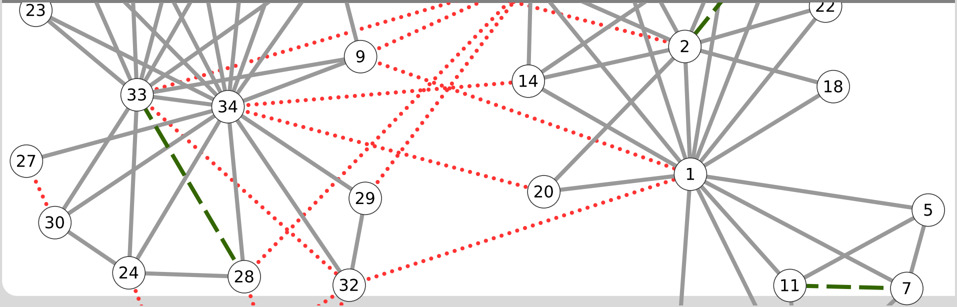
Karlsruhe Institute of Technology

Engineering Exact Quasi-Threshold Editing

Lars Gottesbüren, **Michael Hamann**, Philipp Schoch, Ben Strasser, Dorothea Wagner and Sven Zühlsdorf | June 2020

KARLSRUHE INSTITUTE OF TECHNOLOGY – INSTITUTE OF THEORETICAL INFORMATICS – GROUP ALGORITHMICS I



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Quasi-Threshold Graphs

- Trivially perfect graphs

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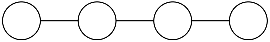
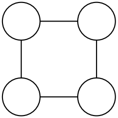
- No P_4 or C_4 as node-induced subgraph





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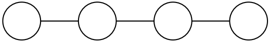

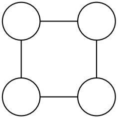

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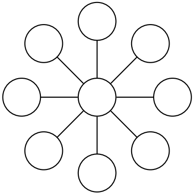

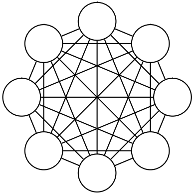

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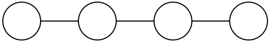

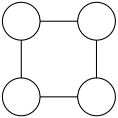

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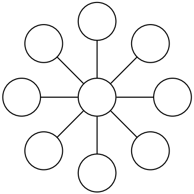

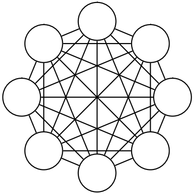

- Certifying recognition in linear time. [Chu08, BHSW15]

Why Quasi-Threshold Graphs?

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- Interesting graph class with natural definition

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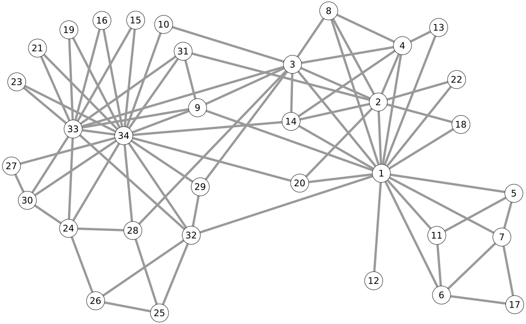

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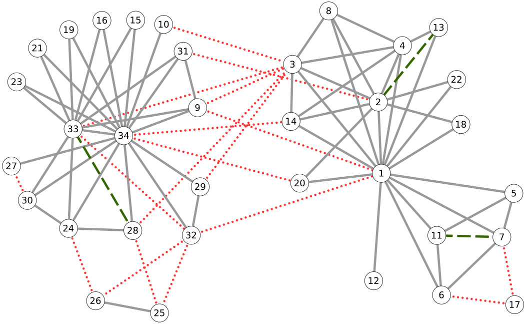

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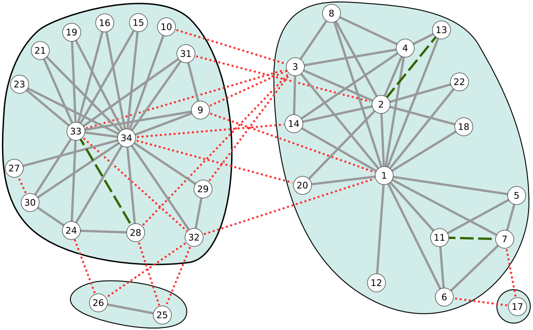

Quasi-Threshold Editing

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Quasi-Threshold Editing Problem

Given a graph G find a quasi-threshold graph with minimum edge editing (insertion + deletion) distance to G.

