From association rules to interpretable classification models - a tutorial

Tomas Kliegr

Department of Information and Knowledge Engineering

Faculty of informatics and statistics

University of Economics, Prague

Tomas Kliegr

Associate professor, Dep. of Information and Knowledge Engineering at VSE Praha

Software projects
- EasyMiner.eu – web-based rule learning system
- Inbeat.eu – rule-based recommender system
- R packages for building and explaining *association rule classifiers* (arc, qCBA, contributor: rCBA, arulesExplain – coming)

Results published in Web Semantics, Knowledge-based systems, Data and Knowledge Engineering, RuleML, ACM RecSys, ECML PKDD, Web Reasoning.

Outline

- Association rules
- Classification based on Association rules
- CBA algorithm
- Evaluation and comparison with other algorithms
- Extensions and implementations
- Summary

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Association rules - introduction

- Serve for discovering interesting patterns in data
- Conjunctive rules

IF milk and diapers THEN beer

- Exhaustive - all rules are discovered that meet user-set pattern and constraints
- Initially developed for analysis of shopping baskets and recommendation.
- The most well-known algorithm is Apriori (Agrawal, 1994)

Association rules – how they can be used

When customer buys item X, then he will also buy item Y

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Association rules – importance

The Apriori algorithm was soon after its publication in 1994 considers as a breakthrough:

"... Association rules are among data mining's biggest successes."

Hastie et al. Elements of Statistical Learning

Association rules – use for classification

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The contribution of the algorithm lied in the ability to process large multidimensional data in short time.

Association rules – use for classification

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Hastie et al. Elements of Statistical Learning

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In 1998, the algorithm was adapted for the ***classification task*** in*:*

Bing Liu, Wynne Hsu, and Yiming Ma. 1998. Integrating classification and association rule mining. In Proceedings of the Fourth International Conference on Knowledge Discovery and Data Mining (KDD'98), Rakesh Agrawal and Paul Stolorz (Eds.). AAAI Press 80-86.

Outline

- Association rules
- Classification based on Association rules
- Algoritmus Classification based on Associations (CBA)
  - Data preparation
  - Training phases
  - Prediction
- Evaluation and comparison with other algorithms
- Extensions and implementations
- Summary

Illustration problem

Dataset contains historical data on worker's comfort
- Two predictors: temperature (Y axis) and room humidity (X axis)
- One target attribute: worker's comfort (1 = worst, 4 = best)

The dataset was designed to allow visualization in 2D
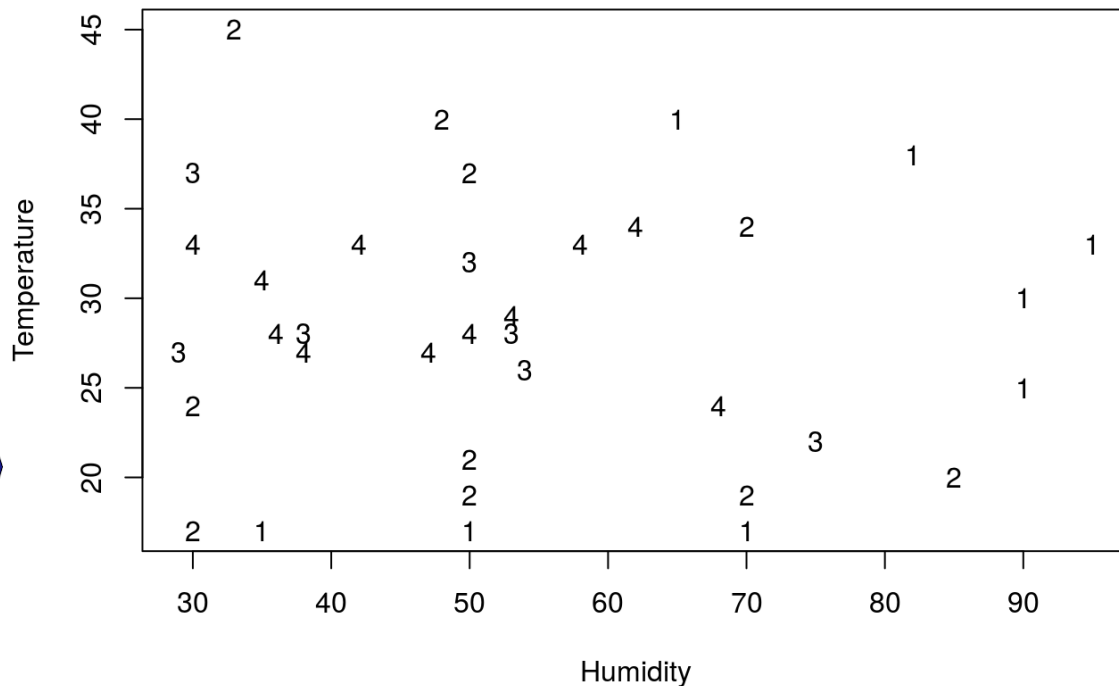
Classification based on Associations
principle of the CBA algorithm (Liu, 1998)

Discretization

⬇

Frequent item sets

⬇

Association rules

⬇

Classification rule lists
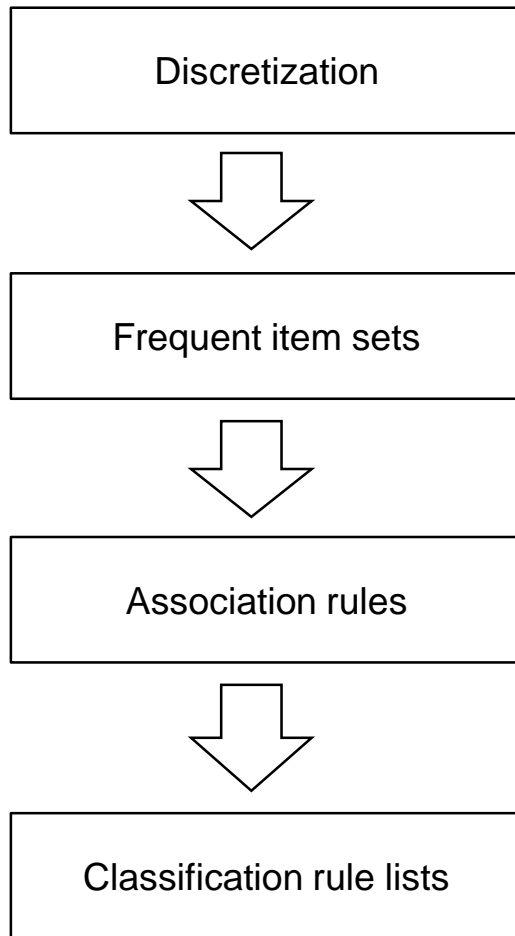
Classification based on Associations (CBA)
only nominal attributes are on the input

