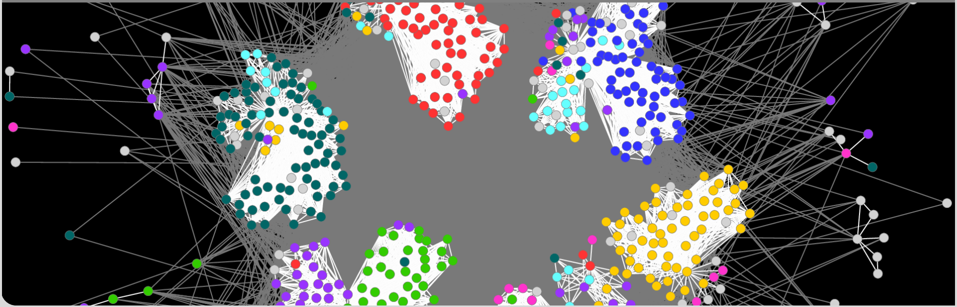
Graph Editing Problems and their Application in Graph Clustering

CALDAM Indo-German Pre-Conference School on Algorithms and Combinatorics

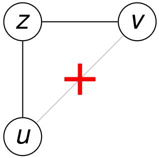
Dorothea Wagner | February 13-14, 2017

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

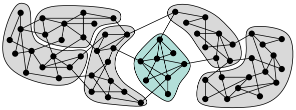


Overview

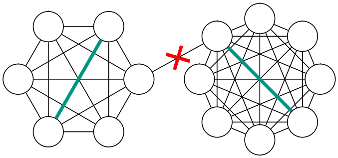
- Introduction to graph editing



- Introduction to graph clustering



- Cluster editing

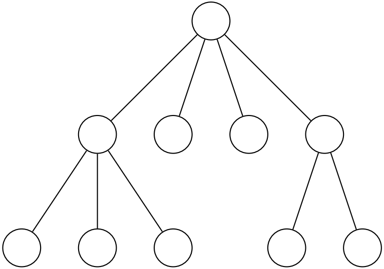


Graph Classes

Graph $\mathcal{G}$ is part of a graph class if it fulfills certain properties.

Examples:

- Trees
- Planar graphs
- Chordal graphs



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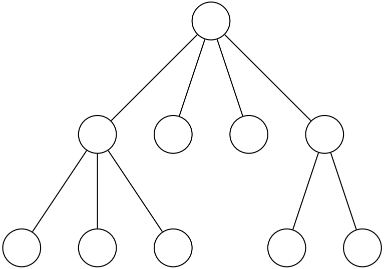

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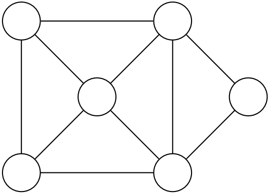

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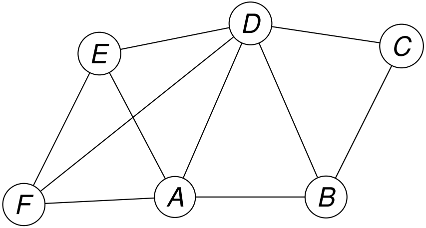

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Given a graph $\mathcal{G}$ – what is the smallest number of operations that need to be applied such that $\mathcal{G}$ is part of a graph class $\mathcal{H}$?

Possible operations:

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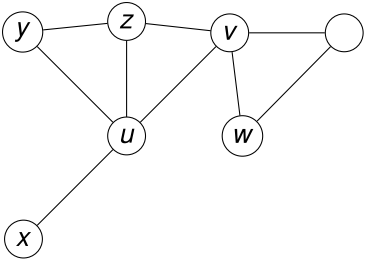

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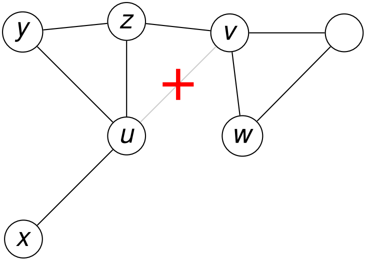

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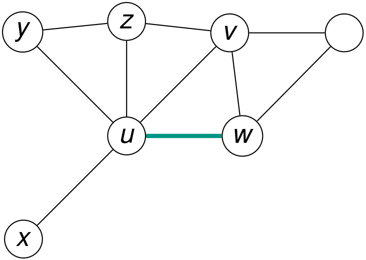

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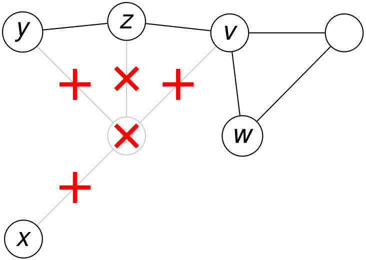

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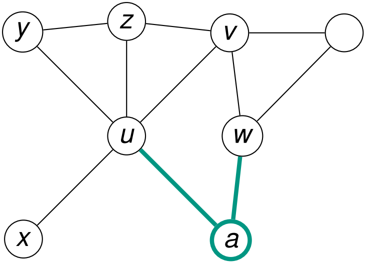

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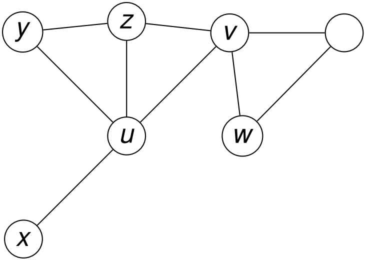


Can assign costs to operations – minimize sum of costs.

Example: Spanning Forest

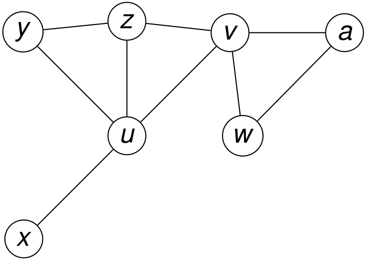
Spanning Forest

Given a graph $G = (V, E)$, find a maximal set $F \subseteq E$ such that $H = (V, F)$ is a forest.

Equivalent:
find a set of minimum size of edges X such that $G \setminus X$ is a forest.

As editing problem:

- Operations: edge deletion
- Target class: forest



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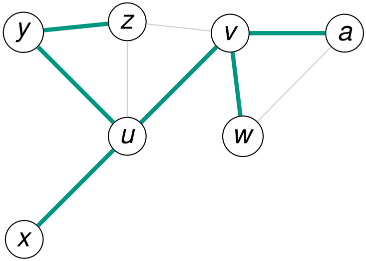

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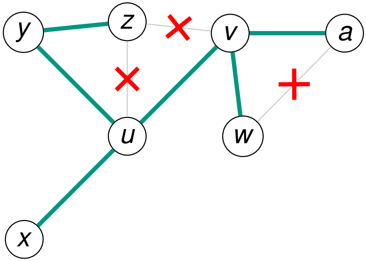

Example: Maximum Spanning Forest

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Given a weighted graph $G = (V, E, \omega)$, find a set $F \subseteq E$ of maximum weight such that $H = (V, F)$ is a forest.

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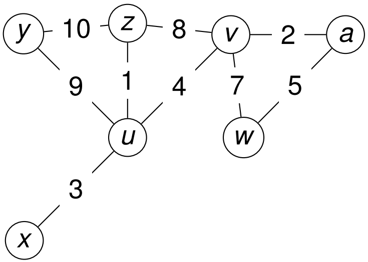
Kruskal's algorithm: $O(m \log n)$



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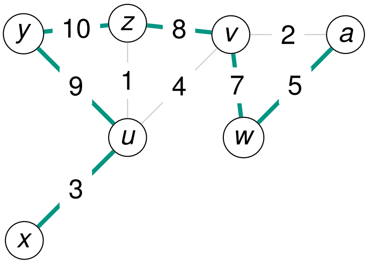

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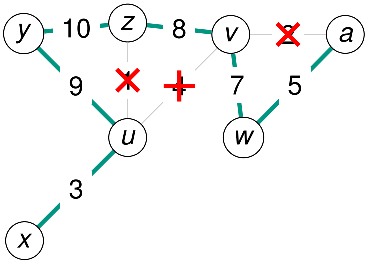


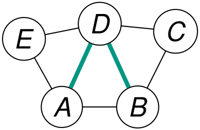
Example: Chordal Completion

Chordal Graph

A graph $G = (V, E)$ is chordal iff all cycles of four or more vertices have a chord, i.e., an edge that is not part of the cycle but connects two vertices of it.

Minimum Chordal Completion:

- Operation: edge insertion
- Target class: chordal graphs



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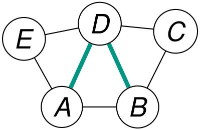

Treewidth

One less than the size of the largest clique in a chordal completion with smallest clique number.

Example: Independent Set

Maximum Independent Set

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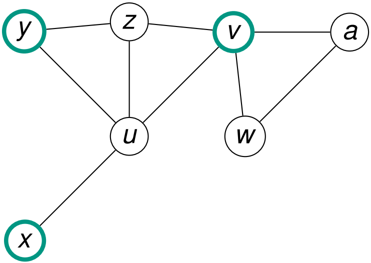

NP-complete.

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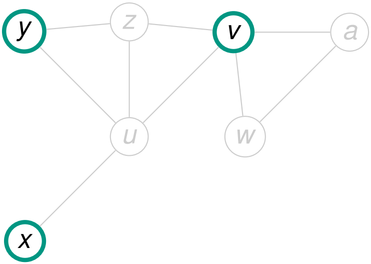

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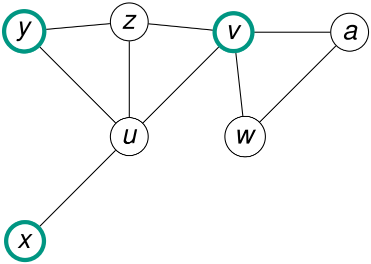

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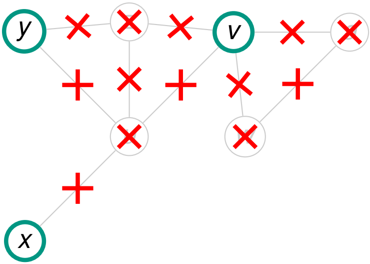

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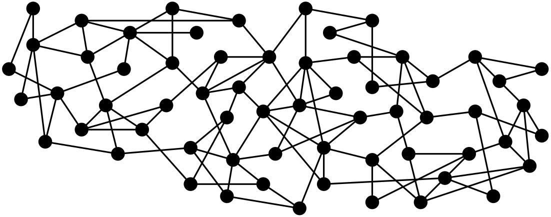
Graph Clustering: A First Intuition



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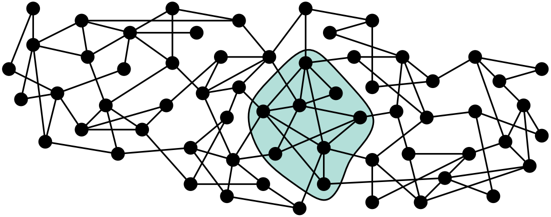

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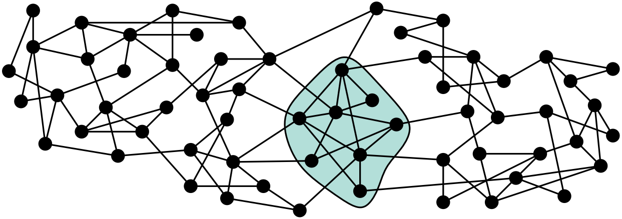