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- Is NP-hard [NG13]
- Is FPT $O\left(6^k\,(|V| + |E|)\right)$ [Cai96]
- Polynomial kernel exists ($O\left(k^7\right)$ vertices) [DP17]
- Heuristics exist [NG13, BHSW15]

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Our contribution:

- Exact algorithms – evaluation of heuristics and exact solutions
- Improved branch-and-bound FPT algorithm and ILP
- For forbidden subgraphs $\mathcal{F}$
- Experimental evaluation for $\{P_4, C_4\}$

Example: P_3-free, $k = 3$

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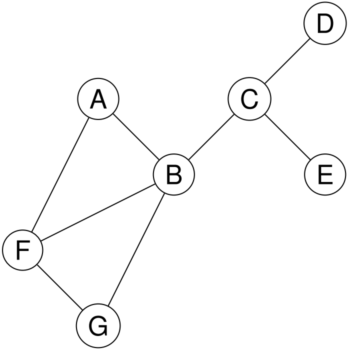
G



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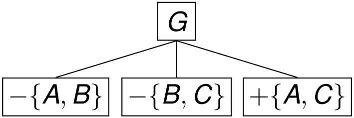

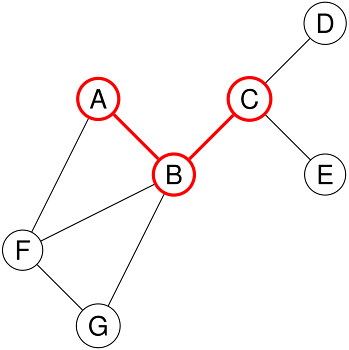

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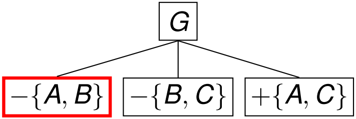

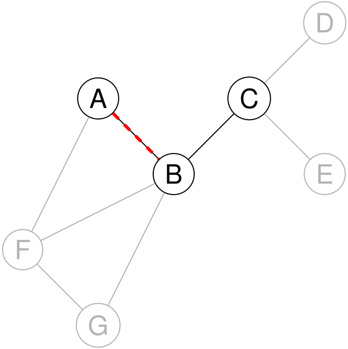

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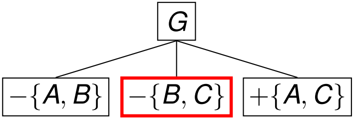

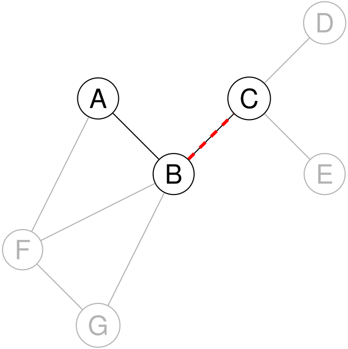

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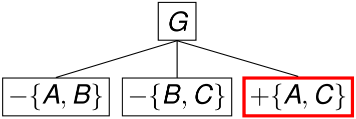

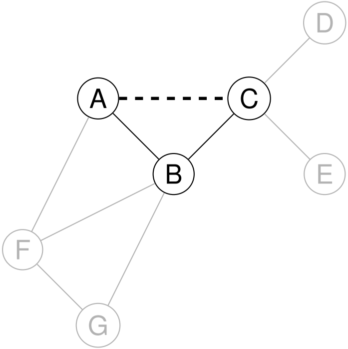

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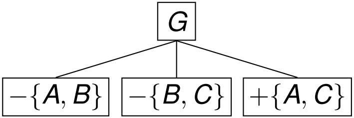

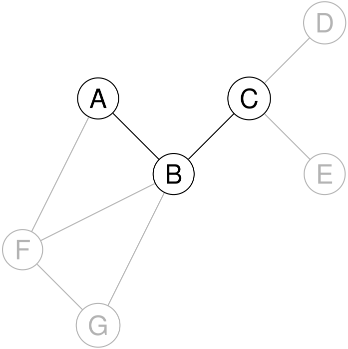

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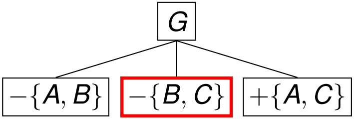

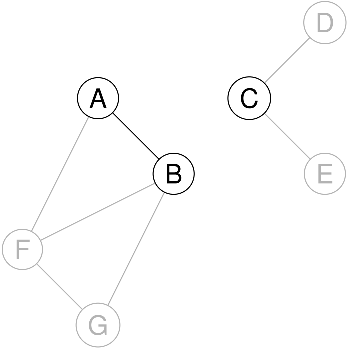

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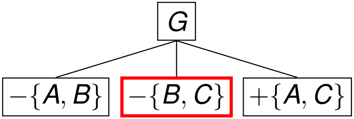

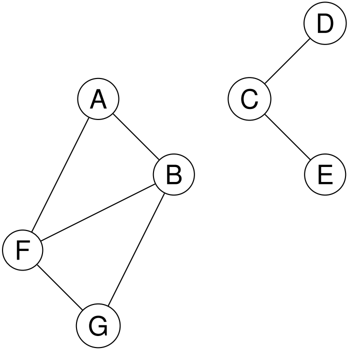

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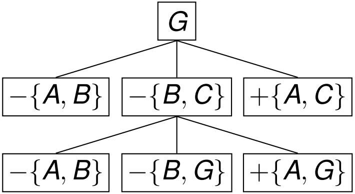

