Subgraph Isomorphism Meets Cutting Planes

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KTH Royal Institute of Technology

NordConsNet 2019
Simula Research Laboratory
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May 21, 2019

Joint work in progress with Jan Elffers, Stephan Gocht, Ciaran McCreesh, . . .

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The Problem

Input

- Pattern graph $\mathcal{P}$ with vertices $V(\mathcal{P}) = \{a, b, c, \ldots\}$
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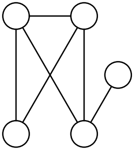
Task

- Find all subgraph isomorphisms $\varphi : V(\mathcal{P}) \to V(\mathcal{T})$
- I.e., if
  1. $\varphi(a) = u$
  2. $\varphi(b) = v$
  3. $(a, b) \in E(\mathcal{P})$

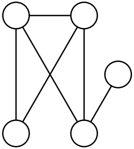
  then must have $(u, v) \in E(\mathcal{T})$

Subgraph Isomorphism Example



Pattern

Subgraph Isomorphism Example



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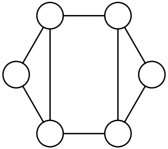


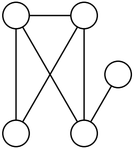
Target

Subgraph Isomorphism Example

Pattern *Target*

No subgraph isomorphism

Subgraph Isomorphism Example



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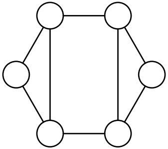

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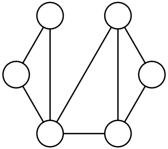
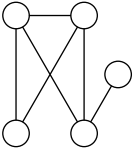


2nd target

No subgraph isomorphism

Subgraph Isomorphism Example



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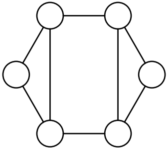

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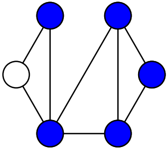

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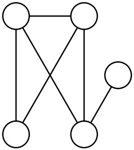
No subgraph isomorphism

Has subgraph isomorphism

Subgraph Isomorphism Example



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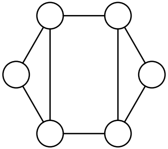

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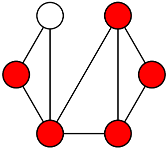

2nd target

No subgraph isomorphism

Has subgraph isomorphism
In fact, two of them

The Challenge

Subgraph isomorphism important in

- biochemistry
- compiler construction
- computer vision
- plagiarism and malware detection
- et cetera...

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But computationally very challenging!

1. How to solve efficiently?
2. How do we know if answer is correct?
   (In particular, that we found **all** subgraph isomorphisms)

This Work

- Analyze Glasgow Subgraph Solver [ADH+19, McC19]

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Graph Notation and Terminology

- Undirected graphs $\mathcal{G}$ with vertices $V(\mathcal{G})$ and edges $E(\mathcal{G})$
- No loops in this talk (for simplicity)
- Neighbours $N_{\mathcal{G}}(v) = \{u \mid (u,v) \in E(\mathcal{G})\}$
- Degree $\deg_{\mathcal{G}}(v) = \left|N_{\mathcal{G}}(v)\right|$
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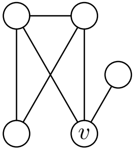

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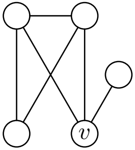

$$\deg(v) = 3$$

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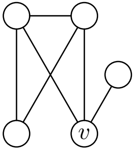

$\deg(v) = 3$
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Preprocessing Using Degree and Degree Sequence

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2. If $\deg_{\mathcal{P}}(a) > \deg_{\mathcal{T}}(u)$, then $a \not\mapsto u$

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2. If $\deg_{\mathcal{P}}(a) > \deg_{\mathcal{T}}(u)$, then $a \not\mapsto u$
3. If $\mathrm{degseq}_{\mathcal{P}}(a) \not\leq \mathrm{degseq}_{\mathcal{T}}(u)$ pointwise, then $a \not\mapsto u$

