Algorithm Selection for Maximum Common Subgraph

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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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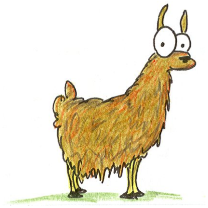
LLAMA (Kotthoff 2013)



Algorithms

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

Labelling

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

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- 3 subproblems
  - no labels
  - vertex labels
  - vertex and edge labels

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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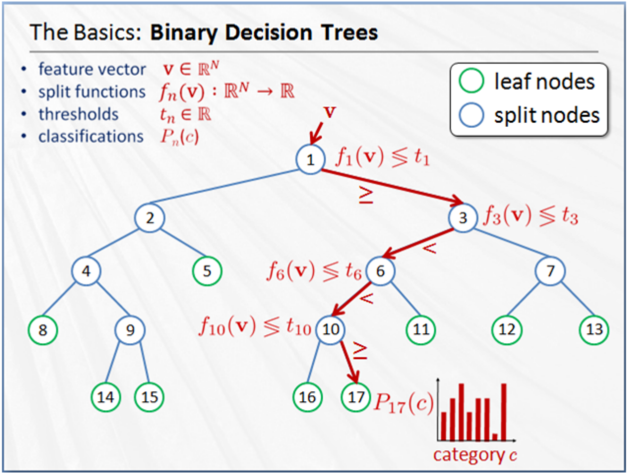
11. ratios of features 1–5

Random forests (Breiman 2001)



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

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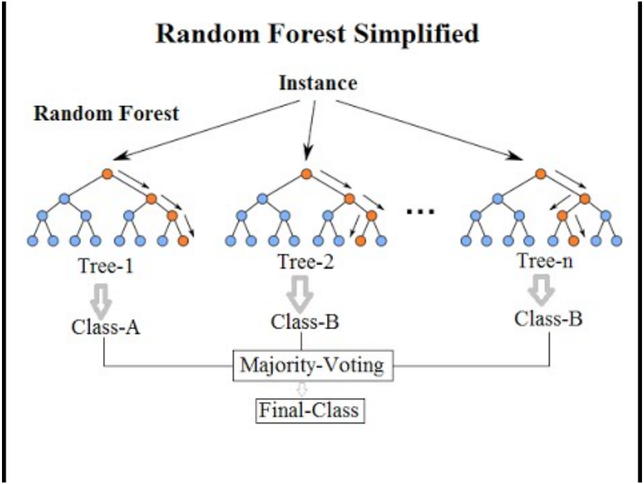
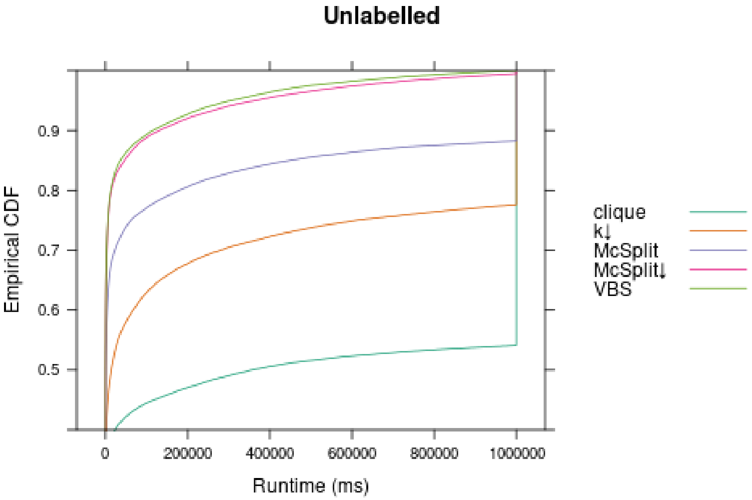
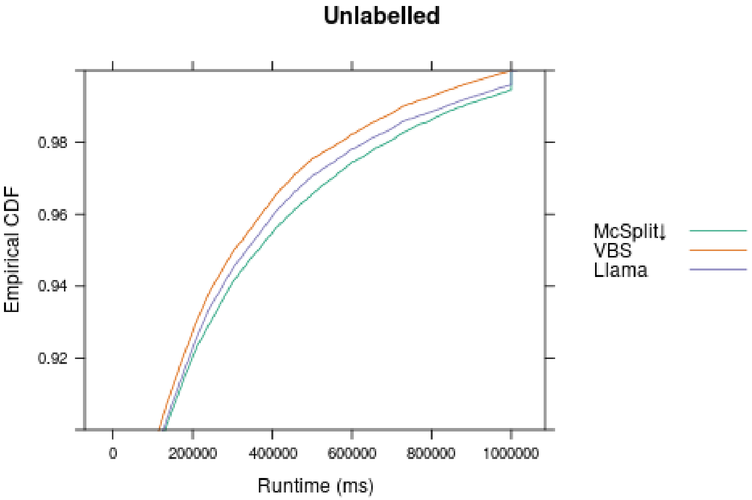


