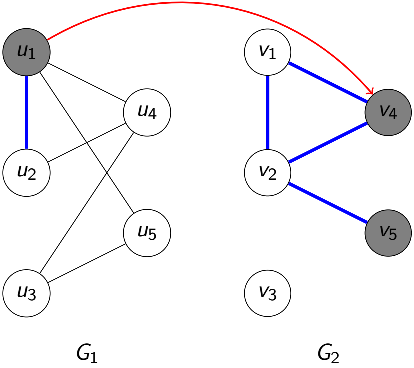
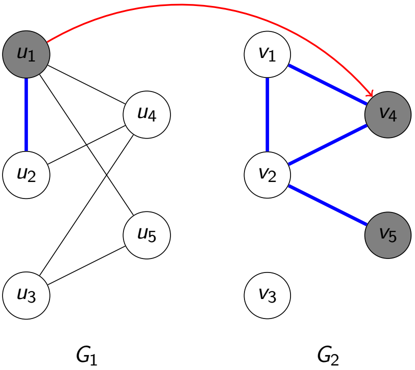


Partial solution:
Upper bound: 4

Label	G_1	G_2
00	u_3	v_3
01	u_4, u_5	$\emptyset$
02	u_2	v_1, v_2
10	$\emptyset$	v_5

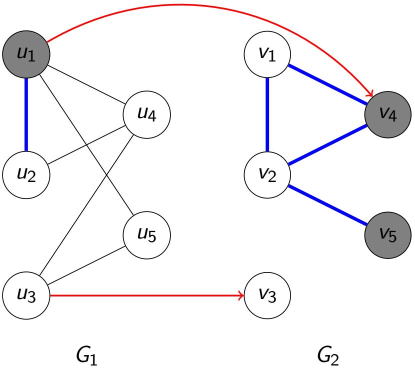
McSplit: a Branch and Bound Algorithm



Partial solution: $u_1 \mapsto v_4$
Upper bound: $1 + 2$

Label	G_1	G_2
00	u_3	v_3
01	u_2	v_1, v_2

McSplit: a Branch and Bound Algorithm



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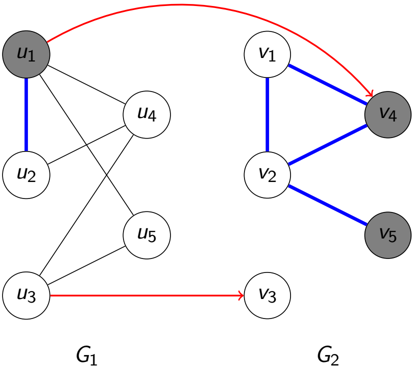
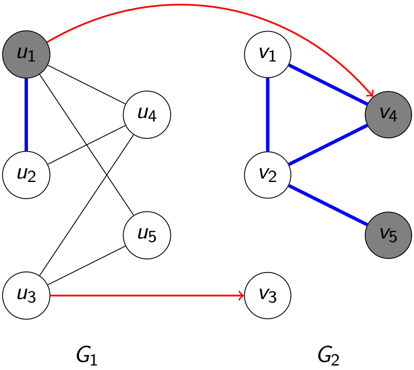