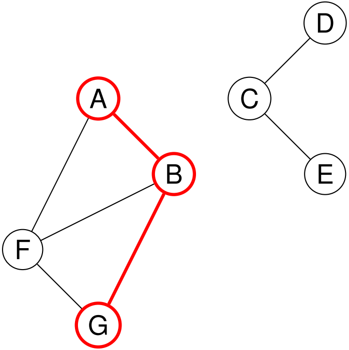

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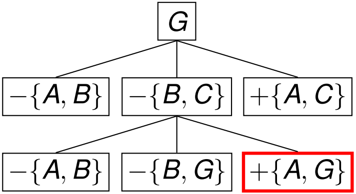

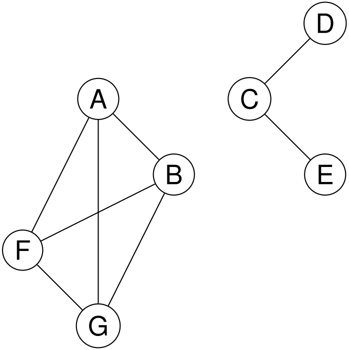

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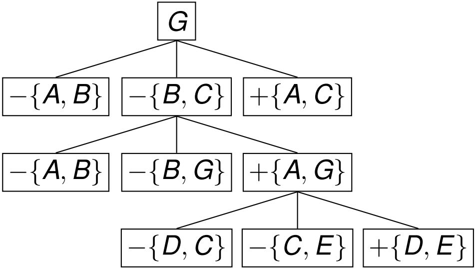

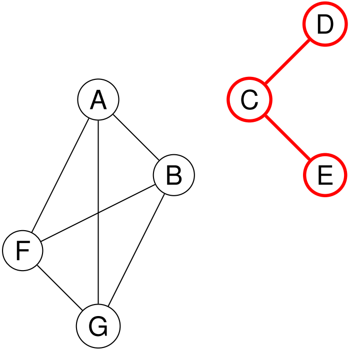

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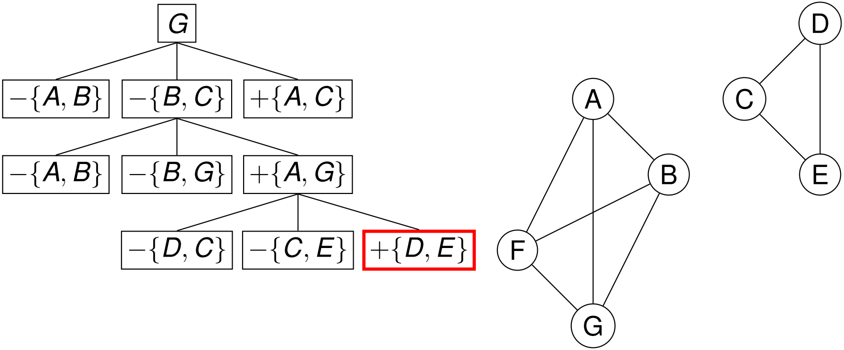

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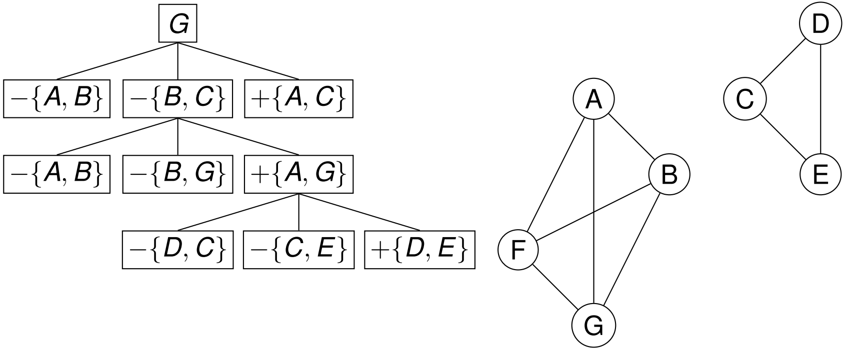

$\Rightarrow$ Found solution.

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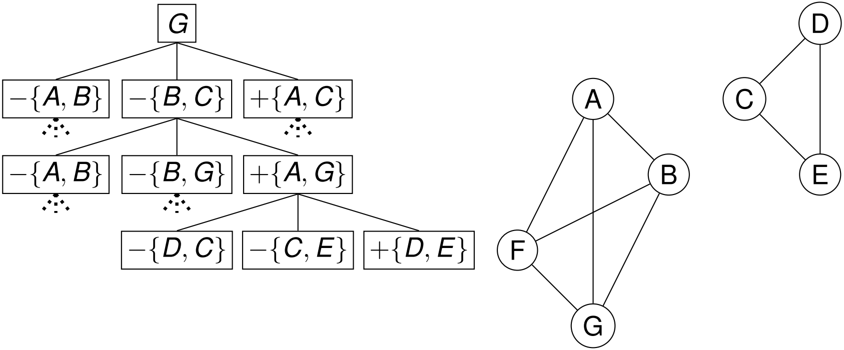

⇒ Found solution. If not: need to search the full tree.
If nothing found at level k: impossible with k edits.