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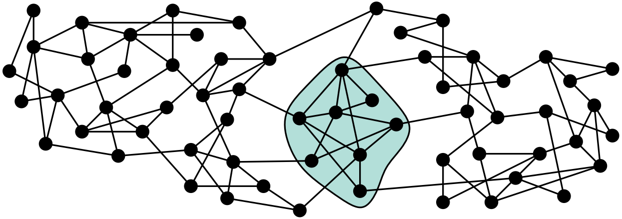

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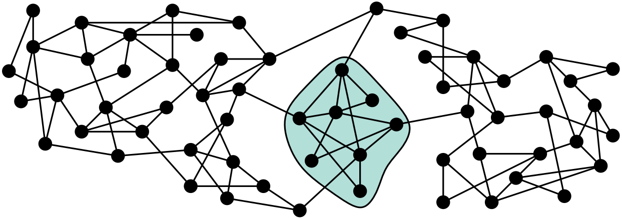

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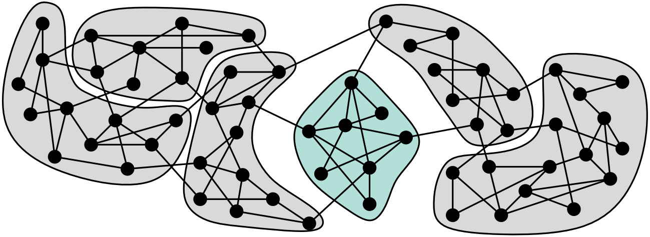

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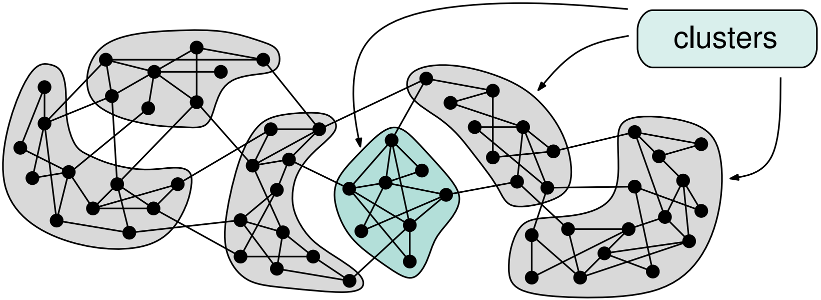

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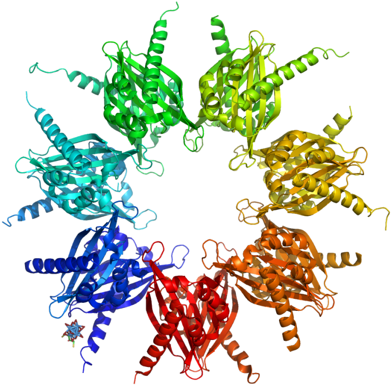
$\longrightarrow$ decomposition into dense subgraphs (= Clustering)

Applications in Biology



molecular structure of a protein

(Ca^{2+}/Calmodulin-dependent kinase II (CaMKII)
source: protein database www.rcsb.org)

cluster $\approx$ functional unit (*domain*) of a protein

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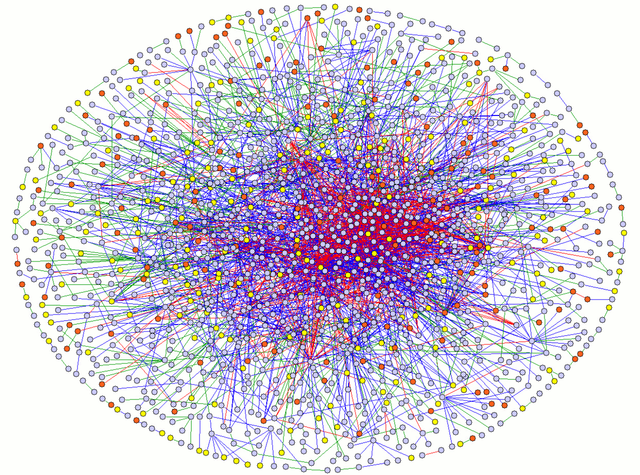

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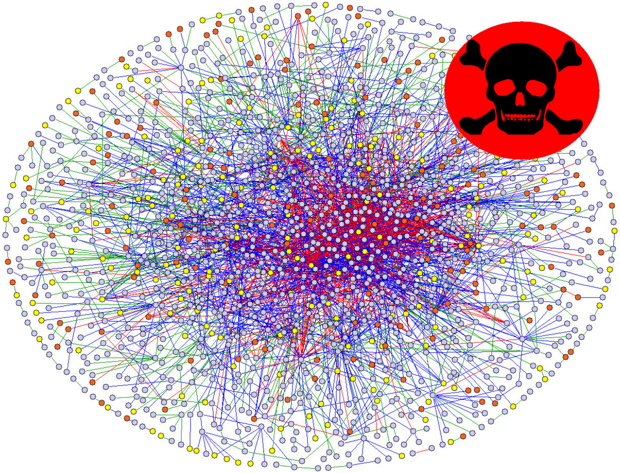

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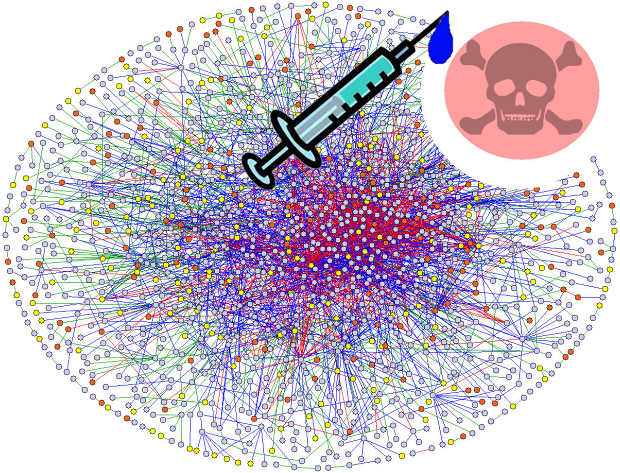

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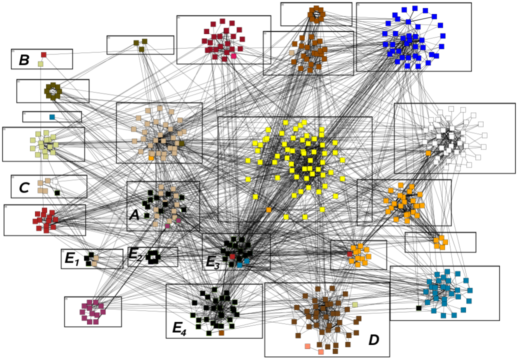
cluster ≈ isolatable seat of disease

Applications in Social Network Analysis



static snapshot: edges = 3 months of emails

From Intuition to Formalization

Paradigm of Graph Clustering

Intra-cluster density vs. **inter-cluster sparsity**

$\Downarrow$

Mathematical Formalization

- quality measures for clusterings
- models for communities – cliques, quasi-cliques, . . .

Many exist, optimization generally (NP-)hard

There is no single, universally best strategy

Postulations to a Measure

Given a graph G and a clustering $\mathcal{C}$, a *quality measure* should behave as follows:

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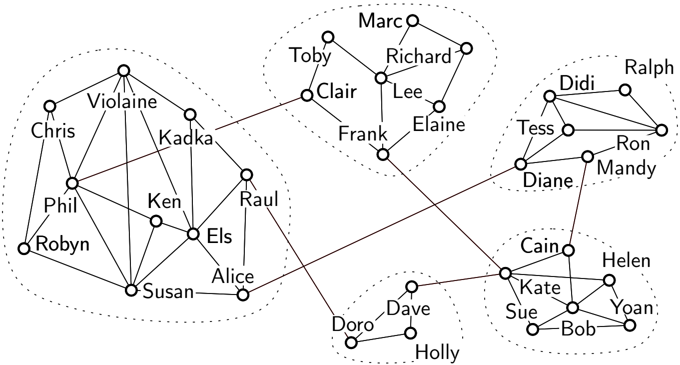
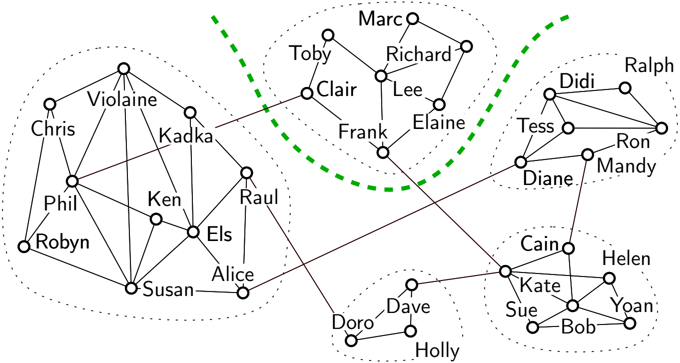
Kleinberg: An impossibility theorem for clustering [Kle02]

Formalization via Bottleneck



Formalization via Bottleneck



Quality of the clustering, upper cluster:

- inter-cluster sparsity: 2 *edges for cutting off* 7 *nodes* **(cheap)**

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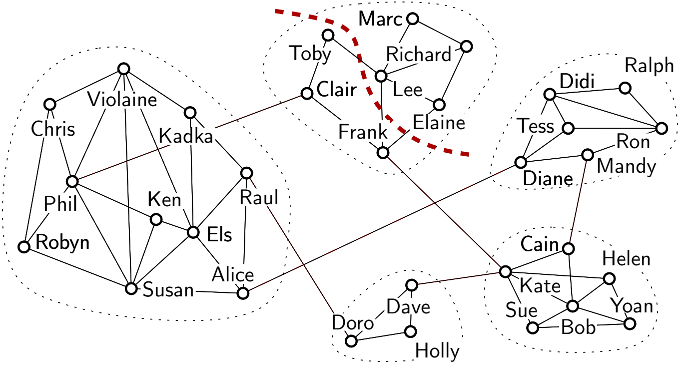


Quality of the clustering, upper cluster:

- inter-cluster sparsity: 2 *edges for cutting off* 7 *nodes* **(cheap)**
- intra-cluster density: best addit. cut:
  3 *edges for cutting off* 4 *nodes* **(expensive)**

Examples: Conductance, Expansion

conductance of a cut $(C, V \setminus C)$:

$$\varphi(C, V \setminus C) := \frac{\omega(E(C, V \setminus C))}{\min\left\{\sum_{v \in C} \omega(v), \sum_{v \in V \setminus C} \omega(v)\right\}}$$

(i.e.: thickness of bottleneck which cuts off C)

inter-cluster conductance $(\mathcal{C}) := 1 - \max_{C \in \mathcal{C}} \ \varphi(C, V \setminus C)$

(i.e.: $1-$ worst bottleneck induced by some $C \in \mathcal{C}$)

intra-cluster conductance $(\mathcal{C}) := \quad \min_{C \in \mathcal{C}} \ \min_{P \uplus Q = C} \ \varphi_{|C}(P, Q)$

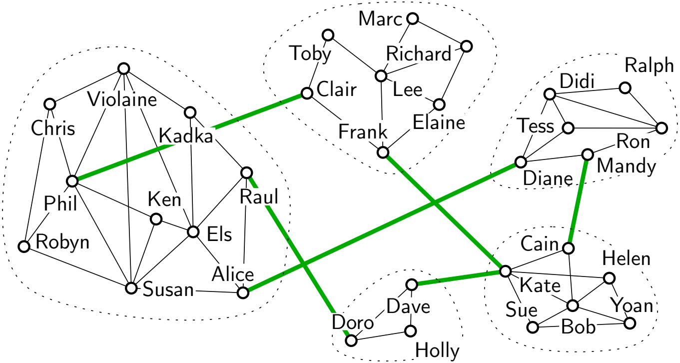
(i.e.: best bottleneck still left uncut inside some $C \in \mathcal{C}$)

expansion of a cut $(C, V \setminus C)$:

$$\psi(C, V \setminus C) := \frac{\omega(E(C, V \setminus C))}{\min\left\{|C|, |V \setminus C|\right\}}$$

