

Outlier Detection and Explanation with Random Forests

Graph mining and outlier detection meets Logic proof tutoring

Karel Vaculík, Leona Nezvalová, Luboš Popelínský

Knowledge Discovery Lab, FI MU Brno

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Outline

- Resolution for theorem proving
- Graph data – student solutions
- New features - generalized subgraph patterns
- Class outlier detection
- Finding anomalous graphs
- Explanation of outliers

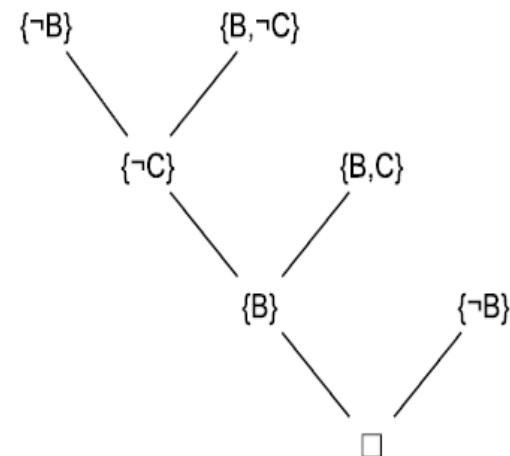
Introduction

Resolution in propositional logic

- Theorem-proving technique based on refutation
- *Resolution rule* produces a new clause implied by two clauses
- *Example:* Prove that the following set of clauses is contradictory

(B or $\neg C$) and $\neg C$ and (B or C) and $\neg B$ and
 $(\neg A, B)$ and (A or C)

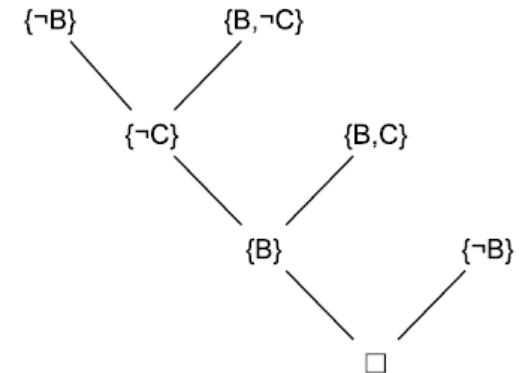
$\{\{B, \neg C\}, \{\neg C\}, \{B, C\}, \{\neg B\}, \{\neg A, B\}, \{A, C\}\}$



Method and goal

$\{\{B, \neg C\}, \{\neg C\}, \{B, C\}, \{\neg B\}, \{\neg A, B\}, \{A, C\}\}$

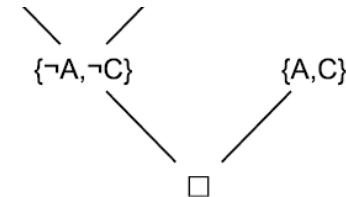
- graph mining, class outlier detection
- teaching enhancement by analysing students' solutions



Data

- 351 students solved resolution proofs via a web-based tool

- 873 resolution proofs classified into two classes
 - 772 correct
 - 101 incorrect



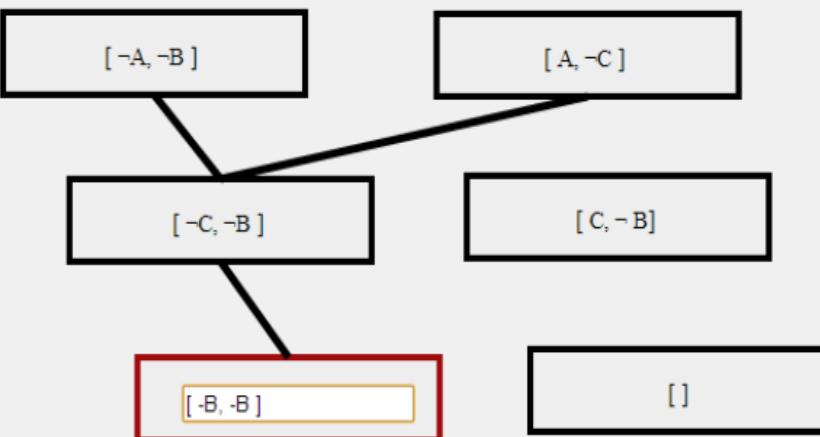
Incorrect ~ at least one error has been detected by an automatic evaluator

