Subgraph Isomorphism Meets Cutting Planes

Towards Verifiably Correct Constraint Programming

Jakob Nordström

University of Copenhagen

KU Leuven
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Joint work with Jan Elffers, Stephan Gocht, and Ciaran McCreesh

The Problem

Input

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

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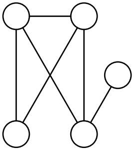
Task

- 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

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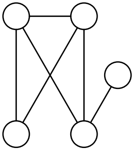

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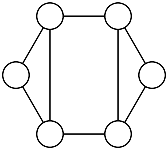

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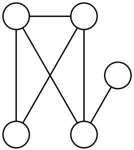

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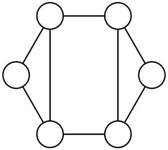

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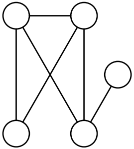
Subgraph Isomorphism Example



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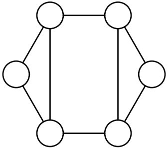

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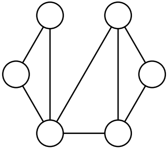
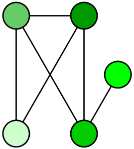


2nd target

No subgraph isomorphism

Subgraph Isomorphism Example



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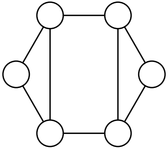

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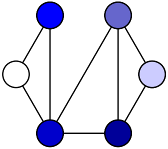

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Has subgraph isomorphism

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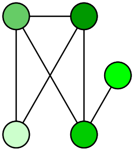

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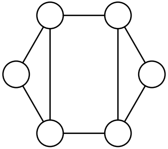

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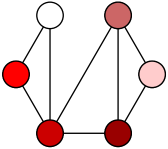

2nd target

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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2. Even more importantly: How do we know answer is correct?

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But computationally very challenging!

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

This Work

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

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- Results likely to extend also to other state-of-the-art solvers
- Intriguing possibility: learn pseudo-Boolean no-goods ⇒ exponential speed-ups!?

Outline

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 $\deg_{\mathcal{G}}(v) = |N_{\mathcal{G}}(v)|$
- Degree sequence
  $\mathrm{degseq}_{\mathcal{G}}(v) = sort_{>}(\{\deg_{\mathcal{G}}(u) \mid u \in N_{\mathcal{G}}(v)\})$

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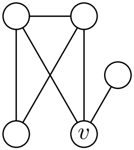

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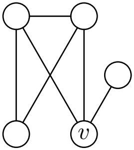

$\deg(v) = 3$

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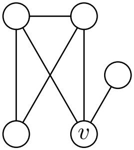

$\deg(v) = 3$
$\mathrm{degseq}(v) = (3,3,1)$

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 shape graph $\mathcal{S}$ with 2 special vertices σ, τ
- Shaped graph $\mathcal{G}^{\mathcal{S}}$ has
  1. vertices $V(\mathcal{G})$
  2. edges (u, v) iff $\mathcal{S}$ subgraph of $\mathcal{G}$ with $\sigma \mapsto u$ & $\tau \mapsto v$

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Further preprocessing

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

  then must have $(u, v) \in E(\mathcal{T}^{\mathcal{S}})$
  ($\mathcal{S}$ “local subgraph” of $\mathcal{P}$ $\Rightarrow$ “local subgraph” also of $\mathcal{T}$)

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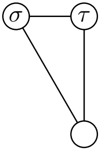
  ($\mathcal{S}$ "local subgraph" of $\mathcal{P} \Rightarrow$ "local subgraph" also of $\mathcal{T}$)
- So repeat degree & degree sequence preprocessing for shaped graphs
- Plus do some other stuff that we're skipping in this talk. . .