Preprocessing Using Shapes

Shapes

- Choose special shape graphs $\mathcal{S}$ with 2 special vertices s, t
- Shaped graph $\mathcal{G}^{\mathcal{S}}$ has
  1. vertices $V\left(\mathcal{G}^{\mathcal{S}}\right) = V(\mathcal{G})$
  2. edges $(u, v) \in E\left(\mathcal{G}^{\mathcal{S}}\right)$ iff $\mathcal{S}$ subgraph of $\mathcal{G}$ with $s \mapsto u$ and $t \mapsto v$

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Further preprocessing

- If
  1. $a \mapsto u$
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  3. $(a, b) \in E\big(\mathcal{P}^{\mathcal{S}}\big)$

  then must have $(u, v) \in E\big(\mathcal{T}^{\mathcal{S}}\big)$

  (Since $\mathcal{S}$ "local subgraph" of $\mathcal{P}$, has to be "local subgraph" also of $\mathcal{T}$)

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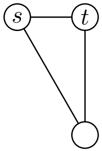
  (Since $\mathcal{S}$ "local subgraph" of $\mathcal{P}$, has to be "local subgraph" also of $\mathcal{T}$)
- So repeat degree & degree sequence preprocessing for shaped graphs
- Plus do some other stuff that we're skipping in this talk

Example of Preprocessing Using Shapes



Shape

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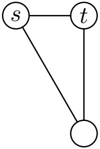

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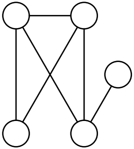

Pattern

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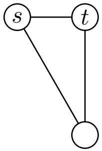

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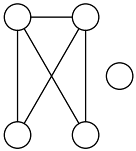

Pattern shaped

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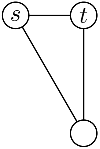

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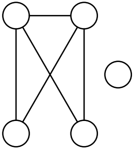

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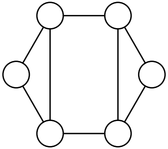
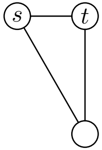


Target

Example of Preprocessing Using Shapes



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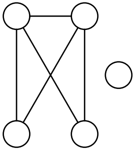

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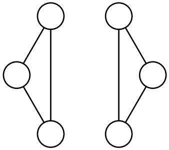

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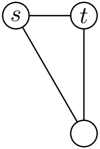

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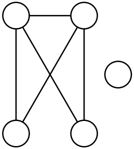

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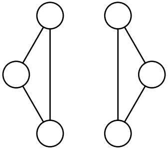

Target shaped

Now obvious that there can be no subgraph isomorphism!

Main Search Loop (Very Rough Outline)

- For every $a \in V(\mathcal{P})$ maintain possible domain $D(a) \subseteq V(\mathcal{T})$

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  1. Shrink domains of $b \in N_{\mathcal{P}}(a)$ for assigned a to $D(b) \cap N_{\mathcal{T}}(u)$
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- Run all-different propagation
  If $\exists A$ with $D(A) = \bigcup_{a \in A} D(a)$ such that
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- Repeat from top of slide
- Backtrack at failure (or when solution found)

Pseudo-Boolean Constraints

In this talk, "pseudo-Boolean" (PB) refers to 0-1 integer linear constraints

Convenient to use non-negative linear combinations of literals, a.k.a. normalized form

$$\sum_i a_i \ell_i \geq A$$

- coefficients a_i: non-negative integers
- degree (of falsity) A: positive integer
- literals ℓ_i: x_i or $\overline{x}_i$ (where $x_i + \overline{x}_i = 1$)

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In what follows:

- all constraints assumed to be implicitly normalized
- "$\sum_i a_i \ell_i \leq A$" is syntactic sugar for "$\sum_i a_i \overline{\ell}_i \geq -A + \sum_i a_i$"
- "$=$" is syntactic sugar for two inequalities "$\geq$" and "$\leq$"

Examples of Pseudo-Boolean Constraints

1. Clauses are pseudo-Boolean constraints

$$x \vee \overline{y} \vee z \quad \Leftrightarrow \quad x + \overline{y} + z \geq 1$$

(So can view CNF formula as collection of pseudo-Boolean constraints)

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2. Cardinality constraints

$$x_1 + x_2 + x_3 + x_4 + x_5 + x_6 \geq 3$$

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3. General constraints

$$x_1 + 2\overline{x}_2 + 3x_3 + 4\overline{x}_4 + 5x_5 \geq 7$$

Cutting Planes [CCT87]