Discretization

Frequent item sets

Association rules

Classification rule lists
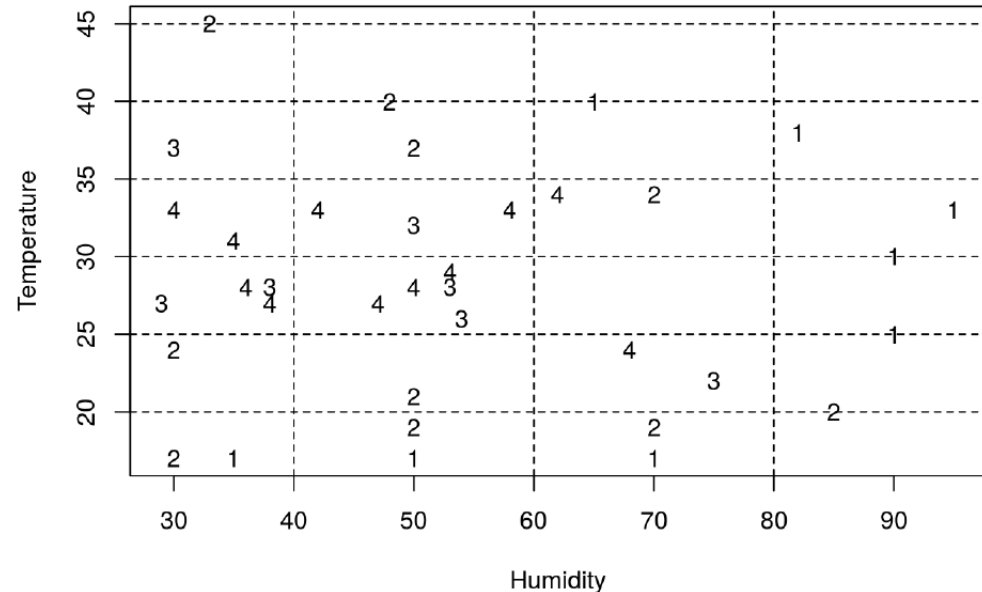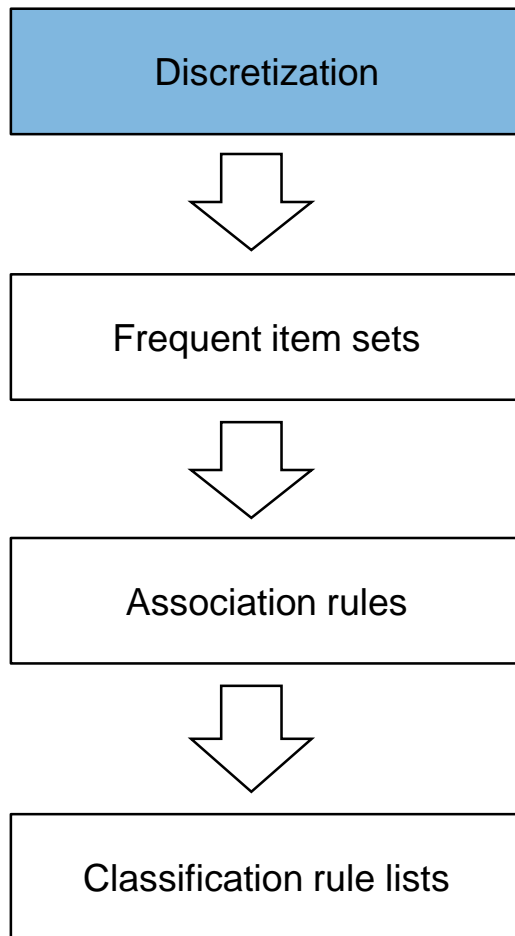
- Algorithms for association rule mining accept only nominal attributes on the input.
- For discretization – conversion of numerical attributes to intervals – one typically uses equidistant method or the entropy-based MDLP algorithm (Fayyad, 93)
- Item is a tuple: `attribute=value`
  `Humidity=(40;60]`

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Classification based on Associations (CBA)
support of item set