The most serious and common error: resolving on two literals at the same time

<input type="button" value="Načítať formulu"/>
<input type="button" value="Pridať klauzulu"/>
<input type="button" value="Vytvoriť čiaru"/>
<input type="button" value="Odstrániť"/>
<input type="button" value="Znovu vybrať typ rezolúcie a klauzúl"/>
<input type="button" value="Vložiť spor"/>
<input type="button" value="Vložiť nekonečno ∞"/>
<input type="button" value="Rozšíriť klauzulu"/>
<input type="button" value="Uložiť a ukončiť'"/>
<input type="button" value="Help"/>
Znak pre negáciu sa vkladá znakom "-"

Rozhodnite, či nasledujúca množina klauzúl je splniteľná prostredníctvom rezolúcie: { $[\neg A, \neg B]$, $[A, \neg C]$, $[B, \neg A]$, $[C, \neg B]$ } použite SLD rezolúciou (Selective Linear Definite)

Zvolil si: SLD rezolúcia (Selective Linear Definite Res.)



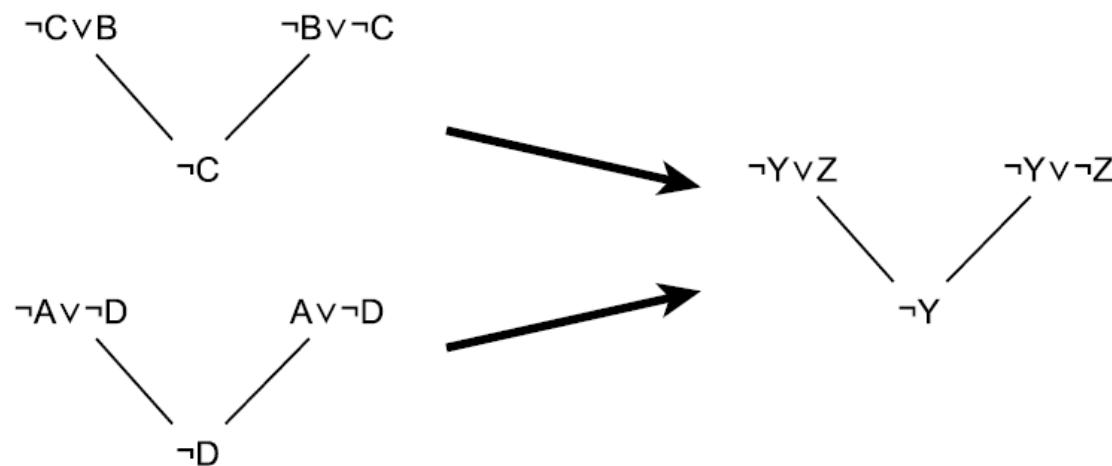
New features : subgraph patterns

- Representation of graphs by their substructures – patterns
 - Pattern_i , appeared in the graph -> true
 - Pattern_i , did not appear in the graph -> false

pattern ₁	pattern ₂	...	pattern _m	class
true	false	...	false	incorrect
...	
false	true	...	true	correct

Generalized Subgraph Patterns

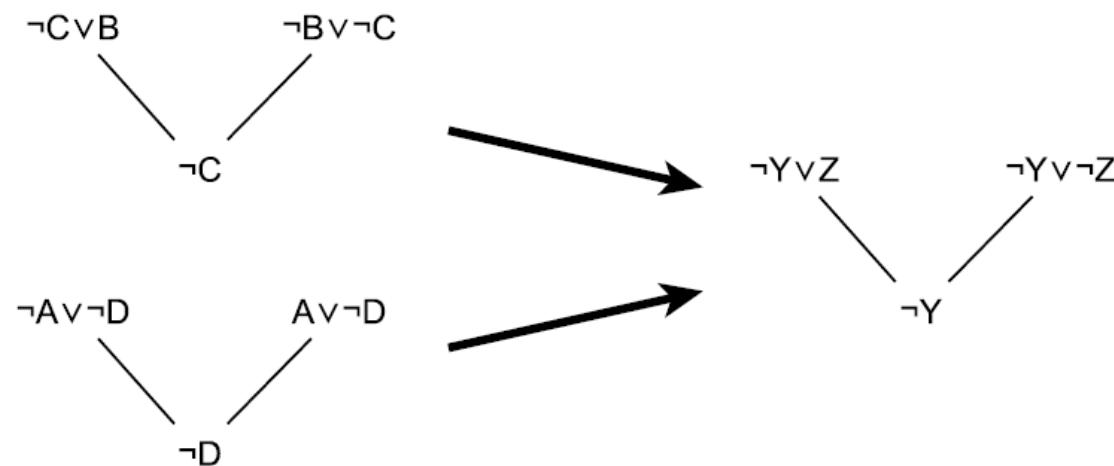
- Representation of graphs by their substructures (patterns)
- Simple subgraphs inappropriate
=> generalized subgraphs