Partial solution: $u_1 \mapsto v_4$
Upper bound: $1 + 2$

Label	G_1	G_2
010	u_2	v_1, v_2
011	u_4, u_5	$\emptyset$

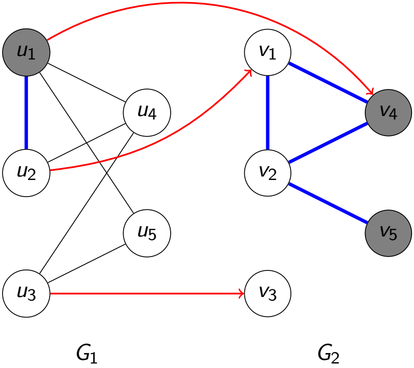
McSplit: a Branch and Bound Algorithm



Partial solution: $u_1 \mapsto v_4$, $u_3 \mapsto v_3$
Upper bound: $2 + 1$

Label	G_1	G_2
010	u_2	v_1, v_2

McSplit: a Branch and Bound Algorithm



Partial solution: $u_1 \mapsto v_4,\ u_3 \mapsto v_3$
Upper bound: $2 + 1$

Label	G_1	G_2
010	u_2	v_1, v_2

Decision: $u_2 \mapsto v_1$
Found a solution!
Backtrack to confirm optimality

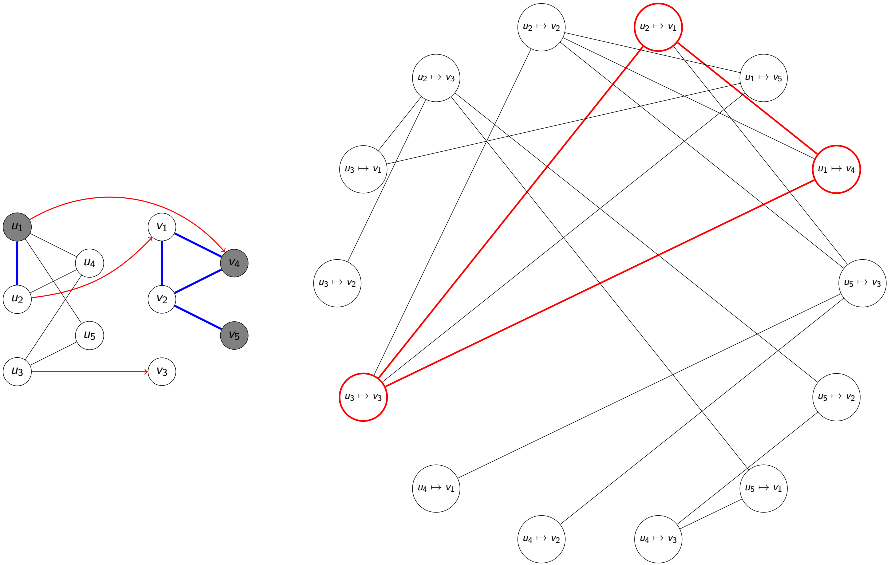
$k\downarrow$

- $k = 0$: search for a complete subgraph isomorphism
- $k = 1$: allow one vertex of the smaller graph to not match anything
- ... and so on
- Developed to handle large instances
- Implements many domain filtering techniques

McSplit↓

- TODO

Clique Encoding



(Per-Instance) Algorithm Selection

Definition (Bischl et al. 2016)

Given a set $\mathcal{I}$ of problem instances, a space of algorithms $\mathcal{A}$, and a performance measure $m \colon \mathcal{I} \times \mathcal{A} \to \mathbb{R}$, the *algorithm selection problem* is to find a mapping $s \colon \mathcal{I} \to \mathcal{A}$ that optimises $\mathbb{E}[m(i, s(i))]$.

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$$(G_1, G_2) \longrightarrow \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}$$

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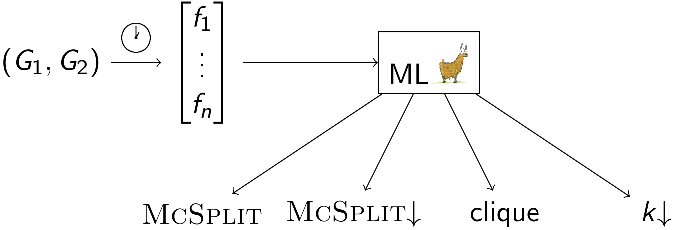

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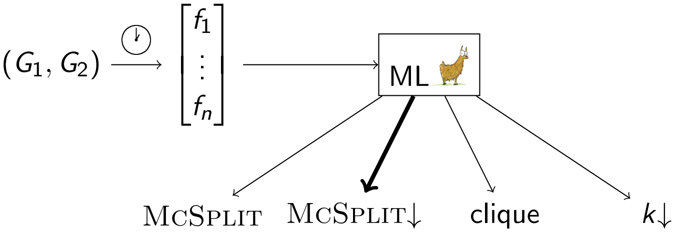