Discretization

⬇

Frequent item sets

⬇

Association rules

⬇

Classification rule lists
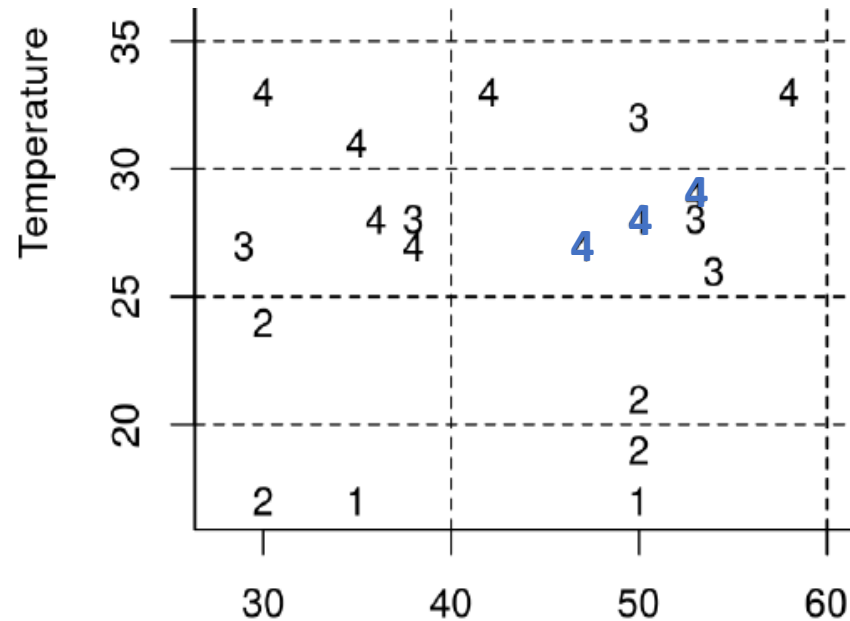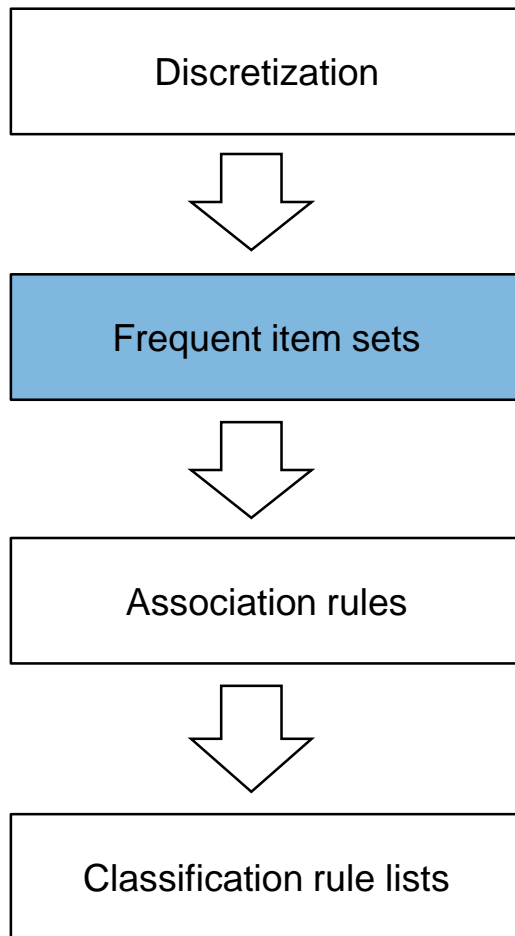
Item set = conjunction of conditions

```
Temp=(25;30] AND Hum=(40;60] AND Comf=4;
```
support = 3

Minimum support: algorithm finds all combinations of items, which are *frequent* - they appear in at least user-set minimum number of input rows.

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Classification based on Associations (CBA)
confidence of association rule

Discretization

Frequent item sets

Association rules

Classification rule lists
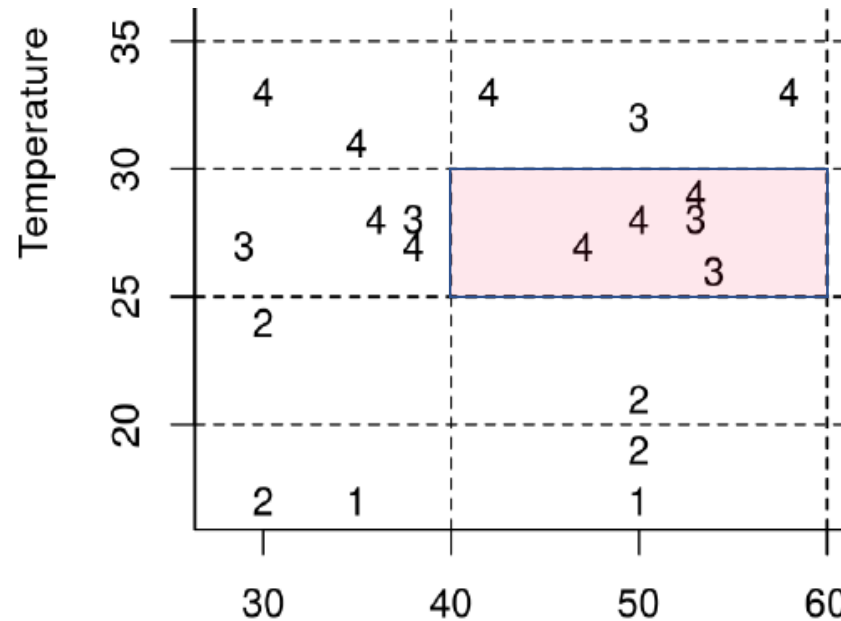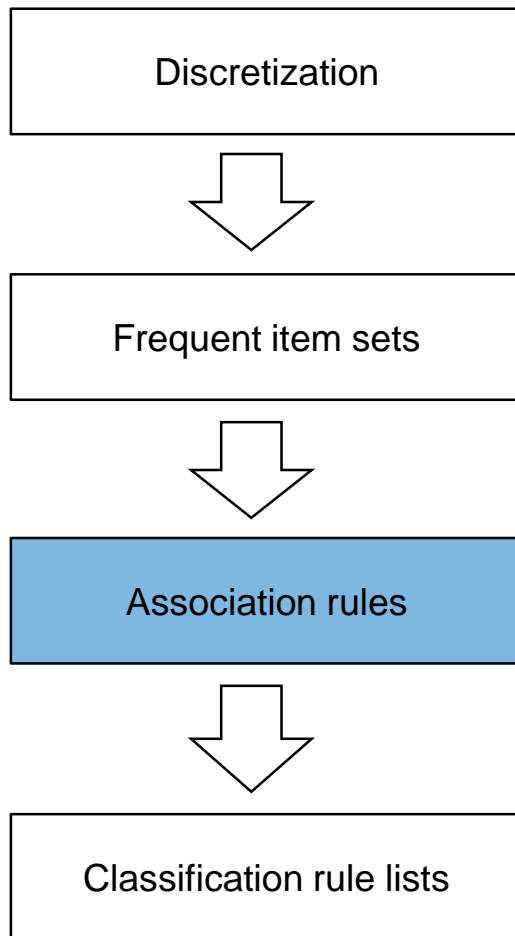
```
Temp=(25;30] AND Hum=(40;60] => Comf=4
   Support = 3; Confidence = 0.6 = 3/5
```