Generalized Subgraph Patterns

Procedure:

1. Extract all 3-node subgraphs (parents with the resolvent)
2. Perform generalization on these subgraphs



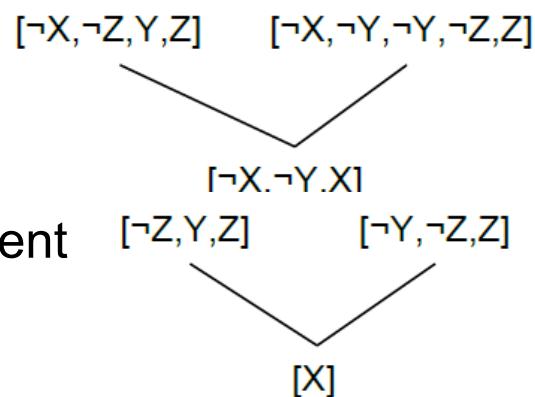
Generalized Subgraph Patterns – Higher Level

- To increase performance of algorithms, we created a new, higher-level, generalization
- This method generalizes patterns created by previous gen. method
- It exploits domain knowledge about general resolution principle
- From 3-node generalized pattern it creates new pattern in following form:
 $[L_{i_1}, L_{i_2}, \dots, L_{i_n}]; [L_{j_1}, L_{j_2}, \dots, L_{j_m}]$
 (*added*) (*dropped*)
- *added*: literals which were added erroneously to the resolvent
- *dropped*: literals from parents which participated in the resolution process

Generalized Subgraph Patterns – Higher Level

Example:

- Go through literals in resolvent and delete those that occur in at least one parent



added = [X], dropped = [-Z, Y, Z, -Y, -Z, Z]

- Rename letters in lists *dropped* and *added*, and sort both lists to get the final pattern

[Z];[-X, -X, -Y, X, X, Y]

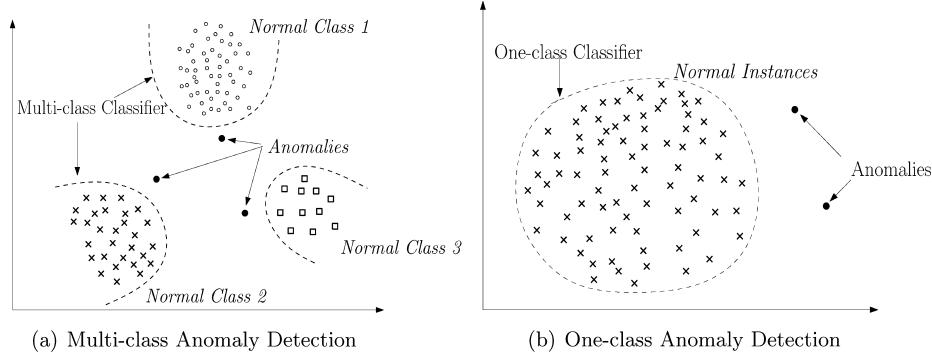
Detection of anomalous solutions

- (1a) Learn a classifier that would discriminate between correct and incorrect solutions, and
Detect rare cases that are incorrectly classified – outliers
 - (1b) Clustering and observing class distribution in clusters
- (2) BETTER: Directly detect outliers without learning a classifier.