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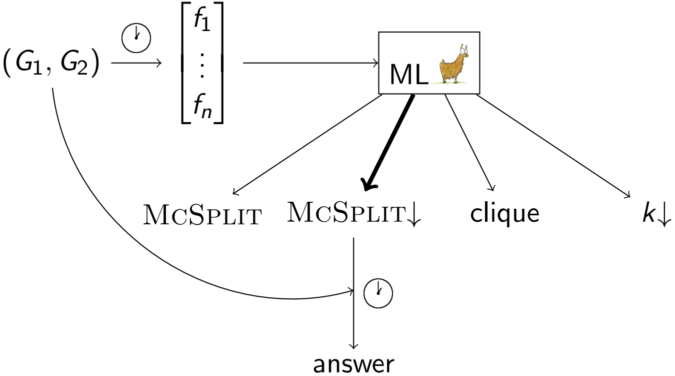

Labelling

Data from Foggia, Sansone and Vento 2001; Santo et al. 2003 (81400 pairs of graphs)

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A graph $G = (V, E, \mu)$ is said to have a *p% (vertex) labelling* if

$$N = \max\left\{2^n : n \in \mathbb{N},\, 2^n < \left\lfloor \frac{p}{100\%} \times |V| \right\rfloor\right\}.$$

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- Typical values explored: 33%, 50%, 75%

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- In my data: 5%, 10%, 15%, 20%, 25%, 33%, 50%

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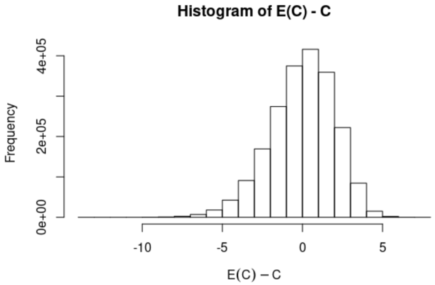
- Typical values explored: 33%, 50%, 75%
- In my data: 5%, 10%, 15%, 20%, 25%, 33%, 50%
- 3 subproblems
  - no labels
  - vertex labels
  - vertex and edge labels

The Number of Vertices Per Label



For each graph and label

- C is the number of vertices with that label
- $\mathrm{E}(C)$ is the number we would expect from a (discrete) uniform distribution

Features (34 in total)

1–8 are from Kotthoff, McCreesh and Solnon 2016

1. number of vertices
2. number of edges
3. mean/max degree
4. density
5. mean/max distance between pairs of vertices
6. number of loops
7. proportion of vertex pairs with distance $\geq 2, 3, 4$
8. connectedness

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9. standard deviation of degrees
10. labelling percentage

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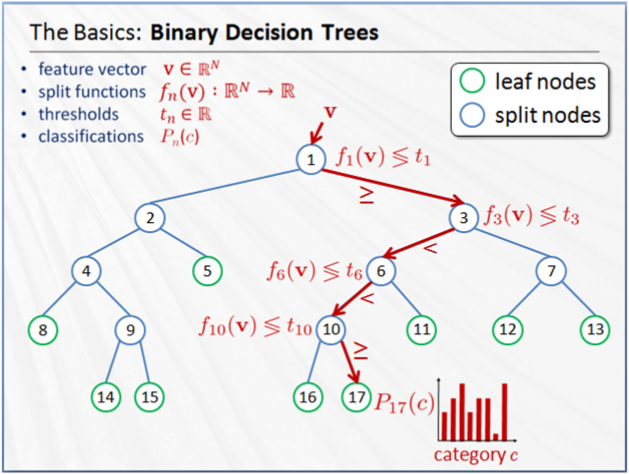
9. standard deviation of degrees
10. labelling percentage
11. ratios of features 1–5

Random Forests (Breiman 2001)



Source: Tae-Kyun Kim & Bjorn Stenger, Intelligent Systems and Networks (ISN) Research Group, Imperial College London

