# Efficient MUS Enumeration of Horn Formulae with Applications to Axiom Pinpointing

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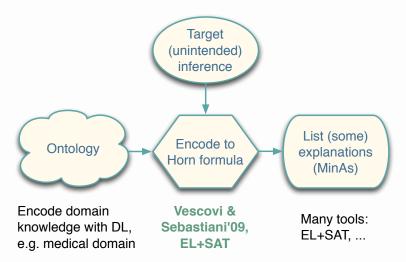
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    - ► E.g. SNOMED CT: Systematized Nomenclature Of MEDicine Clinical Terms → 311,000 concepts

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[BS08]

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VS09]

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- Our goal: efficient enumeration of MUSes of Horn formulae



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- Axiom pinpointing corresponds to group MUS enumeration of Horn formulae:
  - ▶ Group 0 ( $G_0$ ): Set of Horn clauses representing background knowledge, e.g. encode classification of the  $\mathcal{EL}^+$  ontology; ignored for the purpose of reporting MUSes
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  - Additional groups, each with a single unit clause, representing one axiom
  - ► Enumeration of MUSes of group Horn formulae is not output polynomial unless P = NP [BPS07]

# Outline

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## Description logic $\mathcal{EL}^+$

- $N_C$ ,  $N_R$  denote concept & role names, respectively
- Concept descriptions formed using 3 constructors below
- ullet Ontology  ${\mathcal T}$  is a finite set of GCI's and RI's

	Syntax	Semantics
top	Т	4
conjunction	$X \sqcap Y$	$X^{\perp} \cap Y^{\perp}$
existential restriction	∃r.X	
general concept inclusion	$X \sqsubseteq Y$	$X^{\mathcal{I}} \subseteq Y^{\mathcal{I}}$
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- Interpretation:  $\mathcal{I} = (\Delta^{\mathcal{I}}, \cdot^{\mathcal{I}})$ , where
  - $-\Delta^{\mathcal{I}}$  is non-empty set of individuals, and
  - $-\cdot^{\mathcal{I}}$  maps
    - ▶ Each  $C \in N_C$  to  $C^{\mathcal{I}} \subseteq \Delta^{\mathcal{I}}$
    - ▶ Each  $r \in N_R$  to a binary relation  $r^T$  in  $\Delta^T$
  - $-\cdot^{\mathcal{I}}$  is defined inductively for arbitrary concept descriptions:

	Syntax	Semantics
top	Т	$\Delta^{\mathcal{I}}$
conjunction	$X \sqcap Y$	$X^{\mathcal{I}} \cap Y^{\mathcal{I}}$
existential restriction	∃r.X	$\{x \in \Delta^{\mathcal{I}} \mid \exists y \in \Delta^{\mathcal{I}} : (x, y) \in r^{\mathcal{I}} \land y \in X^{\mathcal{I}}\}$
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- Classification: infer all subsumption relations between atomic concepts
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- MinA: minimal set of axioms from which some subsumption relation can be inferred

## Example of medical ontology

```
Endocarditis \sqsubseteq Inflammation \sqcap \existshasLoc.Endocardium, Inflammation \sqsubseteq Disease \sqcap \existsactsOn.Tissue, Endocardium \sqsubseteq Tissue \sqcap \existscontIn.HeartValve, HeartValve \sqsubseteq \existscontIn.Heart, HeartDisease \equiv Disease \sqcap \existshasLoc.Heart, contIn \circ contIn \sqsubseteq contIn, hasLoc \circ contIn \sqsubseteq hasLoc
```

- MinA example:
  - Endocarditis 
     ⊆ HeartDisease explained by axioms above
- Unintended subsumption in (old version of) SNOMED CT: AmputationOfFinger □<sub>O</sub> AmputationOfHand



[BS08]

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  - Compute all MCSes
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  - But, there can be exponentially many MCSes
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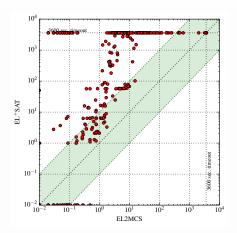
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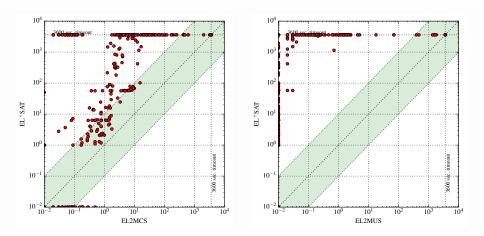


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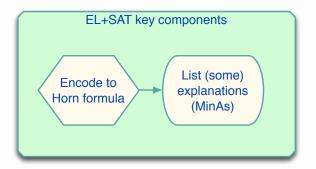
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## What is EL<sup>+</sup>SAT?

