Is it really the time to give up with semantics?

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Progic - Combining Probability and Logic

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Introduction & Motivation



Open KG online with content freely accessible

- BabelNet
- DBpedia
- Freebase
- Wikidata
- YAGO
-

Enterprise KG for commercial usage

- Google
- Amazon
- Facebook
- LinkedIn
- Microsoft

picture from https://www.csee.umbc.edu/courses/graduate/691/fall19/07/1 > < 🗇 > < 🗄 > < 🗄 > = > 🗐 = 🔗 🤇 🗠

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Applications

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- e-Commerce
- Semantic Search
- Fact Checking
- Personalization
- Recommendation
- Medical decision support system
- Question Answering
- Machine Translation

Research Areas

- Information Extraction
- Natural Language Processing
- Machine Learnig (ML)
- Knowledge Representation
- Web

• ...

Robotics



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Machine Learning & Knowledge Graphs



Two perspectives:

• KG as input to ML

• **Goal:** improving the performance in many learning tasks, e.g. QA, image classification, instance disambiguation, etc.

• ML as input to KG

- Goal: improving the KG itself
 - creating new facts
 - creating generalizations
 - prototyping
 - $\bullet\,$ improving the size, coverage, depth and accuracy of KGs $\rightarrow\,$ reducing their production costs

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What is a Knowledge Graph?



Basics

Knowledge Graph: Definition

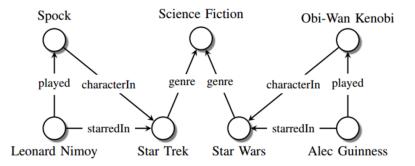
- ^a A graph of data intended to convey knowledge of the real world
 - conforming to a graph-based data model
 - nodes represent entities of interest
 - edges represent potentially different relations between these entities
 - data graph potentially enhanced with schema

^aA. Hogan et al. Knowledge Graphs. ACM Computing Surveys, 54, 1–37. (2021)

KGs: Main Features

- ontologies employed to define and reason about the semantics of nodes and edges
- grounded on the Open World Assumption (OWA)
- RDF, RDFS, OWL represetation languages will be assumed
- very large data collections
- suffer of *incompleteness* and *noise*
 - since often result from a complex building process

Knowledge Graph: Example



Source: Maximilian Nickel et al. A Review of Relational Machine Learning for Knowledge Graphs: From Multi-Relational Link Prediction to Automated Knowledge Graph Construction

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ML, Reasoning and KGs

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ML as input to KG



Incompleteness and noise

Knowledge Graph Refinement

- Link Prediction: predicts missing links between entities
 - regarded as a *learning to rank* problem
- *Triple Classification*: assesses correctness of a statement wrt a KG
 - regarded as a *binary classification* problem

New scalable Machine Learning methods

Very Large Data Collections

- grounded on *numeric-based approaches*
 - vector embedding models largely investigated ²

Isseus:

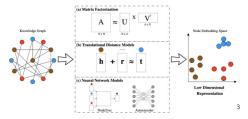
- CWA (or LCWA) mostly adopted vs. OWA
- schema level information and reasoning capabilities almost disregarded
- no interpretable models \Rightarrow hard to motivate results

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ML, Reasoning and KGs

Basics

Numeric-based methods consist of series of numbers without any obvious human interpretation



This may affects:

- the *interpretability* of the results
- the explainability
- and thus also somehow the trustworthiness of results

DRKG - Drug Repurposing Knowledge Graph



³Picture from D. N. Nicholson et al. Constructing knowledge graphs and their biomedical applications, Computational and Structural Biotechnology Journal, Vol. 18, pp. 1414–1428, (2020) ISSN 2001-0370

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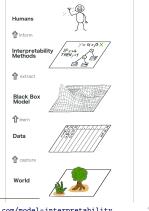
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⁴Picture from https://github.com/topics/knowledge-graph-embeddings 💉 🗆 🕨 🗇

Basics

Symbol-based learning methods usually provide

- *interpretable models* generalizing conclusions
 - e.g. trees, rules, logical formulae, etc.
- may be exploited for a better understanding of the provided results
- could be combined with deductive reasoning to make predictions
- limited in scalability



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⁵Picture from https://jaipancholi.com/model-interpretability C. d'Amato (UniBa) ML, Reasoning and KGs

Numeric-based learning methods:

- Can be enriched by taking into account schema level information and reasoning capabilities?
- If so, may it be beneficial?

Symbol-based learning methods:

- Can be still be applied to KGs?
- Why doing so?