Discovered rules must comply to user-set threshold for **minimum confidence:**

$$\text{Conf}(X \rightarrow Y) = \frac{\text{Number of rows matching X i Y}}{\text{Number of rows matching X}}$$

Classification based on Associations (CBA)
rules are created from frequent item sets

Discretization

⬇

Frequent item sets

⬇

Association rules

⬇

Classification rule lists
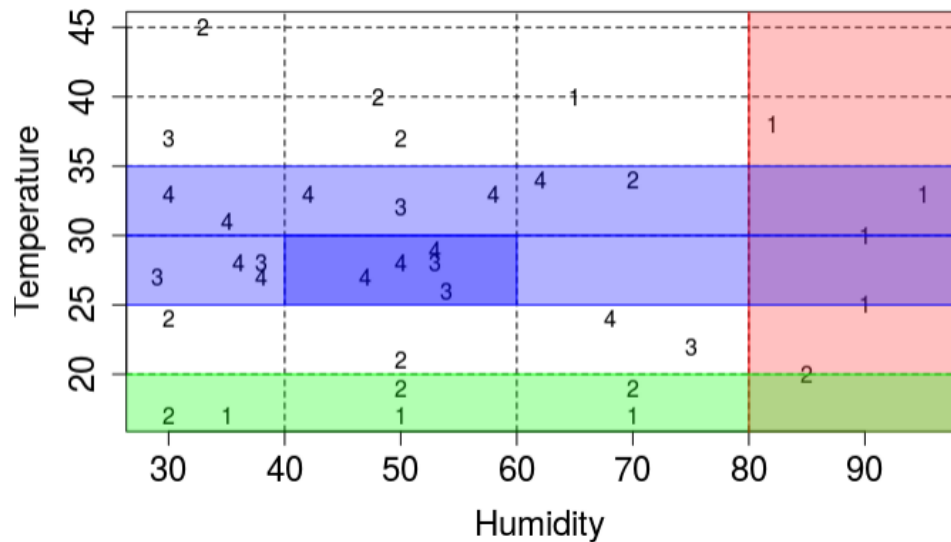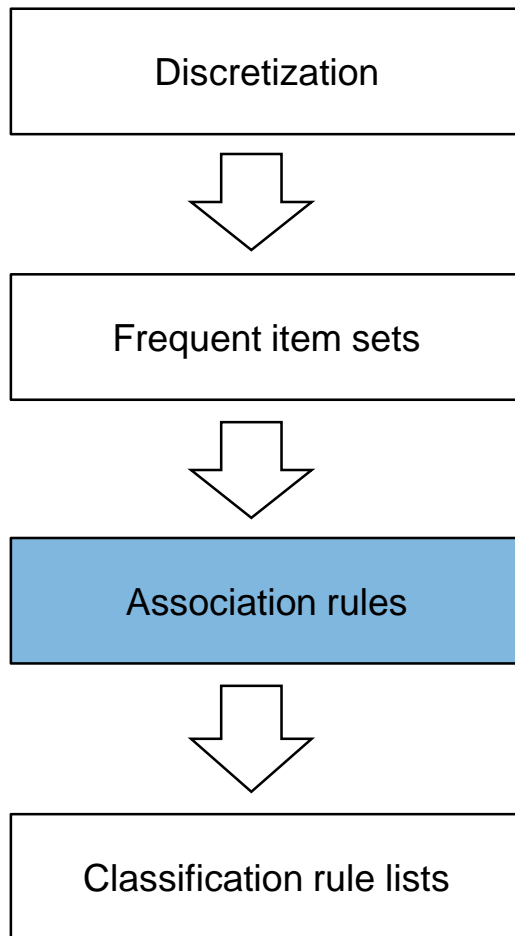
Discovered rules, colours – predicted comfort
minimum confidence = 0.5

1= red, 2 = green, 3 = unassigned, 4 = blue

```
{Humidity=(80;100]}                       => {Comfort=1}
{Temperature=(30;35]}                     => {Comfort=4}
{Temperature=(25;30],Humidity=(40;60]}=> {Comfort=4}
{Temperature=(15;20]}                     => {Comfort=2}
{Temperature=(25;30]}                     => {Comfort=4}
```

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Classification based on Associations (CBA)
the core of CBA is effective choice of rules

Discretization

⬇

Frequent item sets

⬇

Association rules

⬇

Classification rule lists
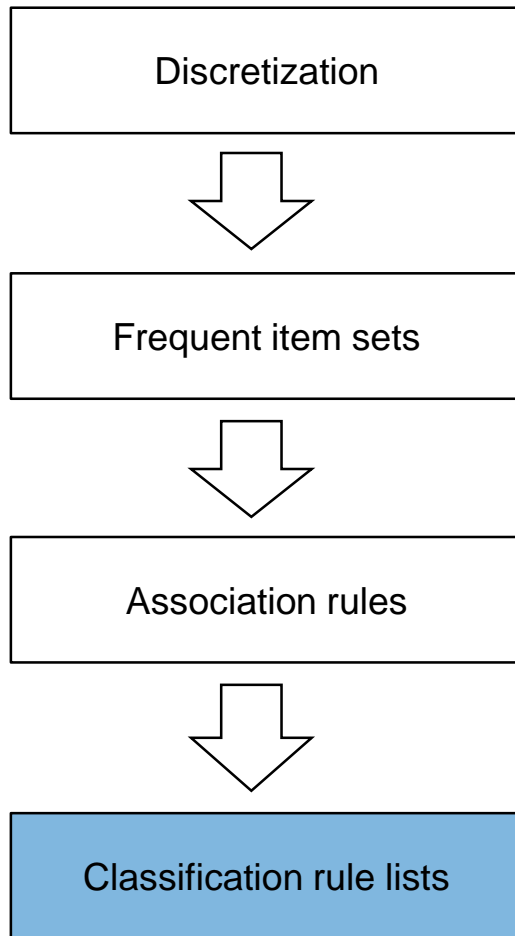
Input: Discovered association rules
… recommended is 70.000 rules

