

Mining the Semantic Web: the Knowledge Discovery Process in the SW

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Grenoble, January 24 - EGC 2017 Winter School

Knowledge Discovery: Definition

Knowledge Discovery (KD)

“the process of automatically searching large volumes of data for *patterns* that can be considered *knowledge about the data*” [Fay'96]

Knowledge

awareness or *understanding of facts*, information, descriptions, or skills, which is acquired through experience or education by perceiving, discovering, or learning

What is a Pattern?

An expression **E** in a given language L
describing a subset F_E of facts F.

E is called pattern if it is simpler than enumerating facts in F_E

Patterns need to be:

- New – *Hidden in the data*
- Useful
- Understandable

Knowledge Discovery and Data Mining

- KD is often related with Data Mining (DM) field
- DM is one step of the "Knowledge Discovery in Databases" process (KDD)[Fay'96]
- DM is the *computational process of discovering patterns in large data sets* involving methods at the intersection of artificial intelligence, machine learning, statistics, and databases.
- **DM goal:** extracting information from a data set and transforming it into an understandable structure/representation for further use

The KDD process



Data fusion (multiple sources)
Data Cleaning (noise, missing val.)
Feature Selection
Dimensionality Reduction
Data Normalization

The most labourous and time consuming step

The **knowledge** gained at the end of the process is given as a **model/data generalization**

Filtering Patterns
Visualization
Statistical Analysis
- Hypothesis testing
- Attribute evaluation
- *Comparing learned models*
- Computing Confidence Intervals

CRISP-DM (Cross Industry Standard Process for Data Mining) alternative process model developed by a consortium of several companies

All data mining methods use ***induction-based learning***

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Data Mining Tasks...

- **Predictive Tasks**: predict the value of a particular attribute (called target or dependent variable) based on the value of other attributes (called explanatory or independent variables)

Goal: learning a model that minimizes the error between the predicted and the true values of the target variable

- Classification → *discrete* target variables
- Regression → *continuous* target variables

...Data Mining Tasks...

Examples of Classification tasks

- Predict customers that will respond to a marketing campaign
- Develop a profile of a “successful” person

Examples of Regression tasks

- Forecasting the future price of a stock

... Data Mining Tasks...

- **Descriptive tasks:** discover patterns (correlations, clusters, trends, trajectories, anomalies) summarizing the underlying relationship in the data
 - **Association Analysis:** discovers (*the most interesting*) patterns describing strongly associated features in the data/relationships among variables
 - **Cluster Analysis:** discovers groups of closely related facts/observations. Facts belonging to the same cluster are more similar each other than observations belonging other clusters

...Data Mining Tasks...

Examples of Association Analysis tasks

- Market Basket Analysis
 - Discovering interesting relationships among retail products. To be used for:
 - Arrange shelf or catalog items
 - Identify potential cross-marketing strategies/cross-selling opportunities

Examples of Cluster Analysis tasks

- Automatically grouping documents/web pages with respect to their main topic (e.g. sport, economy...)

... Data Mining Tasks

- Anomaly Detection: identifies facts/observations (Outlier/change/deviation detection) having characteristics significantly different from the rest of the data. A good anomaly detector has a high detection rate and a low false alarm rate.
 - Example: Determine if a credit card purchase is fraudulent → **Imbalance learning setting**

Approaches:

- Supervised: build models by using input attributes to predict output attribute values
- Unsupervised: build models/patterns without having any output attributes

The KDD process



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A closer look at the Evaluation step

Given

- DM task (i.e. Classification, clustering etc.)
- A particular problem for the chosen task