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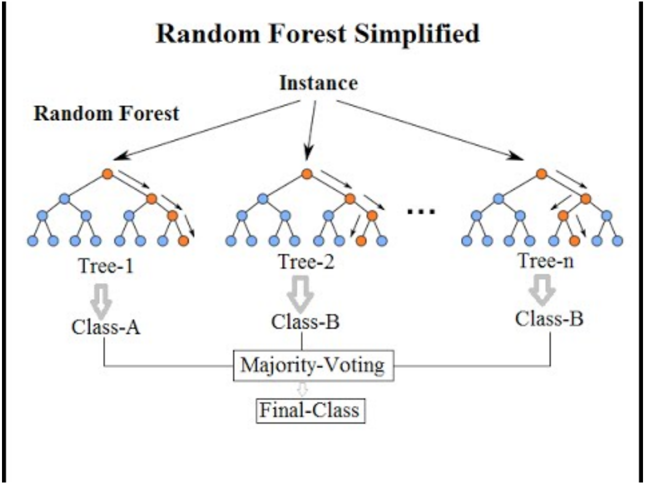
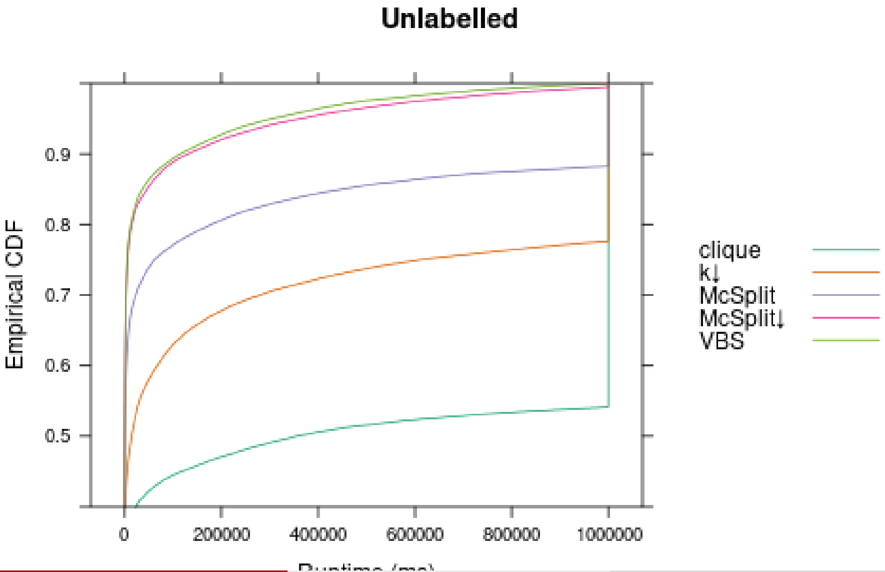
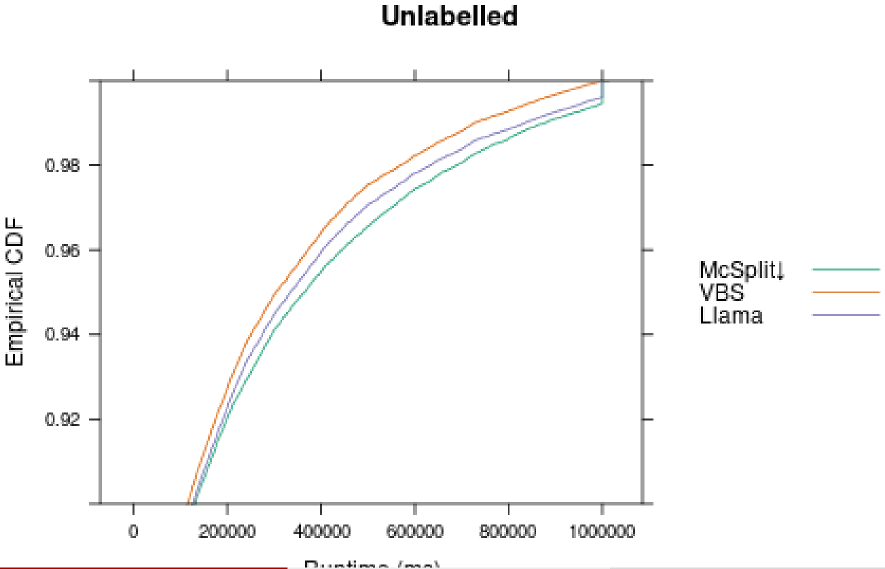