CBA
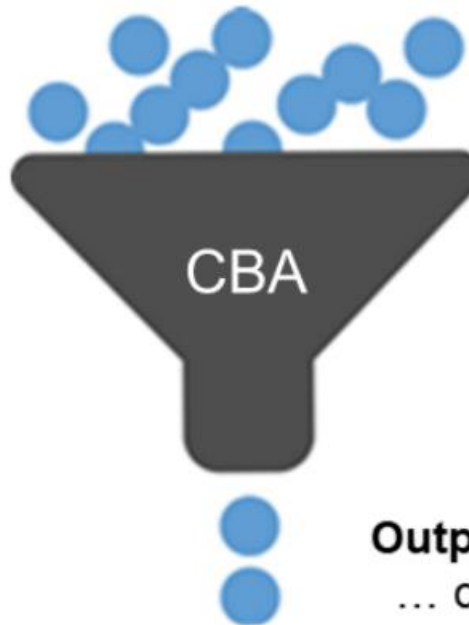
Principle:
Rules selected using heuristics

Objectives
- Improve accuracy
- Reduce number of rules

Output: Classification rule list
… on average about 70 rules

Classification based on Associations (CBA)
rule list is used to create the classifier

Discretization

⬇

Frequent item sets

⬇

Association rules

⬇

Classification rule lists
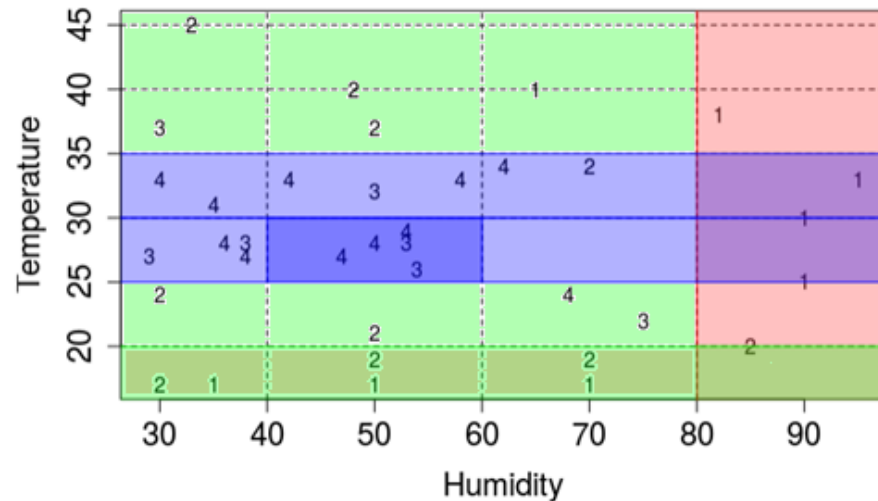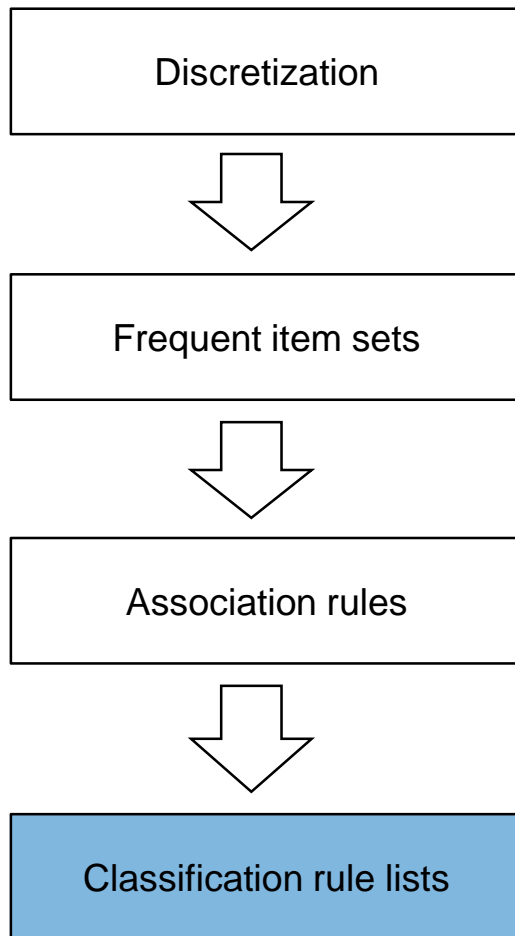
The last rule in the classifier is called default rule (light green), it ensures that all conceivable instances are covered by the classifier.

Classification based on Associations (CBA)
use for prediction
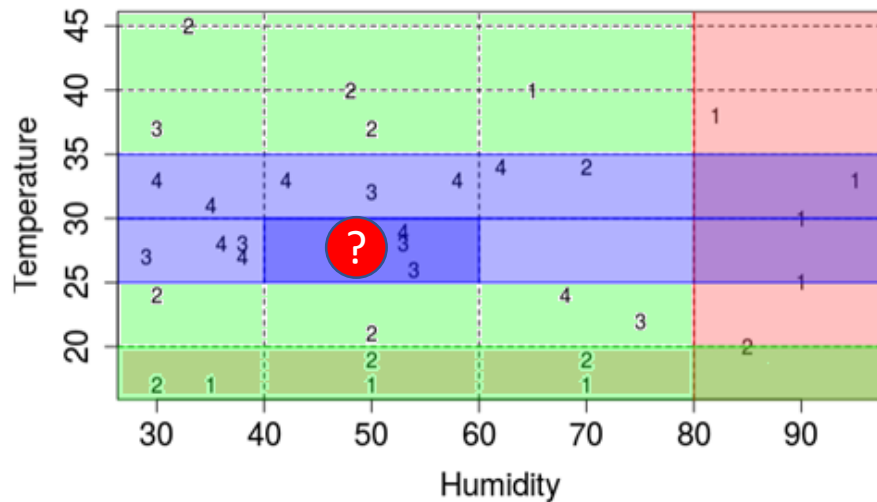
- The first rule in the order of confidence, support and length (more general rules are preferred)