Example of Preprocessing Using Shapes



Shape

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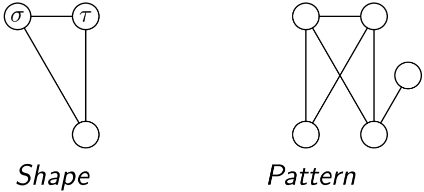

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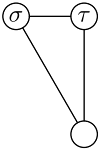

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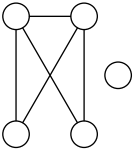

Pattern shaped

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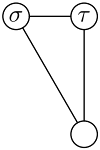

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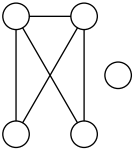

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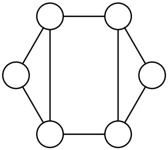
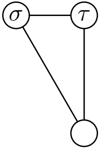


Target

Example of Preprocessing Using Shapes



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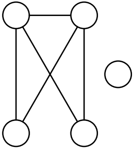

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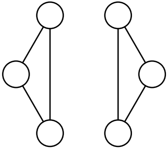

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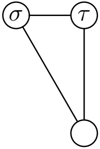

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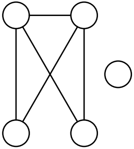

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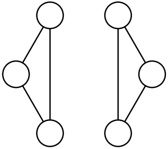
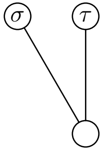


Target shaped

Now obvious that there can be no subgraph isomorphism!

Second Example of Preprocessing Using Shapes



Shape

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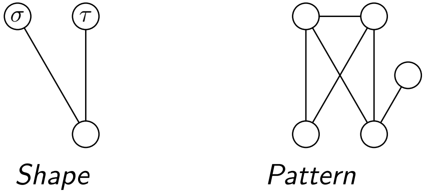

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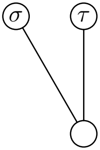

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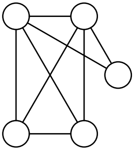

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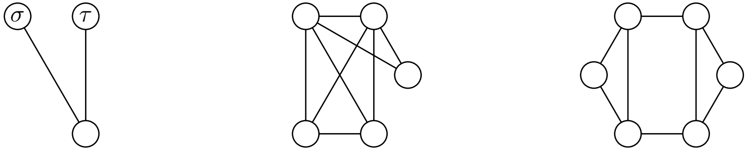

Shape

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Target

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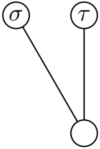

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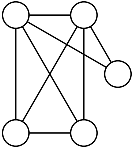

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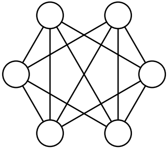

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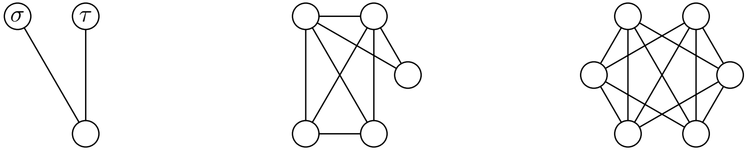

Shape *Pattern shaped* *Target shaped*

Maybe not as obviously enlightening. . .

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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- Run all-different propagation
  If $\exists A$ with $D(A) = \bigcup_{a \in A} D(a)$ such that
  1. $|D(A)| < |A| \Rightarrow$ contradiction
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- Repeat from top of slide

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- Run all-different propagation
  If $\exists A$ with $D(A) = \bigcup_{a \in A} D(a)$ such that
  1. $|D(A)| < |A| \Rightarrow$ contradiction
  2. $|D(A)| = |A| \Rightarrow$ erase $D(A)$ from other domains
- 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

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

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

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:

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

More About Cutting Planes

A toy example:

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

More About Cutting Planes

A toy example:

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

More About Cutting Planes

A toy example:

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

$$\frac{8x + 6y + 3z + 2w \geq 7}{3x + 2y + z + w \geq 3} \text{ Division}$$

- 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 $V(\mathcal{T}) = \{u, v, w, \ldots\}$
- No loops (for simplicity)