Data have been classified => common outlier detection does not help

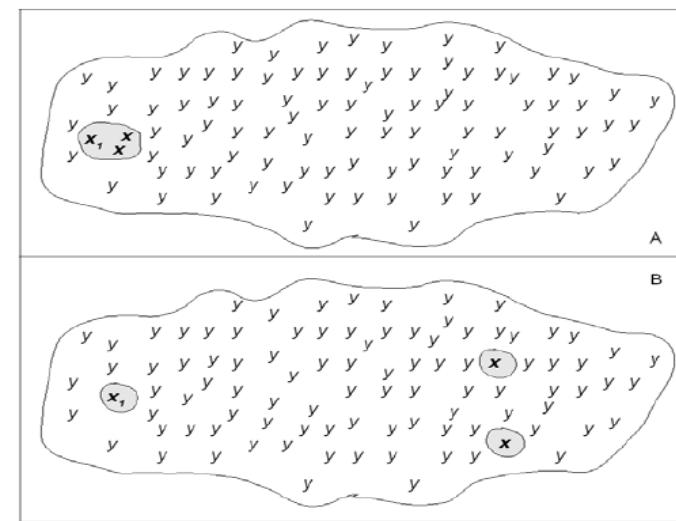
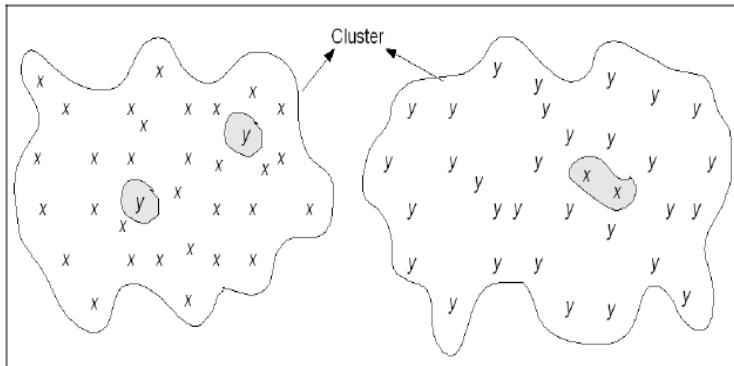
=> Class-based outlier detection

Class outliers



(a) Multi-class Anomaly Detection

(b) One-class Anomaly Detection



A

B

Class Outlier Detection

CODB (Hewahi and Saad 2007) – distance and density based

- weka-peka (Pekarčíková 2013)
 - Based on Random Forests
 - Analysis of proximity matrix

Class Outlier Detection via Random Forest

weka-peka (Pekarčíková 2013)

- Learn Random Forest
- After each tree is built, all of the data are run down the tree, and **proximities** are computed for each pair of cases:
If two cases occupy the same terminal node, their proximity is increased by one.
- At the end of the run, the proximities are normalized by dividing by the number of trees.

Class Outlier Detection via Random Forest

weka-peka (Pekarčíková 2013)

$$FO(p) = FO1(p) + FO2(p) + cFO3(p)$$

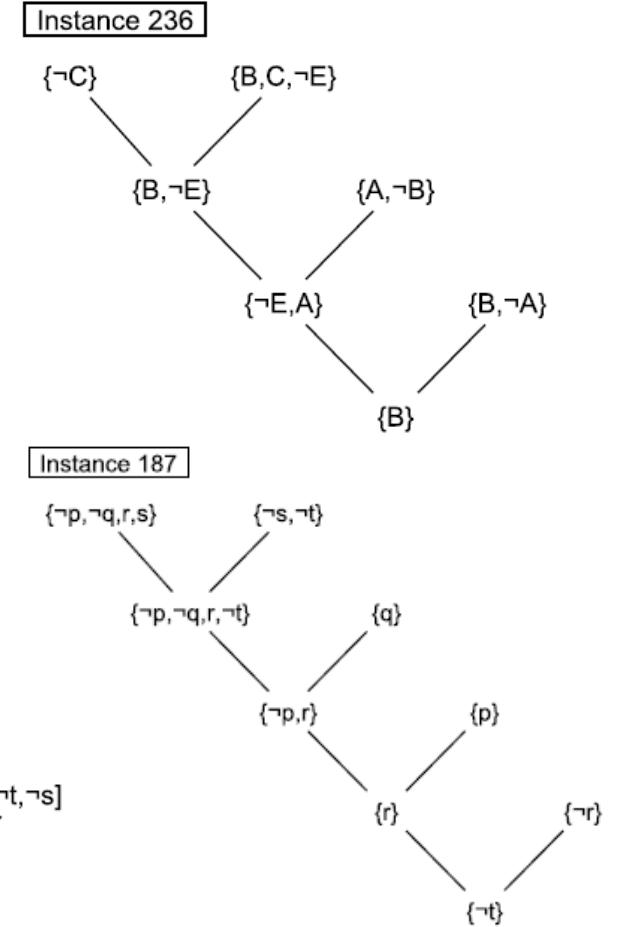
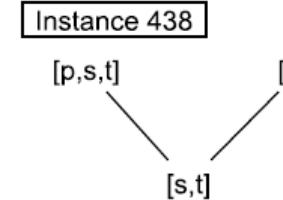
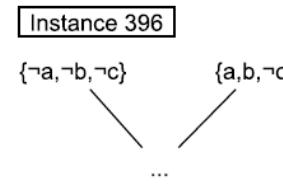
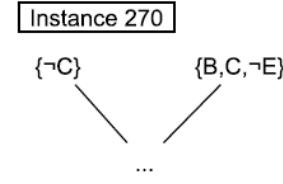
- $1/FO1(p)$... proximity of p to elements from the same class
- $FO2(p)$ frequency of incorrect classification of p
- $FO3(p)$ proximity p to all elements, i.e. when ignoring the class attribute