Temperature	Humidity	Comfort
27	48	?

```
##      lhs                                              rhs              sup   conf  len
## [1] {Humidity=(80;100]}                           => {Comfort=1}  0.11  0.80  1
## [2] {Temperature=(30;35]}                         => {Comfort=4}  0.14  0.64  1
## [3] {Temperature=(25;30],Humidity=(40;60]}        => {Comfort=4}  0.08  0.60  2
## [4] {Temperature=(15;20]}                         => {Comfort=2}  0.11  0.57  1
## [5] {Temperature=(25;30]}                         => {Comfort=4}  0.14  0.50  1
## [6] {}                                            => {Comfort=2}  0.28  0.28  x
```

Classification based on Associations (CBA)
use for prediction
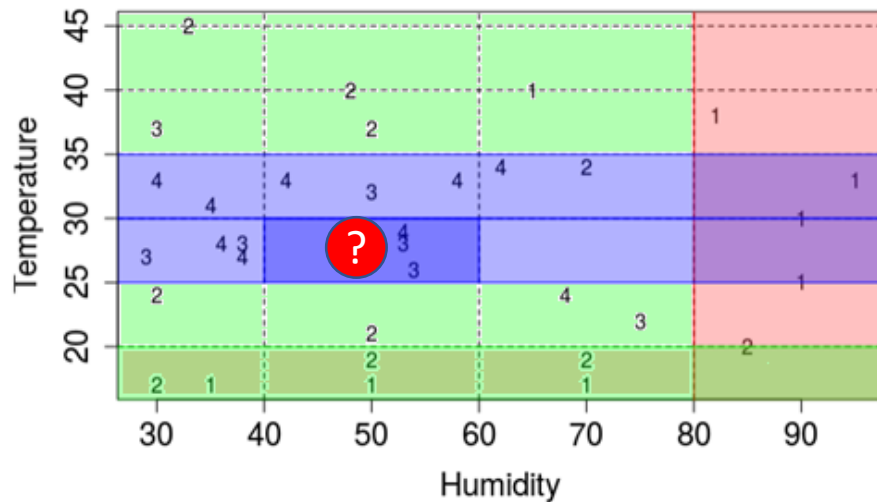
- The first rule in the order of confidence, support and length (more general rules are preferred)

Temperature	Humidity	Comfort
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Outline

- Association rules
- Classification based on Association rules
- CBA algorithm
- Evaluation and comparison with other algorithms
  - Association rule classification
  - Other rule-based classifiers and decision trees
  - Other frequently used classifiers
- Extensions and implementations
- Summary

Evaluation - other association classifiers

- In last 20 years multiple algorithms derived from CBA were proposed
- The design goal was typically achieving higher model accuracy, using one of the following methods:
  - Instead of classification with one strongest rule in CBA **single**, some methods combine **multiple** rules to classify each instance
  - Instead of **crisp** rules in CBA, use probabilistic approach with **fuzzy rules**
  - CBA is a **deterministic** algorithm, generating always the same output with given inputs. Some algorithms use **stochastic methods**, such as genetic or evolutional algorithms.

Categories **single**, **crisp** and **det** are used to compare interpretability of algorithms on the next slide.

Evaluation - other association classifiers

algorithm	year	single	crisp	det	assoc	acc	rules	time
CBA	1998	yes	yes	yes	yes	.80	185	35s
CBA 2	2001	yes	yes	yes	yes	.79	184	2 m
2SLAVE	2001	no?	no	no	no	.77	16	22m
CMAR	no	2001	yes	yes	yes	.79	1419	6m
CPAR	no	2003	yes	yes	yes	.82	788	11s
LAFAR	2003	no	no	no	yes	.75*	47*	5h*
FH-GBML	2005	no	no	no	no	.77	11	3h
CFAR	2008	yes	no	yes	yes	.71*	47*	17m*
SGERD	2008	no?	no	no	no	.74	7	3s
FARC-HD	2011	no?	no	no	yes	.84	39	1h 20m

Values for acc, rules and time sourced from: Alcala-Fdez, Jesús, Rafael Alcala, and Francisco Herrera. "A fuzzy association rule-based classification model for high-dimensional problems with genetic rule selection and lateral tuning." IEEE Transactions on Fuzzy systems 19.5 (2011): 857-872.

single denotes one rule classification

crisp do conditions in the rules comprising the classifier have crisp boundaries (as opposed to fuzzy)

det. Is algorithm deterministic without any random element, such as genetic algorithm

assoc is the algorithm based on association rules

acc, **rules**, **time** average accuracy, number of rules and train time on across 26 datasets in Alcala, 2011.