(i.e.: in φ, replace $\omega(v)$ by 1; *intra-* and *inter-cluster expansion* analogously)

Formalization: Counting Edges



Measuring clustering quality by counting edges:

- inter-cluster sparsity: 6 *edges of ca. 800 node pairs* **(few)**

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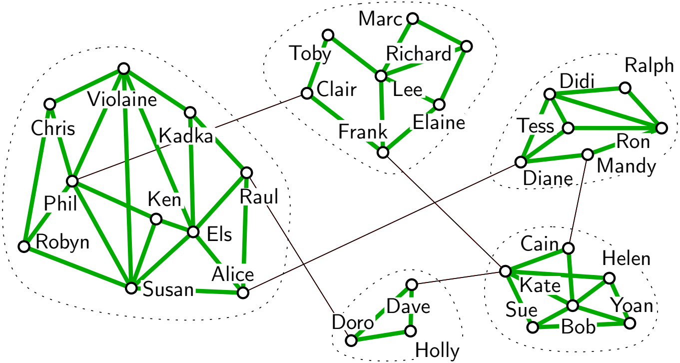

Measuring clustering quality by counting edges:

- inter-cluster sparsity: 6 *edges of ca. 800 node pairs* **(few)**
- intra-cluster density: 53 *edges of* 99 *node pairs* **(many)**

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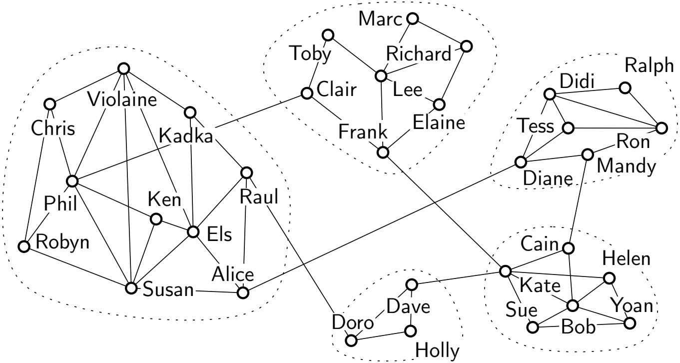
Example: Coverage



- *coverage:* $\mathrm{cov}(\mathcal{C}) := \dfrac{\text{\# intra-cluster edges}}{\text{\# edges}} \approx 0.9$

  (i.e.: fraction of covered edges)

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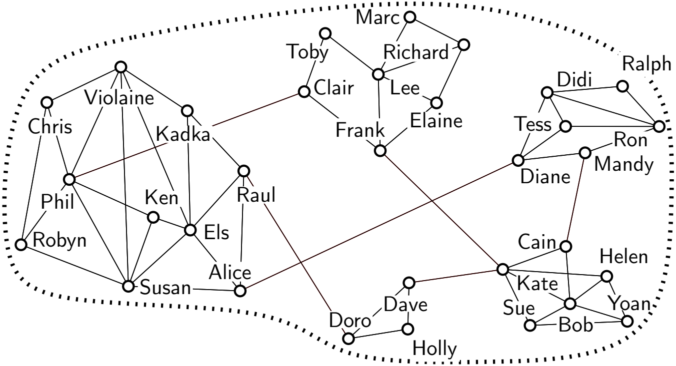

- *coverage:* $\text{cov}(\mathcal{C}) := \dfrac{\text{\# intra-cluster edges}}{\text{\# edges}} \approx 0.9$

  (i.e.: fraction of covered edges)

- **only one cluster $\Rightarrow$ *coverage* = 1.0**

A Promising Remedy

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"... if we subtract from [coverage] the ***expected*** *value [...], we do get a useful measure."* [NG04]

A Promising Remedy

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Modularity

$$\text{mod}(\mathcal{C}) := \quad \mathit{cov}(\mathcal{C}) \quad - \mathbb{E}(\mathit{cov}(\mathcal{C}))$$

$$= \frac{\text{\# intra-cluster edges}}{|\#\mathit{edges}|} - \frac{1}{4|\#\mathit{edges}|^2} \sum_{C \in \mathcal{C}} \left(\sum_{v \in C} \deg(v) \right)^2$$

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NP-hard to optimize [BDG⁺08]

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Modularity in Practice

- easy to use & implement
- reasonable behavior on many practical instances
  $\rightsquigarrow$ heavily used in various fields:
  - ecosystem exploration
  - collaboration analyses
  - biochemistry
  - structure of the internet (AS-graph, www, routers)
- close to human intuition of quality [GGHW10]

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- scaling behavior (double instance, result differs) [folklore]
- non-locality of optimal clustering [folklore]
- resolution limit (no tiny and large clusters at the same time) [FB07]
- large sparse graph $\rightsquigarrow$ high values, balanced clusters [GdMC10]

Surprise

$G = (V, E)$, $|E| = m$, clustering $\mathcal{C}$, i_e intracluster edges
Random $\mathcal{G}$ with m edges

Surprise

$$S(\mathcal{C}) := \text{Prob}(\mathcal{G} \text{ has at least } i_e \text{ intracluster edges in } \mathcal{C}) = \sum_{i=i_e}^{m} \frac{\binom{i_p}{i} \cdot \binom{p-i_p}{m-i}}{\binom{p}{m}},$$

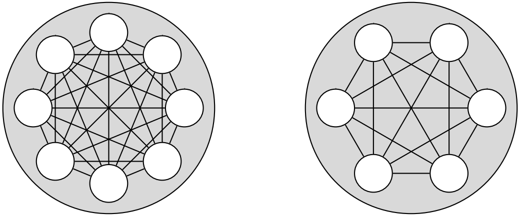
where $p := \binom{n}{2}$ and i_p #intra-cluster node pairs. [AMM05]

Urn model: i_p white, $p - i_p$ black balls, draw m balls w/o replacement

- NP-hard to optimize [FKW14]

Cluster Editing

Ideal clustering: Disjoint cliques.



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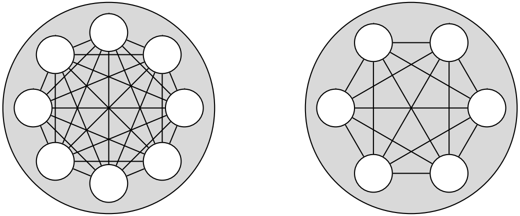

Idea: Edge editing to disjoint cliques – **Cluster Editing**.

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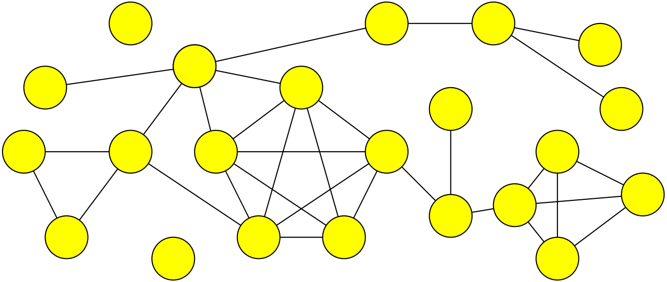
Cluster Editing

“How many edges must be inserted or deleted to arrive at disjoint cliques?”



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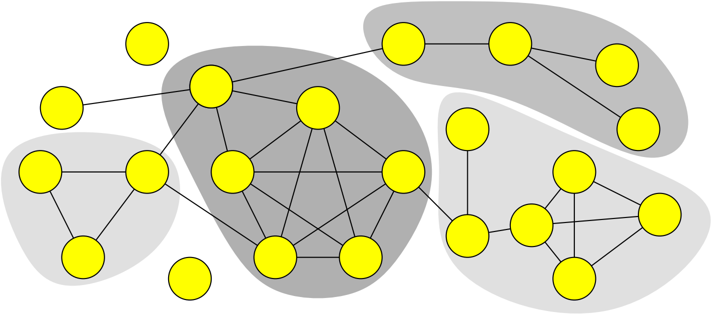

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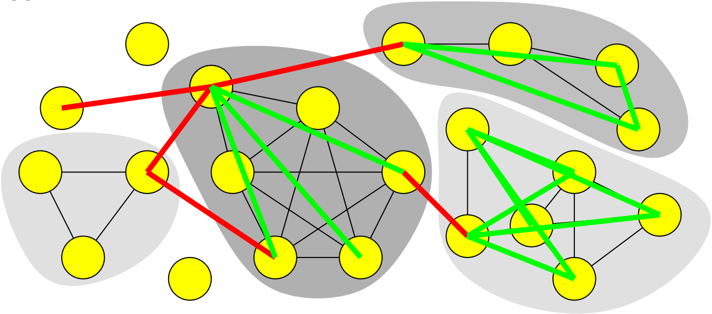

editing set has size 5 + 12 = 17 (bad)

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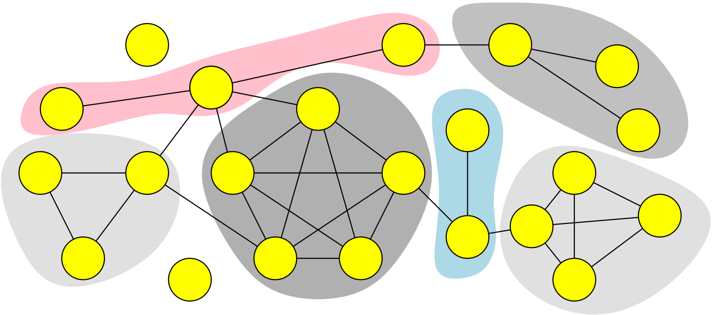

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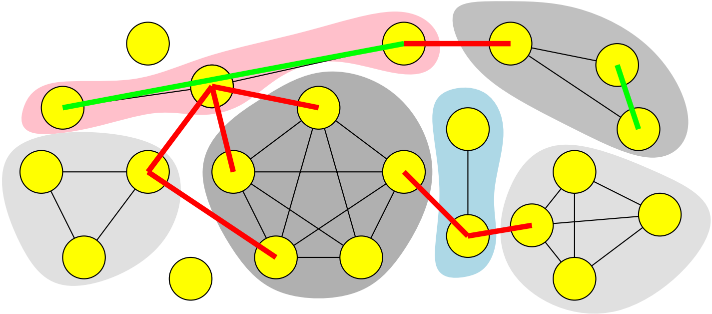
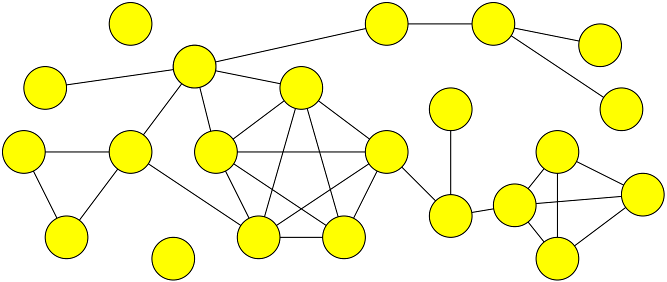


editing set has size 7 + 3 = 10 (better)

Cluster Editing

"How many edges must be inserted or deleted to arrive at disjoint cliques?"