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- No loops (for simplicity)

Pseudo-Boolean encoding

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

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

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

Key Finding

All reasoning steps in Glasgow Subgraph Solver can be formalized efficiently in the cutting planes proof system

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   - that knows nothing about graphs
   - in time comparable to the solver execution

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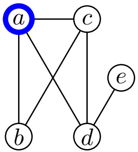
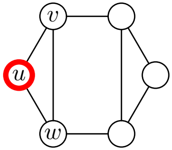
All reasoning steps in Glasgow Subgraph Solver can be formalized efficiently in the cutting planes proof system

Means that

1. Solver can justify each step by writing local formal derivation
2. Local derivations can be concatenated to global proof of correctness
3. Proof checkable by stand-alone verifier
   - that knows nothing about graphs
   - ~~in time comparable to the solver execution~~
     in time not much larger than solver execution
     (work in progress on optimizing this)

Example: Degree Preprocessing with PB Reasoning





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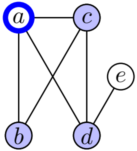
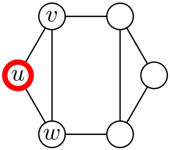


$$\overline{x}_{a \mapsto u} + x_{b \mapsto v} + x_{b \mapsto w} \geq 1$$

$$\overline{x}_{a \mapsto u} + x_{c \mapsto v} + x_{c \mapsto w} \geq 1$$

$$\overline{x}_{a \mapsto u} + x_{d \mapsto v} + x_{d \mapsto w} \geq 1$$



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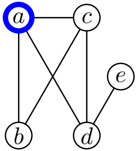

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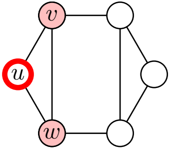

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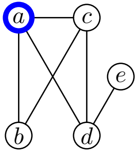

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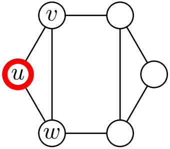

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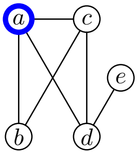

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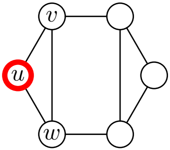
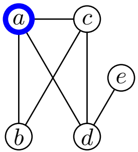


Sum up all constraints & divide by 3 to obtain

Example: Degree Preprocessing with PB Reasoning



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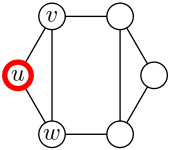
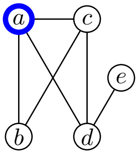


Sum up all constraints & divide by 3 to obtain

$$3\overline{x}_{a\mapsto u} + 10 \geq 11$$

Example: Degree Preprocessing with PB Reasoning



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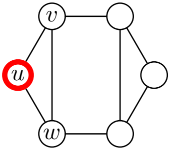

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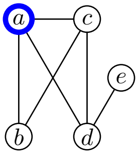

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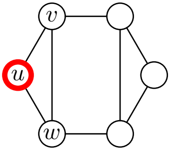
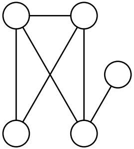


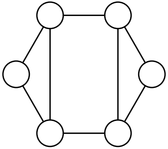
Sum up all constraints & divide by 3 to obtain

$$3\overline{x}_{a\mapsto u} \geq 1$$
$$\overline{x}_{a\mapsto u} \geq 1$$

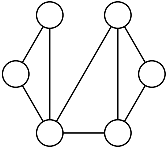
Graph Input Format



Pattern



Target 1



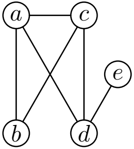
Target 2

```
5
3 1 3 4
3 0 3 4
1 3
3 0 1 2
2 0 1
```

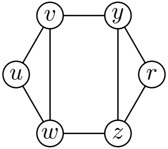
```
6
3 1 4 5
3 0 2 3
3 1 3
3 1 2 4
3 0 3 5
2 0 4
```

```
6
2 4 5
3 2 3 4
2 1 3
3 1 2 4
4 0 1 3 5
2 0 4
```

