Subgraph Isomorphism Meets Cutting Planes

Towards Verifiably Correct Constraint Programming

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Joint work with 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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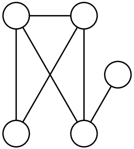
Task

- 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



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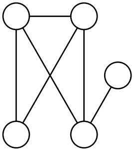

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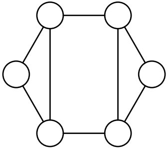

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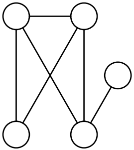

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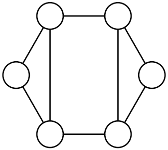

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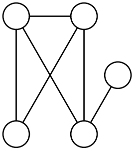

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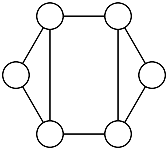

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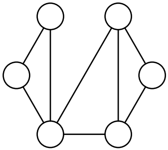

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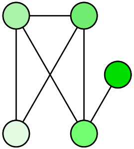
No subgraph isomorphism

Subgraph Isomorphism Example



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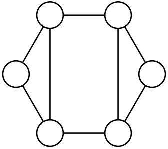

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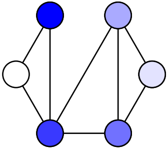

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Has subgraph isomorphism

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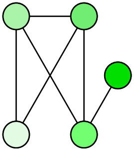

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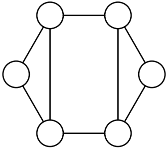

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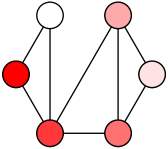

2nd target

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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. 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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- And to constraint programming in general... [EGMN20]
- Intriguing possibility: learn pseudo-Boolean no-goods $\Rightarrow$ 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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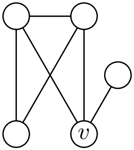

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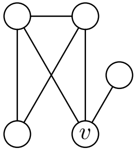

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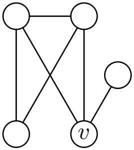

$\deg(v) = 3$
$\mathrm{degseq}(v) = (3, 3, 1)$

Preprocessing Using Degree and Degree Sequence

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1. If $\left|V(\mathcal{P})\right| > \left|V(\mathcal{T})\right|$, then no solution
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. $a \mapsto u$
  2. $b \mapsto v$
  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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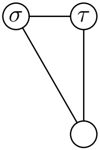
  ($\mathcal{S}$ "local subgraph" of $\mathcal{P} \Rightarrow$ "local subgraph" also of $\mathcal{T}$)
- So repeat degree & degree sequence preprocessing for shaped graphs
- Plus do some other stuff that we're skipping in this talk. . .

Example of Preprocessing Using Shapes



Shape

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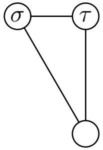

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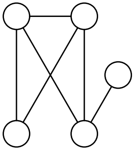

Pattern

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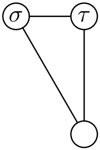

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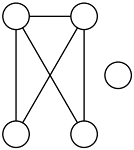

Pattern shaped

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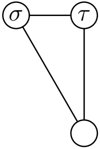

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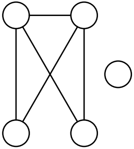

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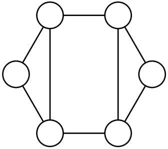

Target

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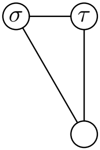

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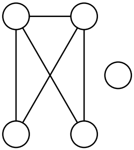

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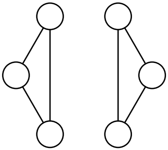

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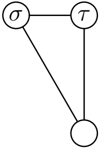

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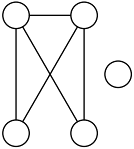

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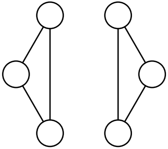
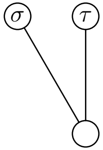


Target shaped

Now obvious that there can be no subgraph isomorphism!