Task: find clustering with minimum cluster editing set [BB13, BBK08]

- NP-complete
- popular in biology

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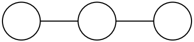
Forbidden Subgraphs

Disjoint cliques $\Leftrightarrow$ no P_3 as node-induced subgraph



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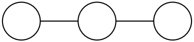
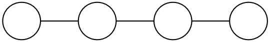
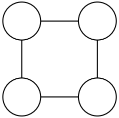
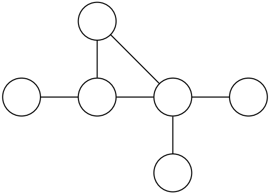


Generalization:
No P_4 or C_4 as node-induced subgraph
= *Quasi-Threshold Graph*







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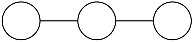
Disjoint cliques ⇔ no P_3 as node-induced subgraph



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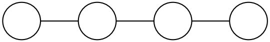

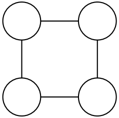

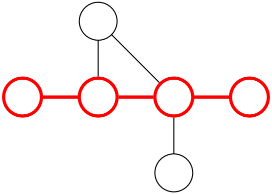

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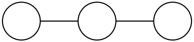

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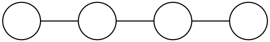

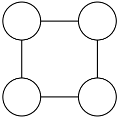

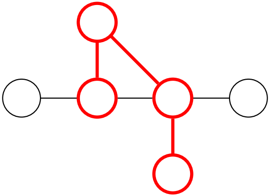

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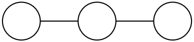

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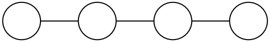
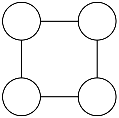
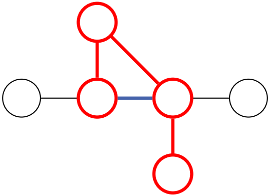
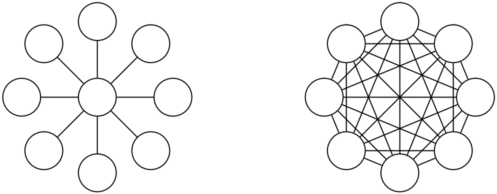






Quasi-Threshold Graphs

- Trivially perfect graphs
- Dense? Sparse? – Both!



- Max. diameter 2
- Central hub per component

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Why Quasi-Threshold Editing?

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- Components of quasi-threshold graphs are communities [NG13]

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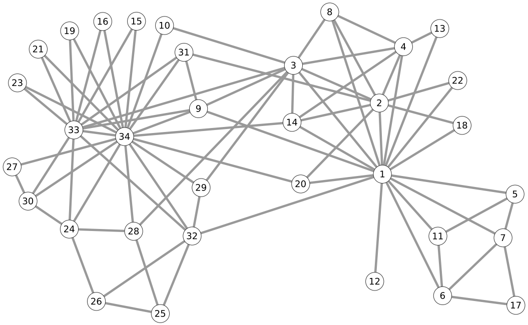

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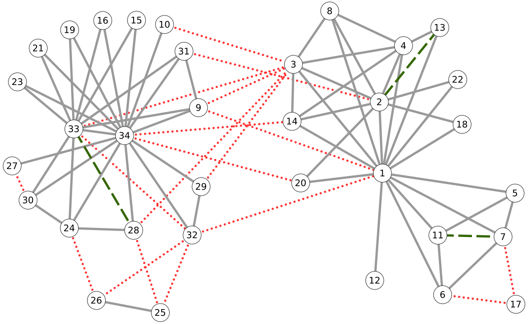

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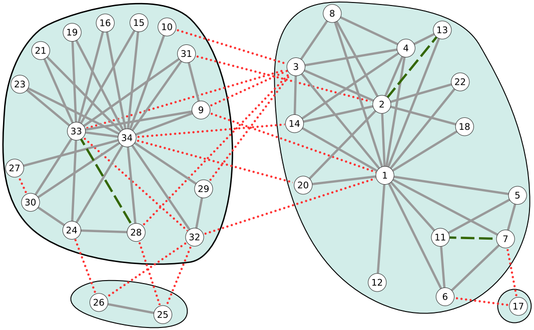

Algorithmic Results

- General
- Cluster Editing
- Quasi-Threshold Editing
- Threshold Editing

Approaches

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P_3-free editing and P_4/C_4-free editing are NP-complete
$\Rightarrow$ no efficient exact algorithms in general

Alternative approaches:

- Average case instead of worst case analysis
- Randomization
- Approximative solutions
- Fixed parameter tractability (FPT)
- Empirical studying of heuristics on benchmarks

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Fixed Parameter Tractability

Goal: Limit the explosion of the running time: $O(f(k) \cdot n^{O(1)})$.
Challenge: Identifying a suitable, “small” parameter k.

$\oplus$: Optimal, provable running time
$\ominus$: Exponential running time

Hope:

- Obtain a small kernel in polynomial time
- “Tolerable” $f(k)$

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Formal Definition

Parameterized Problem

$L \subseteq \Sigma^* \times \Sigma^*$ (usually $\subseteq \Sigma^* \times \mathbb{N}$)

Fixed-parameter tractable

$L \in \mathcal{FPT}$ iff $(x, k) \in L$ can be decided in time $f(k) \cdot |x|^{O(1)}$ where f is a computable function only depending on k.

Kernelization

$(x, k) \mapsto (x', k')$, with

- $k' \leq k$, $|x'| \leq g(k)$
- $(x, k) \in L$ iff $(x', k') \in L$
- Reduction in polynomial time

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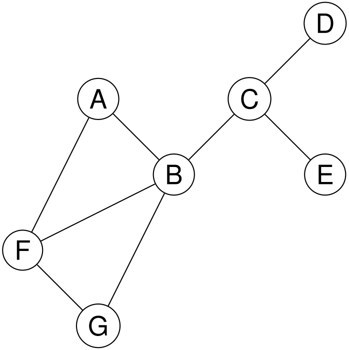
General Results

Graph classes defined by a finite set of (finite) forbidden induced subgraphs:

- Editing FPT in number of edits k, $O\left(\nu^{2k} \cdot n^{\nu+1}\right)$, ν maximum number of nodes in a forbidden subgraph. [Cai96]

Example: P_3-free, $k = 3$

$\boxed{G}$



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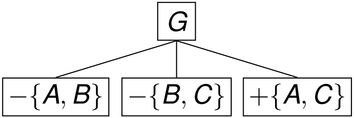

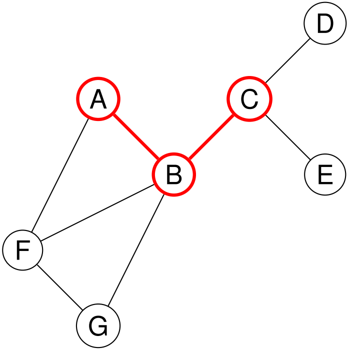

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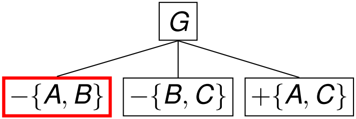

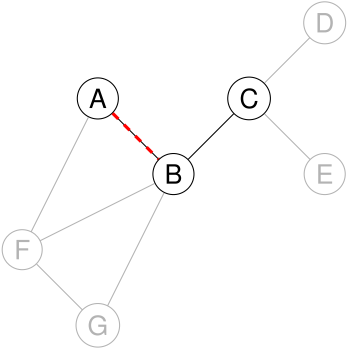

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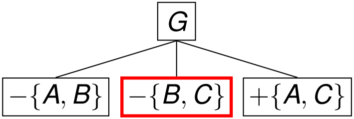

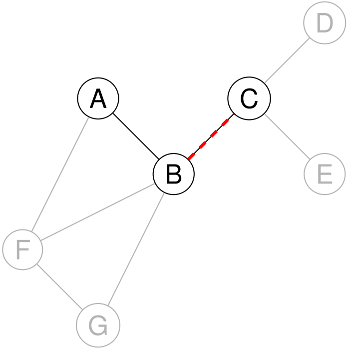

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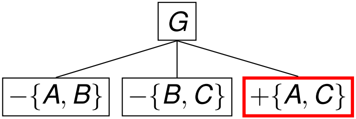

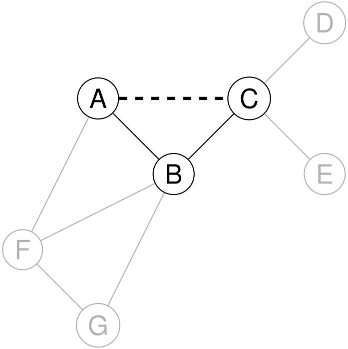

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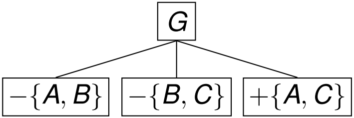

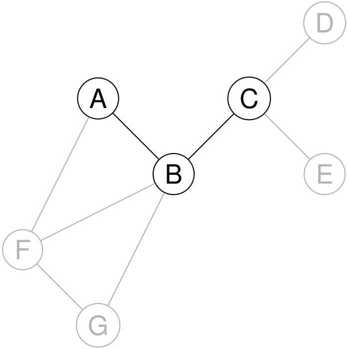

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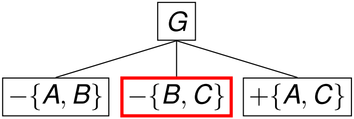

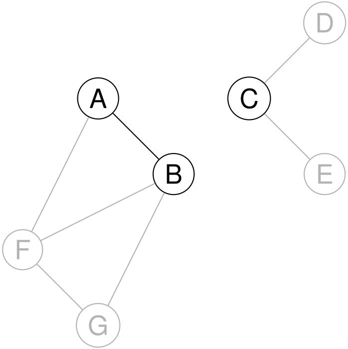

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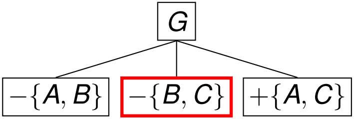

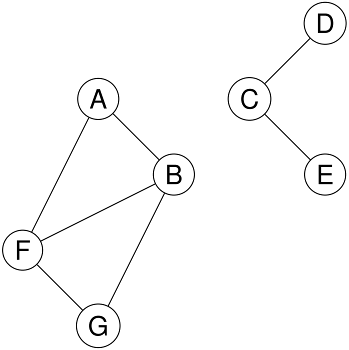

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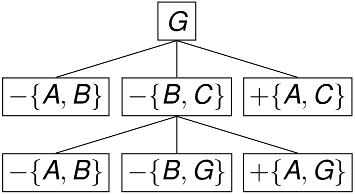

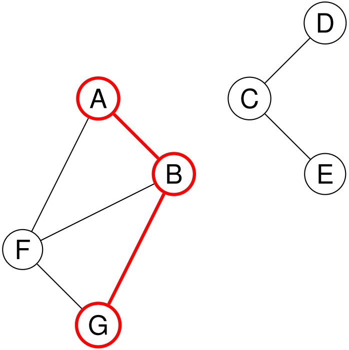

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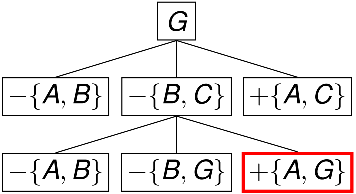
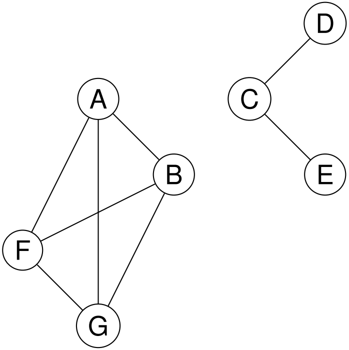
Example: P_3-free, $k = 3$