• Two main components: Horn encoder & MinA enumerator

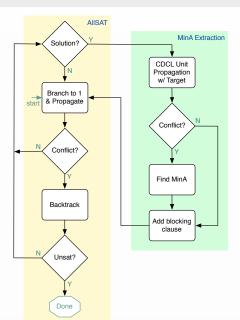
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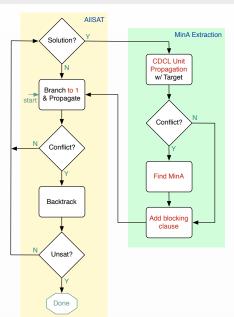
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  - Corresponds to SAT with preferences

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- Horn formulae decided by unit propagation with CDCL SAT solver
  - In MiniSat, unit propagation takes worst-case quadratic time, due to implementation of watched literals
  - Also, unnecessary propagation of 0-valued variables
  - We can do better: use dedicated LTUR algorithm

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- Computing each MinA corresponds to deletion-based MUS extraction
  - We can do better: use insertion-based MUS extraction (more later)
- Blocking of MCSes/MSSes does not eliminate supersets of MCSes (or subsets of MSSes)
  - Why? Clause learning only uses decision variables; learned clauses only contain negative literals; supersets of MCSes not blocked



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- 1. Partial MUS enumeration paradigm
  - Implements implicit hitting set dualization

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4. Dedicated Horn decision procedure – LTUR

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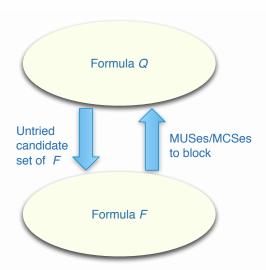
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- 4. Dedicated Horn decision procedure LTUR

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5. Dedicated MUS extraction algorithm for Horn formulae

## Partial MUS enumeration – eMUS / MARCO



## Partial MUS enumeration – eMUS / MARCO (cont.)

```
Input: CNF formula F
Output: Reports the set of MUSes of F
I \leftarrow \{p_i \mid c_i \in F\}
                                                  # Variable p_i picks clause c_i
Q \leftarrow \emptyset
while true do
    (st, P) \leftarrow \mathsf{MaximalModel}(Q)
                                             # Hit MCSes w/o repeating MUSes height
    if not st then return
    F' \leftarrow \{c_i \mid p_i \in P\}
                                                         # Pick selected clauses
    M \leftarrow \mathsf{ComputeMUS}(F')
    ReportMUS(M)
     b \leftarrow \{ \neg p_i \mid c_i \in M \}
                                                              # Block computed MUS
  b \leftarrow \{p_i \mid p_i \in I \setminus P\}
                                                          # Block computed MCS/MSS
 Q \leftarrow Q \cup \{b\}
```

# MUS/MCS blocking

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                                              # Negative clause blocking MUS
  b \leftarrow \{p_i \mid p_i \in I \setminus P\}
                                          # Positive clause blocking MCS/MSS
 Q \leftarrow Q \cup \{b\}
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```
G_0 = \{ (\neg a \lor \neg b), (b), (\neg c \lor \neg d \lor \neg e) \}
G_1 = \{ (a) \}
G_2 = \{ (c) \}
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  - Blocking clauses:  $(\neg p_1)$ ,  $(\neg p_2 \lor \neg p_3 \lor \neg p_4)$

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- Alternative: blocking clause  $(p_1 \lor p_2)$  [PMS13,LM13,LPMMS15]

# An example with eMUS / MARCO (cont.)

```
G_0 = \{ (\neg a \lor \neg b), (b), (\neg c \lor \neg d \lor \neg e) \}  MUS = \{ \{(a)\}, \{(c), (d), (e)\} \} MCS = \{ \{(a)\}, \{(a)\}, \{(a), (e)\} \} G<sub>2</sub> = \{(c)\} G<sub>3</sub> = \{(d)\} G<sub>4</sub> = \{(e)\}
```