Numeric-based learning methods:

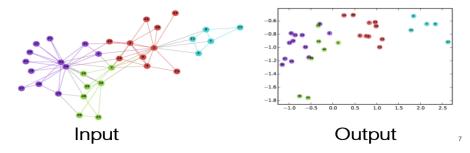
- Can be enriched by taking into account schema level information and reasoning capabilities?
- If so, may it be beneficial?

Symbol-based learning methods:

- Can be still be applied to KGs?
- Why doing so?

KG Embedding Models...

KGE models 6 convert data graph into an optimal low-dimensional space



Graph structural information and properties preserved as much as possible

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⁰Cai, H. et al.: A comprehensive **survey** of graph embedding: problems, techniques, and applications. IEEE TKDE 30(09), pp. 1616-1637 (2018).

Picture from https://laptrinhx.com/node2vec-graph-embedding-method-2620064815/ < = + < = + = = =

...KG Embedding Models

Goal	Optimizer		
Learning embeddings s.t.			
 score of a valid (positive) triple is higher than 	Lookup Layer	Scoring Layer $f(s, p, o) \in \mathbb{R}$	Loss Functions £
 the score of an invalid (negative) triple 	Negatives Generation		

⁸Picture from "ECAI-20 Tutorial: Knowledge Graph Embeddings: From Theory to:Practice" + (= +

Idea: Enhance KGE through Background Knowledge Injection

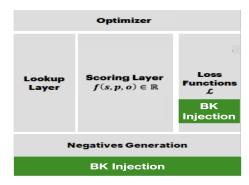
By two components:

Reasoning: used for generating negative triples

Axioms: domain, range, disjointWith, functionalProperty;

BK Injection: defines constraints on functions, corresponding to the considered axioms, *guiding the way embedding are learned*

Axioms: equivClass, equivProperty, inverseOf and subClassOf.



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Other KG Embedding Methods Leveraging BK

- Jointly embedding KGs and logical rules Guo, S. et al. @ ACL 2016
 - triples represented as atomic formulae
 - rules represented as complex formulae modeled by t-norm fuzzy logics
- Adversarial training exploiting Datalog clauses encoding assumptions to regularize neural link predictors [Minervini, P. et al. @ UAI 2017]

A specific form of BK required, not directly applicable to KGs

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An approach to learn embeddings exploiting BK [d'Amato et al. @ ESWC 2021]⁹



Could be applied to more complex KG embedding methods with additional formalization

TRANSOWL...

TransOWL maintains TransE setting

 ${\rm TRANSE^{10}}$ learns the vector embedding by minimizing Margin-based loss function

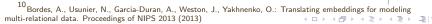
$$L = \sum_{\substack{\langle s, \rho, o \rangle \in \Delta \\ \langle s', \rho, o' \rangle \in \Delta'}} \left[\gamma + f_{\rho}(\mathsf{e}_{s}, \mathsf{e}_{o}) - f_{\rho}(\mathsf{e}_{s'}, \mathsf{e}_{o'}) \right]_{+}$$

where $[x]_+ = \max\{0, x\}$, and $\gamma \ge 0$

Score function

similarity (negative L_1 or L_2 distance) of the translated subject embedding $(e_s + e_p)$ to the object embedding e_o :

$$f_p(e_s, e_o) = - \|(e_s + e_p) - e_o\|_{\{1,2\}}$$



...TRANSOWL

- Derive *further triples to be considered for training* via schema axioms
 - equivClass, equivProperty, inverseOf and subClassOf
- More complex loss function
 - adding a number of terms consistently with the constraints

$$L = \sum_{\substack{\langle h,r,t\rangle \in \Delta\\ \langle h',r,t'\rangle \in \Delta'}} [\gamma + f_r(h,t) - f_r(h',t')]_+ + \sum_{\substack{\langle t,q,h\rangle \in \Delta_{inverseOf}\\ \langle t',q,h'\rangle \in \Delta'_{inverseOf}}} [\gamma + f_q(t,h) - f_q(t',h')]_+ \\ + \sum_{\substack{\langle h,s,t\rangle \in \Delta_{equivProperty}\\ \langle h',s,t'\rangle \in \Delta'_{equivProperty}}} [\gamma + f_s(h,t) - f_s(h',t')]_+ + \sum_{\substack{\langle h,vpeOf,l\rangle \in \Delta \cup \in \Delta_{equivClass}\\ \langle h',vpeOf,l'\rangle \in \Delta' \cup \Delta'_{equivClass}}} [\gamma + f_{typeOf}(h,l) - f_{typeOf}(h',l')]_+ \\ + \sum_{\substack{\langle h,subClassOf,p\rangle \in \Delta_{subClass}\\ \langle h',subClassOf,p'\rangle \in \Delta'_{subClass}}} [(\gamma - \beta) + f(h,p) - f(h',p')]_+$$

where $q \equiv r^-$, $s \equiv r$ (properties), $l \equiv t$ and $t \sqsubseteq p$ (classes) and $f(h, p) = ||e_h - e_p||$

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TRANSROWL...