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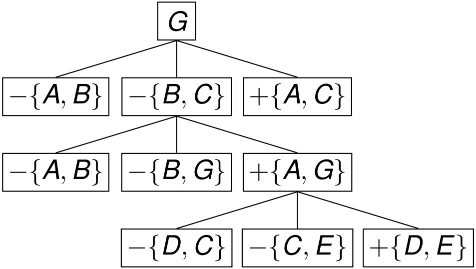

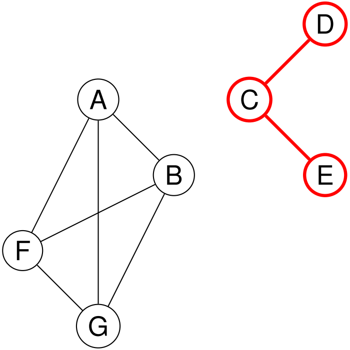

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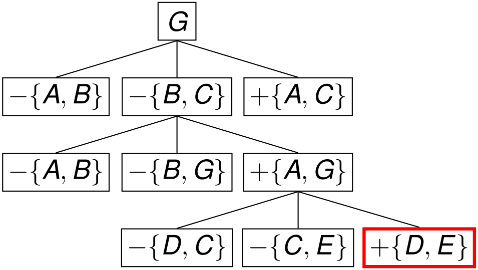

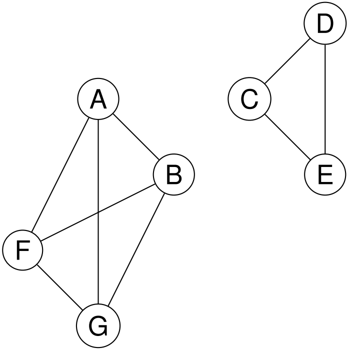

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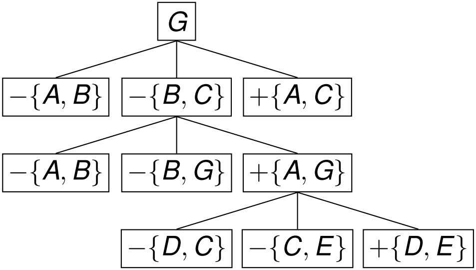
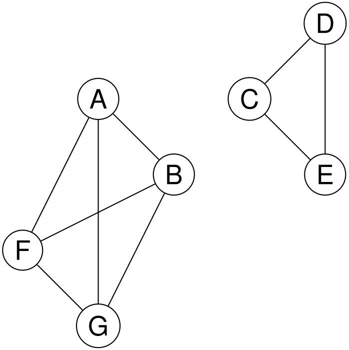
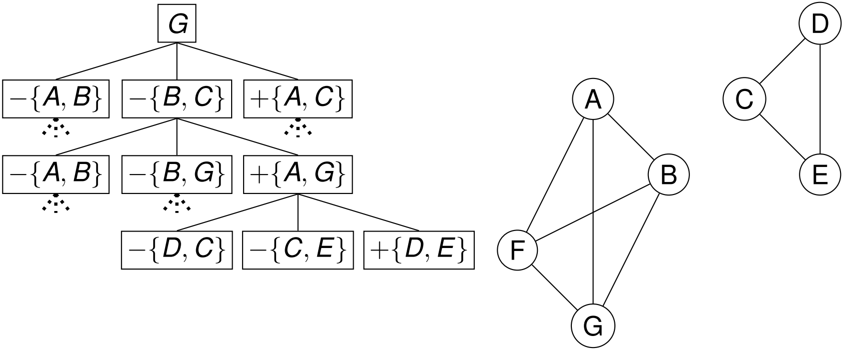




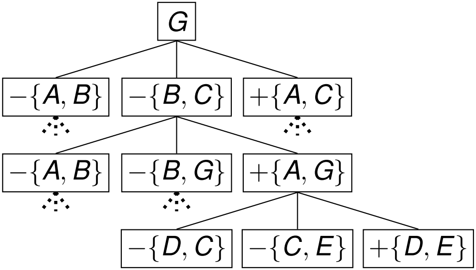
$\Rightarrow$ Found solution.

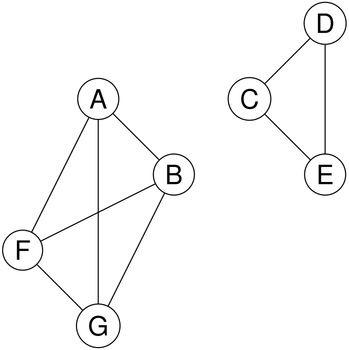
Example: P_3-free, $k = 3$



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

Example: P_3-free, $k = 3$





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

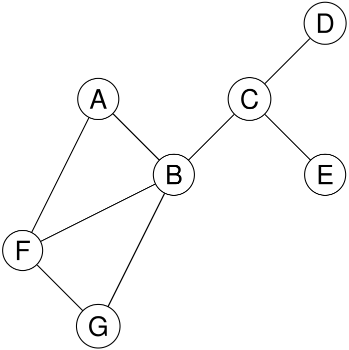
- Time $O(3^k \cdot \text{poly}(n))$
- Best known: $O(1.62^k + m + n)$ [Böc12]

FPT-based editing

- Show for a graph that k is exact solution:
  - show solution with k
  - show impossibility with $k-1$
- Branching rules can be optimized automatically [GGHN03]
- Bounding possible to limit explored branches.

Lower Bounds: P_3-free, $k = 3$

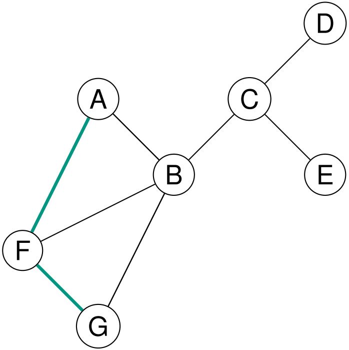
$\boxed{G}$



Lower Bound: 0
Remaining operations: 3

Lower Bounds: P_3-free, $k = 3$

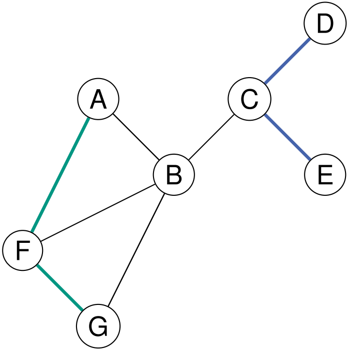
$\boxed{G}$



Lower Bound: 1
Remaining operations: 3

Lower Bounds: P_3-free, $k = 3$

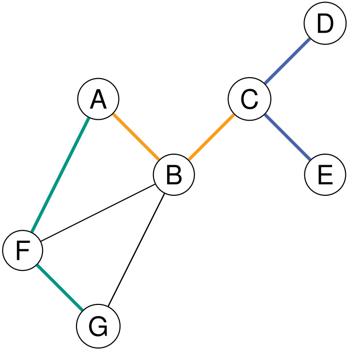
$\boxed{G}$



Lower Bound: 2
Remaining operations: 3

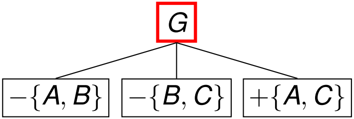
Lower Bounds: P_3-free, $k = 3$

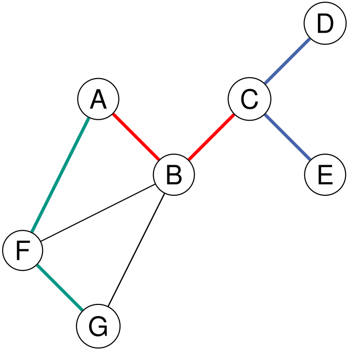
$\boxed{G}$



Lower Bound: 3
Remaining operations: 3

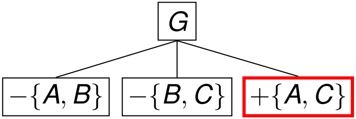
Lower Bounds: P_3-free, $k = 3$

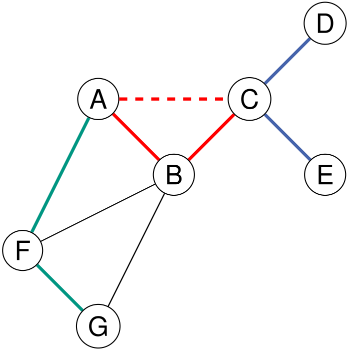




Lower Bound: 3
Remaining operations: 3

Lower Bounds: P_3-free, $k = 3$





Lower Bound: 3
Remaining operations: 2

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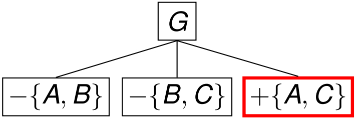
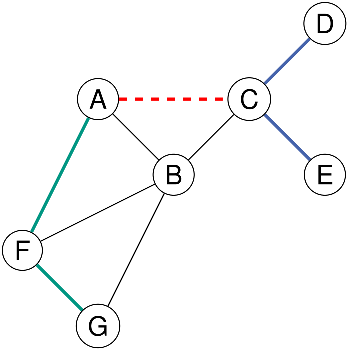
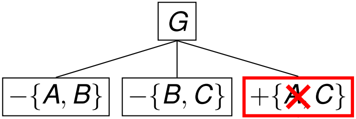
Lower Bounds: P_3-free, $k = 3$

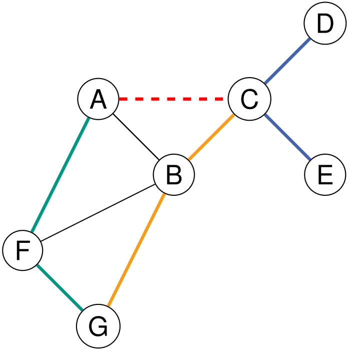




Lower Bound: 2
Remaining operations: 2

Lower Bounds: P_3-free, $k = 3$





Lower Bound: 3
Remaining operations: 2

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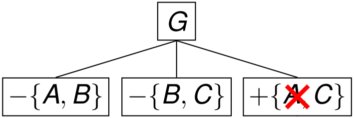

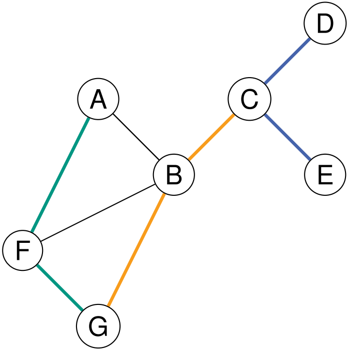

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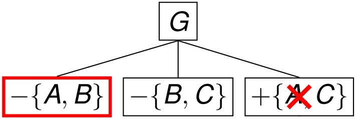