#### Blocking with negative clauses

Q	MxM model	MUS	MCS	Blocking clause	OK?
Ø	$p_1 = \ldots = 1$	$\{G_1\}$		$B_1 = (\neg p_1)$	1
$\{B_1\}$	$p_2=\ldots=1$	$\{G_2, G_3, G_4\}$		$B_2 = (\neg p_2 \vee \neg p_3 \vee \neg p_4)$	1
$\{B_1,B_2\}$	$p_3=p_4=1$		$\{G_1,G_2\}$	$B_3 = (\neg p_3 \vee \neg p_4)$	✓
$\{B_1, B_2, B_3\}$	$p_2=p_3=1$		$\{G_1,G_4\}$	$B_4 = (\neg p_2 \vee \neg p_3)$	1
$\{B_1,\ldots,B_4\}$	$p_2=p_4=1$		$\{G_1,G_3\}$	$B_5 = (\neg p_2 \vee \neg p_4)$	✓
$\{B_1,\ldots,B_5\}$	$p_3 = 1$		$\{G_1, G_2, G_4\}$	$B_6=(\neg p_3)$	X
$\{B_1,\ldots,B_6\}$	$p_4 = 1$		$\{G_1,G_2,G_3\}$	$B_7 = (\neg p_4)$	X
$\{B_1,\ldots,B_7\}$	$p_1=\ldots=0$				

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#### • Distinct blocking of MUSes and MCSes

[PMS13,LM13,LPMMS13]

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$\{B_1\}$	$p_2=\ldots=1$	$\{G_2, G_3, G_4\}$		$B_2 = (\neg p_2 \vee \neg p_3 \vee \neg p_4)$	1
$\{B_1,B_2\}$	$p_3=p_4=1$		$\{G_1,G_2\}$	$B_3=(p_1\vee p_2)$	1
$\{B_1, B_2, B_3\}$	$p_2=p_3=1$		$\{G_1,G_4\}$	$B_4 = (p_1 \vee p_4)$	1
$\{B_1,\ldots,B_4\}$	$p_2=p_4=1$		$\{G_1,G_3\}$	$B_5=(p_1\vee p_3)$	1
$\{B_1,\ldots,B_5\}$	Ø		$\{G_1, G_2, G_3\}$		

## Computing maximal models

```
Input: Q a CNF formula
Output: (st, P): with st a Boolean and P a MxM (if it exists)
 # P: under-approximation of maximal model
 # U: remaining target set of literals
# B: backbone literals
(P, U, B) \leftarrow (\{\{x\} \mid \neg x \notin L(Q)\}, \{\{x\} \mid \neg x \in L(Q)\}, \emptyset)
(st, P, U) \leftarrow InitialAssignment(Q \cup P)
if not st then return (false, \emptyset)
while U \neq \emptyset do
    I \leftarrow \mathsf{SelectLiteral}(U)
   (st, \mu) = SAT(Q \cup P \cup B \cup \{I\})
# Else, update B with backbone literal from U)
 (U,B) \leftarrow (U \setminus \{I\}, B \cup \{\neg I\})
return (true, P)
                                                               # P is a MxM of Q
```

#### **LTUR**

- Simplified implementation of Dowling&Gallier's algorithm [DG84,M88]
- Variables assigned value 0, by default
- Can be viewed as one-sided unit propagation, i.e. propagate only variables that must be assigned value 1
- There is no branching
- Either no conflicts or a single conflict
- Data structures:
  - Use adjacency lists (for negative literals)
  - Use clause counters for the negative literals
- Run time:  $\mathcal{O}(||F||)$
- And, LTUR can be used incrementally



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  - $-\mathcal{O}(|F|)$  calls to SAT oracle
  - For Horn formulae, with LTUR:  $\mathcal{O}(|F| \cdot ||F||)$

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- But, LTUR can be used incrementally!
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  - For Horn formulae, with LTUR:  $\mathcal{O}(|M| \cdot ||F||)$
- Thus, for Horn formulae, with an incremental decision procedure, insertion-based is preferable to deletion-based!
  - Also, QuickXplain/Progression cannot improve over insertion-based

