A Machine Learning Perspective for Ontology Mining

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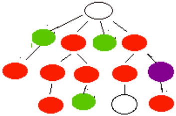
- **Ontologies ⇒ basic element for realizing the semantic interoperability**
  - on the Web and in other contexts



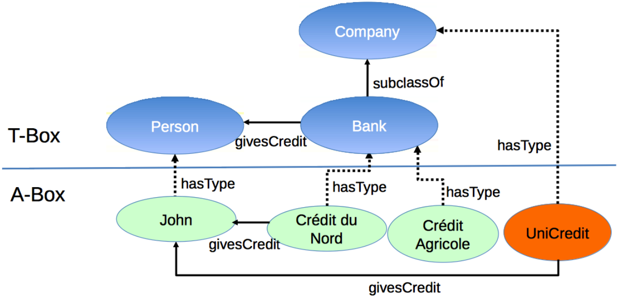
Examples of existing real ontologies

- Schema.org
- Gene Ontology
- Foundational Model of Anatomy ontology
- Financial Industry Business Ontology (by OMG Finance Domain Task Force)
- GoodRelations
- ...

Reasoning on Description Logics Ontologies

OWL adopted ⇒ **Description Logics** theoretical foundation

Ontologies are equipped with deductive reasoning capabilities ⇒ allowing to make explicit, knowledge that is implicit within them



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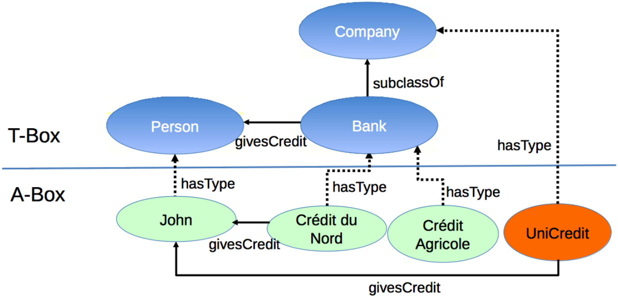
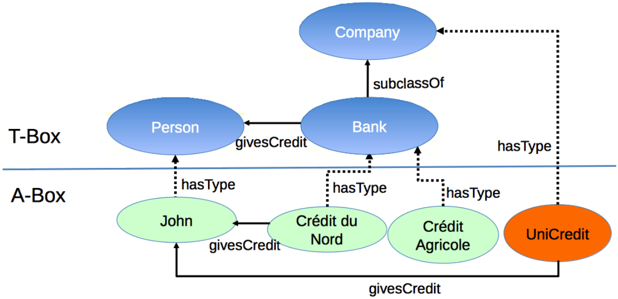


Deduction:
"Crédit du Nord", "Crédit Agricole" are also `Company`

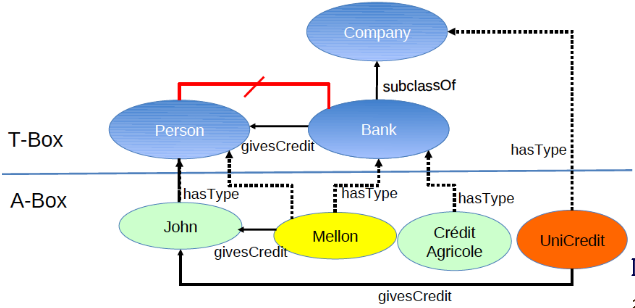
Reasoning on Description Logics Ontologies



Incompleteness

"*UniCredit*" is a `Bank`

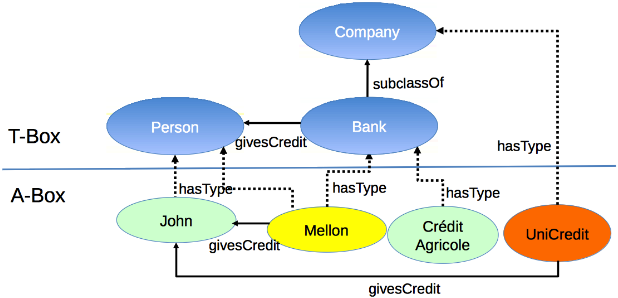
Reasoning on Description Logics Ontologies