Several DM algorithms can be used to solve the problem

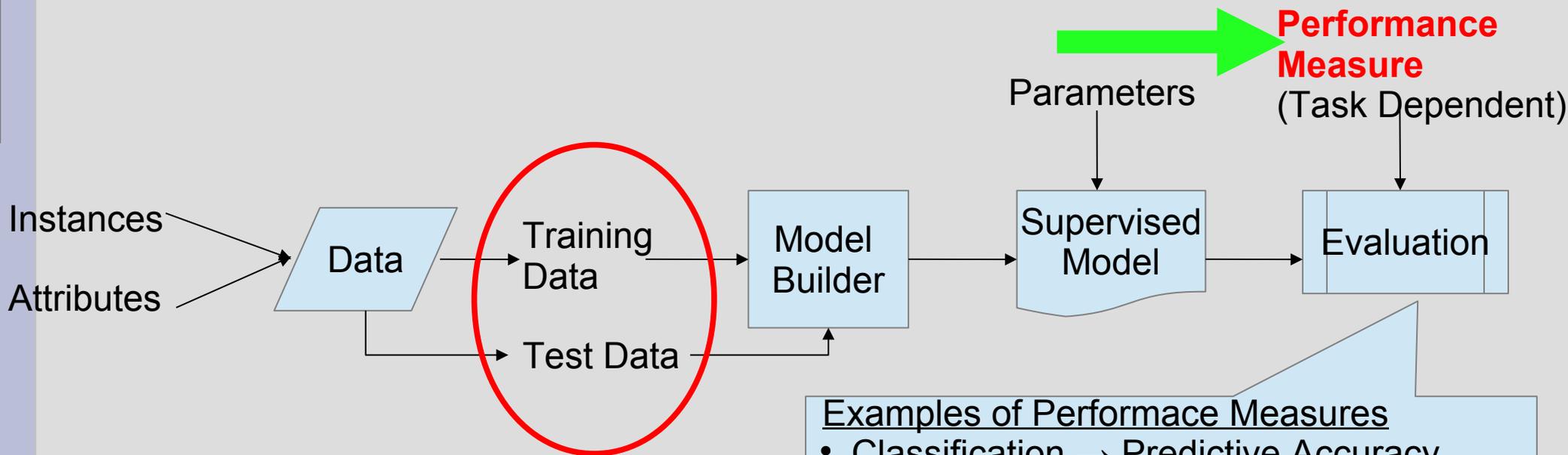


- 1) How to assess the performance of an algorithm?**
- 2) How to compare the performance of different algorithms solving the same problem?

Evaluating the Performance of an Algorithm

Assessing Algorithm Performances

Components for supervised learning [Roiger'03]



Examples of Performance Measures

- Classification → Predictive Accuracy
- Regression → Mean Squared Error (MSE)
- Clustering → Cohesion Index
- Association Analysis → Rule Confidence
-

Test data missing in unsupervised setting

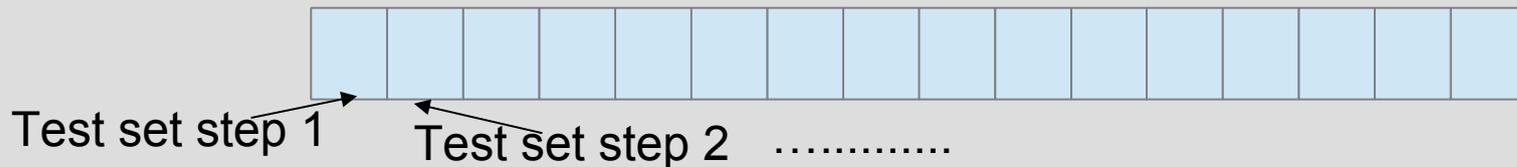
Supervised Setting: Building Training and Test Set

Necessary to predict performance bounds based with whatever data (**independent test set**)

- Split data into **training** and **test set**
 - The **repeated and stratified k-fold cross-validation** is the most widely used technique
 - Leave-one-out or bootstrap used for small datasets
- Make a model on the training set and evaluate it out on the test set [Witten'11]
 - e.g. Compute predictive accuracy/error rate

K-Fold Cross-validation (CV)

- **First step**: split data into k subsets of equal size
- **Second step**: use each subset in turn for testing, the remainder for training



- Subsets often *stratified* → reduces variance
- Error estimates averaged to yield the overall error estimate
- Even better: **repeated stratified cross-validation**
 - E.g. 10-fold cross-validation is repeated 15 times and results are averaged → reduces the variance

Leave-One-Out cross-validation

- **Leave-One-Out** → a particular form of cross-validation:
 - Set number of folds to number of training instances
 - I.e., for n training instances, build classifier n times
 - The results of all n judgements are averaged for determining the final error estimate
- Makes best use of the data for training
- Involves no random subsampling
- There's no point in repeating it → the same result will be obtained each time