#### Insertion-based MUS extraction

```
Input: H denotes the G_0 clauses; I denotes the set of (individual) group clauses
Output: M denotes the computed MUS
# LTUR_prop / LTUR_undo: incremental LTUR propagation / undo
(M, c_r) \leftarrow (H, 0)
LTUR_prop(M, M)
                                      # Start by propagating G_0 clauses
while true do
    if c_r > 0 then
        M \leftarrow M \cup \{c_r\}
                           # Add transition clause c_r to M
        if not LTUR_prop(M, \{c_r\}) then
            LTUR_{undo}(M, M)
           return M \setminus H # Remove G_0 clauses from computed MUS
    S \leftarrow \emptyset
    while true do
        c_r \leftarrow \mathsf{SelectRemoveClause}(I)
                                               # Target transition clause
        S \leftarrow S \cup \{c_r\}
        if not LTUR_prop(M \cup S, {c_r}) then
           I \leftarrow S \setminus \{c_r\}
                                          # Update working set of groups
           LTUR\_undo(M, S)
           break
                                    # c_r represents a transition clause
                                                      4 D > 4 P > 4 E > 4 E > E 9 Q P
```

# Outline

- Medical ontologies:
  - GALEN, with two variants: FULL-GALEN and NOT-GALEN
  - GENE
  - NCI
  - SNOMED CT

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- x2: apply COI, re-encode to ontology and encode to Horn formula
- Compute cluster, with 3600s time limit and 4 GByte memory limit



### Experimental setup – goal & tools

- Goal:
  - Compute all MinAs/MUSes or as many MinAs/MUSes as possible within the given timeout
- Our tool:
  - EL2MUS: uses EL<sup>+</sup>SAT encoder as front-end to HgMUS
- Other SAT-based tools:
  - EL<sup>+</sup>SAT: developed in 2009, updated in 2014, 2015

[VS09, VS15]

EL2MCS: developed in 2015

AMMS15

- SATPin: developed in 2015

[MP15]

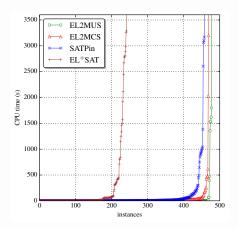
- Other (non SAT-based) tools:
  - CEL only computes 10 MinAs, developed in 2006

[BLS06]

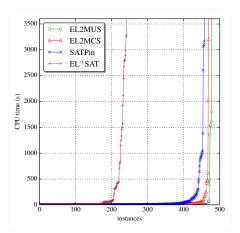
– JUST – cannot handle all  $\mathcal{EL}^+$  constructs, developed in 2014

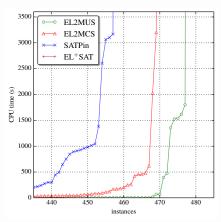
[L14]

# Cactus plots – COI instances

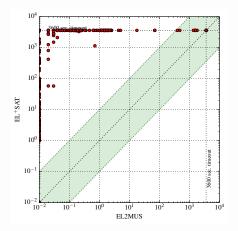


## Cactus plots – COI instances

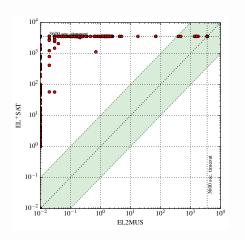


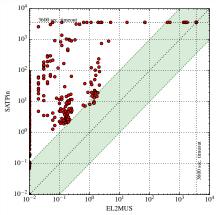


## Scatter plots – COI instances

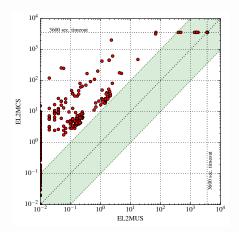


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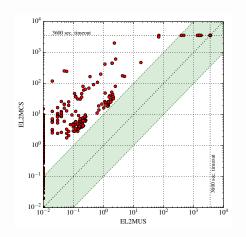