Source: Random Forests(r), Explained, Ilan Reinstein, KDnuggets

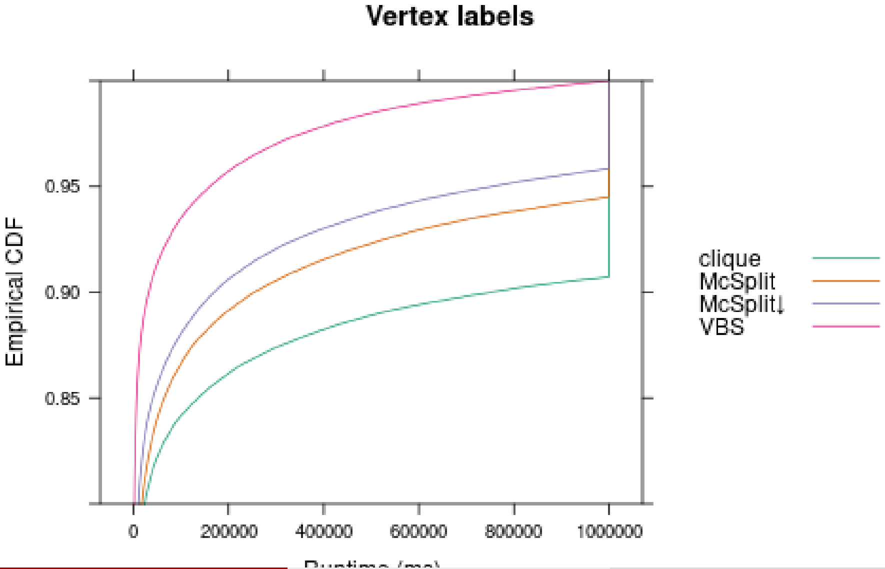
Results


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

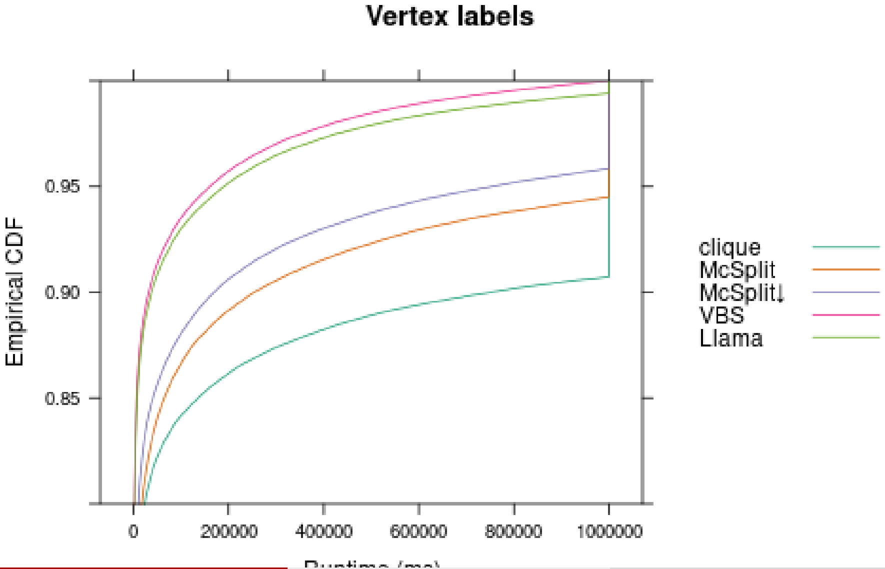
Results (27%)


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

Results


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

Results (86%)