Outlier detection by weka-peka

Instance	Error E3	Outlier score
270	no	131.96
396	no	131.96
236	no	73.17
187	no	61.03
438	yes	54.43
389	yes	52.50
74	yes	15.91
718	yes	15.91

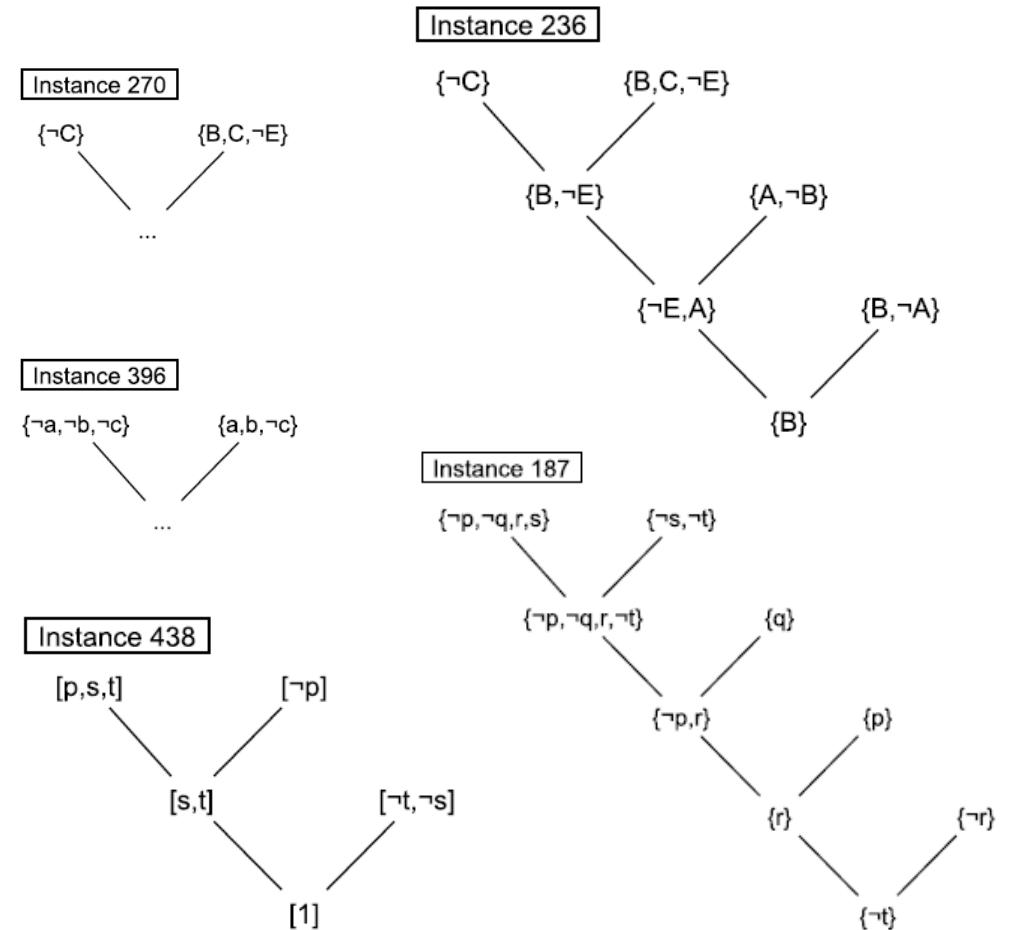
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Goal now: to explain/interpret outliers

References

VACULÍK, Karel, NEZVALOVÁ, Leona a Lubomír POPELÍNSKÝ. Graph Mining and Outlier Detection Meet Logic Proof Tutoring. Proc. of EDM 2014 Ws Graph-based Educational Data Mining

VACULÍK, Karel, Leona NEZVALOVÁ a Lubomír POPELÍNSKÝ. Educational data mining for analysis of students' solutions. 16th International Conference, AIMA 2014. London: Springer, 2014.