Inconsistency

Mellon cannot be a Person **and** a Bank

Reasoning on Description Logics Ontologies

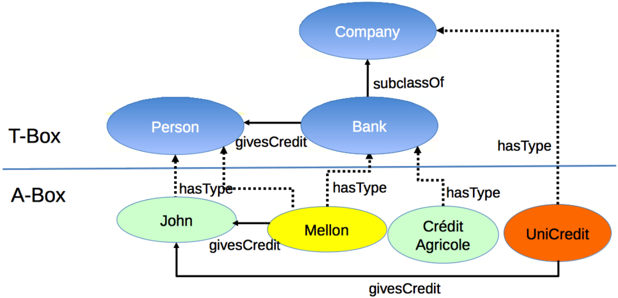


Noise

$\texttt{Person} \equiv \neg\texttt{Bank}$ missing

Reasoning on Description Logics Ontologies

Question: would it be possible to discover new/additional knowledge by exploiting *the evidence coming from the assertional data*?



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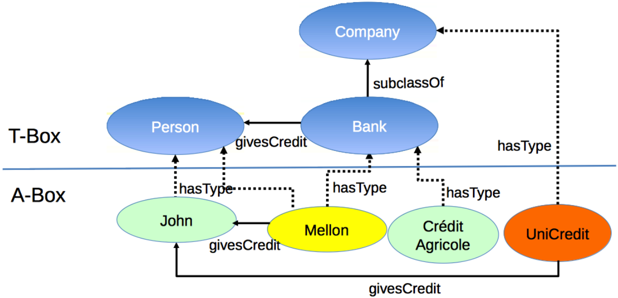

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Idea: exploiting **Machine Learning methods** for **Ontology Mining** related tasks *[d'Amato et al. @SWJ'10]*

Definition (Ontology Mining)

All activities that allow for

discovering hidden knowledge from
ontological knowledge bases

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Special Focus on:

- (similarity-based) *inductive learning methods*
  - use specific examples to reach general conclusions
  - are known to be very efficient and fault-tolerant

Ontology Mining Tasks

- Instance Retrieval (Instance Level)
- Ontology Enrichment (Schema Level)
- Concept Drift and Novelty Detection (Ontology Dynamic)

from an inductive perspective

Focus on: similarity-based methods

Ontology Mining Tasks

- **Instance Retrieval (Instance Level)**
- Ontology Enrichment (Schema Level)
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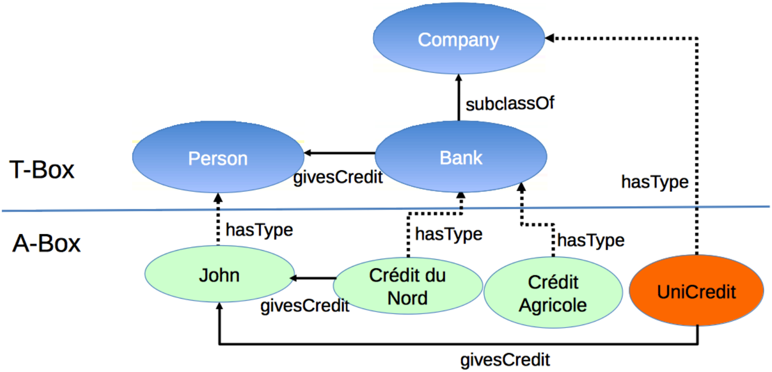
from an inductive perspective

Introducing Instance Retrieval I

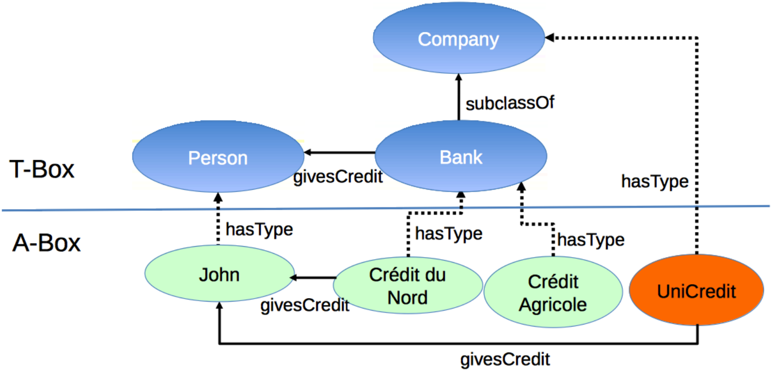
Instance Retrieval → Finding the extension of a query concept