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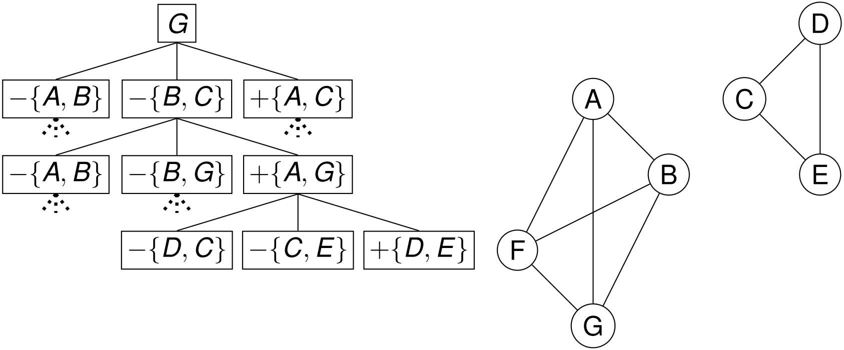

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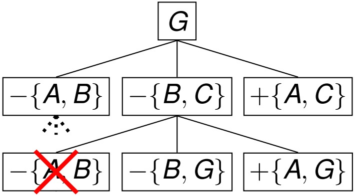
- Time $O(3^k \cdot \text{poly}(n))$
- Best known: $O(1.62^k + m + n)$ [Böc12]

Branch-and-Bound Algorithm

- Increasing values of k to find exact k
  - show impossibility with $k - 1$
  - show solution with k
- Blocking: avoid duplicate enumeration [Dam08]
- Bounding: limit explored branches.



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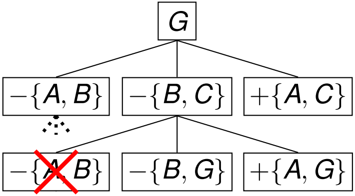
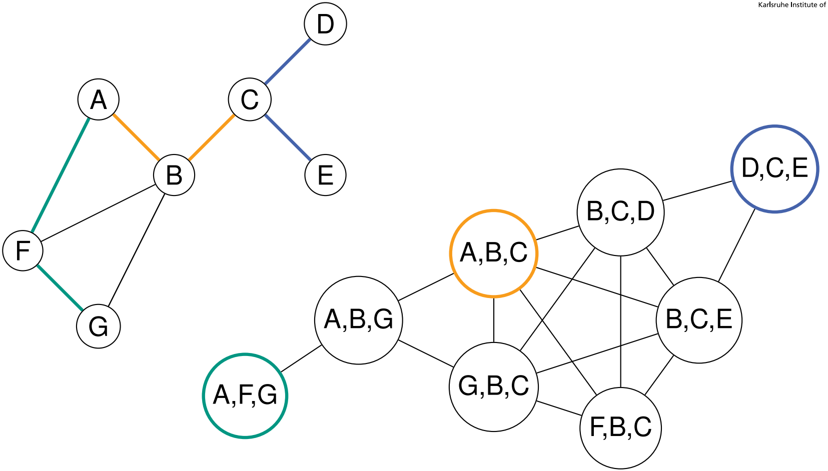


Our contribution:

- Good lower bounds
- Heuristic for selecting subgraphs to branch on

Lower Bound



- Implicit conflict graph representation
- Use two-improvements and plateau search
- Incremental updates, exploit blocked edges

[ARW12]

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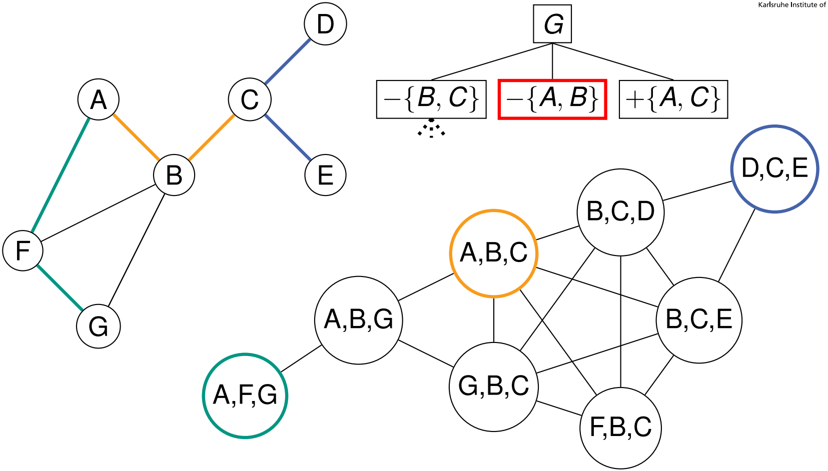