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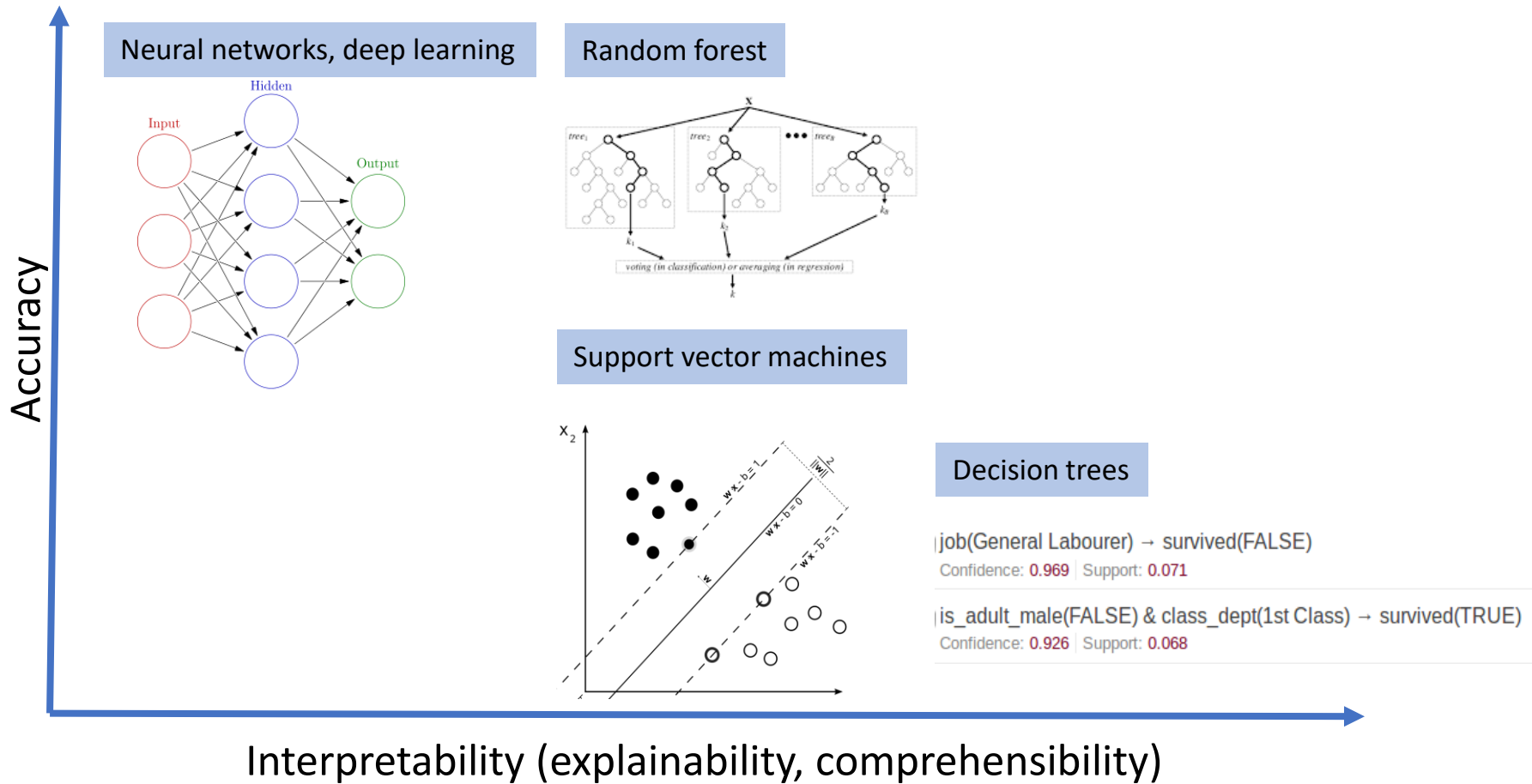
- Best algorithm FARC—HD, has on average 4% higher accuracy, but generates less understandable fuzzy rules
- CBA creates more understandable models than other algorithms for classification on the basis of association rules.

Evaluation - other rule-based classifiers

dataset	RIP	J48	PART	FURIA	CBA
anneal	0.94 (14)	0.94 (40)	0.95 (37)	0.99 (24)	0.96 (27)
australian	0.85 (4)	0.86 (9)	0.86 (6)	0.86 (9)	0.85 (109)
autos	0.79 (15)	0.79 (32)	0.78 (22)	0.78 (22)	0.79 (57)
breast-w	0.96 (6)	0.94 (10)	0.96 (10)	0.96 (16)	0.95 (51)
diabetes	0.75 (4)	0.74 (8)	0.74 (11)	0.75 (8)	0.76 (30)
glass	0.67 (8)	0.65 (15)	0.69 (16)	0.72 (15)	0.71 (28)
hepatitis	0.79 (4)	0.81 (4)	0.78 (6)	0.81 (8)	0.79 (32)
hypothyroid	0.99 (5)	1 (12)	0.99 (8)	1 (14)	0.98 (29)
ionosphere	0.91 (6)	0.87 (7)	0.88 (5)	0.89 (11)	0.92 (53)
iris	0.92 (4)	0.94 (4)	0.93 (5)	0.93 (5)	0.92 (6)
labor	0.88 (3)	0.71 (4)	0.84 (5)	0.74 (6)	0.84 (11)
lymph	0.77 (8)	0.74 (8)	0.78 (11)	0.87 (16)	0.81 (38)
sonar	0.74 (6)	0.68 (7)	0.73 (7)	0.79 (10)	0.74 (44)
vehicle	0.67 (21)	0.72 (44)	0.73 (35)	0.72 (24)	0.69 (147)
average	0.83 (8)	0.81 (5)	0.83 (13)	0.84 (13)	0.84 (47)

- CBA is fast and gives a equally good result as other rule based classifiers, but can be faster
- CBA generates more rules

Comparison with other classifiers

Accuracy (vertical axis)

Interpretability (explainability, comprehensibility) (horizontal axis)

Neural networks, deep learning

Input — Hidden — Output

Random forest

Support vector machines

Decision trees

job(General Labourer) → survived(FALSE)
Confidence: 0.969 | Support: 0.071

is_adult_male(FALSE) & class_dept(1st Class) → survived(TRUE)
Confidence: 0.926 | Support: 0.068

Based on:

Explainable Artificial Intelligence – Program Update, DARPA, US, 2017.

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Comparison with other classifiers

82%

Accuracy

8%

76%

Random forest

JRip rule learner

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Confidence: 0.969 | Support: 0.071

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Interpretability (explainability, comprehensibility)

Based on:

Explainable Artificial Intelligence – Program Update, DARPA, US, 2017.