# Scatter plots – COI instances (cont.)

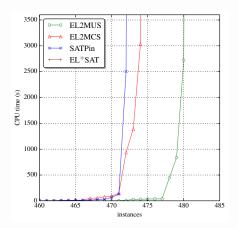


# Scatter plots – COI instances (cont.)

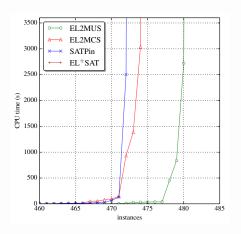


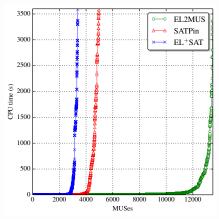
% wins	EL <sup>+</sup> SAT	SATPin	EL2MCS
EL+SAT	_	20.29%	17.66%
SATPin	79.71%	-	19.13%
EL2MCS	82.34%	80.41%	_
EL2MUS	100.0%	100.0%	100.0%
$> 10^{1}$ x	98.09%	96.78%	98.41%
$> 10^{2}$ x	97.55%	72.07%	58.07%
$> 10^{3}$ x	96.46%	47.75%	14.09%
> 10 <sup>4</sup> x	74.05%	06.49%	00.00%
$> 10^{5}$ x	31.10%	00.45%	00.00%

## Cactus plots - x2 instances

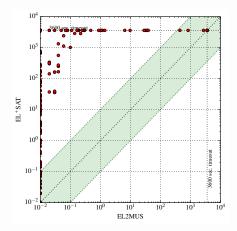


#### Cactus plots – x2 instances

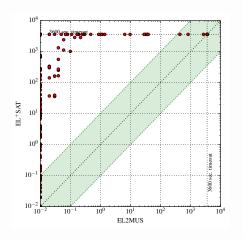


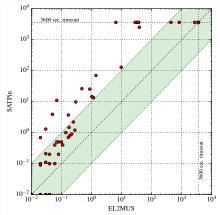


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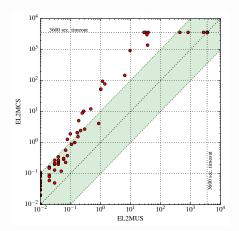


## Scatter plots – x2 instances

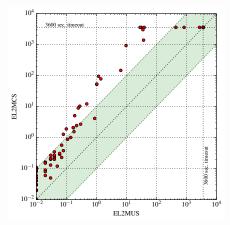




# Scatter plots – x2 instances (cont.)

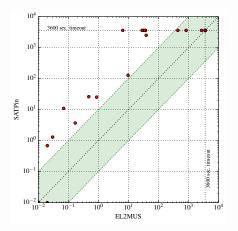


## Scatter plots – x2 instances (cont.)

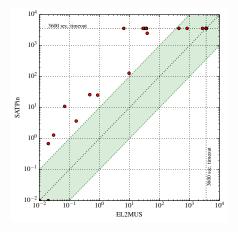


% wins	EL <sup>+</sup> SAT	SATPin	EL2MCS
EL <sup>+</sup> SAT	-	00.00%	00.00%
SATPin	100.0%	-	91.55%
EL2MCS	100.0%	08.45%	_
EL2MUS	100.0%	67.69%	99.32%
19 TO inst	EL <sup>+</sup> SAT	SATPin	EL2MCS
# MUSes	788	1484	0
Δ MUSes	9160	8864	9948

#### SNOMED CT x2 instances - EL2MUS vs. SATPin

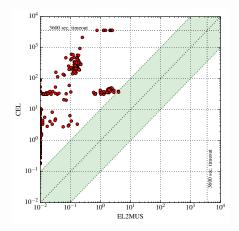


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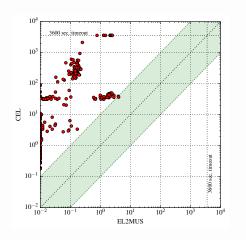


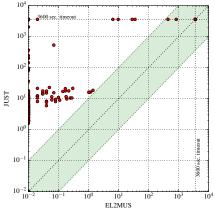
$\#$ instances with run time $\geq$ 3600s	19	
$\#$ instances with run time $\le 0.1$ s	65	
# EL2MUS wins		
Total instances	100	

#### Non-SAT based tools – vs CEL on COI instances



#### Non-SAT based tools – vs Just on x2 instances





## Outline

#### Conclusions & research directions

- Novel MUS enumeration algorithm for group Horn formulae
  - Exploits partial MUS enumeration, MCS extraction, (old) LTUR, insertion-based MUS extraction, etc.
- Application in axiom pinpointing of  $\mathcal{EL}^+$  ontologies
- Orders of magnitude speedups for the larger instances (i.e. COI)
- Clear performance gains for the smaller instances (i.e. x2)
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- Develop standalone axiom pinpointing tool
  - Collaboration with SATPin authors
- Integrate recent advances in MUS & MCS extraction

#### Thank You