Second Example of Preprocessing Using Shapes



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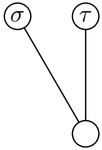

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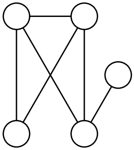

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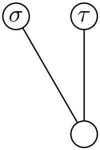

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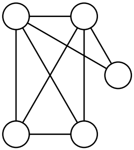

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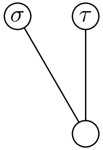

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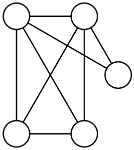

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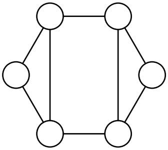

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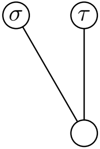

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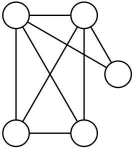

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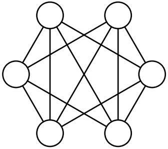

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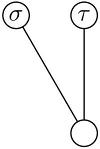

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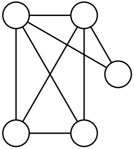

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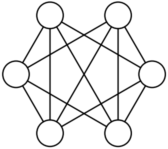

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Maybe not as obviously enlightening. . .

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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- For every $a \in V(\mathcal{P})$ maintain possible domain $D(a) \subseteq V(\mathcal{T})$
- Pick a with smallest domain & iterate over $a \mapsto u$ for $u \in D(a)$

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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- 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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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:

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

More About Cutting Planes

A toy example:

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

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

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

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Pseudo-Boolean encoding

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

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

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

Key Finding

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

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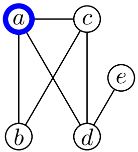
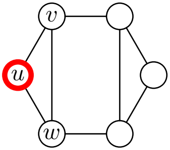
3. Proof checkable by stand-alone verifier
    - that knows nothing about graphs
    - ~~in time comparable to the solver execution~~
      in time hopefully not too much larger than solver execution (work in progress on optimizing this)
4. Further interesting features:
    - Even for buggy solver, a correct proof is always accepted
    - Even for formally verified solver that gets whacked by cosmic radiation/hardware failure, wrong proof will always be rejected

Example: Degree Preprocessing with PB Reasoning





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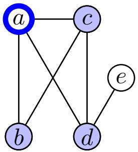
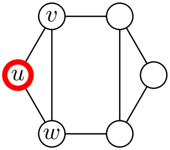


$$\overline{x}_{a \mapsto u} + x_{b \mapsto v} + x_{b \mapsto w} \geq 1$$

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

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



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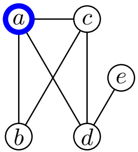

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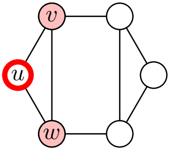

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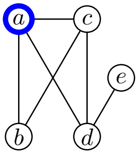

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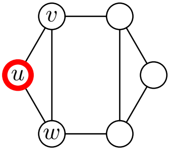

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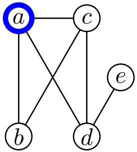

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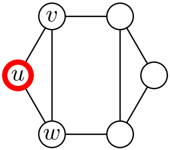

Sum up all constraints & divide by 3 to obtain

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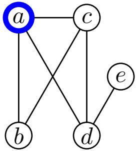

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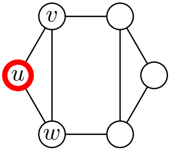

Sum up all constraints & divide by 3 to obtain

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

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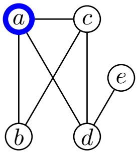

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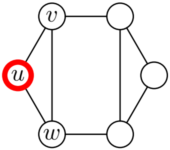

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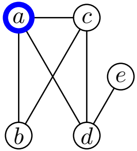

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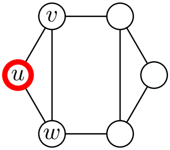