TRANSROWL

- \bullet adopts the same approach of $\mathrm{TRANSOWL}$
- is derived from TRANSR ¹¹

 $\begin{aligned} \mathrm{TRANSE} &\Rightarrow \text{poor modeling } \textit{reflexive} \text{ and } \textit{non 1-to-1 relations (e.g. typeOf)} \\ \mathrm{TRANSR} &\Rightarrow \text{more suitable to handle such specificity} \end{aligned}$

 TRANSR adopts TRANSE loss function

Score function

preliminarily projects e_s and e_o to the different *d*-dimensional space of the relational embeddings e_p through a suitable matrix $M \in \mathbb{R}^{k \times d}$:

$$f_p'(\mathsf{e}_s,\mathsf{e}_o) = - \| (\mathsf{M}\mathsf{e}_s + \mathsf{e}_p) - \mathsf{M}\mathsf{e}_o \|_{\{1,2\}}.$$

¹¹Lin, Y., Liu, Z., Sun, M., Liu, Y., Zhu, X.: Learning entity and relation embeddings for knowledge graph completion. In: AAAI 2015 Proceedings. (2015)

...TRANSROWL

- $\bullet~\mathrm{TRANSOWL}$ loss function adopted plus weighting parameters
 - equivClass, equivProperty, inverseOf and subClassOf
- $\bullet~\mathrm{TRANSR}$ score function adopted

$$\begin{split} \mathcal{L} &= \sum_{\substack{\langle h,r,t \rangle \in \Delta \\ \langle h',r,t' \rangle \in \Delta'}} [\gamma + f'_r(h,t) - f'_r(h',t')]_+ + \lambda_1 \sum_{\substack{\langle t,q,h \rangle \in \Delta_{inverseOf} \\ \langle t',q,h' \rangle \in \Delta_{inverseOf'}}} [\gamma + f'_q(t,h) - f'_q(t',h')]_+ \\ + \lambda_2 \sum_{\substack{\langle h,s,t \rangle \in \Delta_{equivProperty} \\ \langle h',s,t' \rangle \in \Delta_{equivProperty'}}} [\gamma + f'_s(h,t) - f'_s(h',t')]_+ + \lambda_3 \sum_{\substack{\langle h,typeOf,l \rangle \in \Delta \cup \Delta_{equivClass} \\ \langle h',typeOf,l' \rangle \in \Delta' \cup \Delta'_{equivClass}}} [\gamma + f'_{typeOf}(h,l) - f'_{typeOf}(h',l')]_+ \\ + \lambda_4 \sum_{\substack{\langle t,subClassOf,p \rangle \in \Delta_{subClass} \\ \langle t',subClassOf,p' \rangle \in \Delta_{subClass}'}} [(\gamma - \beta) + f'(t,p) - f'(t',p')]_+ \end{split}$$

where

- $q \equiv r^-$, $s \equiv r$ (properties), $l \equiv t$ and $t \sqsubseteq p$ (classes)
- the parameters λ_i , $i \in \{1, ..., 4\}$, weigh the influence that each function term has during the learning phase

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$\mathrm{TRANSROWL}^{R}...$

 ${\rm TRANSROWL}^R$ adopts axiom-based regularization of the loss function, as for ${\rm TRANSE}^{R}{}_{^{12}}$

- by adding specific constraints to the loss function rather than
- explicitly derive additional triples during training

 $TRANSE^{R}$ adopt TRANSE score and loss function adds to the loss function axiom-based regularizers for inverse and equivalent property constraints

Loss function

$$L = \sum_{\substack{\langle h, r, t \rangle \in \Delta \\ (h', r', t') \in \Delta'}} [\gamma + f_r(h, t) - f_r(h', t')]_+ + \lambda \sum_{r \equiv q^- \in \mathcal{T}_{\mathsf{inverseOf}}} \|r + q\| + \lambda \sum_{r \equiv p \in \mathcal{T}_{\mathsf{equivProp}}} \|r - p\|$$