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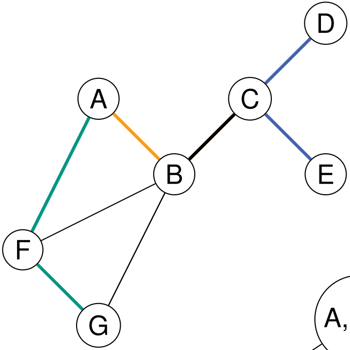

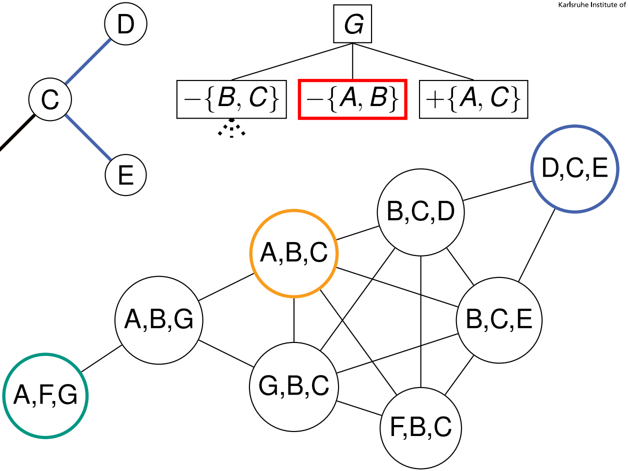

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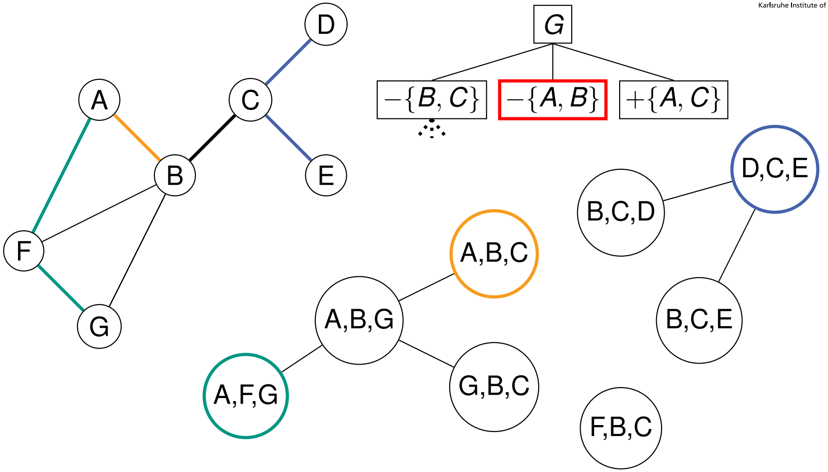

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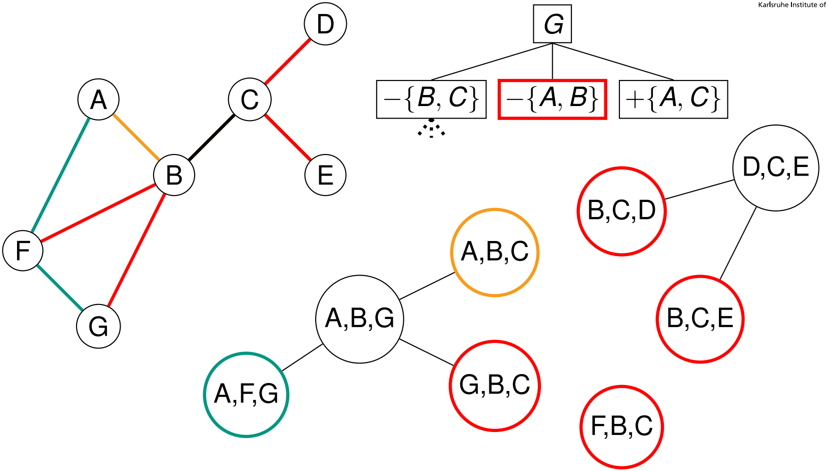

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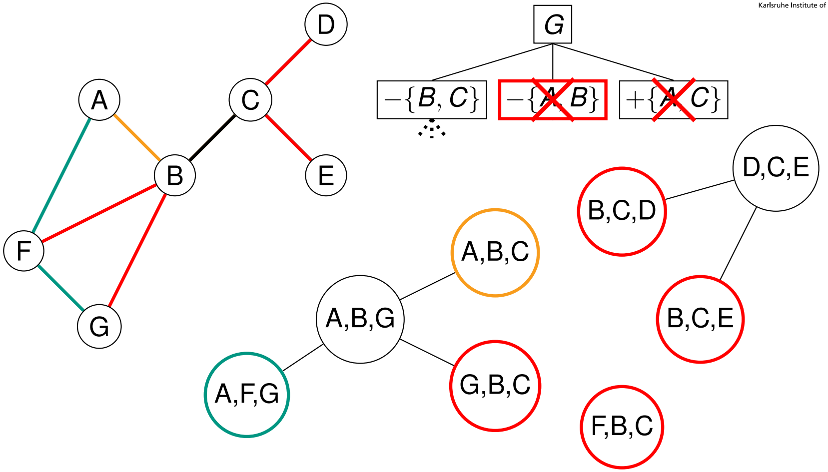