Sum up all constraints & divide by 3 to obtain

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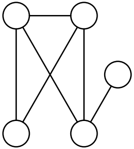
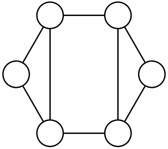
Graph Input Format



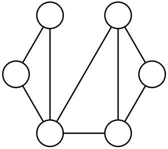
Pattern

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



Target 1

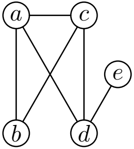
```
6
3 1 4 5
3 0 2 3
3 1 3
3 1 2 4
3 0 3 5
2 0 4
```



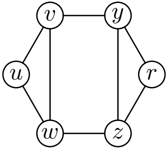
Target 2

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

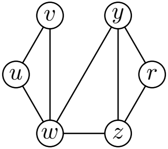
Graph Input Format



Pattern



Target 1



Target 2

Pattern	Target 1	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)

Formulas: Extension of *OPB* (`www.cril.univ-artois.fr/PB12/format.pdf`)
Proofs: *VeriPB* (`github.com/StephanGocht/VeriPB`, [EGMN20])

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

- `f [nProblemConstraints] 0`
  Load input formula from (specified) file
- `p [sequence of operations in reverse polish notation] 0`
  Derive constraint by addition, scalar multiplication and division
- `u [PB constraint]`
  Add PB constraint as valid if negation unit propagates to contradiction
- `j [constraintId] [PB constraint]`
  Add PB constraint as valid if implied by constraint on given line
- `d [constraintId1] [constraintId2] [constraintId3] ... 0`
  Delete constraints from database of derived PB constraints
- `v [literal] [literal] ... 0`
  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

```
pseudo-Boolean proof version 1.0
f 88 0
* cannot map a to u due to degrees in graph pairs 0
p 26 27 + 28 + 11 + 13 + 0
j 89 1 ~xa_u >= 1 ;
d 89 0
* cannot map a to r due to degrees in graph pairs 0
p 29 30 + 31 + 12 + 16 + 0
j 91 1 ~xa_r >= 1 ;
d 91 0
* cannot map c to u due to degrees in graph pairs 0
p 56 57 + 58 + 11 + 13 + 0
j 93 1 ~xc_u >= 1 ;
d 93 0
* cannot map c to r due to degrees in graph pairs 0
p 59 60 + 61 + 12 + 16 + 0
j 95 1 ~xc_r >= 1 ;
d 95 0
* cannot map d to u due to degrees in graph pairs 0
p 74 75 + 76 + 11 + 13 + 0
j 97 1 ~xd_u >= 1 ;
d 97 0
* cannot map d to r due to degrees in graph pairs 0
p 77 78 + 79 + 12 + 16 + 0
j 99 1 ~xd_r >= 1 ;
d 99 0
* [0] guessing a=z
* unit propagating a=z
* hall set or violator size 3/3
p 1 5 + 7 + 12 + 13 + 16 + 0
* hall set or violator size 4/4
p 1 5 + 7 + 3 + 12 + 13 + 15 + 16 + 0
* unit propagating b=r
* hall set or violator size 3/3
p 1 3 + 5 + 12 + 15 + 16 + 0
* unit propagating c=y
* [1] propagation failure on a=z
u  1 ~xa_z >= 1 ;
* [0] guessing a=v
* unit propagating a=v
* hall set or violator size 3/3
p 1 5 + 7 + 11 + 12 + 13 + 0
* hall set or violator size 4/4
p 1 5 + 7 + 3 + 11 + 12 + 13 + 14 + 0
* unit propagating b=u
* hall set or violator size 3/3
p 1 3 + 5 + 11 + 13 + 14 + 0
* unit propagating c=w
* [1] propagation failure on a=v
u  1 ~xa_v >= 1 ;
* [0] guessing a=w
* unit propagating a=w
* hall set or violator size 3/3
p 1 5 + 7 + 11 + 13 + 16 + 0
* hall set or violator size 4/4
p 1 5 + 7 + 3 + 11 + 13 + 14 + 16 + 0
* unit propagating b=u
* hall set or violator size 3/3
p 1 3 + 5 + 11 + 13 + 14 + 0
* unit propagating c=v
* [1] propagation failure on a=w
u  1 ~xa_w >= 1 ;
* [0] guessing a=y
* unit propagating a=y
* hall set or violator size 3/3
p 1 5 + 7 + 11 + 12 + 16 + 0
* hall set or violator size 4/4
p 1 5 + 7 + 3 + 11 + 12 + 15 + 16 + 0
* unit propagating b=r
* hall set or violator size 3/3
p 1 3 + 5 + 12 + 15 + 16 + 0
* unit propagating c=z
* [1] propagation failure on a=y
u  1 ~xa_y >= 1 ;
* asserting that we've proved unsat
u >= 1 ;
c 117 0
```