Graph Input Format



Pattern



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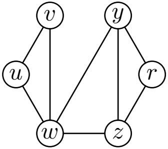

Target 2

	v,y	v,w
a,b	v,w	u,v
a,c	u,v	y,r
a,d	y,r	y,z
b,c	y,z	y,w
c,d	r,z	r,z
d,e	z,w	z,w
	u,w	u,w

Pseudo-Boolean Encoding for Mapping Pattern to Target 1

```
* #variable= 30 #constraint= 88
* pattern vertex domain constraints
1 a_v 1 a_y 1 a_w 1 a_u 1 a_r 1 a_z >= 1 ;
-1 a_v -1 a_y -1 a_w -1 a_u -1 a_r -1 a_z >= -1 ;
1 c_v 1 c_y 1 c_w 1 c_u 1 c_r 1 c_z >= 1 ;
-1 c_v -1 c_y -1 c_w -1 c_u -1 c_r -1 c_z >= -1 ;
1 d_v 1 d_y 1 d_w 1 d_u 1 d_r 1 d_z >= 1 ;
-1 d_v -1 d_y -1 d_w -1 d_u -1 d_r -1 d_z >= -1 ;
1 b_v 1 b_y 1 b_w 1 b_u 1 b_r 1 b_z >= 1 ;
-1 b_v -1 b_y -1 b_w -1 b_u -1 b_r -1 b_z >= -1 ;
1 e_v 1 e_y 1 e_w 1 e_u 1 e_r 1 e_z >= 1 ;
-1 e_v -1 e_y -1 e_w -1 e_u -1 e_r -1 e_z >= -1 ;
* injectivity constraint for target vertices
-1 a_v -1 c_v -1 d_v -1 b_v -1 e_v >= -1 ;
-1 a_y -1 c_y -1 d_y -1 b_y -1 e_y >= -1 ;
-1 a_w -1 c_w -1 d_w -1 b_w -1 e_w >= -1 ;
-1 a_u -1 c_u -1 d_u -1 b_u -1 e_u >= -1 ;
-1 a_r -1 c_r -1 d_r -1 b_r -1 e_r >= -1 ;
-1 a_z -1 c_z -1 d_z -1 b_z -1 e_z >= -1 ;
* adjacency for edge a -- c mapping a to v
1 ~a_v 1 c_y 1 c_w 1 c_u >= 1 ;
* adjacency for edge a -- d mapping a to v
1 ~a_v 1 d_y 1 d_w 1 d_u >= 1 ;
* adjacency for edge a -- b mapping a to v
1 ~a_v 1 b_y 1 b_w 1 b_u >= 1 ;
* adjacency for edge a -- c mapping a to y
1 ~a_y 1 c_v 1 c_r 1 c_z >= 1 ;
* adjacency for edge a -- d mapping a to y
1 ~a_y 1 d_v 1 d_r 1 d_z >= 1 ;
* adjacency for edge a -- b mapping a to y
1 ~a_y 1 b_v 1 b_r 1 b_z >= 1 ;
* adjacency for edge a -- c mapping a to w
1 ~a_w 1 c_v 1 c_u 1 c_z >= 1 ;
* adjacency for edge a -- d mapping a to w
1 ~a_w 1 d_v 1 d_u 1 d_z >= 1 ;
* adjacency for edge a -- b mapping a to w
1 ~a_w 1 b_v 1 b_u 1 b_z >= 1 ;
* adjacency for edge a -- c mapping a to u
1 ~a_u 1 c_v 1 c_w >= 1 ;
* adjacency for edge a -- d mapping a to u
1 ~a_u 1 d_v 1 d_w >= 1 ;
* adjacency for edge a -- b mapping a to u
1 ~a_u 1 b_v 1 b_w >= 1 ;
* adjacency for edge a -- c mapping a to r
1 ~a_r 1 c_y 1 c_z >= 1 ;
* adjacency for edge a -- d mapping a to r
1 ~a_r 1 d_y 1 d_z >= 1 ;
* adjacency for edge a -- b mapping a to r
1 ~a_r 1 b_y 1 b_z >= 1 ;
* adjacency for edge a -- c mapping a to z
1 ~a_z 1 c_y 1 c_w 1 c_r >= 1 ;
* adjacency for edge a -- d mapping a to z
1 ~a_z 1 d_y 1 d_w 1 d_r >= 1 ;
* adjacency for edge a -- b mapping a to z
1 ~a_z 1 b_y 1 b_w 1 b_r >= 1 ;
* adjacency for edge c -- a mapping c to v
1 ~c_v 1 a_y 1 a_w 1 a_u >= 1 ;
 . . .
```