The bootstrap

- **CV** uses *sampling without replacement*
 - The same instance, once selected, cannot be selected again for a particular training/test set
- **Bootstrap** uses *sampling with replacement*
 - Sample a dataset of n instances n times *with replacement* to form a new dataset
 - Use this new dataset as the training set
 - Use the remaining instances not occurring in the training set for testing
 - Also called the *0.632 bootstrap* → The training data will contain approximately 63.2% of the total instances

Estimating error with the bootstrap

The error estimate of the true error on the test data will be very pessimistic

- Trained on just ~63% of the instances
- Therefore, combine it with the resubstitution error:

$$err = 0.632 \cdot e_{\text{test instances}} + 0.368 \cdot e_{\text{training instances}}$$

- The resubstitution error (error on training data) gets less weight than the error on the test data
- **Repeat the bootstrap procedure** several times with different replacement samples; **average the results**



Comparing Algorithms Performances For Supervised Approach

Comparing Algorithms Performance

Frequent question: which of two learning algorithms performs better?

Note: this is domain dependent!

Obvious way: compare the error rates computed by the use of k-fold CV estimates

Problem: variance in estimate on a single 10-fold CV

Variance can be reduced using repeated CV

However, we still don't know whether the results are reliable

Significance tests

- Significance tests tell how confident we can be that there really is a difference between the two learning algorithms
- **Statistical hypothesis test exploited** → used for testing a statistical hypothesis
 - **Null hypothesis:** there is no significant (“real”) difference (between the algorithms)
 - *Alternative hypothesis:* there is a difference
- Measures how much evidence there is in favor of rejecting the null hypothesis for a specified level of significance
 - Compare two learning algorithms by comparing e.g. the average error rate over several cross-validations (see [Witten'11] for details)

DM methods and SW: A closer Look

DM methods and SW: a closer look

- Classical DM algorithms originally developed for propositional representations
- Some upgrades to (multi-)relational and graph representations defined

Semantic Web: characterized by

- Rich/expressive representations (RDFS, OWL)
 - How to cope with them when applying DM algorithms?
- Open world Assumption (OWA)
 - DM algorithms grounded on CWA
 - Are metrics for classical DM tasks still applicable?

Exploiting DM methods in SW: Problems and Possible Solutions

Classification

Exploiting DM methods in SW: Problems and Possible Solutions...

- Approximate inductive instance retrieval
 - assess the class membership of the individuals in a KB w.r.t. a query concept [d'Amato'08, Fanizzi'12, Rizzo'15]
- (Hyierarchical) Type prediction
 - Assess the type of instances in RDF datasets [Melo'16]
- Link Prediction
 - Given an individual and a role R , predict the other individuals a that are in R relation with [Minervini'14-'16]

Regarded as a **classification task** → (semi-)automatic ontology population

...Exploiting DM methods in SW: Problems and Possible Solutions...

Classification task → assess the class membership of individuals in an ontological KB w.r.t. the query concept

What is the value added?

- Perform some form of reasoning on inconsistent KB
- Possibly induce new knowledge not logically derivable

State of the art classification methods cannot be straightforwardly applied

- generally applied to feature vector representation
 - upgrade expressive representations
- implicit Closed World Assumption made
 - cope with the OWA (made in DLs)

...Exploiting DM methods in SW: Problems and Possible Solutions...

Problem Definition

Given:

- a populated ontological knowledge base $KB = (T, A)$
- a query concept Q
- a training set with $\{+1, -1, 0\}$ as target values (OWA taken into account)

Learn a classification function f such that: $\forall a \in \text{Ind}(A)$:

- $f(a) = +1$ if a is instance of Q
- $f(a) = -1$ if a is instance of $\neg Q$
- $f(a) = 0$ otherwise

...Exploiting DM methods in SW: Problems and Possible Solutions...

Dual Problem

- given an individual $a \in \text{Ind}(A)$, determine concepts C_1, \dots, C_k in KB it belongs to

the multi-class classification problem is decomposed into a set of ternary classification problems (one per target concept)

...Exploiting DM methods in SW: Problems and Possible Solutions...