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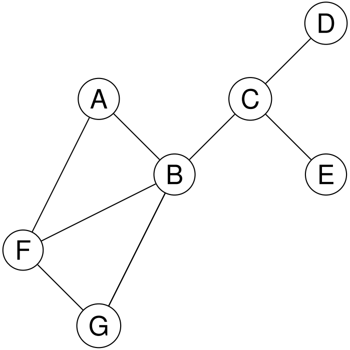
[ARW12]

Optimizing Branching Decisions

- Prune early: even before recursion
- First node pair = most likely edited node pair in **all** solutions



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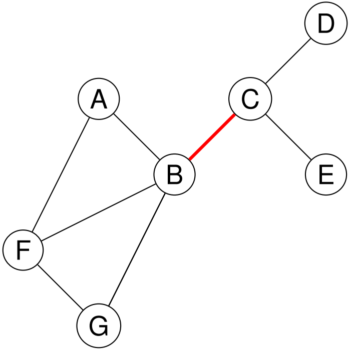
Idea: Prefer node pairs that are part of many forbidden subgraphs



Integer Linear Programming

- Binary variables $X_{uv} \forall u, v \in V_G$
- $X_{uv} = 1 \iff$ edge $\{u, v\}$ exists

$$\text{minimize} \sum_{\{u,v\} \in E_G} (1 - x_{uv}) + \sum_{\{u,v\} \in \overline{E_G}} x_{uv}$$

$$\text{subject to} \sum_{\{u,v\} \in E_H} (1 - x_{\pi(u)\pi(v)}) + \sum_{\{u,v\} \in \overline{E_H}} x_{\pi(u)\pi(v)} \geq 1$$

$$\forall H \in \mathcal{F}, \forall \pi : V_H \hookrightarrow V_G$$

- Row generation
- LP relaxation is upper bound for lower bound

Experiments

Implementation:

- $\{P_4, C_4\}$-free editing
- Implemented in C++, parallelization using work stealing
- Gurobi for ILP
- `https://github.com/kit-algo/fpt-editing`

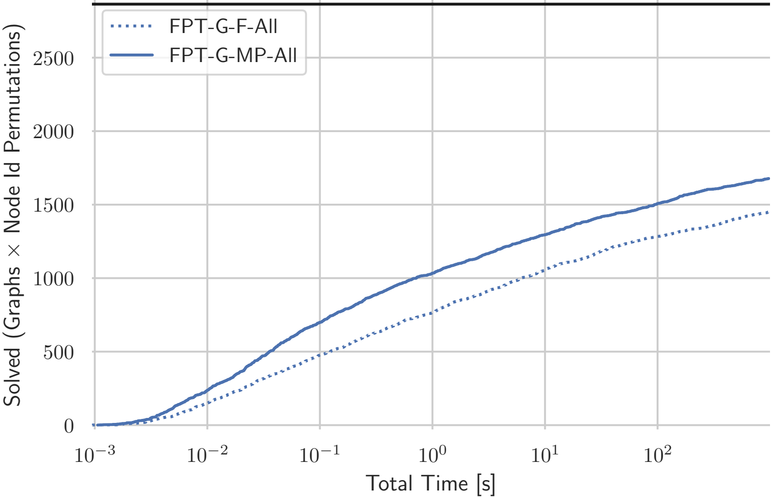
Data:

- 716 of 3964 connected components of COG protein similarity data – remaining need < 20 edits
- 4 node id permutations

Setup:

- $2 \cdot 8$ core Intel Xeon E5-2670 (Sandy Bridge), 64 GB RAM
- 1000 seconds time limit

FPT Running Time



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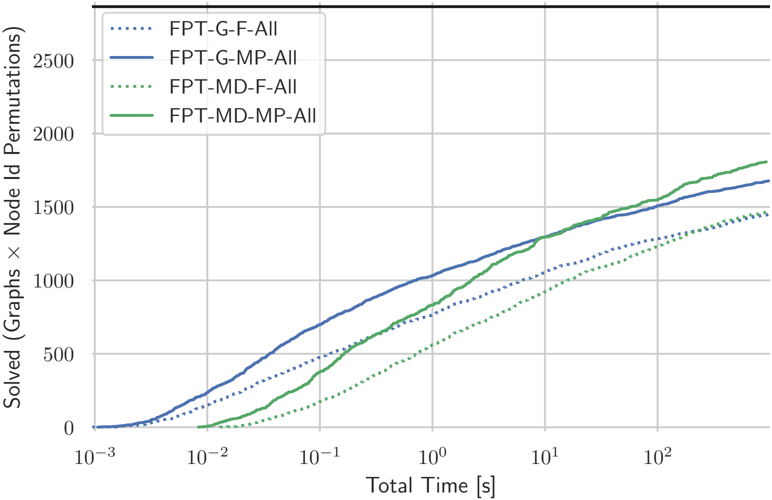