Proof Logging Format and Rules (Excerpt)

Formula format: `http://www.cril.univ-artois.fr/PB12/format.pdf` with some extensions

Every constraint gets line number, which can be used to refer to the constraint

- `f [nProblemConstraints] 0`
  Load input formula from (specified) file
- `l [nVars] 0`
  Load literal axioms $x \geq 0$ *and* $\overline{x} \geq 0$ *for all variables* x
- `p [sequence in reverse polish notation] 0`
  Derive constraint by addition, scalar multiplication and division
- `u opb [PB constraint]`
  Add PB constraint as valid if negation unit propagates to contradiction
- `v [literal] [literal] ...`
  Check that partial assignment propagates to solution; add the disjunction of the negations of these literals to mark solution as found
- `c [ConstraintId] 0`
  Verify that constraint on line `ConstraintId` *is* $0 \geq A$ *for some positive* A

Proof of No Subgraph Isomorphism for Pattern & Target 1

```
* cannot map a to u due to degrees
p 0 26 + 27 + 28 + 11 + 13 + 0
* cannot map a to r due to degrees
p 0 29 + 30 + 31 + 12 + 16 + 0
* cannot map c to u due to degrees
p 0 44 + 45 + 46 + 11 + 13 + 0
* cannot map c to r due to degrees
p 0 47 + 48 + 49 + 12 + 16 + 0
* cannot map d to u due to degrees
p 0 62 + 63 + 64 + 11 + 13 + 0
* cannot map d to r due to degrees
p 0 65 + 66 + 67 + 12 + 16 + 0
* [0] guessing a=z and propagating
* hall set or violator size 3/3
p 0 1 + 3 + 5 + 12 + 13 + 16 + 0
* hall set or violator size 4/4
p 0 1 + 3 + 5 + 7 + 12 + 13 + 15 + 16 + 0
* unit propagating b=r
* hall set or violator size 3/3
p 0 1 + 3 + 7 + 12 + 15 + 16 + 0
* unit propagating c=y
* [1] propagation failure on a=z
u opb -1 a_z >= 0 ;
* [0] guessing a=v and propagating
* hall set or violator size 3/3
p 0 1 + 3 + 5 + 11 + 12 + 13 + 0
* hall set or violator size 4/4
p 0 1 + 3 + 5 + 7 + 11 + 12 + 13 + 14 + 0
* unit propagating b=u
* hall set or violator size 3/3
p 0 1 + 3 + 7 + 11 + 13 + 14 + 0
* unit propagating c=w
* [1] propagation failure on a=v
u opb -1 a_v >= 0 ;
* [0] guessing a=w and propagating
* hall set or violator size 3/3
p 0 1 + 3 + 5 + 11 + 13 + 16 + 0
* hall set or violator size 4/4
p 0 1 + 3 + 5 + 7 + 11 + 13 + 14 + 16 + 0
* unit propagating b=u
* hall set or violator size 3/3
p 0 1 + 3 + 7 + 11 + 13 + 14 + 0
* unit propagating c=v
* [1] propagation failure on a=w
u opb -1 a_w >= 0 ;
* [0] guessing a=y and propagating
* hall set or violator size 3/3
p 0 1 + 3 + 5 + 11 + 12 + 16 + 0
* hall set or violator size 4/4
p 0 1 + 3 + 5 + 7 + 11 + 12 + 15 + 16 + 0
* unit propagating b=r
* hall set or violator size 3/3
p 0 1 + 3 + 7 + 12 + 15 + 16 + 0
* unit propagating c=z
* [1] propagation failure on a=y
u opb -1 a_y >= 0 ;
* [0] out of guesses
* asserting that we've proved unsat
u opb >= 1 ;
c 171 0
```