Vertex labels
Empirical CDF
0.85
0.90
0.95
0
200000
400000
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800000
1000000
clique
McSplit
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VBS
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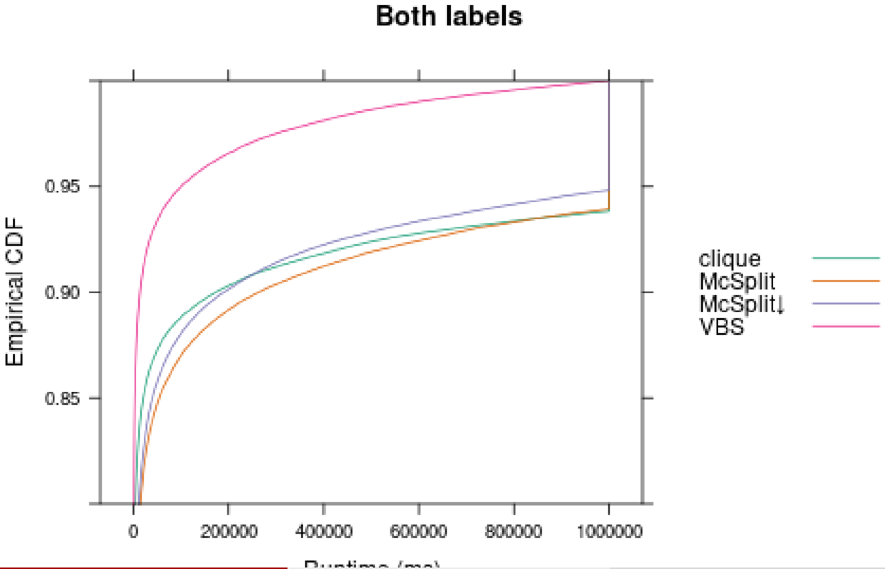
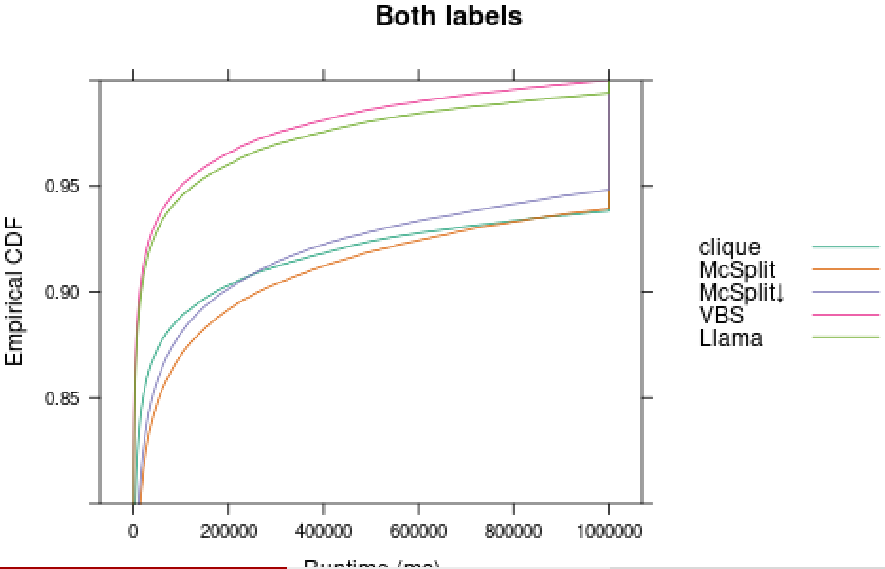
Results


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

Results (88%)


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

Errors

- Out-of-bag error
- For each algorithm
  - $1 -$ recall

Definition

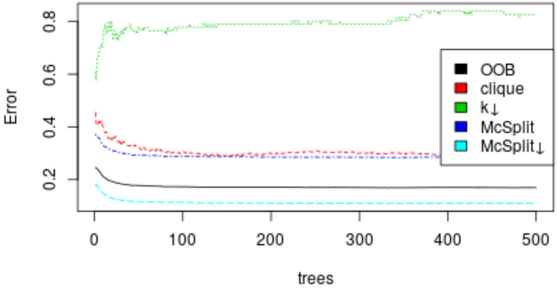
For an algorithm A, *recall* (sensitivity) is

$$\frac{\text{the number of instances that were correctly predicted as } A}{\text{the number of instances where } A \text{ is the correct prediction}}.$$