CODB:

Hewahi N.M. and Saad M.K. *Class Outliers Mining: Distance-Based Approach*. International Journal of Intelligent Systems and Technologies, Vol. 2, No. 1, pp 55-68, 2007.

	pattern	text
1	{}	; {neg Z,Z}
2	{}	; {}
3	{}	; {neg Z}
4	...(cykli)	; ... (cykli)
5	{neg Z}	; {neg Y,Y}
6	{neg Y,Z}	; {neg X,X}
7	{}	; {Z}
8	{}	; {neg Y,neg Z,Y,Z}
9	{Y}	; {neg Y,neg Z,Z}
10	{}	; {Z,Z}
11	{neg Y}	; {neg Z,Y,Z}
12	{}	; {neg Z,neg Z}
13	{Z}	; {neg Y,Y}
14	{}	; {neg Y,neg Z,Y}
15	{}	; {neg Y,Y,Z,Z}
16	{Z}	; {neg X,neg Y,X,Y}
17	{neg Z}	; {neg X,neg Y,X,Y}
18	{}	; {neg X,neg Y,neg Z,X,Y,Z}
19	{Y}	; {neg X,X,Z}
20	{}	; {neg Y,Z}

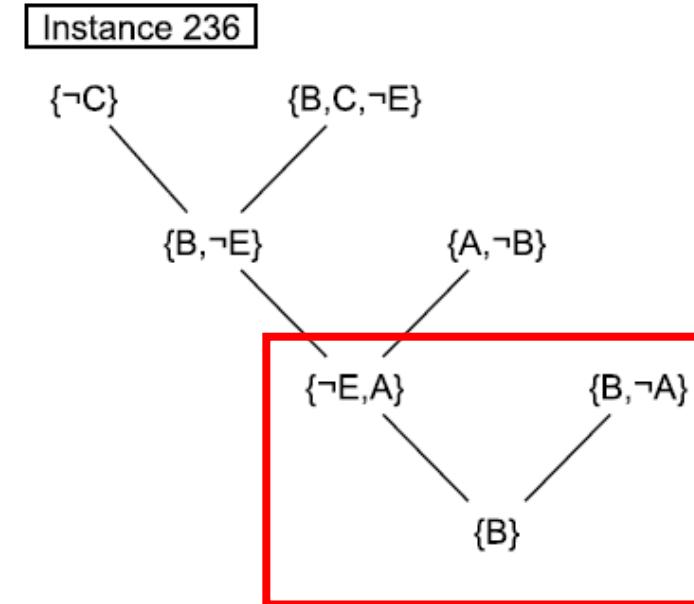
AScore

- Let P be a pattern and suppose its value is *true* for the outlier
- Compute AScore of P as the fraction of remaining instances from the same class as the outlier whose value of P is equal to *false*
- Similarly for P equal to *false*, but AScore ranges from 0 to -1

Outlier Explanation

Instance	Error E3	Outlier score	Significant patterns* [(Ascore) added; dropped]	Significant missing patterns* [(Ascore) added; dropped]
270	no	131.96	(0.96) <i>looping</i>	(-0.99) {};{¬Z,Z}
396	no	131.96	(0.96) <i>looping</i>	(-0.99) {};{¬Z,Z}
236	no	73.17	(0.99) {};{¬Y, ¬Z, Y}	
187	no	61.03	(0.99) {}; (0.99) {};	{¬Z};{¬Y, Y} {¬Y, ¬Z, Y}
438	yes	54.43	(1.00) {};	{Z};{¬X, ¬Y, X, Y} (-0.94) {};
389	yes	52.50	(1.00) {};	{¬Y, ¬Z, Y} (-0.94) {};{¬Z, Z} (-0.81)
74	yes	15.91	(0.98) {}; (0.98) {};	{¬Z};{¬X, ¬Y, X, Y} (-0.94) {¬X, ¬Y, ¬Z, X, Y, Z} {};
718	yes	15.91	(0.98) {}; (0.98) {};	{¬Z};{¬X, ¬Y, X, Y} (-0.94) {¬X, ¬Y, ¬Z, X, Y, Z} {};