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...TRANSROWL^R

- $\bullet \ {\rm TransR}$ score function adopted
- additional regularizers needed for equivalentClass and subClassOf axioms
- further constraints on the projection matrices associated to relations

Loss function

$$L = \sum_{\substack{\langle h, r, t \rangle \in \Delta \\ \langle h', r', t' \rangle \in \Delta'}} [\gamma + f'_r(h, t) - f'_r(h', t')]_+ \\ + \lambda_1 \sum_{r \equiv q^- \in \mathcal{T}_{\text{inverseOf}}} \|r + q\| + \lambda_2 \sum_{r \equiv q^- \in \mathcal{T}_{\text{inverseOf}}} \|M_r - M_q\| \\ + \lambda_3 \sum_{r \equiv p \in \mathcal{T}_{\text{equivProp}}} \|r - p\| + \lambda_4 \sum_{r \equiv p \in \mathcal{T}_{\text{equivProp}}} \|M_r - M_p\| \\ + \lambda_5 \sum_{e' \equiv e'' \in \mathcal{T}_{\text{equivClass}}} \|e' - e''\| + \lambda_6 \sum_{s' \subseteq s'' \in \mathcal{T}_{\text{subClass}}} \|1 - \beta - (s' - s'')\|$$

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Lesson Learnt from Experiments...

Goal: Assessing the benefit of exploiting BK

• Comparing¹³ TRANSOWL, TRANSROWL, TRANSROWL^{*R*} over to the original models TRANSE and TRANSR as a baseline

Perfomances tested on:

- Link Prediction task
- Triple Classification task
- Standard metrics adopted

KGs adopted:

KG	#Triples	#Entities	#Relationships
DBpedia15K	180000	12800	278
DBpedia100K	600000	100000	321
DBpediaYAGO	290000	88000	316
NELL ¹⁴	150000	68000	272

13 All methods implemented as publicly available systems https://github.com/Keehl-Mihael/TransROWL-HRS

14 equivalentClass and equivalentProperty missing; limited number of typeOf-triples; abundance of subClassOf-triples: ->> < <->

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...Lesson Learnt from Experiments

- Best performance achieved by TRANSROWL, in most of the cases, and TRANSROWL^R
- TRANSROWL slightly superior performance of TRANSROWL^R

As for NELL , the models showed oscillating performances wrt the baselines

- NELL was aimed at testing in condition of larger incompleteness
 - equivalentClass and equivalentProperty missing
 - low number of typeOf-triples per entity

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Numeric-based learning methods:

• Can be enriched by taking into account schema level information and reasoning capabilities?

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• If so, may it be beneficial?

Symbol-based learning methods:

- Can be still be applied to KGs?
- Why doing so?

Symbol-based learning methods for Learning Disjointness Axioms

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A fine grained schema level information can bring better insight of the data

Disjointness axioms often missing

Problems:

introduction of noise

 $\mathcal{K} = \{ Journal Paper \sqsubseteq Paper, Conference Paper \sqsubseteq Paper, Conference Paper(a), Author(a) \}$ \mathcal{K} is Consistent !!! Cause Axiom: Author $\equiv \neg$ Conference Paper missing

counterintuitive inferences

 $\mathcal{K} = \{ Journal Paper \sqsubseteq Paper, Conference Paper \sqsubseteq Paper, Conference Paper(a) \}$

 $\mathcal{K} \models JournalPaper(a)$? Answer: Unknown Cause Axiom: JournalPaper $\equiv \neg$ ConferencePaper missing

• hard collecting negative examples when adopting numeric approaches

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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

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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?

Idea: Exploiting (Conceptual) clustering methods for the purpose

Definition (Problem Definition)

Given

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

Find

- *n* pairwise disjoint clusters $\{C_1, \ldots, C_n\}$
- for each i = 1, ..., n, a concept description D_i that describes C_i , such that:

•
$$\forall a \in C_i : \mathcal{K} \models D_i(a)$$

- $\forall b \in C_j, j \neq i$: $\mathcal{K} \models \neg D_i(b)$.
- Hence $\forall D_i, D_j, i \neq j$: $\mathcal{K} \models D_j \sqsubseteq \neg D_i$.