- Instance Retrieval (Bank) = {"Crédit du Nord","Crédit Agricole"}



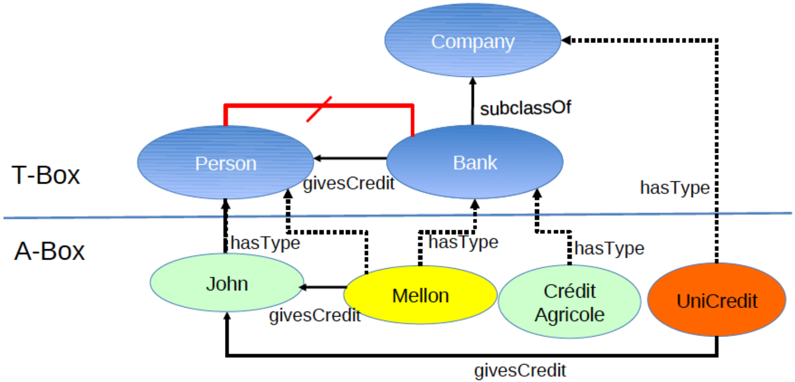
Introducing Instance Retrieval I

Problem: Instance Retrieval in incomplete/inconsistent/noisy ontologies



Introducing Instance Retrieval II

Problem: Instance Retrieval in incomplete/<u>inconsistent</u>/noisy ontologies



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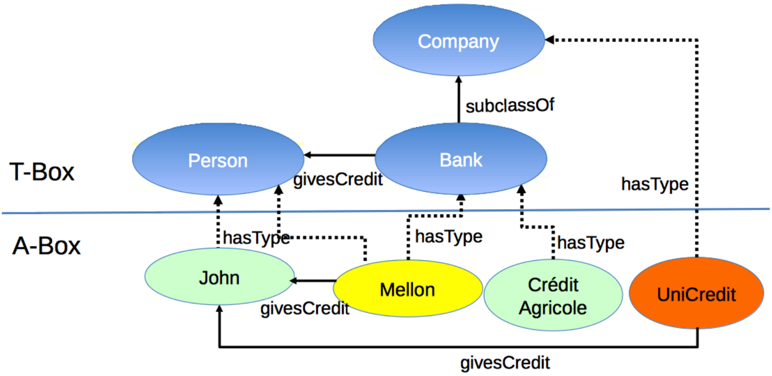

Issues & Solutions I

IDEA

Casting the problem as a Machine Learning **classification problem**

assess the class membership of individuals in a Description Logic (DL) KB w.r.t. the query concept

State of art classification methods cannot be straightforwardly applied

- generally applied to *feature vector* representation
  $\rightarrow$ *upgrade DL expressive representations*
- implicit *Closed World Assumption* made in ML
  $\rightarrow$ *cope with the Open World Assumption made in DLs*
- classes considered as *disjoint*
  $\rightarrow$ *cannot assume disjointness of all concepts*

Issues & Solutions II

Adopted Solutions:

- Defined new semantic similarity measures for DL representations
  - to cope with the high expressive power of DLs
  - to deal with the semantics of the compared objects (concepts, individuals, ontologies)
  - to convey the underlying semantics of KB
- Formalized a set of criteria that a similarity function has to satisfy in order to be defined *semantic [d'Amato et al. @ EKAW 2008]*
- Definition of the classification problem taking into account the OWA
- Multi-class classification problem decomposed into a set a smaller classification problems

Definition (Problem Definition)

Given:

- a populated ontological knowledge base $\mathcal{K} = \langle \mathcal{T}, \mathcal{A} \rangle$
- a query concept Q
- a training set with $\{+1, -1, 0\}$ as target values

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

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

Dual Problem

- given an individual $a \in Ind(\mathcal{A})$, tell concepts $C_1, \ldots, C_k$ in $\mathcal{K}$ it belongs to
- the multi-class classification problem is *decomposed* into a set of *ternary classification problems* (one per target concept)

Developed methods

Pioneering the Problem

- relational K-NN for DL KBs *[d'Amato et al. ESWC'08]*

Improving the efficiency

- kernel functions for kernel methods to be applied to DLs KBs *[Fanizzi, d'Amato et al. @ ISMIS'06, JWS 2012; Bloehdorn and Sure @ ISWC'07]*

Scaling on large datasets

- Statistical Relational Learning methods for large scale and data sparseness *[Huang et al. @ ILP'10, Minervini et a. @ ICMLA'15]*

Lesson Learnt from experiments I

Experiments performed on ontologies publicly available

Results compared with a standard deductive reasoner

Need for new metrics $\rightarrow$ **Defined** *to distinguish induced assertions from mistakes*