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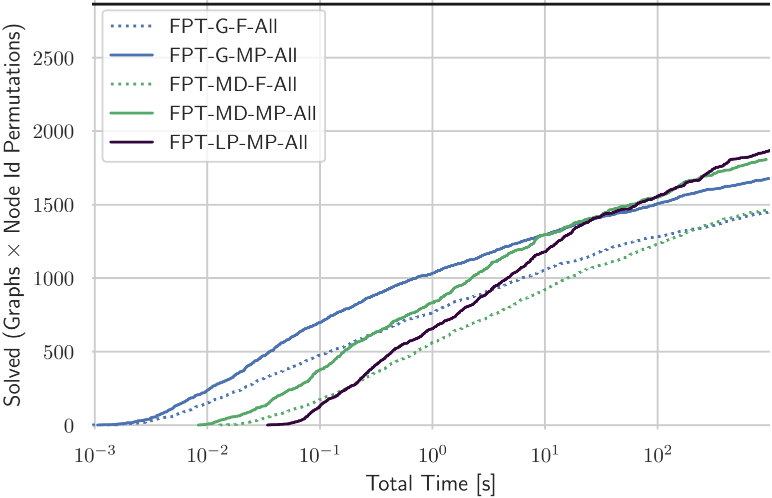

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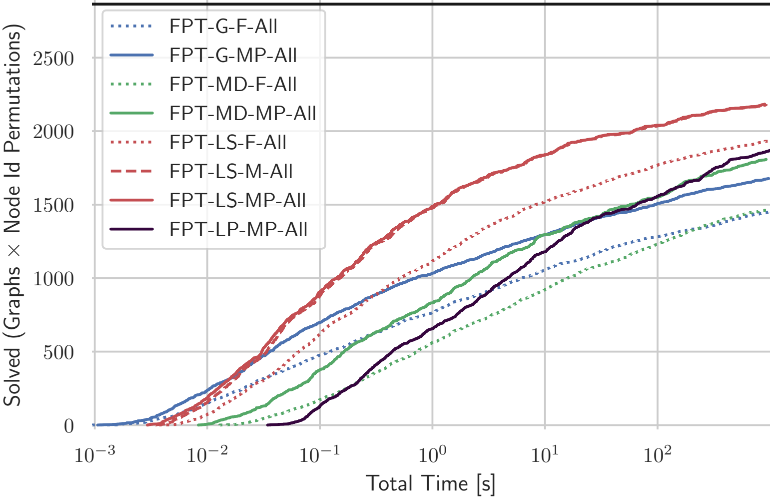
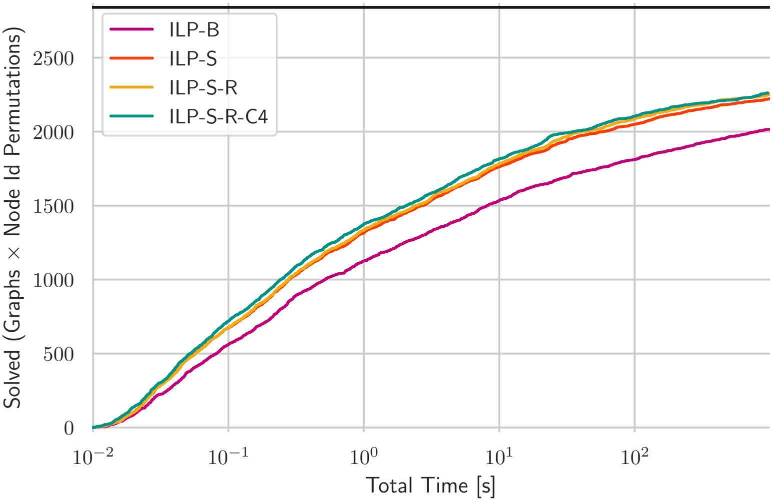
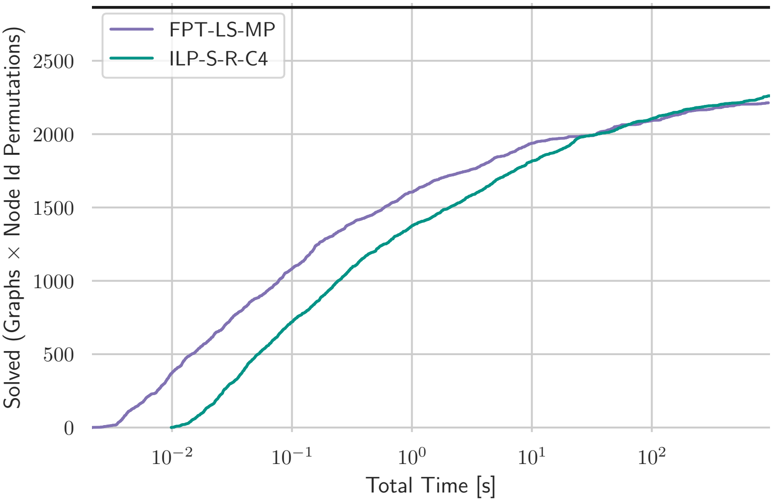