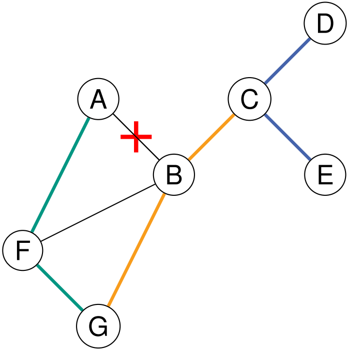

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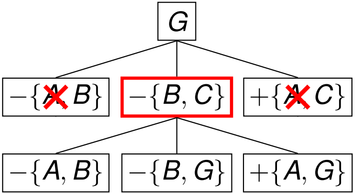
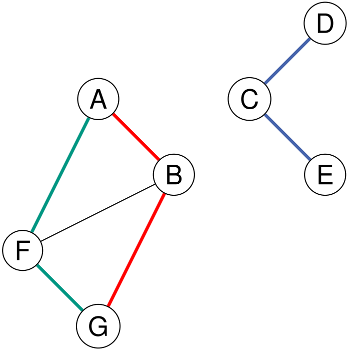
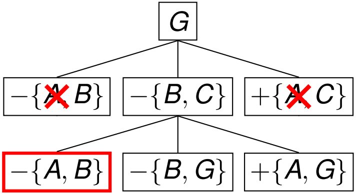
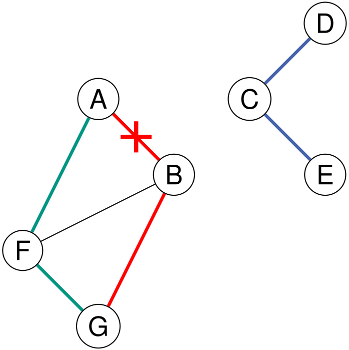




Lower Bound: 2
Remaining operations: 2

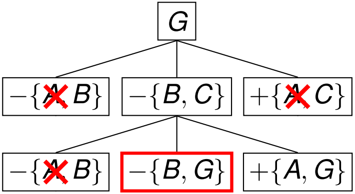
Lower Bounds: P_3-free, $k = 3$

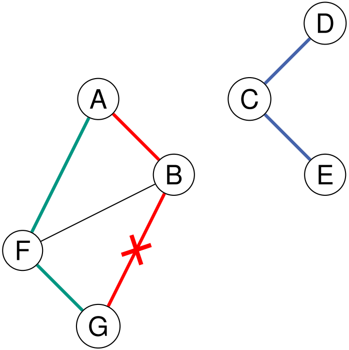




Lower Bound: 2
Remaining operations: 1

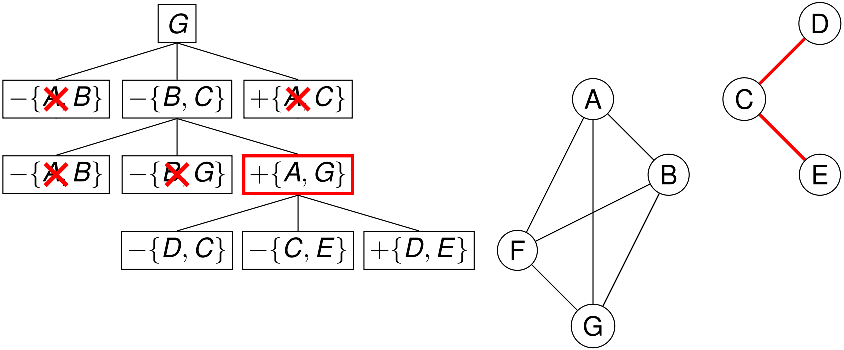
Lower Bounds: P_3-free, $k = 3$





Lower Bound: 2
Remaining operations: 1

Lower Bounds: P_3-free, $k = 3$



Lower Bound: 1
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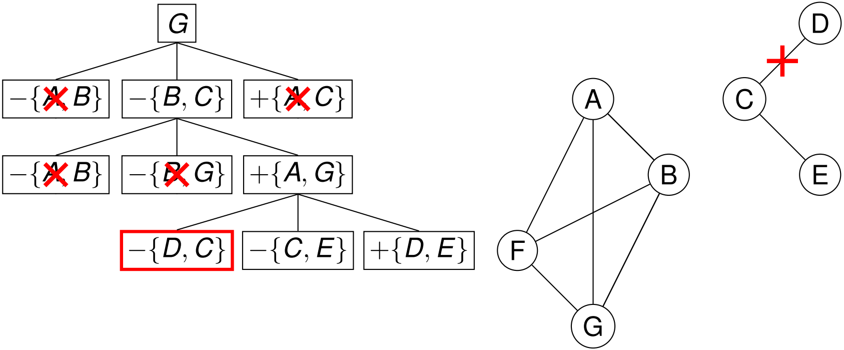
Lower Bounds: P_3-free, $k = 3$



Lower Bound: 0
Remaining operations: 0

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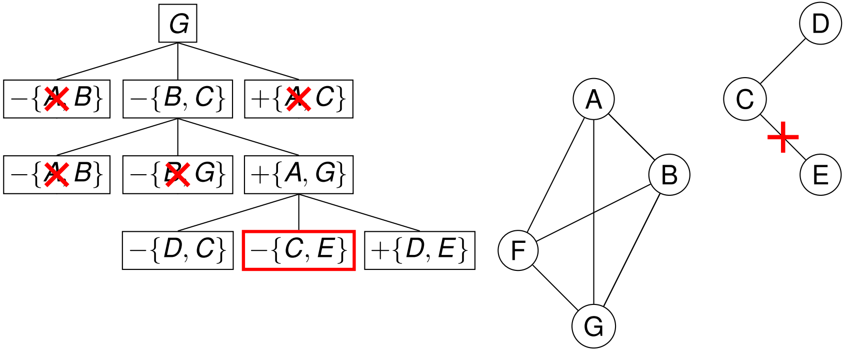
Lower Bounds: P_3-free, $k = 3$



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Remaining operations: 0

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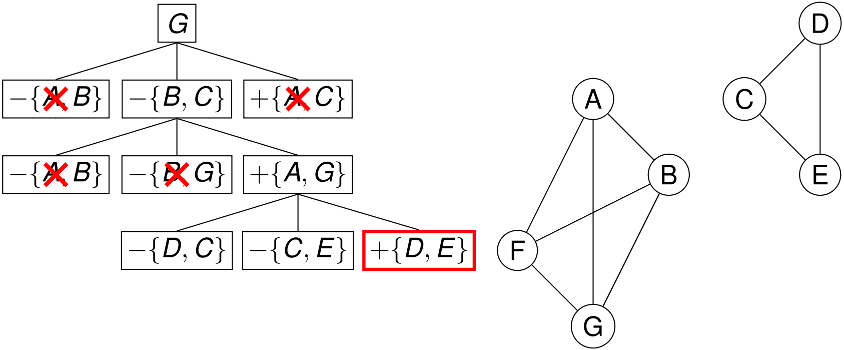

Lower Bound: 0
Remaining operations: 0

Cluster Editing

- There is a $2k$-kernel ($k =$ number of edits) [CM12]
- Heuristics exist [BB13]

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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Karlsruhe Institute of Technology

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Quasi-Threshold Recognition:

- Certifying recognition in linear time. [Chu08]
- Simpler certifying recognition algorithm [BHSW15]

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Exact editing:

- Is NP-hard [NG13]
- Is FPT $O\left(6^k\left(|V|+|E|\right)\right)$ [Cai96]
- Polynomial kernel exists ($O\left(k^7\right)$ vertices) [DP15]

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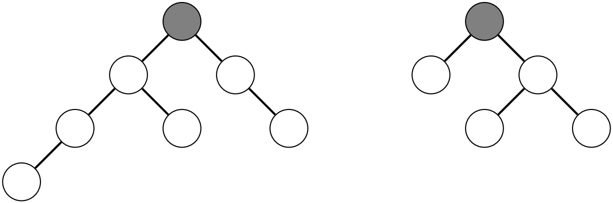
Heuristic editing:

- First editing heuristic – $\Omega\left(|V|^2\right)$ [NG13]
- Faster editing heuristic: Quasi-Threshold Mover (QTM) [BHSW15]

Skeleton Forests



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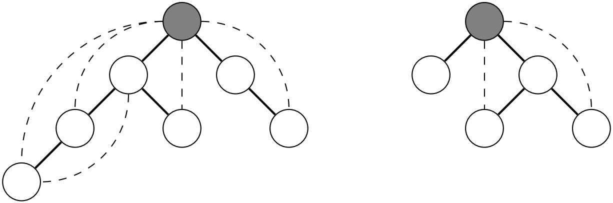
Skeleton Forests



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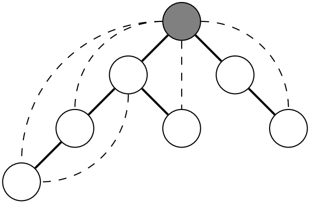

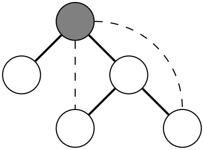

Quasi-Threshold Graphs

Quasi-threshold graphs are exactly the transitive closure of rooted forests.

Certifying Algorithms

Certifying Algorithm

A certifying algorithm is an algorithm that produces, with each output, a certificate or witness (easy-to-verify proof) that the particular output has not been compromised by a bug. [MMNS11]

Quasi-Threshold Recognition:

- Positive proof: A skeleton forest such that the graph is its transitive closure.
- Negative proof: An induced P_4 or C_4.

Quasi-Threshold Recognition

$p(u)$ parent of node u, init with -1;
foreach *$u \in V$ sorted by degree in decreasing order* **do**
    foreach *non-processed neighbor c of u* **do**
        if $p(u) = p(c)$ **then**
            Set $p(c)$ to u;
        else
            Construct P_4 or C_4;
    Mark u as processed;

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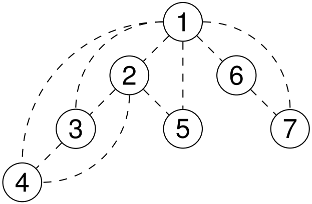

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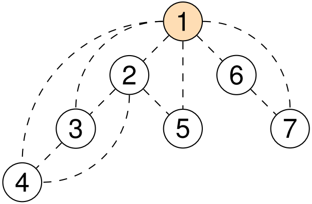

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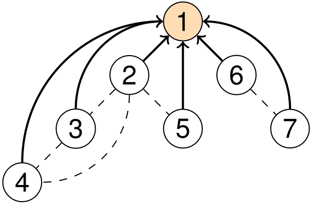

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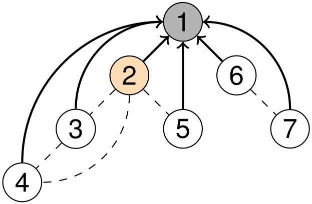

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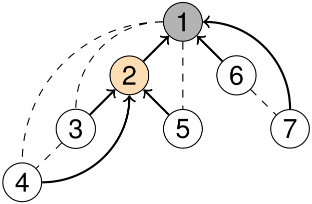

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Karlsruhe Institute of Technology

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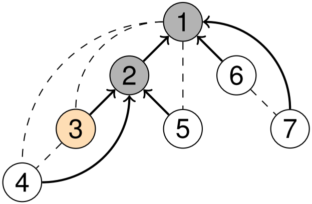

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Quasi-Threshold Recognition

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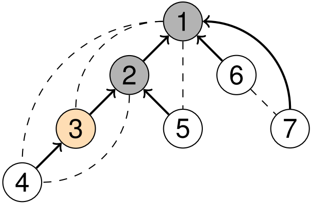

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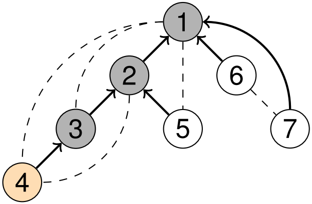

Quasi-Threshold Recognition

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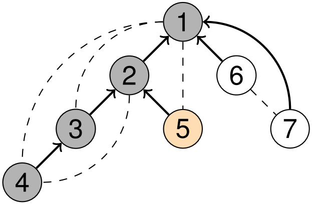

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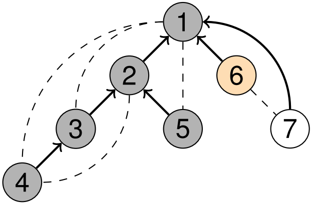