Literal axioms $$\frac{}{\ell_i \geq 0}$$

Linear combination $$\frac{\sum_i a_i \ell_i \geq A \qquad \sum_i b_i \ell_i \geq B}{\sum_i (c_A a_i + c_B b_i)\ell_i \geq c_A A + c_B B} \quad [c_A, c_B \geq 0]$$

Division $$\frac{\sum_i a_i \ell_i \geq A}{\sum_i \lceil a_i / c \rceil \ell_i \geq \lceil A/c \rceil} \quad [c > 0]$$

More About Cutting Planes

A toy example:

$$\frac{6x + 2y + 3z \geq 5 \qquad x + 2y + w \geq 1}{(6x + 2y + 3z) + 2(x + 2y + w) \geq 5 + 2 \cdot 1} \text{ Linear combination}$$

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$$\frac{6x + 2y + 3z \geq 5 \qquad x + 2y + w \geq 1}{8x + 6y + 3z + 2w \geq 7} \text{ Linear combination}$$

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- Literal axioms and linear combinations sound also over the reals
- Division is where the power of cutting planes lies
- Exponentially stronger than resolution/CDCL [Hak85, CCT87]

Subgraph Isomorphism as a Pseudo-Boolean Formula

Recall:

- Pattern graph $\mathcal{P}$ with $V(\mathcal{P}) = \{a, b, c, \ldots\}$
- Target graph $\mathcal{T}$ with $V(\mathcal{T}) = \{u, v, w, \ldots\}$
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Pseudo-Boolean encoding

$$\sum_{v \in V(\mathcal{T})} x_{a \mapsto v} = 1 \qquad \text{[every } a \text{ maps somewhere]}$$

$$\sum_{b \in V(\mathcal{P})} \overline{x}_{b \mapsto u} \geq \left|V(\mathcal{P})\right| - 1 \qquad \text{[mapping is one-to-one]}$$

$$\overline{x}_{a \mapsto u} + \sum_{v \in N(u)} x_{b \mapsto v} \geq 1 \qquad \text{[edge } (a, b) \text{ maps to edge } (u, v)\text{]}$$

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Means that

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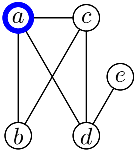
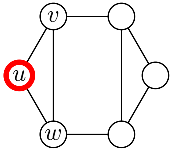
3. Proof checkable by stand-alone verifier
   - that knows nothing about graphs
   - ~~in time comparable to the solver execution~~
     in time hopefully not much larger than solver execution

Example: Degree Preprocessing with PB Reasoning





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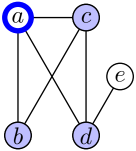

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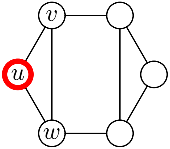

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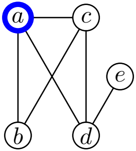

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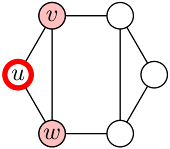

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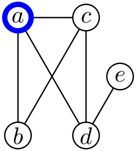

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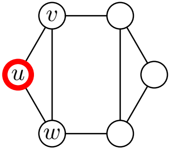

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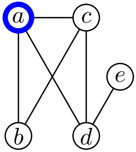

$$
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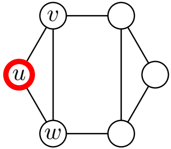

Sum up all constraints & divide by 3 to obtain

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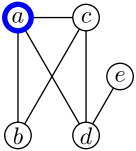

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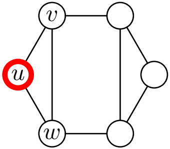

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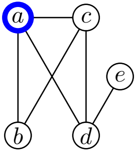

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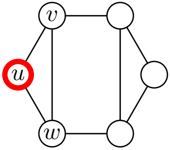

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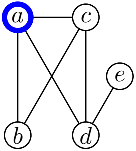

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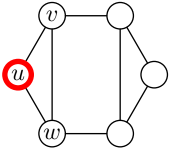

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- Remains to be seen whether this will fly in practice for subgraph isomorphism. . .

Take-Home Message

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- **This work:** Glasgow Subgraph Solver captured by cutting planes
- Consequences:
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Thank you for your attention!

References I

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