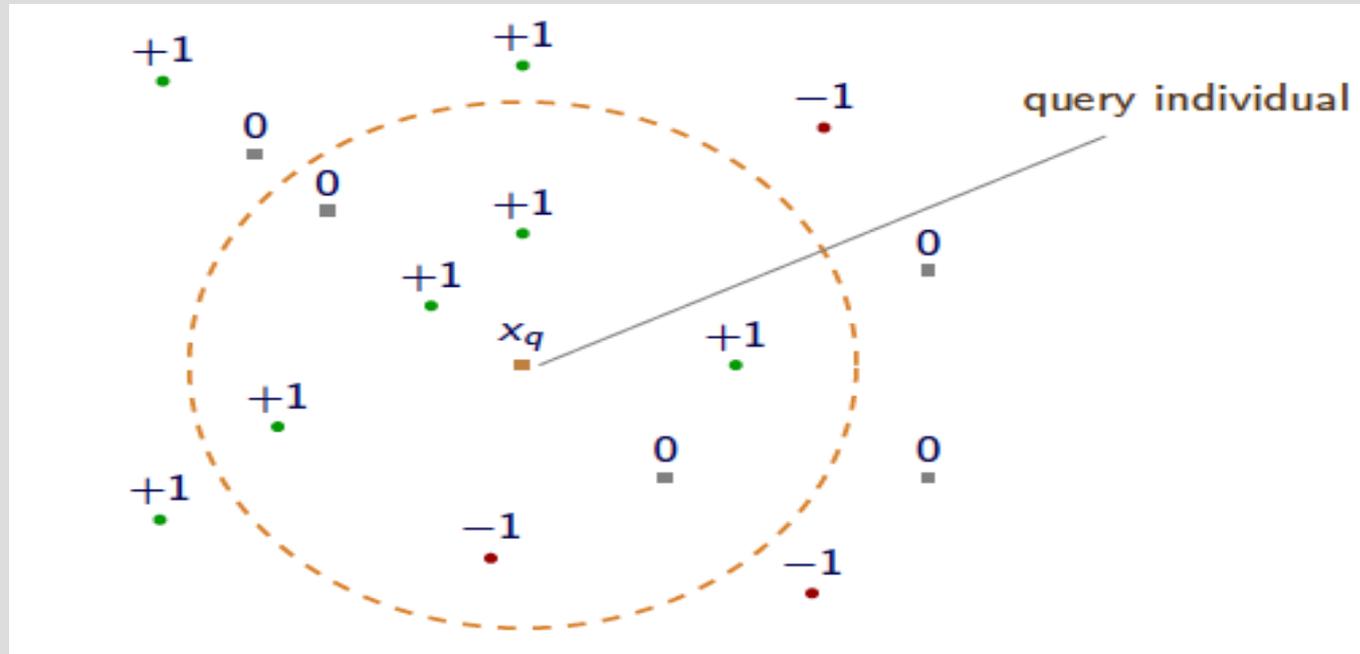
Example: Nearest Neighbor based Classification

Query concept: Bank $k = 7$

Training set with Target values: $\{+1, 0, -1\}$

Similarity Measures for DLs [d'Amato et al. @ EKAW'08]

$f(x_q) \leftarrow +1$



...Exploiting DM methods in SW: Problems and Possible Solutions...

Evaluating the Classifier

- Inductive Classification compared with a standard reasoner
- **Registered mismatches:** Ind. $\{+1,-1\}$ - Deduction: no results
- **Evaluated as mistake** if **precision** and **recall** used while it could turn out to be a **correct inference** if judged by a human

Defined new metrics to distinguish **induced assertions** from **mistakes**
[d'Amato'08]

M Match Rate

C Comm. Err. Rate

O Omis. Err. Rate

I Induct. Rate

		Reasoner		
		+1	0	-1
Inductive Classifier	+1	M	I	C
	0	O	M	O
	-1	C	I	M

...Exploiting DM methods in SW: Problems and Possible Solutions...

