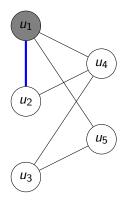
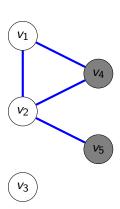
Algorithm Selection for Maximum Common Subgraph

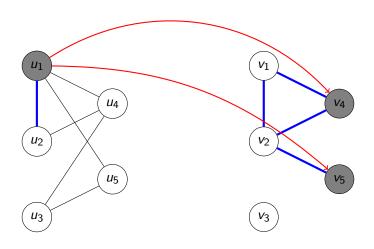
Paulius Dilkas

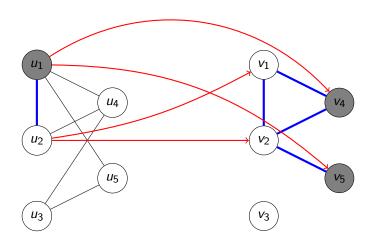
School of Computing Science University of Glasgow

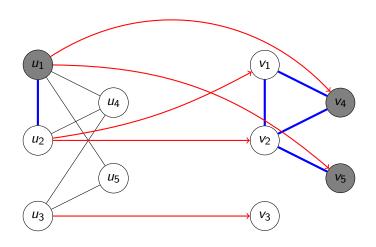
23rd March 2018

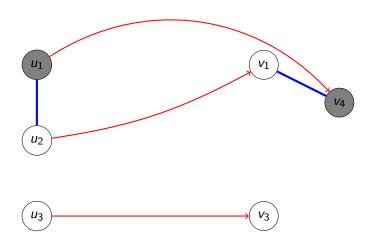


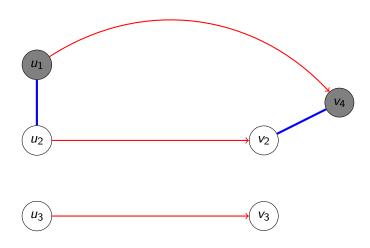


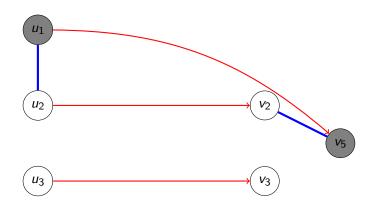












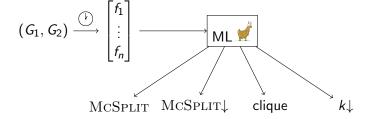
Algorithms

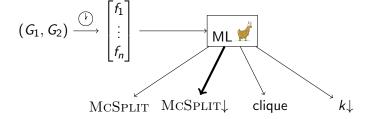
- ► McSplit, McSplit↓
 - ► McCreesh, Prosser and Trimble 2017
- clique encoding
 - ▶ McCreesh, Ndiaye et al. 2016
- ▶ k↓
 - ► Hoffmann, McCreesh and Reilly 2017

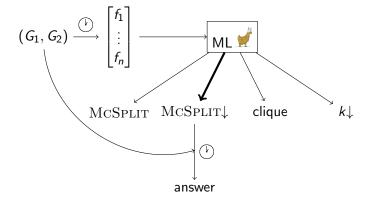
 (G_1, G_2)

$$(G_1, G_2) \xrightarrow{\text{(i)}} \begin{bmatrix} f_1 \\ \vdots \\ f_n \end{bmatrix}$$

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







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

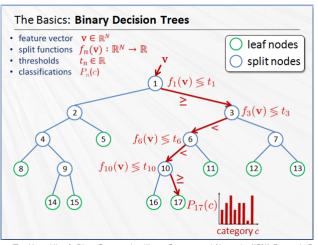
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 - 9. standard deviation of degrees
- 10. labelling percentage

Features (34 in total)

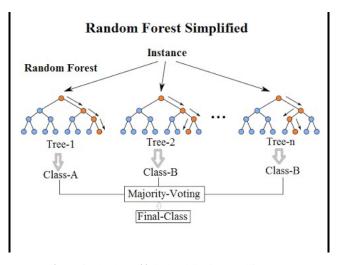
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 - 8. connectedness
 - 9. standard deviation of degrees
- 10. labelling percentage
- 11. ratios of features 1-5