ILP Variants

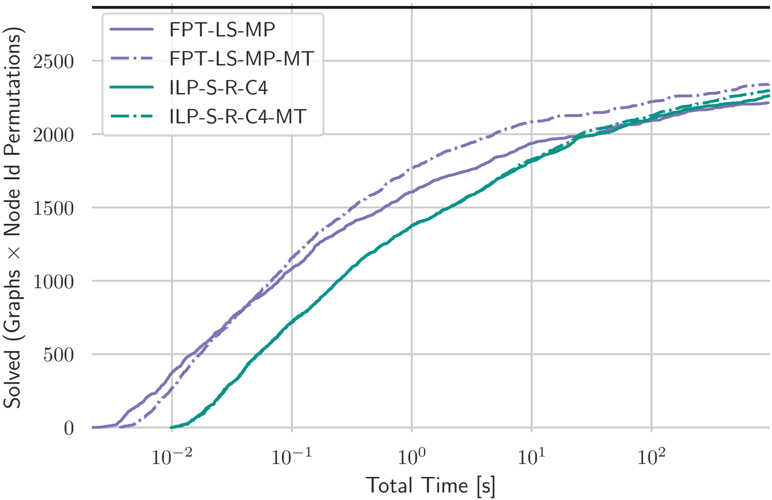


FPT vs. ILP

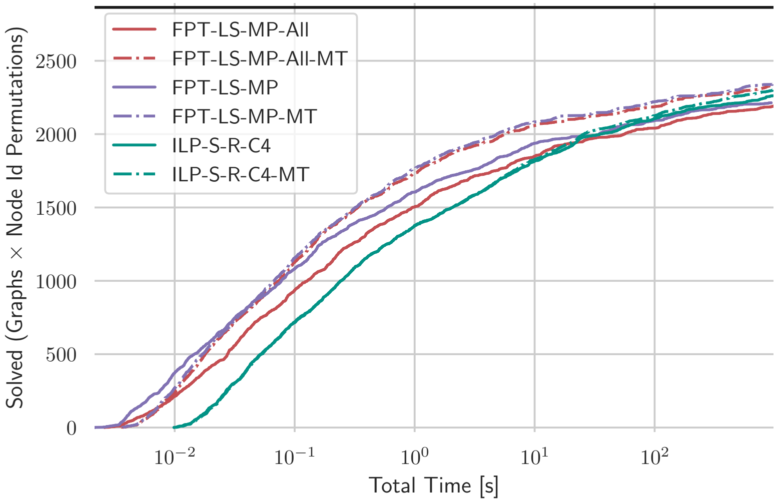


FPT-LS-MP
ILP-S-R-C4
Solved (Graphs × Node Id Permutations)
2500
2000
1500
1000
500
0
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
Total Time [s]

FPT vs. ILP

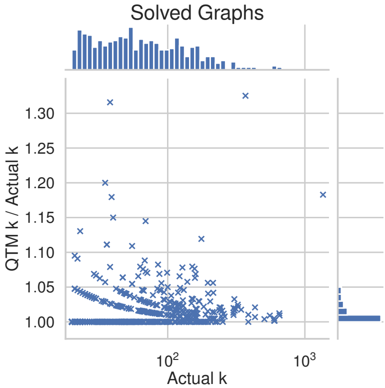

FPT-LS-MP
FPT-LS-MP-MT
ILP-S-R-C4
ILP-S-R-C4-MT
Solved (Graphs × Node Id Permutations)
0
500
1000
1500
2000
2500
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
Total Time [s]

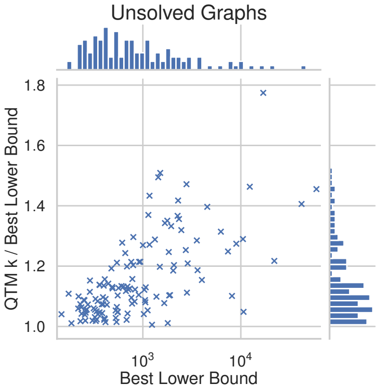
FPT vs. ILP



FPT-LS-MP-All
FPT-LS-MP-All-MT
FPT-LS-MP
FPT-LS-MP-MT
ILP-S-R-C4
ILP-S-R-C4-MT
Solved (Graphs × Node Id Permutations)
2500
2000
1500
1000
500
0
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
Total Time [s]

Comparison with QTM Heuristic





Not shown: Outlier at $k = 64$ where QTM needs 202 edits

Summary

- Carefully engineered branch and bound algorithm beats Gurobi

Future work:

- Adapt for edit costs
- Evaluate for other forbidden subgraphs

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Number of Solutions