Pattern Discovery

...Exploiting DM methods in SW: Problems and Possible Solutions

- [Semi-automatic ontology enrichment](#) [d'Amato'10,Völker'11, Völker'15,d'Amato'16]
 - exploiting the evidence coming from the data → discovering hidden knowledge patterns in the form of relational association rules
 - new axioms may be suggested → existing ontologies can be extended

Regarded as a **pattern discovery task**

Associative Analysis: the Pattern Discovery Task

Problem Definition:

Given a dataset

find

- all possible *hidden pattern* in the form of **Association Rule** (AR)
- having support and confidence greater than a minimum thresholds

Definition: **An AR is** an implication expression of the form $X \rightarrow Y$ where X and Y are disjoint itemsets

An AR expresses a co-occurrence relationship between the items in the antecedent and the consequence not a causality relationship

Basic Definitions

- An *itemset* is a **finite set of assignments** of the form $\{A_1 = a_1, \dots, A_m = a_m\}$ where A_i are attributes of the dataset and a_i the corresponding values
- **The support** of an itemset is the number of instances/tuples in the dataset containing it.

Similarly, support of a rule is $s(X \rightarrow Y) = |(X \cup Y)|$;

- **The confidence of a rule** provides how frequently items in the consequence appear in instances/tuples containing the antecedent

$$c(X \rightarrow Y) = |(X \cup Y)| / |(X)| \quad (\text{seen as } p(Y|X))$$

Discovering Association Rules: General Approach

Articulated in two main steps [Agrawal'93, Tan'06]:

1. **Frequent Patterns Generation/Discovery** (generally in the form of *itemsets*) wrt a minimum frequency (support) threshold
 - Apriori algorithm → The most well known algorithm
 - the most expensive computation;
2. **Rule Generation**
 - Extraction of all the high-confidence association rules from the discovered frequent patterns.

Apriori Algorithm: Key Aspects

- Uses a level-wise generate-and-test approach
- Grounded on the **non-monotonic property of the support of an itemset**
 - The support of an itemset never exceeds the support of its subsets
- **Basic principle:**
 - if an itemset is frequent → all its subsets must also be frequent
 - If an itemset is infrequent → all its supersets must be infrequent too
 - Allow to sensibly cut the search space

Apriori Algorithm in a Nutshell

Goal: Finding the frequent itemsets \leftrightarrow the sets of items that satisfying the min support threshold

Iteratively find frequent itemsets with length from 1 to k (k-itemset)

Given a set L_{k-1} of frequent (k-1) itemset, join L_{k-1} with itself to obtain L_k the candidate k-itemsets

Prune items in L_k that are not frequent (Apriori principle)

If L_k is not empty, generate the next candidate (k+1) itemset **until** the frequent itemset is empty

Apriori Algorithm: Example...

Suppose having the transaction table
(Boolean values considered for simplicity)

Apply APRIORI algorithm

ID	List of Items
T1	{I1,I2,I5}
T2	{I2,I4}
T3	{I2,I3}
T4	{I1,I2,I4}
T5	{I1,I3}
T6	{I2,I3}
T7	{I1,I3}
T8	{I1,I2,I3,I5}
T9	{I1,I2,I3}

...Apriori Algorithm: Example...

Output After Pruning

Itemset	Sup. Count.
{1}	6
{2}	7
{3}	6
{4}	2
{5}	2

Min. Supp. 2
Pruning

Itemset	Sup. Count.
{1}	6
{2}	7
{3}	6
{4}	2
{5}	2

L_1

Join for
candidate
generation

Itemset	Sup. Count.
{1,2}	4
{1,3}	4
{1,4}	1
{1,5}	2
{2,3}	4
{2,4}	2
{2,5}	2
{3,4}	0
{3,5}	1
{4,5}	0

L_2

Min. Supp. 2

Pruning

...Apriori Algorithm: Example

Apply Apriori principle

Itemset	Sup. Count
{1,2}	4
{1,3}	4
{1,5}	2
{2,3}	4
{2,4}	2
{2,5}	2

Output After Pruning

Join for candidate generation

Itemset	Prune Infrequent
{1,2,3}	No
{1,2,5}	No
{1,2,4}	Yes {1,4}
{1,3,5}	Yes {3,5}
{2,3,4}	Yes {3,4}
{2,3,5}	Yes {3,5}
{2,4,5}	Yes {4,5}

L₃

Min. Supp. 2
Pruning

Itemset	Sup. Count.
{1,2,3}	2
{1,2,5}	2

Output After Pruning

Join for candidate generation

Itemset	Prune Infrequent
{1,2,3,5}	Yes {3,5}

L₄

Empty Set

STOP



Generating ARs from frequent itemsets

- For each frequent itemset “I”
 - generate all non-empty subsets S of I
- For every non empty subset S of I
 - compute the rule $r := “S \rightarrow (I-S)”$
- **If** $\text{conf}(r) \geq \text{min confidence}$
 - **then** output r

Generating ARs: Example...