Random forests (Breiman 2001)



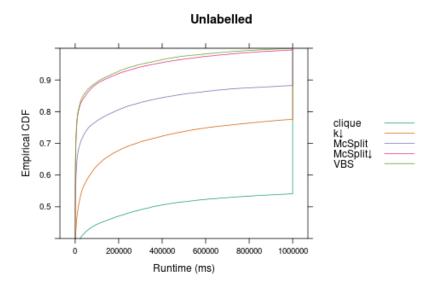
Source: Tae-Kyun Kim & Bjorn Stenger, Intelligent Systems and Networks (ISN) Research Group, Imperial College London

Random forests (Breiman 2001)

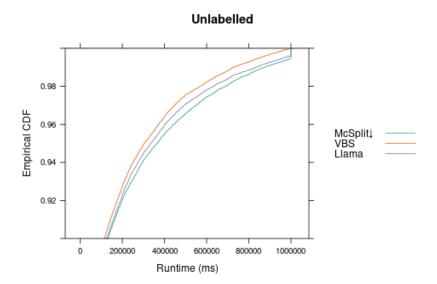


Source: Random Forests(r), Explained, Ilan Reinstein, KDnuggets

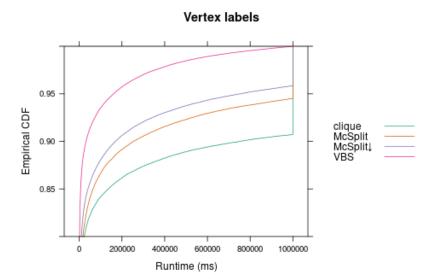
Results



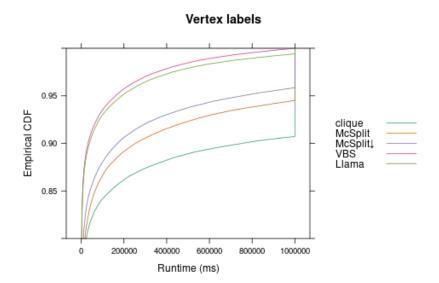
Results (27%)



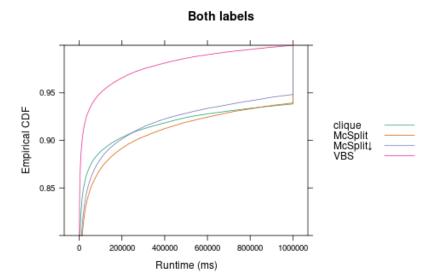
Results



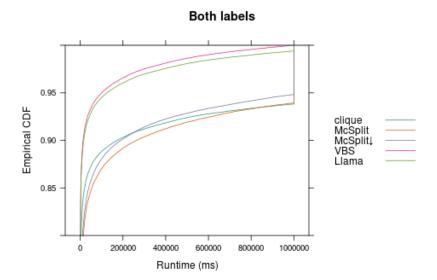
Results (86%)

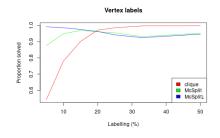


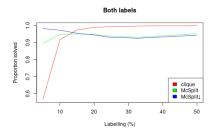
Results

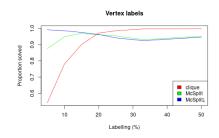


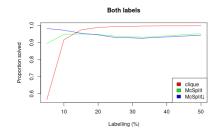
Results (88%)

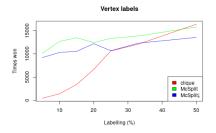


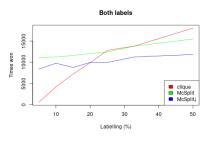












Other Accomplishments

- Identified important features:
 - ► labelling, standard deviation of degrees
- ▶ Extended $k \downarrow$ to support vertex labels
 - using neighbourhood degree sequences
- ightharpoonup Defined and developed new algorithms capable of switching between $\operatorname{McSplit}$ and the clique encoding