Source: Random Forests(r), Explained, Ilan Reinstein, KDnuggets

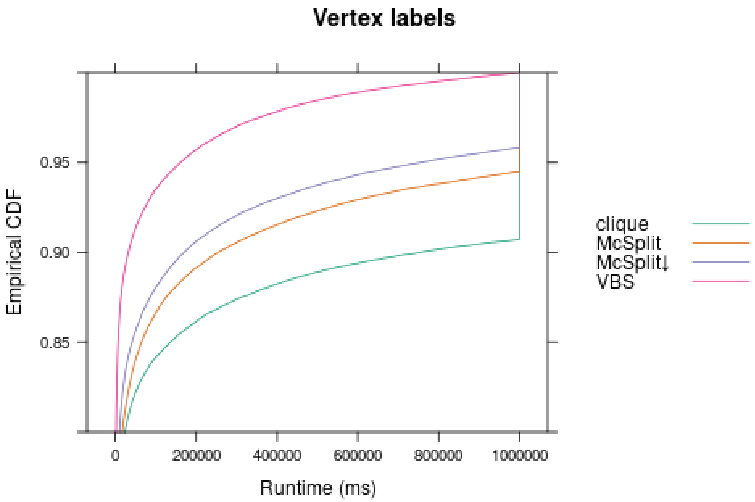
Results


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

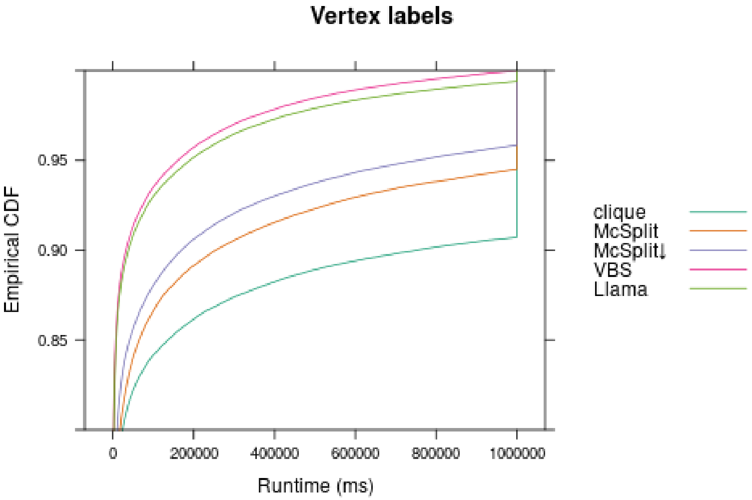
Results (27%)