		REASONER		
		+1	0	-1
INDUCTIVE CLASSIFIER	+1	*M*	*I*	*C*
	0	*O*	*M*	*O*
	-1	*C*	*I*	*M*

M **Match Rate**
O **Ommission Error Rate**
C **Commission Error Rate**
I **Induction Rate**

Lesson Learnt from experiments II

- *Commission error* almost zero on average
- *Omission error rate* very low and only in some cases
  - Not null for ontologies in which disjoint axioms are missing
- *Induction Rate* not zero
  - **new knowledge (not logically derivable) induced** $\Rightarrow$ can be used for *semi-automatizing the ontology population task*

	match	commission	omission	induction
SWM	97.5 ± 3.2	0.0 ± 0.0	2.2 ± 3.1	0.3 ± 1.2
LUBM	99.5 ± 0.7	0.0 ± 0.0	0.5 ± 0.7	0.0 ± 0.0
NTN	97.5 ± 1.9	0.6 ± 0.7	1.3 ± 1.4	0.6 ± 1.7
FINANCIAL	99.7 ± 0.2	0.0 ± 0.0	0.0 ± 0.0	0.2 ± 0.2

Ontology Mining Tasks

- Instance Retrieval (Instance Level)
- **Ontology Enrichment (Schema Level)**
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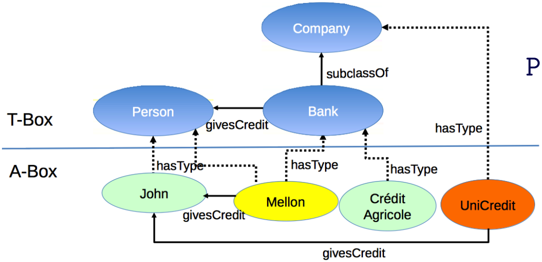
from an inductive perspective

Ontology Enrichment as a Disjointness Axioms Discovery Problem

Disjointness axioms often missing within ontologies

Problems:

- introduction of noise



Noise

$\texttt{Person} \equiv \neg\texttt{Bank}$ **missing**

- counterintuitive inferences

$\mathcal{K} = \{ JournalPaper \sqsubseteq Paper,\ ConferencePaper \sqsubseteq Paper,\ ConferencePaper(a)\ \}$

$\mathcal{K} \models JournalPaper(a)$?

Answer: Unknown

Observation: extensions of disjoint concepts do not overlap

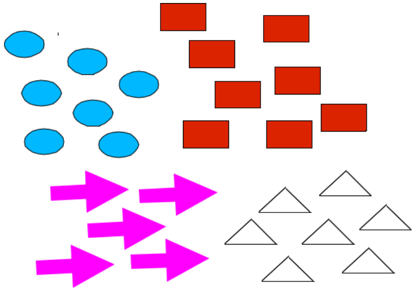
Question: would it be possible to *automatically capture* disjointness axioms by analyzing the data configuration/distribution?

Idea: Exploiting **(Conceptual) clustering methods** for the purpose

Basics on Clustering Methods

Clustering methods: unsupervised inductive learning methods that organize a collection of unlabeled resources into meaningful clusters such that

- intra-cluster *similarity* is high
- inter-cluster *similarity* is low



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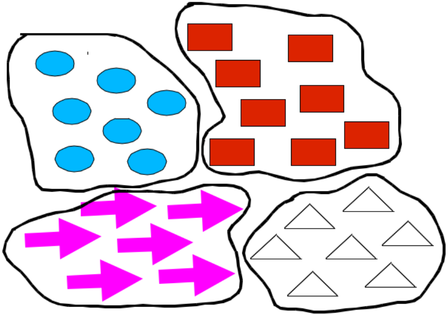

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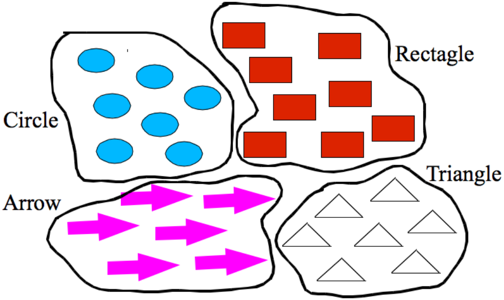

Observation: extensions of disjoint concepts do not overlap

Question: would it be possible to *automatically capture* them by analyzing the data configuration/distribution?