*Only patterns with $|AScore| > 0.8$ are displayed

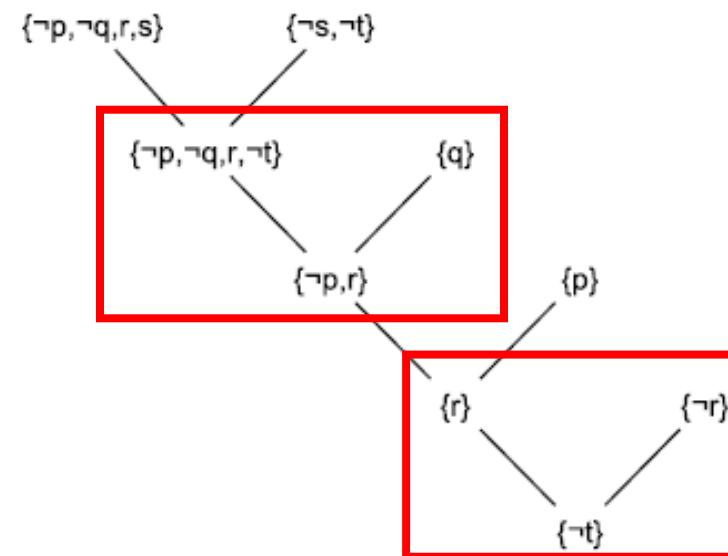


Outlier Explanation

Instance	Error E3	Outlier score	Significant patterns* [(Ascore) added; dropped]	Significant missing patterns* [(Ascore) added; dropped]
270	no	131.96	(0.96) <i>looping</i>	(-0.99) {};{¬Z,Z}
396	no	131.96	(0.96) <i>looping</i>	(-0.99) {};{¬Z,Z}
236	no	73.17	(0.99) {};{¬Y, ¬Z,Y}	
187	no	61.03	(0.99) {¬Z};{¬Y,Y} (0.99) {},{¬Y, ¬Z,Y}	
438	yes	54.43	(1.00) {Z};{¬X, ¬Y,X,Y}	(-0.94) {};{¬Y, ¬Z,Y,Z}
389	yes	52.50	(1.00) {};{¬Y, ¬Z,Y}	(-0.94) {};{¬Y, ¬Z,Y,Z} (-0.81) {};{¬Z,Z}
74	yes	15.91	(0.98) {¬Z};{¬X, ¬Y,X,Y} (0.98) {},{¬X, ¬Y, ¬Z,X,Y,Z}	(-0.94) {};{¬Y, ¬Z,Y,Z}
718	yes	15.91	(0.98) {¬Z};{¬X, ¬Y,X,Y} (0.98) {},{¬X, ¬Y, ¬Z,X,Y,Z}	(-0.94) {};{¬Y, ¬Z,Y,Z}

*Only patterns with $|AScore| > 0.8$ are displayed

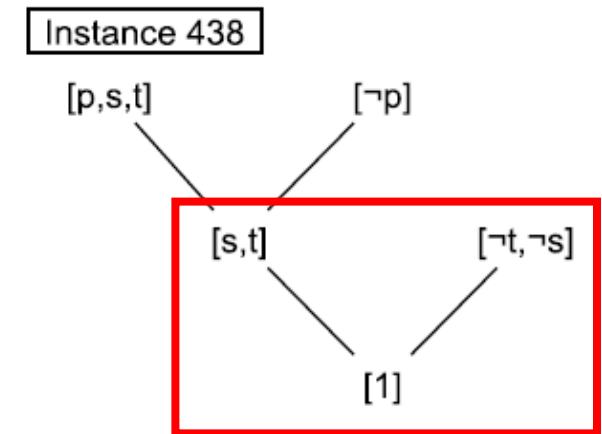
Instance 187



Outlier Explanation

Instance	Error E3	Outlier score	Significant patterns* [(Ascore) added; dropped]	Significant missing patterns* [(Ascore) added; dropped]
270	no	131.96	(0.96) looping	(-0.99) {};{¬Z,Z}
396	no	131.96	(0.96) looping	(-0.99) {};{¬Z,Z}
236	no	73.17	(0.99) {};{¬Y, ¬Z, Y}	
187	no	61.03	(0.99) {¬Z};{¬Y, Y} (0.99) {};{¬Y, ¬Z, Y}	
438	yes	54.43	(1.00) {Z};{¬X, ¬Y, X, Y}	(-0.94) {};{¬Y, ¬Z, Y, Z}
389	yes	52.50	(1.00) {};{¬Y, ¬Z, Y}	(-0.94) {};{¬Y, ¬Z, Y, Z} (-0.81) {};{¬Z, Z}
74	yes	15.91	(0.98) {¬Z};{¬X, ¬Y, X, Y} (0.98) {};{¬X, ¬Y, ¬Z, X, Y, Z}	(-0.94) {};{¬Y, ¬Z, Y, Z}
718	yes	15.91	(0.98) {¬Z};{¬X, ¬Y, X, Y} (0.98) {};{¬X, ¬Y, ¬Z, X, Y, Z}	(-0.94) {};{¬Y, ¬Z, Y, Z}