Proof for Subgraph Isomorphisms for Pattern & Target 2

```
proof using f l p u c v 0
f 88 0
l 30 0
* cannot map a to v due to degrees
p 0 17 + 18 + 19 + 12 + 13 + 0
* cannot map a to u due to degrees
p 0 23 + 24 + 25 + 11 + 12 + 0
* cannot map a to r due to degrees
p 0 29 + 30 + 31 + 14 + 16 + 0
* cannot map c to v due to degrees
p 0 35 + 36 + 37 + 12 + 13 + 0
* cannot map c to u due to degrees
p 0 41 + 42 + 43 + 11 + 12 + 0
* cannot map c to r due to degrees
p 0 47 + 48 + 49 + 14 + 16 + 0
* cannot map d to v due to degrees
p 0 53 + 54 + 55 + 12 + 13 + 0
* cannot map d to u due to degrees
p 0 59 + 60 + 61 + 11 + 12 + 0
* cannot map d to r due to degrees
p 0 65 + 66 + 67 + 14 + 16 + 0
* [0] guessing a=z and propagating
* hall set or violator size 3/3
p 0 1 + 3 + 5 + 12 + 14 + 16 + 0
* hall set or violator size 4/4
p 0 1 + 3 + 5 + 7 + 12 + 14 + 15 + 16 + 0
* unit propagating b=r
* hall set or violator size 3/3
p 0 1 + 3 + 7 + 14 + 15 + 16 + 0
* unit propagating c=y
```

```
* unit propagating d=w
* [1] guessing e=u and propagating
* found solution a=z b=r c=y d=w e=u
v a_z b_r c_y d_w e_u
* [2] incorrect guess
u opb -1 a_z -1 e_u >= -1 ;
* [1] guessing e=v
* unit propagating e=v
* found solution a=z b=r c=y d=w e=v
v a_z b_r c_y d_w e_v
* [2] incorrect guess
 . . .
* [1] guessing e=u and propagating
* found solution a=y b=r c=z d=w e=u
v a_y b_r c_z d_w e_u
* [2] incorrect guess
u opb -1 a_y -1 e_u >= -1 ;
* [1] guessing e=v and propagating
* found solution a=y b=r c=z d=w e=v
v a_y b_r c_z d_w e_v
* [2] incorrect guess
u opb -1 a_y -1 e_v >= -1 ;
* [1] out of guesses
* [1] incorrect guess
u opb -1 a_y >= 0 ;
* [0] out of guesses
* asserting that we've proved unsat
u opb >= 1 ;
c 178 0
```

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- Subgraph isomorphism algorithm performs tree-like search
- Can we learn from failures and cut away larger parts of search space?

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

Take-Home Message

- Subgraph isomorphism important problem with many applications
- Can often be efficiently solved, but what about correctness?
- **This work:** Glasgow Subgraph Solver captured by pseudo-Boolean reasoning using cutting planes
- Consequences:
  1. Efficiently verifiable certificates of correctness
  2. Potential for exponential speed-up from PB no-goods?
- **Caveat:** Still work in progress. . .
- **Question:** Can cutting planes formalize algorithms for other hard combinatorial problems in similar way?

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Thank you for your attention!

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