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Definition (Problem Definition)

Given

- an ontological knowledge base $\mathcal{K} = \langle \mathcal{T}, \mathcal{A} \rangle$
- a set of individuals $\mathbf{I} \subseteq \mathsf{Ind}(\mathcal{A})$

Find

- n pairwise disjoint clusters $\{\mathbf{C}_1, \ldots, \mathbf{C}_n\}$
- for each $i = 1, \ldots, n$, a concept description D_i that describes $\mathbf{C}_i$, such that:
    - $\forall a \in \mathbf{C}_i : \ \mathcal{K} \models D_i(a)$
    - $\forall b \in \mathbf{C}_j, j \neq i : \ \mathcal{K} \models \neg D_i(b)$.
- Hence $\forall D_i, D_j, i \neq j : \ \mathcal{K} \models D_j \sqsubseteq \neg D_i$.

Clustering Individuals of An Ontology: Developed Methods

Purely Logic-based

- KLUSTER *[Kietz & Morik, 94]*
- CSKA *[Fanizzi et al., 04]*
  - Produce a *flat output*
  - *Suffer from noise* in the data

Similarity-based ⇒ *noise tolerant*

- Evolutionary Clustering Algorithm around Medoids *[Fanizzi et al. @ IJSWIS 2008]*
  - automatically assess the best number of clusters
- k-Medoid (hierarchical and fuzzy) clustering algorithm *[Fanizzi et al. @ ESWC'08, Fundam. Inform.'10]*
  - number of clusters required

Developed Methods for:

Supervised Concept Learning

- Separate-and-conquer approach
  - YinYang *[Iannone et al. @ Appl. Intell. J. 2007]*
  - DL-FOIL *[Fanizzi et al. @ ILP 2008]*
  - DL-Learner *[Lehmann et al. @ MLJ 2010, SWJ 2011]*
- Divide-and-conquer approach
  - TermiTIS *[Fanizzi et al. @ ECML 2010, Rizzo et al. @ ESWC 2015]*
- can be exploited for learning intentional cluster descriptions - do not tackle the problem of learning disjointness axioms

Learning Disjointness Axioms

- Statistical-based approach
  - NAR - exploiting negative association rules *[Fleischhacker et al. @ OTM'11]*
  - PCC - exploiting Pearson's correlation coeff. *[Völker at al.@JWS 2015]*
- do not exploit any background knowledge

Terminological Cluster Tree

Defined a method for eliciting disjointness axioms *[Rizzo et.al.@ESWC'17]*

- solving a clustering problem via learning Terminological Cluster Trees
- providing a concept description for each cluster

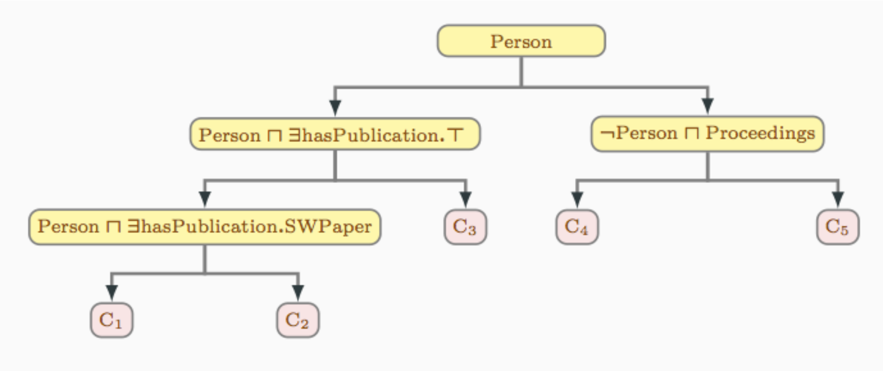
Definition (Terminological cluster tree (TCT))

A binary logical tree where

- a node stands for a cluster of individuals $\mathbf{C}$
- each inner node contains a description D (over the signature of $\mathcal{K}$)
- each departing edge corresponds to positive (left) and negative (right) examples of D

Example of TCT

Given $\mathbf{I} \subseteq \mathsf{Ind}(\mathcal{A})$, an example of TCT describing individuals in the Semantic Web research community



Collecting Disjointness Axioms

Given a TCT **T**:

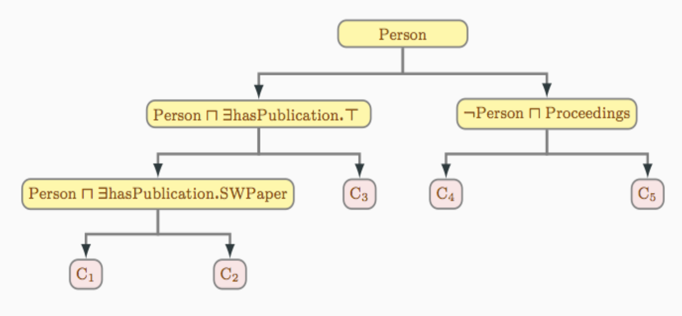
Step I:

- Traverse the **T** to collect the concept descriptions describing the clusters at the leaves
- A set of concepts **CS** is obtained

Step II:

- A set of candidate axioms **A** is generated from **CS**:
  - an axiom $D \sqsubseteq \neg E$ ($D, E \in \mathbf{CS}$) is generated if
    - $D \not\equiv E$ (or $D \not\sqsubseteq E$ or viceversa)
    - $E \sqsubseteq \neg D$ has not been generated

Collecting Disjointness Axioms: Example



CS = { Person, Person $\sqcap$ $\exists$hasPublication.$\top$, $\neg$(Person $\sqcap$ $\exists$hasPublication.$\top$), Person$\exists$hasPublication.SWPaper, $\neg$Proceedings, $\neg$Person $\sqcap$ Proceedings, $\cdots$ }

Axiom1: $Person \sqcap \exists hasPublication.SWPaper \sqsubseteq \neg(\neg Proceedings)$
Axiom2: $\cdots$

Inducing a TCT

Given the set of individuals **I** and $\top$ concept

Divide-and-conquere approach adopted

- **Base Case:** test the STOPCONDITION
  - the cohesion of the cluster **I** exceeds a threshold ν
    - distance between *medoids* below a threshold ν
- **Recursive Step** (STOPCONDITION does not hold):
  - a set **S** of refinements of the current (parent) description C generated
  - the BESTCONCEPT $E^* \in$ **S** is selected and installed as *current node*
    - the one showing the *best cluster separation* $\Leftrightarrow$ with max distance between the *medoids* of its positive P and negative N individuals
  - **I** is SPLIT in:
    - $I_{left} \subseteq$ **I** $\leftrightarrow$ individuals with the smallest distance wrt the *medoid* of P
    - $I_{right} \subseteq$ **I** $\leftrightarrow$ individuals with the smallest distance wrt the *medoid* of N

Note: *Number of clusters not required* - obtained from data distribution

Lesson Learnt from experiments I

Experiments performed on ontologies publicly available

- Goal I: Re-discover a target axiom (existing in $\mathcal{K}$)
  - Setting:
    - A copy of each ontology is created removing a target axiom
    - Threshold $\nu = 0.9, 0.8, 0.7$
    - Metrics # discovered axioms and #cases of inconsistency
  - Results:
    - target axioms rediscovered for almost all cases
    - *additional* disjointness *axioms discovered* in a significant number
    - limited number of inconsistencies found

Ontology	TCT 0.9		TCT 0.8		TCT 0.7	
	#inc.	#ax's	#inc.	#ax's	#inc.	#ax's
BioPax	2	53	2	53	3	52
NTN	10	70	9	73	10	75
Financial	0	125	0	126	0	127
GeoSkills	2	345	1	347	4	347
Monetary	0	432	0	432	0	433
DBPedia3.9	45	45	44	44	43	43

Lesson Learnt from experiments II

Goal II:

- Re-discover randomly selected target axioms added according to the **Strong Disjointness Assumption** *[Schlobach et al. @ ESWC 2005]*
  - two sibling concepts in a subsumption hierarchy considered as disjoint
- comparative analysis with statistical-based methods *[Völker at al. @ JWS 2015, Fleischhacker et al. @ OTM'11]*
  - PCC - based on *Pearson's correlation coefficient*
  - NAR - exploiting *negative association rules*
- Setting:
  - A copy of each ontology created removing 20%, 50%, 70% of the disjointness axioms
    - The copy used to induce TCT - $\nu = 0.9, 0.8, 0.7$ - # Run: 10 times
  - **Metrics**: rate of **rediscovered** target axioms, #cases of inconsistency, # addional discovered axioms

Lesson Learnt from experiments III

- Results:
  - *almost all axioms rediscovered*
    - Rate decreases when larger fractions of axioms removed, *as expected*
  - *TCT outperforms PCC and NAR* wrt *additionally discovered axioms* whilst introducing limited inconsistency
    - TCT allows to express complex disjointness axioms
    - PCC and NAR tackle only disjointness between concept names