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

Results


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

Results (86%)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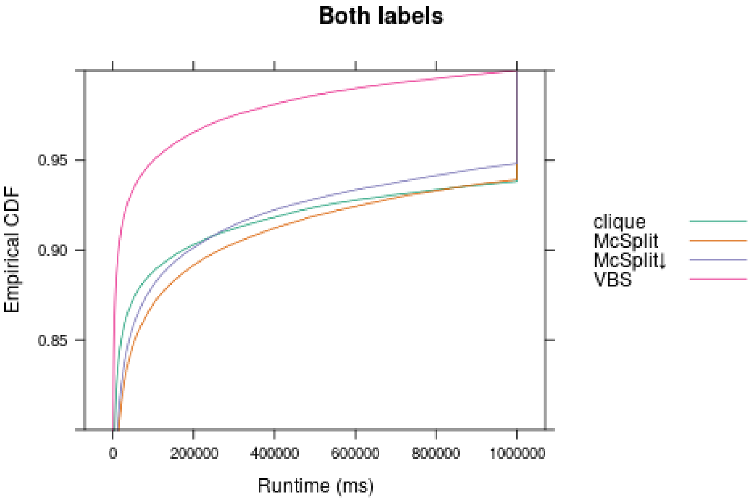
Both labels
Empirical CDF
0.85
0.90
0.95
Runtime (ms)
0
200000
400000
600000
800000
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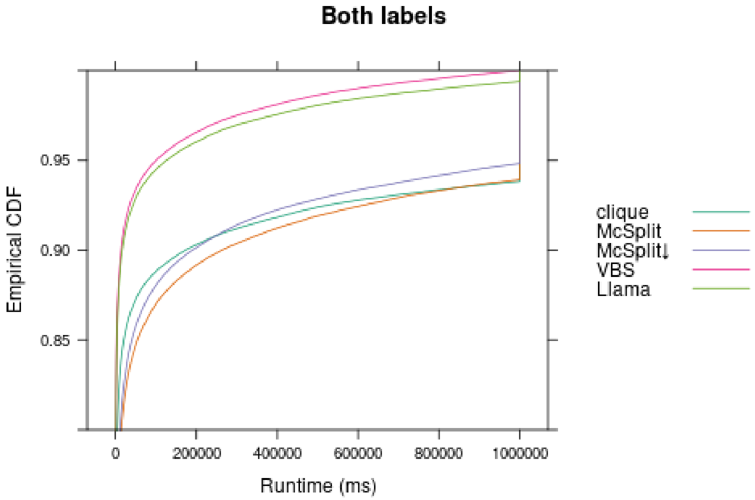
clique
McSplit
McSplit↓
VBS

Results (88%)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Errors

- Out-of-bag error
- For each algorithm
  - $1 - \text{recall}$

Definition

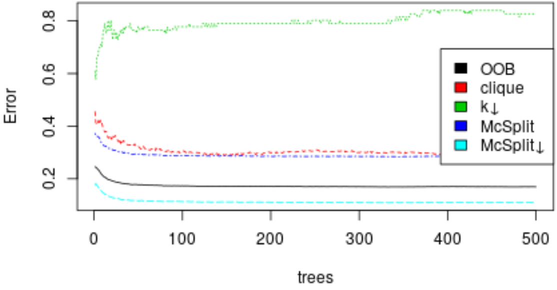
For an algorithm A, *recall* (sensitivity) is

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

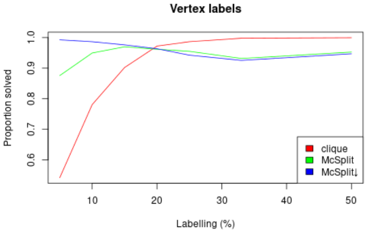
Errors (%)

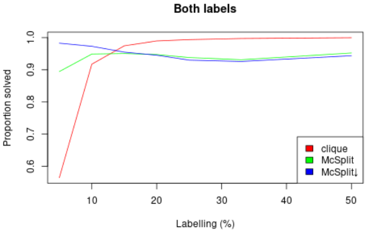
Error	Labelling: no	vertex	both
out-of-bag	17	13	14
clique	30	8	7
McSplit	29	22	29
McSplit $\downarrow$	11	11	11
$k \downarrow$	80		

Convergence of errors for unlabelled graphs



What happens when labelling changes?





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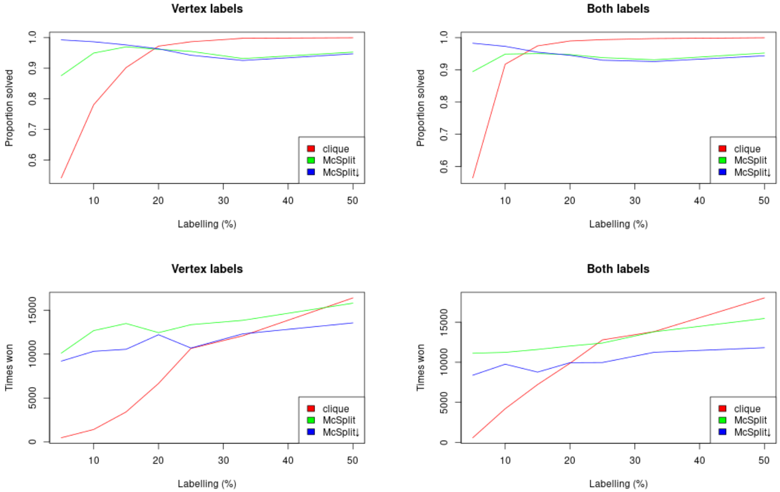

Future work

- Relationships between clique algorithm's performance and properties of the association graph
- How the association graph changes after making a decision
- Can $k \downarrow$ and clique work together?