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Karlsruhe Institute of Technology

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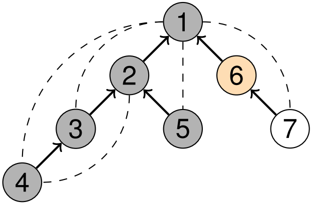

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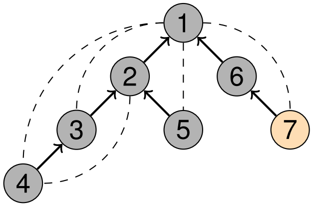

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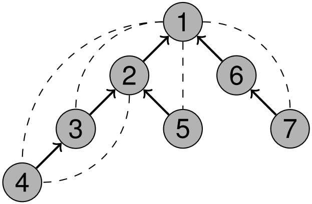

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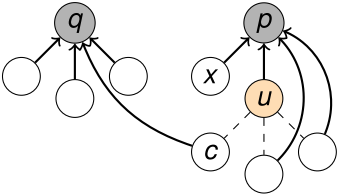

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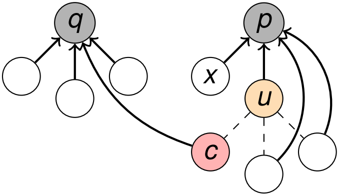

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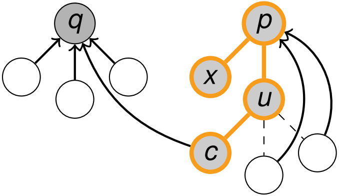
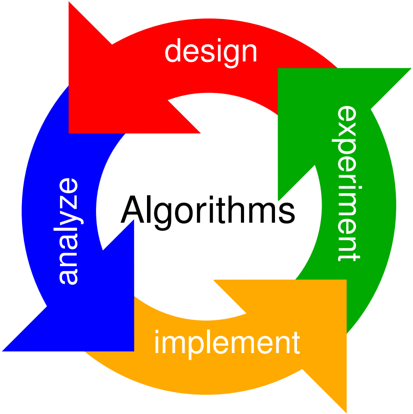


Algorithm Engineering



Initial Editing Heuristic

- Use recognition
- Resolve errors locally

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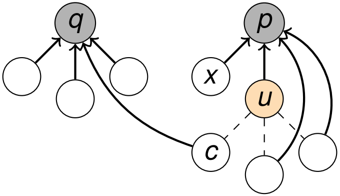

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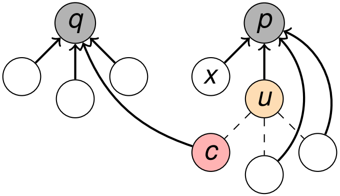

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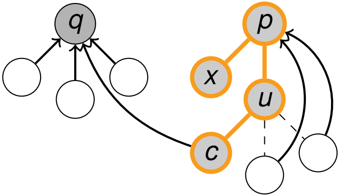

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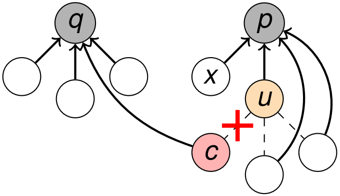

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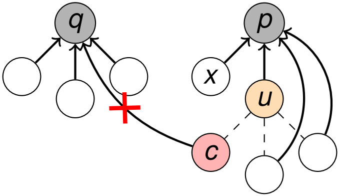

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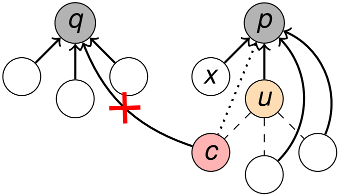

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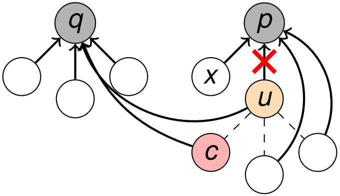

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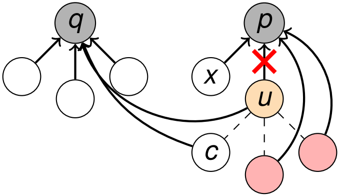

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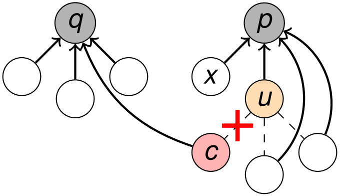

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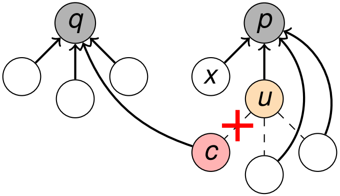

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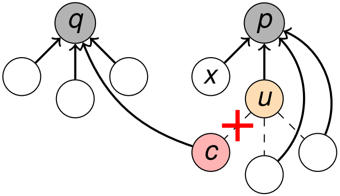

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- Time: Triangle counting $O(\alpha \cdot |E|)$ + linear

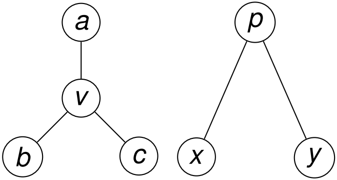
QTM: Basic Idea

Modify skeleton forest using local moving

For each node apply move:

- Choose parent
- Adopt children

such that #edits is minimum among choices.



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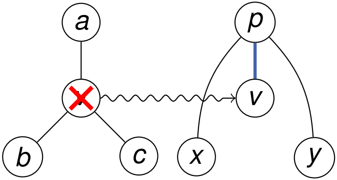

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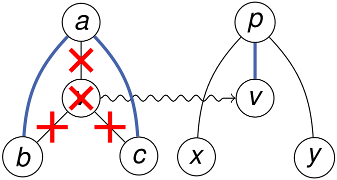

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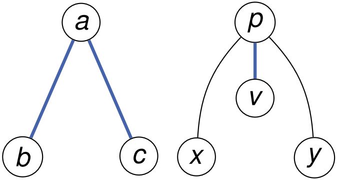

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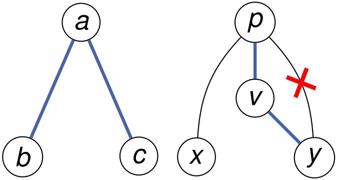

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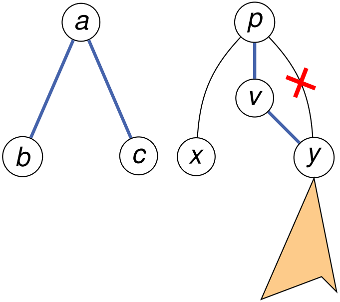

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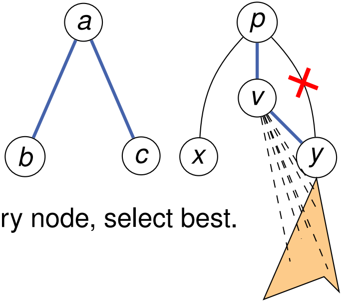

Count (non-)neighbors below and above every node, select best.

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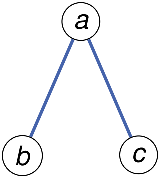

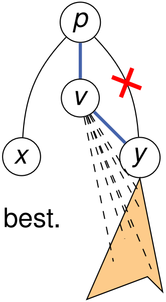

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Simple idea:

- Count (non-)neighbors below and above each node using a (single) DFS
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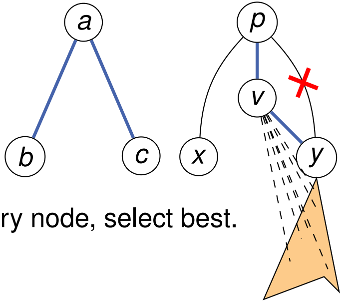

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Problem: time $O(|V|)$ per node, $O(|V|^2)$ per round.

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Parents: neighbors and nodes with children that should be adopted

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How to evaluate children:

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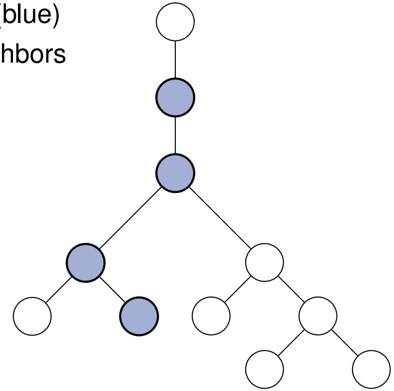

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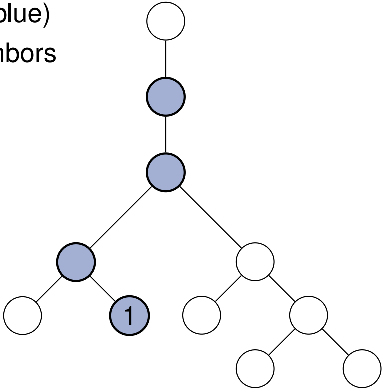

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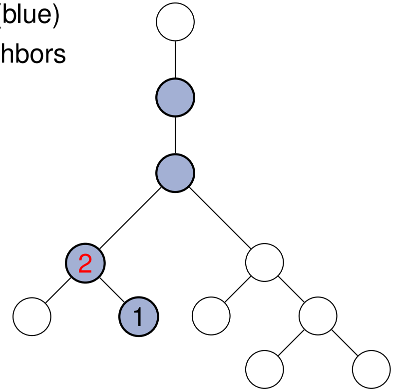

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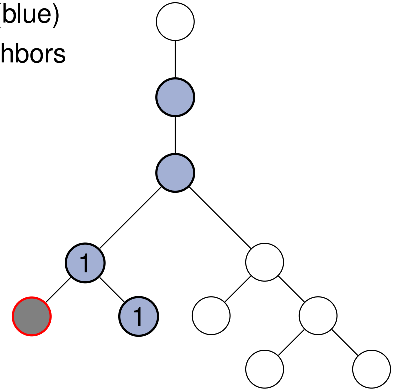

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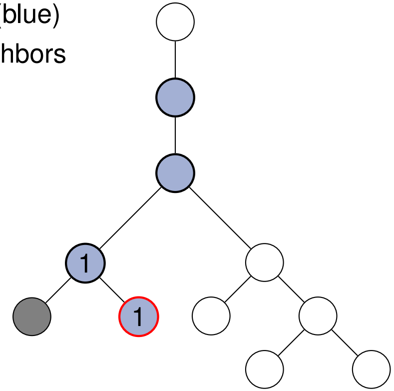

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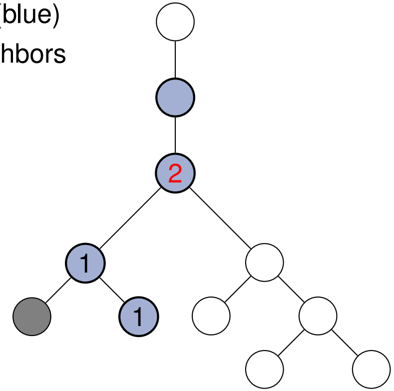

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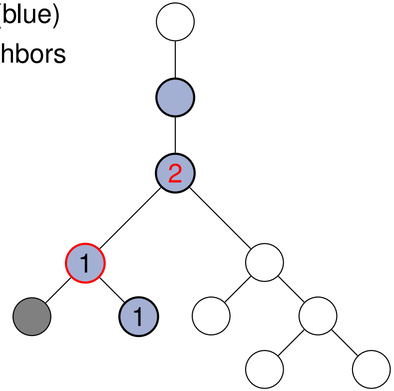