Given:

$L = \{ \{I1\}, \{I2\}, \{I3\}, \{I4\}, \{I5\}, \{I1,I2\}, \{I1,I3\}, \{I1,I5\}, \{I2,I3\}, \{I2,I4\}, \{I2,I5\}, \{I1,I2,I3\}, \{I1,I2,I5\} \}$.

Let us fix 70% for the Minimum confidence threshold

- Take $I = \{I1,I2,I5\}$.
- All nonempty subsets are $\{I1,I2\}, \{I1,I5\}, \{I2,I5\}, \{I1\}, \{I2\}, \{I5\}$.

The resulting ARs and their confidence are:

- R1: $I1 \text{ AND } I2 \rightarrow I5$

$\text{Conf}(R1) = \text{supp}\{I1,I2,I5\}/\text{supp}\{I1,I2\} = 2/4 = 50\%$ **REJECTED**

...Generating ARs: Example...

Min. Conf. Threshold 70%; $I = \{I1, I2, I5\}$.

- All nonempty subsets are $\{I1, I2\}$, $\{I1, I5\}$, $\{I2, I5\}$, $\{I1\}$, $\{I2\}$, $\{I5\}$.

The resulting ARs and their confidence are:

- R2: $I1 \text{ AND } I5 \rightarrow I2$

$\text{Conf}(R2) = \text{supp}\{I1, I2, I5\} / \text{supp}\{I1, I5\} = 2/2 = 100\%$ RETURNED

- R3: $I2 \text{ AND } I5 \rightarrow I1$

$\text{Conf}(R3) = \text{supp}\{I1, I2, I5\} / \text{supp}\{I2, I5\} = 2/2 = 100\%$ RETURNED

- R4: $I1 \rightarrow I2 \text{ AND } I5$

$\text{Conf}(R4) = \text{sc}\{I1, I2, I5\} / \text{sc}\{I1\} = 2/6 = 33\%$ REJECTED

...Generating ARs: Example

Min. Conf. Threshold 70%; $I = \{I1, I2, I5\}$.

- All nonempty subsets: $\{I1, I2\}, \{I1, I5\}, \{I2, I5\}, \{I1\}, \{I2\}, \{I5\}$.

The resulting ARs and their confidence are:

- R5: $I2 \rightarrow I1 \text{ AND } I5$

$$\text{Conf}(R5) = \text{sc}\{I1, I2, I5\} / \text{sc}\{I2\} = 2/7 = 29\% \text{ REJECTED}$$

- R6: $I5 \rightarrow I1 \text{ AND } I2$

$$\text{Conf}(R6) = \text{sc}\{I1, I2, I5\} / \{I5\} = 2/2 = 100\% \text{ RETURNED}$$

Similarly for the other sets I in L (Note: it does not make sense to consider an itemset made by just one element i.e. $\{I1\}$)

On improving Discovery of ARs

Apriori algorithm may degrade significantly for dense datasets

Alternative solutions:

- FP-growth algorithm outperforms Apriori
 - Does not use the generate-and-test approach
 - Encodes the dataset in a compact data structure (FP-Tree) and extract frequent itemsets directly from it
- Usage of additional interestingness metrics (besides support and confidence) (see [Tan'06])
 - Lift, Interest Factor, correlation, IS Measure

Pattern Discovery on RDF data sets for Making Predictions

Discovering ARs from RDF data sets → for making predictions

Problems:

- Upgrade to Relational Representation (need variables)
- OWA to be taken into account
- Background knowledge should be taken into account
- ARs are exploited for making predictions
 - New metrics, considering the OWA, for evaluating the results, are necessary

Proposal [Galarraga'13-'15]

- Inspired to the general framework for discovering frequent **Datalog patterns** [Dehaspe'99; Goethals et al'02]
- Grounded on level-wise **generate-and-test** approach

Pattern Discovery on RDF data sets for Making Predictions

Start: initial general pattern, single atom → role name (plus variable names)