Fernández-Delgado, Manuel, et al. "Do we need hundreds of classifiers to solve real world classification problems?." The Journal of Machine Learning Research 15.1 (2014): 3133-3181.

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Outline

- Association rules
- Classification based on Association rules
- CBA algorithm
- Evaluation and comparison with other algorithms
- Extensions and implementations
  - Reducing the size of the model
  - Combinatorial explosion and its solution
  - Software
- Summary

Combinatorial explosion

Recovering information lost during discretization

Quantitative CBA performs additional optimization of the list of rules generated by CBA. QCBA achieves consistent reduction of model size by 50% without reduction of accuracy
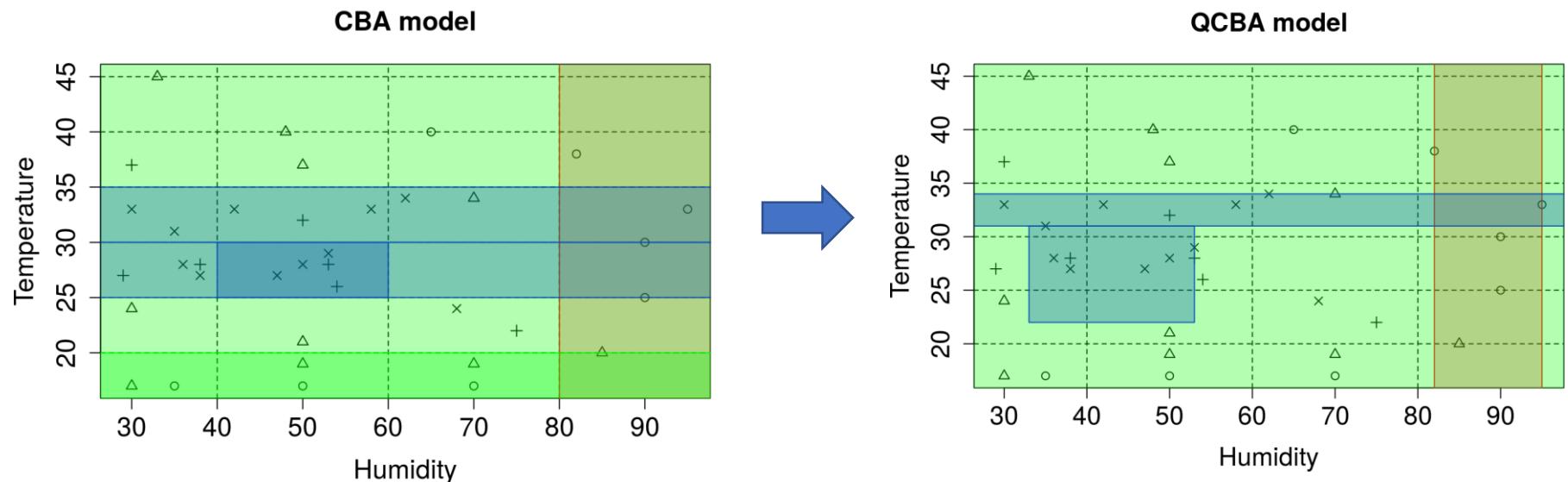
Kliegr, Tomas. "Quantitative CBA: Small and Comprehensible Association Rule Classification Models." arXiv preprint arXiv:1711.10166 (2017).
Tutorial on QCBA: https://nb.vse.cz/~klit01/qcba/tutorial.html

Combinatorial explosion

Automatic tuning of metaparameters

- Incorrect setting of minimum confidence and support thresholds affects quality of classifier

- We can't use grid search, because of the risk of combinatorial explosion

Solution 1: Generic algorithm

Implemented in R package *rCBA*

Solution 2: Set of heuristics combined with „time outs"

Implemented in R package *arc*

Assume m=70 binary attributes
140 rules of length 1
9660 rules of length 2
2.5 * 10^33 rules of length 70

Availability of implementations

software name	1st release	license	note
R implementations			
arulesCBA	2016	GPL-3	from author of popular arules R package
rCBA	2015	Apache 2.0	
arc	2016	AGPL-3	
Other implementations			
DM-II	2001?	commercial	original implementation Liu et al. (1998)
LUCS-KDD	2004	not stated	endorsed by author of original impl.
KEEL	2010?[7]	GPLv3	not available in RKEEL

Software from our group:
- arc (R Package with CBA implementation)
- pyARC (Python version of arc)
- qCBA (postprocess CBA models with Quantitative CBA)
- EasyMiner (Web framework with user interface, with CBA backend)

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Summary

- We introduced principles of association rule classification algorithms composed of association rules

- High number of input rules is a strength and challenge
    + Candidate rules are fast to generate
    + High number of candidates to select from
    - Sensitivity to minimum support
    - More rules on the output than for other rule models

- There are multiple algorithms and implementations that reduce or remove these limitations

- Goal: achieving the right balance between speed, explainability and accuracy of models

Publications

- Fürnkranz, Johannes, and Tomáš Kliegr. "The Need for Interpretability Biases." International Symposium on Intelligent Data Analysis. Springer, Cham, 2018.

- Vojíř, S., Zeman, V., Kuchař, J., & Kliegr, T. (2018). EasyMiner. eu: Web framework for interpretable machine learning based on rules and frequent itemsets. Knowledge-Based Systems, 150, 111-115.

- Fürnkranz, Johannes, Tomáš Kliegr, and Heiko Paulheim. "On Cognitive Preferences and the Plausibility of Rule-based Models." arXiv preprint arXiv:1803.01316 (2018).

- Kliegr, Tomáš, Štěpán Bahník, and Johannes Fürnkranz. "A review of possible effects of cognitive biases on interpretation of rule-based machine learning models." arXiv preprint arXiv:1804.02969 (2018).

- Kliegr, Tomas. "Quantitative CBA: Small and Comprehensible Association Rule Classification Models." arXiv preprint arXiv:1711.10166 (2017).

Thanks for your attention