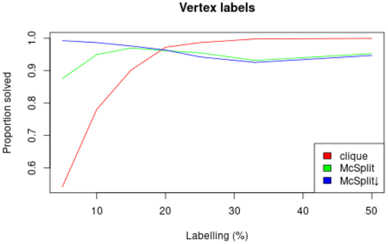
Errors (%)

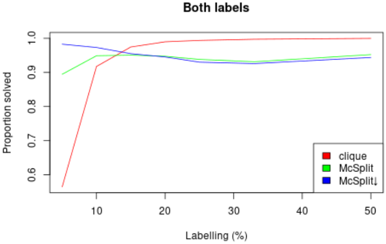
Error	Labelling		
	no	vertex	both
out-of-bag	17	13	14
clique	30	8	7
McSplit	29	22	29
McSplit $\downarrow$	11	11	11
$k \downarrow$	80		

Convergence of Errors for Unlabelled Graphs



What Happens When Labelling Changes?





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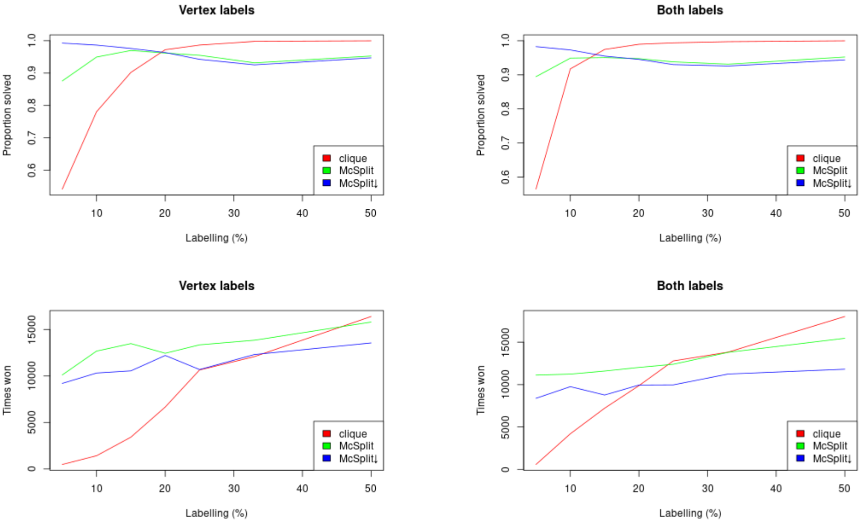

Idea 1: Switch After Making d Decisions

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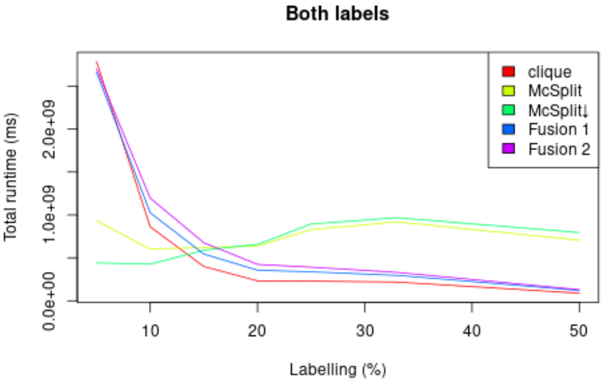
- Vertices of the association graph can be constructed from McSplit label classes, edges from the original input graphs
- Only a few extra lines of code:

$$|incumbent_{\mathsf{clique}}| \leftarrow |incumbent_{\textsc{McSplit}}| - |M|$$

and then

$$incumbent_{\textsc{McSplit}} \leftarrow incumbent_{\textsc{McSplit}} \cup incumbent_{\mathsf{clique}}$$

Not That Good...



Idea 2: Map Partially Solved Instances to Unsolved Instances

- ...