Proof for Subgraph Isomorphisms for Pattern & Target 2

```
pseudo-Boolean proof version 1.0
f 88 0
* cannot map a to v due to degrees in graph pairs 0
p 17 18 + 19 + 12 + 13 + 0
j 89 1 ~xa_v >= 1 ;
d 89 0
* cannot map a to u due to degrees in graph pairs 0
p 23 24 + 25 + 11 + 12 + 0
j 91 1 ~xa_u >= 1 ;
d 91 0
* cannot map a to r due to degrees in graph pairs 0
p 29 30 + 31 + 14 + 16 + 0
j 93 1 ~xa_r >= 1 ;
d 93 0

 .  .  .

* [1] guessing e=u
* unit propagating e=u
# 3
* found solution a=z b=r c=y d=w e=u
v xa_z xb_r xc_y xd_w xe_u
# 2
* [2] backtracking
u  1 ~xa_z 1 ~xe_u >= 1 ;
w 3
* [1] guessing e=v
* unit propagating e=v
# 3
* found solution a=z b=r c=y d=w e=v
v xa_z xb_r xc_y xd_w xe_v
# 2
* [2] backtracking
u  1 ~xa_z 1 ~xe_v >= 1 ;
w 3
# 1
* [1] incorrect guess
u  1 ~xa_z >= 1 ;
w 2
* [0] guessing a=w
* unit propagating a=w
* hall set or violator size 3/3
p 1 3 + 5 + 12 + 14 + 16 + 0
* [1] propagation failure on a=w
u  1 ~xa_w >= 1 ;
* [0] guessing a=y
* unit propagating a=y
* hall set or violator size 3/3
p 1 5 + 7 + 12 + 14 + 16 + 0
* hall set or violator size 4/4
p 1 5 + 7 + 3 + 12 + 14 + 15 + 16 + 0
* unit propagating b=r
* hall set or violator size 3/3
p 1 3 + 5 + 14 + 15 + 16 + 0
* unit propagating c=z
* unit propagating d=w
# 2
* [1] guessing e=v
* unit propagating e=v
# 3
* found solution a=y b=r c=z d=w e=v
v xa_y xb_r xc_z xd_w xe_v
# 2
* [2] backtracking
u  1 ~xa_y 1 ~xe_v >= 1 ;
w 3
* [1] guessing e=u
* unit propagating e=u
# 3
* found solution a=y b=r c=z d=w e=u
v xa_y xb_r xc_z xd_w xe_u
# 2
* [2] backtracking
u  1 ~xa_y 1 ~xe_u >= 1 ;
w 3
# 1
* [1] incorrect guess
u  1 ~xa_y >= 1 ;
w 2
* asserting that we've proved unsat
u >= 1 ;
c 129 0
```

Better Subgraph Solvers by Learning No-Goods?

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

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- E.g., can do all-different propagation, which CDCL can't

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- Pseudo-Boolean solvers *Sat4j* [LP10] and *RoundingSat* [EN18] can be exponentially stronger
- E.g., can do all-different propagation, which CDCL can't
- 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:** Further optimizations still needed...
- **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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