Exploiting the $\mathcal{K}$ as well as the data distribution improves **disjointness axioms discovery**

Ontology Mining Tasks

- Instance Retrieval (Instance Level)
- Ontology Enrichment (Schema Level)
- **Concept Drift and Novelty Detection** (Ontology Dynamic)

from an inductive perspective

Concept Drift and Novelty Detection

- Ontologies evolve over the time ⇒ *New assertions* added.
- **Concept Drift**
  - change of a concept towards a more general/specific one w.r.t. the evidence provided by new annotated individuals
    - almost all `Worker` work for more than 10 hours per days ⇒ `HardWorker`
- **Novelty Detection**
  - isolated cluster in the search space that requires to be defined through new emerging concepts to be added to the KB
    - subset of `Worker` *employed* in a company ⇒ `Employee`
    - subset of `Worker` *working for* several companies ⇒ `Free-lance`

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Idea: *automatically capturing* them by analyzing the data configuration/distribution

Research Direction

Exploiting **(Conceptual) clustering methods** for the purpose

Lesson Learnt from Experiments

Developed Methods

- Evolutionary Clustering around Medoids *[Fanizzi et al. @ IJSWIS 2008]*
  - automatically assess the best number of clusters
- k-Medoid (hierarchical and fuzzy) clustering algorithm *[Fanizzi et al. @ ESWC'08, Fundam. Inform.'10]*
  - number of clusters required

Clustering algorithms applied on ontologies publicly available

- *evaluated by the use of standard validity clustering indexes* (e.g. Generalized Dunns index, cohesion index, Silhouette index)

Necessity of a domain expert/gold standard particularly **for validating the concept novelty/drift**

Conclusions

Machine Learning methods

- could be usefully exploited for ontology mining
- suitable in case of incoherent/noisy KBs
- **can be seen as an additional layer on top of deductive reasoning** for realizing *new/additional forms of approximated reasoning capabilities*

Future directions:

- Semi-Supervised Learning methods particularly appealing for LOD
- Special focus on scalability issues

That's all!

Thank you

Nicola Fanizzi

Giuseppe Rizzo

Floriana Esposito

Refinement Operators

Downward refinement operators specializing a concept C

ρ_1 $C' = C \sqcap (\neg)A$;

ρ_2 $C' = C \sqcap (\neg)(\exists)R.\top$;

ρ_3 $C' = C \sqcap (\neg)(\forall)R.\top$;

ρ_4 $\exists R.C'_i \in \rho(\exists R.C_i) \land C'_i \in \rho(C_i)$;

ρ_5 $\forall R.C'_i \in \rho(\forall R.C_i) \land C'_i \in \rho(C_i)$.

Distance measure between individuals

Distance Function (adapted from [d'Amato et al.@ESWC2008]):

$$d_n^{\mathcal{C}} : \mathsf{Ind}(\mathcal{A}) \times \mathsf{Ind}(\mathcal{A}) \rightarrow [0, 1]$$

$$d_n^{\mathcal{C}}(a, b) = \left[\sum_{i=1}^{m} w_i \left[1 - \pi_i(a)\pi_i(b)\right]^n \right]^{1/n}$$

Context: a set of atomic concepts $\mathcal{C} = \{B_1, B_2, \ldots, B_m\}$

Projection Function:

$$\forall\ a \in \mathsf{Ind}(\mathcal{A})(\mathcal{A}) \qquad \pi_i(a) = \begin{cases} 1 & \text{if } \mathcal{K} \models B_i(a) \\ 0 & \text{if } \mathcal{K} \models \neg B_i(a) \\ 0.5 & \text{otherwise} \end{cases}$$

2nd Experiment - Outcomes

Ontology	*f*	TCT 0.9		TCT 0.8		TCT 0.7		PCC		NAR	
		#inc.	#ax's	#inc.	#ax's	#inc.	#ax's	#inc.	#ax's	#inc.	#ax's
BioPax	20%	235	3859	357	4235	365	4256				
	50%	125	3576	357	4176	432	4115	257	280	352	2990
	70%	125	3432	235	3875	417	4154				
NTN	20%	312	3128	343	3126	354	3124				
	50%	234	3023	234	3034	235	3034	32	957	376	3766
	70%	156	2987	176	2679	123	2675				
Financial	20%	76	165	87	325	96	276				
	50%	37	143	56	307	53	259	124	1112	542	5366
	70%	33	143	43	276	40	221				
GeoSkills	20%	234	14289	357	14297	432	14345				
	50%	231	14123	356	14154	417	14256	456	13384	456	13299
	70%	234	14122	358	14154	377	14187				
Monetary	20%	535	13456	573	13453	623	13460				
	50%	315	13236	432	13236	532	13236	543	13384	423	13456
	70%	247	13127	231	13127	312	13127				
DBPedia3.9	20%	1345	29730	1432	30143	1432	30567				
	50%	1346	29730	1431	30143	1433	30567	1243	30470	1243	30365
	70%	1343	19730	1432	30143	1432	30567				