Proceed: at each level with

- **specializing** the patterns (use of suitable operators)
 - Add an atom sharing at least one variable/constant
- **evaluating** the generated specializations for **possible pruning**

Stop: stopping criterion met

A rule is a list of atoms (interpreted as a conjunction) where the **first one** represents **the head**

The specialization operators represent the way for exploring the search space

Pattern Discovery on Populated Ontologies for Making Predictions

Pros: **Scalable method**

Limitations:

- Any background/ontological KB taken into account
- No reasoning capabilities exploited
- Only role assertions could be predicted

Upgrade: Discovery of ARs from ontologies [d'Amato'16]

- Exploits the available background knowledge
- Exploits deductive reasoning capabilities

Discovered ARs can make concept and role predictions

Pattern Discovery on Populated Ontologies for Making Predictions

Start: initial general pattern

- **concept name** (plus a variable name) or a **role name** plus variable names)

Proceed: at each level with:

- **specializing** the patterns (use of suitable operators)
 - Add a concept or role atom sharing at least one variable
- **evaluating** the generated specializations for **possible pruning**

Stop: stopping criterion met

A rule is a list of atoms (interpreted as a conjunction) where the **first one** represents **the head**

Pattern Discovery on Populated Ontologies for Making Predictions

For a given pattern all possible specializations are generated by applying the operators:

- **Add a concept atom:** adds an atom with a concept name as a predicate symbol and an **already appearing** variable as argument
- **Add a role atom:** adds an atom with a role name as a predicate symbol; **at least one variable already appears** in the pattern

The Operators are applied so that always **connected and non-redundant rules** are obtained

Additional operators for taking into account constants could be similarly considered

Pattern Discovery on Populated Ontologies for Making Predictions

Language Bias (ensuring decidability)

- **Safety condition:** all variables in the head must appear in body
- **Connection:** atoms share at least one variable or constant
- **Interpretation under DL-Safety condition:** all variables in the rule bind only to known individuals in the ontology
- **Non Redundancy:** there are no atoms that can be derived by other atoms

Example (Redundant Rule)

Given K made by the TBox $T = \{\text{Father} \sqsubseteq \text{Parent}\}$ and the rule
 $r := \text{Father}(x) \wedge \text{Parent}(x) \Rightarrow \text{Human}(x)$

r **redundant** since $\text{Parent}(x)$ is entailed by $\text{Father}(x)$ w.r.t. K .

Pattern Discovery on Populated Ontologies for Making Predictions

Specializing Patterns: Example

- Pattern to be specialized: $C(x) \wedge R(x,y)$

Non redundant Concept D

Refined Patterns

$C(x) \wedge R(x,y) \wedge D(x)$

$C(x) \wedge R(x,y) \wedge D(y)$

Non redundant Role S

Fresh Variable z

Refined Patterns

$C(x) \wedge R(x,y) \wedge S(x,z)$

$C(x) \wedge R(x,y) \wedge S(z,x)$

$C(x) \wedge R(x,y) \wedge S(y,z)$

$C(x) \wedge R(x,y) \wedge S(z,y)$

Non redundant Role S

All Variables Bound

Refined Patterns

$C(x) \wedge R(x,y) \wedge S(x,x)$

$C(x) \wedge R(x,y) \wedge S(x,y)$

$C(x) \wedge R(x,y) \wedge S(y,x)$

$C(x) \wedge R(x,y) \wedge S(y,y)$

Pattern Discovery on Populated Ontologies for Making Predictions

- Rule predicting concept/role assertions
- The method is actually able to prune redundant and inconsistent rules
 - thanks to the exploitation of the background knowledge and reasoning capabilities

Problems to solve/research directions:

- Scalability
 - investigate on additional **heuristics for cutting the search space**
 - Indexing methods for caching the results of the inferences made by the reasoner
- Output only a subset of patterns by the use a suitable **interestingness measures** (potential inner and post pruning)

Conclusions

- Surveyed the classical KDD process
 - Data mining tasks
 - Evaluation of algorithms
- Analyzed some differences of the KD process when RDF/OWL knowledge bases are considered
 - Expressive representation language
 - OWA vs. CWA
 - New metrics for evaluating the algorithms
- Analyzed existing solutions
- Open issues and possible research directions

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