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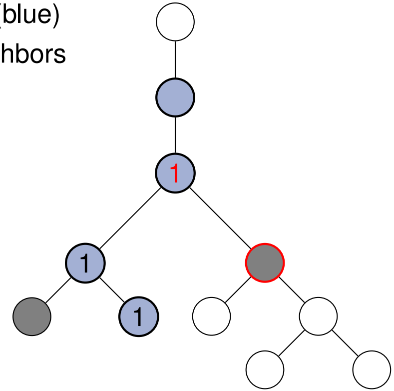

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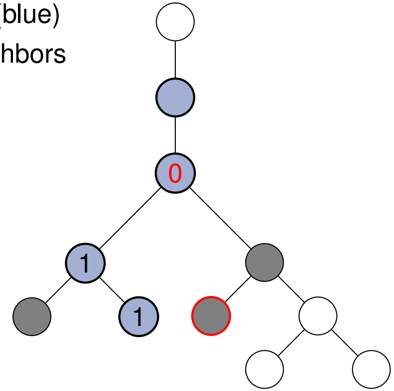

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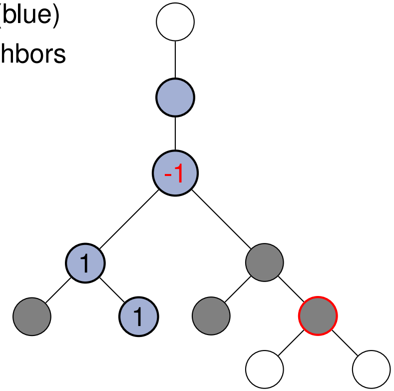

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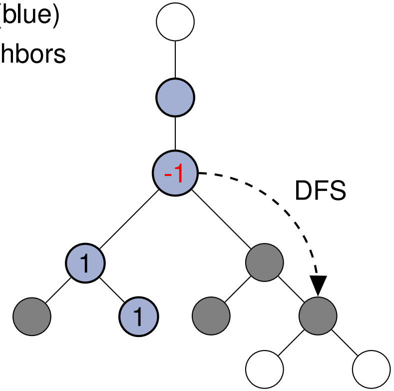

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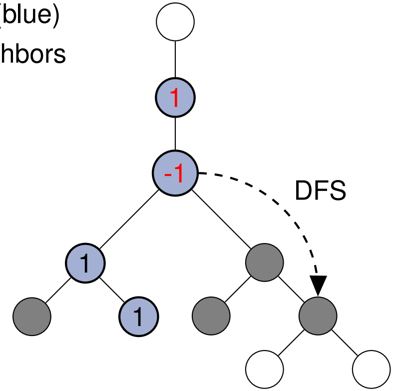

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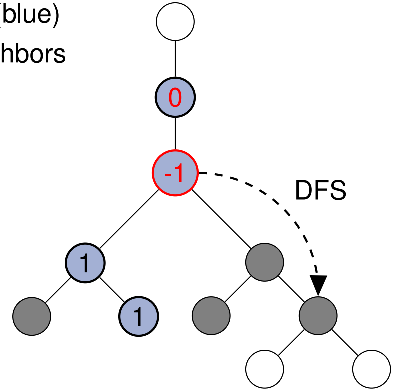

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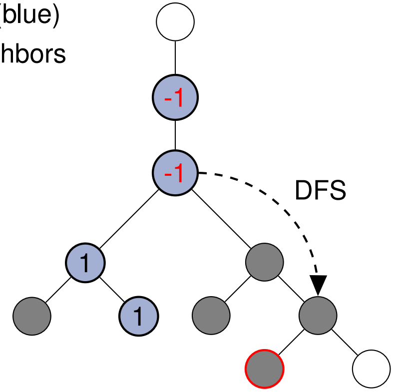

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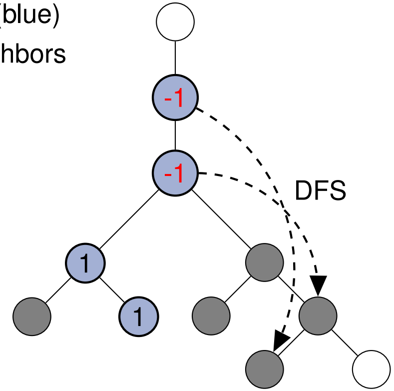


QTM: Fast Local Moving

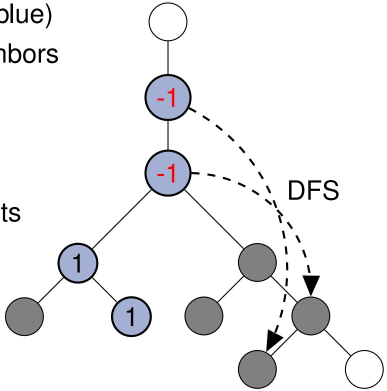
Parents: neighbors and nodes with children that should be adopted
Adopt children that have more neighbors than non-neighbors

How to evaluate children:

- Start at neighbors of node to move (blue)
- Bottom-up scan with surplus of neighbors
- Limited DFS when surplus exists
  $\rightsquigarrow$ visit $O(1)$ nodes per neighbor

Find best parent:

- Bottom-up scan from potential parents



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  $\leadsto$ visit $O(1)$ nodes per neighbor

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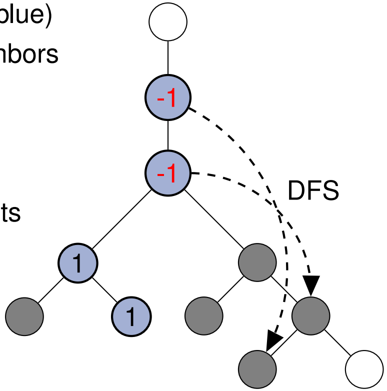
Time:

- Amortized $O(d \log(d))$ per node
- $O(|E| \log d_{\max})$ per round
- 4 rounds enough in practice



Evaluation: Comparison to previous heuristic

On large networks previous heuristic too slow.

QTM:

Name	$\|V\|$ [K]	$\|E\|$ [K]	Edits [K]	Time [s]
Caltech [TMP12]	0.77	16.66	11.6	<0.1
Orkut [LK14]	3 072	117 185	103 426	866.4
uk-2002 [BV04]	18 520	261 787	31 218	1 638.0

Evaluation: Synthetic networks

Generation:

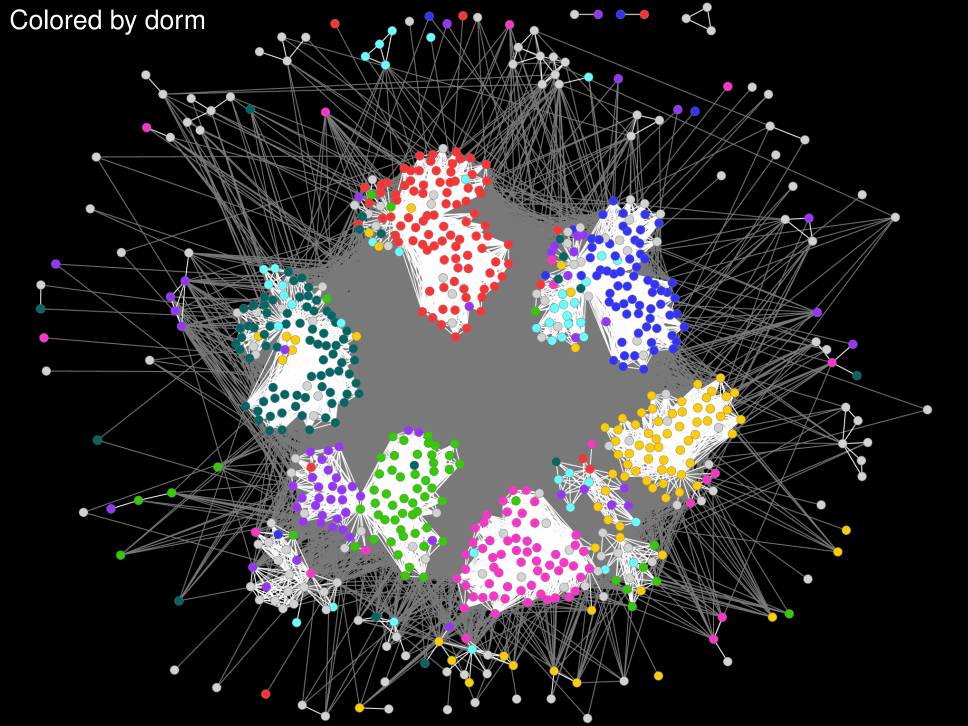
- Generate quasi-threshold graphs
- Introduce edit difference by random edge deletions and insertions

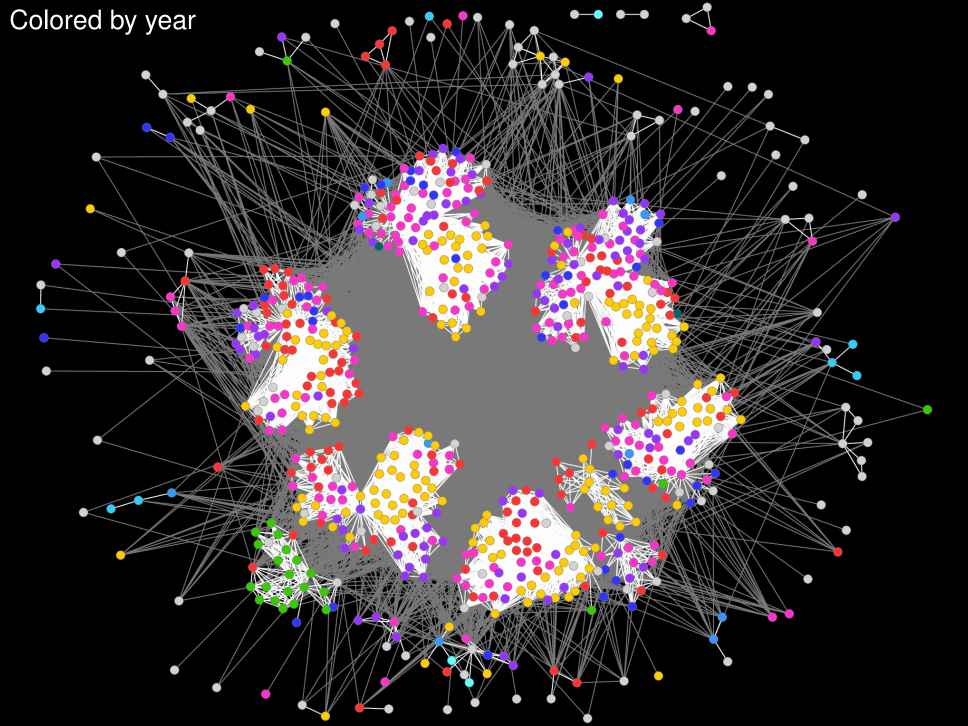
Result:

- QTM results as close or closer than generated quasi-threshold graphs

Case study: Caltech network

- Caltech Facebook network from September 2005 [TMP12]
- Nodes: 769 university members (mostly students)
- Edges: friendship on Facebook
- Anonymized node attributes:
  - Dormitory
  - Class year
  - Gender
  - Major
  - High school
- Dormitory, year correlated with edges


Colored by dorm


Colored by year

Conclusion

- Many problems can be formulated using graph editing
- Clustering – different formalizations using edge editing
- Both exact (FPT) and heuristic algorithms available

Conclusion

Karlsruhe Institute of Technology

- Many problems can be formulated using graph editing
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Outlook

- Many more possible editing problems, e.g. P_5, C_5 – no good heuristics known
- Other variants using core-periphery structure even allow overlapping communities [BHK15]

Thank you!

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