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Learning Disjointness Axioms: Developed Methods

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 and reasoning capabilities

Disjointness axioms learning/discovery can be hardly performed without symbol-based methods

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Terminological Cluster Tree

Defined a method ¹⁵ for eliciting disjointness axioms [*Rizzo et.al.@ SWJ'21*] ¹⁶

- 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

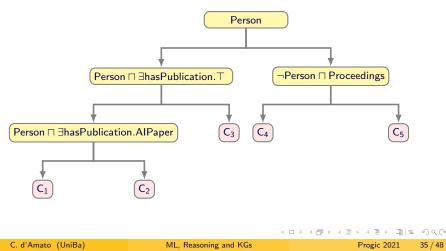
- a leaf node stands for a cluster of individuals C
- each inner node contains a description D (over the signature of \mathcal{K})
- each departing edge corresponds to positive (left) and negative (right) examples of *D*

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¹⁵Implemented system publicly available at https://github.com/Giuseppe-Rizzo/TCTnew

Example of TCT

Given $\mathsf{I}\subseteq\mathsf{Ind}(\mathcal{A}),$ an example of TCT describing the AI research community



Collecting Disjointness Axioms

Given a TCT T:

Step I:

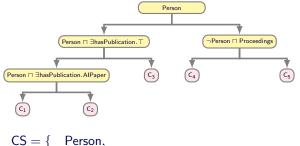
- Traverse the T to collect the concept descriptions describing the clusters at the leaves
- A set of concepts CS is obtained

Step II:

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

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Collecting Disjointness Axioms: Example



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

Axiom1: $Person \sqcap \exists hasPublication. AIPaper \sqsubseteq \neg(\neg Person \sqcap Proceedings)$ Axiom2: ···

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Inducing a TCT

Given the set of individuals I and \top concept

Divide-and-conquere approach adopted

- Base Case: test the $\operatorname{STOPCONDITION}$
 - $\bullet\,$ the cohesion of the cluster I exceeds a threshold $\nu\,$
 - $\bullet\,$ distance between $\textit{medoids}\,$ below a threshold ν
- **Recursive Step** (STOPCONDITION does not hold):
 - a set S of $\underline{refinements}$ 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 ⇔ 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*
 - $I_{\textit{right}} \subseteq I \leftrightarrow$ individuals with the smallest distance wrt the *medoid* of N
 - reasoner employed for collecting P and N

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

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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 $\nu = 0.9, 0.8, 0.7$
 - $\bullet~$ 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	
Ontology	#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

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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 <u>statistical-based</u> 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
 - $\bullet\,$ The copy used to induce TCT ν = 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

Example of axioms

Successfully discovered axioms

 ExternalReferenceUtilityClass □ ∃TAXONREF.⊤ disjoint with xref

Activity disjoint with Person □ ∃nationality.United_states

 Person □ hasSex.Male (≡ Man) disjoint with SupernaturalBeing □ God (≡ God)

Not discovered axioms

• Actor disjoint with Artefact

(concepts with few instances)

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Conclusions

Conclusions:

- Exploiting BK to learn embeddings models may improve link prediction and triple classification results
- Symbol-based learning methods useful for supplementing schema level information
- Deductive reasoning important for the full usage of BK

Further Research Directions:

- More robust enhanaced KG embedding solutions needed for tackling KG incompleteness (case of NELL)
- Scalability of symbol-based learning methods still need to be improved
- Empower KG embedding methods with explanation tools
- Integrate further reasoning approaches (e.g. common sense reasoning)

Thank you



Nicola Fanizzi Giuseppe Rizzo Nicola Flavio Quatraro

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Distance measure between individuals adopted for TCT

Distance Function (adapted from [d'Amato et al.@ESWC2008]): $d_n^{\mathcal{C}}: \operatorname{Ind}(\mathcal{A}) \times \operatorname{Ind}(\mathcal{A}) \to [0, 1]$

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

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

Projection Function:

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

Downward refinement operators specializing a concept C

- $C' = C \sqcap (\neg)(\exists) R.\top;$
- $C' = C \sqcap (\neg)(\forall) R.\top;$
- $\forall R.C'_i \in \rho(\forall R.C_i) \land C'_i \in \rho(C_i).$

Ontologies per Experiments on TCT

Ontology	DL Language	#Concepts	#Roles	<i>#Individuals</i>	#Disj. Ax.s
BioPax	ALCIF(D)	74	70	323	85
NTN	SHIF(D)	47	27	676	40
Financial	ALCIF(D)	60	16	1000	113
GeoSkills	$\mathcal{ALCHOIN}(D)$	596	23	2567	378
Monetary	ALCHIF(D)	323	247	2466	236
DBPedia3.9	$\mathcal{ALCHI}(D)$	251	132	16606	11

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