Experiment II - Outcomes

Ontology	*f*	TCT – *standard mode*			TCT – *early stopping*		
		TCT 0.9	TCT 0.8	TCT 0.7	TCT 0.9	TCT 0.8	TCT 0.7
BioPax	20%	0.90 ± 0.12	0.76 ± 0.13	0.74 ± 0.13	0.80 ± 0.23	0.65 ± 0.23	0.70 ± 0.13
	50%	0.85 ± 0.13	0.74 ± 0.13	0.74 ± 0.13	0.63 ± 0.23	0.63 ± 0.23	0.63 ± 0.23
	70%	0.85 ± 0.13	0.74 ± 0.12	0.74 ± 0.14	0.69 ± 0.13	0.67 ± 0.13	0.66 ± 0.14
NTN	20%	0.99 ± 0.08	0.95 ± 0.06	0.95 ± 0.08	0.70 ± 0.15	0.67 ± 0.15	0.67 ± 0.14
	50%	0.97 ± 0.03	0.93 ± 0.10	0.93 ± 0.01	0.55 ± 0.13	0.54 ± 0.13	0.54 ± 0.15
	70%	0.90 ± 0.10	0.89 ± 0.11	0.89 ± 0.10	0.55 ± 0.13	0.55 ± 0.13	0.55 ± 0.13
Financial	20%	0.99 ± 0.08	0.99 ± 0.08	0.99 ± 0.08	0.60 ± 0.10	0.59 ± 0.11	0.59 ± 0.11
	50%	0.97 ± 0.03	0.97 ± 0.03	0.97 ± 0.03	0.56 ± 0.10	0.56 ± 0.10	0.56 ± 0.10
	70%	0.95 ± 0.05	0.95 ± 0.05	0.95 ± 0.05	0.56 ± 0.10	0.56 ± 0.10	0.56 ± 0.10
GeoSkills	20%	0.99 ± 0.08	0.99 ± 0.08	0.99 ± 0.08	0.70 ± 0.15	0.69 ± 0.11	0.69 ± 0.11
	50%	0.92 ± 0.10	1.00 ± 0.00	1.00 ± 0.00	0.65 ± 0.23	0.65 ± 0.23	0.65 ± 0.23
	70%	0.92 ± 0.10	0.92 ± 0.10	0.92 ± 0.10	0.65 ± 0.23	0.63 ± 0.22	0.62 ± 0.23
Monetary	20%	0.99 ± 0.08	1.00 ± 0.00	1.00 ± 0.00	0.65 ± 0.23	0.63 ± 0.20	0.62 ± 0.23
	50%	0.94 ± 0.13	1.00 ± 0.00	1.00 ± 0.00	0.63 ± 0.12	0.66 ± 0.15	0.65 ± 0.11
	70%	0.94 ± 0.13	0.91 ± 0.14	0.91 ± 0.13	0.62 ± 0.12	0.60 ± 0.13	0.60 ± 0.12
DBPedia3.9	20%	1.00 ± 0.00	1.00 ± 0.00	1.00 ± 0.00	0.70 ± 0.12	0.68 ± 0.13	0.67 ± 0.12
	50%	1.00 ± 0.00	1.00 ± 0.00	1.00 ± 0.00	0.65 ± 0.23	0.68 ± 0.13	0.64 ± 0.12
	70%	0.96 ± 0.08	0.90 ± 0.08	0.90 ± 0.08	0.65 ± 0.22	0.68 ± 0.13	0.64 ± 0.12

Example of axioms

Successfully discovered axioms

- ExternalReferenceUtilityClass $\sqcap \exists$TAXONREF.$\top$
  disjoint with
  xref
- Activity
  disjoint with
  Person $\sqcap \exists$nationality.United_states
- Person $\sqcap$ hasSex.Male ($\equiv$ Man)
  disjoint with
  SupernaturalBeing $\sqcap$ God ($\equiv$ God)