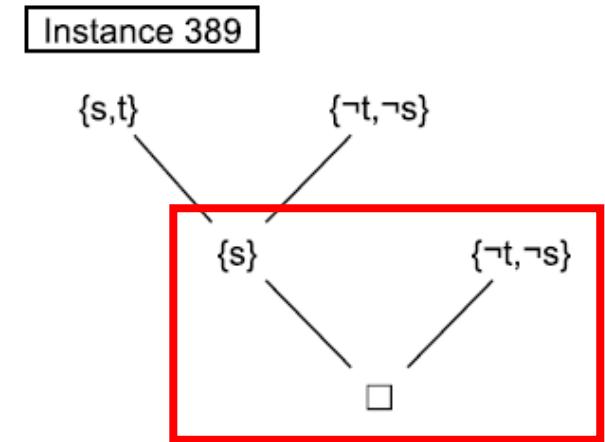
*Only patterns with $|AScore| > 0.8$ are displayed



Outlier Explanation

Instance	Error E3	Outlier score	Significant patterns* [(Ascore) added; dropped]		Significant missing patterns* [(Ascore) added; dropped]	
270	no	131.96	(0.96)	<i>looping</i>	(-0.99)	{ }; {¬Z, Z}
396	no	131.96	(0.96)	<i>looping</i>	(-0.99)	{ }; {¬Z, Z}
236	no	73.17	(0.99)	{ }; {¬Y, ¬Z, Y}		
187	no	61.03	(0.99)	{¬Z}; {¬Y, Y}		
			(0.99)	{ }; {¬Y, ¬Z, Y}		
438	yes	54.43	(1.00)	{Z}; {¬X, ¬Y, X, Y}	(-0.94)	{ }; {¬Y, ¬Z, Y, Z}
389	yes	52.50	(1.00)	{ }; {¬Y, ¬Z, Y}	(-0.94)	{ }; {¬Y, ¬Z, Y, Z}
			(-0.81)	{ }; {¬Z, Z}		
74	yes	15.91	(0.98)	{¬Z}; {¬X, ¬Y, X, Y}	(-0.94)	{ }; {¬Y, ¬Z, Y, Z}
			(0.98)	{ }; {¬X, ¬Y, ¬Z, X, Y, Z}		
718	yes	15.91	(0.98)	{¬Z}; {¬X, ¬Y, X, Y}	(-0.94)	{ }; {¬Y, ¬Z, Y, Z}
			(0.98)	{ }; {¬X, ¬Y, ¬Z, X, Y, Z}		

*Only patterns with $|AScore| > 0.8$ are displayed



Sapling Random Forest (LOF)

- Train trees (sapling) to distinguish normal instances from outliers
- Only subset of normal instances are used (k-nearest neighbours vs. random)
- Find explanation in resulting paths
- Knowledge about classes not taken into account

Tree Reduction

- Original classes replaced with two new classes
 - Normal class – includes labeled class of given instance
 - Outlier class – includes others original classes
- Analysis of the trees that classify instance to Outlier class
- Change attribut values on the path in given tree for given instance and check if resulting class change → attribut is part of explanation
- Find explanation in resulting paths and calculate support

Results

Instance	Error E3	Outlier score	AScore	Sapling Random Forest (LOF)	Tree Reduction
270	no	131.96	pattern_1 (-0.99) pattern_4 (0.96)	pattern_1=0 (1)	pattern_1=0 (0.81)
396	no	131.96	pattern_1 (-0.99) pattern_4 (0.96)	pattern_1=0 (1)	pattern_1=0 (0.81)
236	no	73.17	pattern_14 (0.99)	pattern_2=0 (0.8)	pattern_14=1 (0.46) pattern_14=1 && pattern_5=0 (0.22)
187	no	61.03	pattern_14 (0.99) pattern_5 (0.99)	pattern_2=0 (0.95)	pattern_14=1 (0.76)
438	yes	54.43	pattern_16 (1.00) pattern_8 (-0.94)	pattern_2=0 (0.75)	pattern_1=1 && pattern_8=0 && pattern_17=0 (0.23) pattern_8=0 && pattern_17=0 (0.20)
389	yes	52.50	pattern_14 (1.00) pattern_8 (-0.94) pattern_1 (-0.81)	pattern_1=0 (1)	pattern_8=0 (0.26) pattern_8=0 && pattern_16=0 && pattern_17=0 (0.21) pattern_8=0 && pattern_16=0 && pattern_18=0 (0.21)
74	yes	15.91	pattern_17 (0.98) pattern_18 (0.98) pattern_8 (-0.94)	pattern_2=0 (0.7)	pattern_8=0 && pattern_16=0 (0.29) pattern_1=1 && pattern_8=0 && pattern_16=0 (0.26)