A perspective on Neuro-symbolic Approaches for Knowledge Graph Refinement and Explanation

Claudia d'Amato

Computer Science Department
University of Bari "Aldo Moro", Bari, Italy

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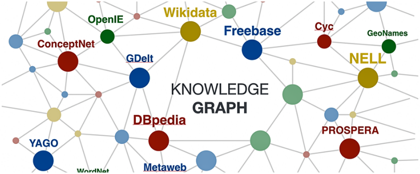


[1]

Applications

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

Research Fields

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

[1] picture from https://www.csee.umbc.edu/courses/graduate/691/fall19/07/

ML and KGs

Two perspectives:

KG as input to ML

Goal: improving the performance in many learning tasks, e.g.

- Question Answering (QA)
- image classification
- instance disambiguation
- text summarization
- ....

ML as input to KG

Goal: improving the KG itself

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

ML as input to KG

(KG Refinement: Link Prediction)

(Explanation of Link Predictions on KGs)

(KG Refinement at Schema Level)

ML as input to KG

(**KG Refinement: Link Prediction**)

(Explanation of Link Predictions on KGs)

(KG Refinement at Schema Level)

Incompleteness and **noise**

$\Downarrow$

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

Very Large Data Collections

$\Downarrow$

New scalable Machine Learning methods

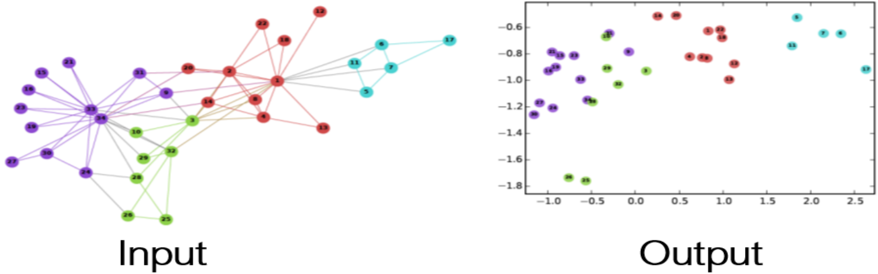
- grounded on numeric-based approaches
  - KG vector embedding models (KGE) largely investigated [Cai *et al.*, 2018]

ML/KGE for KGs: Issues

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

KG Embedding Models...

KGE models convert data graph into an optimal low-dimensional space [Cai *et al.*, 2018]



[2]

Graph structural information and properties preserved as much as possible

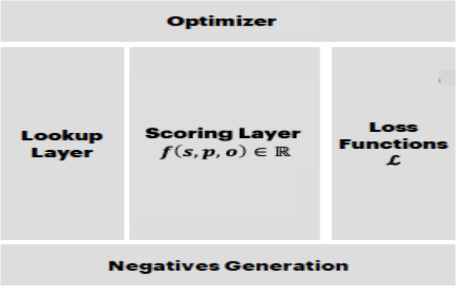
[2] Picture from https://laptrinhx.com/node2vec-graph-embedding-method-2620064815/

...KG Embedding Models

Goal

Learning embeddings s.t.

- score of a valid (positive) triple is higher than
- the score of an invalid (negative) triple



[3]

Negative examples generated by **random corruption of triples**

- false negatives may be generated
- only triple directly observable are considered

[3] Picture from "ECAI-20 Tutorial: Knowledge Graph Embeddings: From Theory to Practice"

KG Refinement by KG Embedding Methods:

Injecting Semantics

Enhancing KGE by Injecting Background Knowledge

[d'Amato *et al.*, 2021c,b]

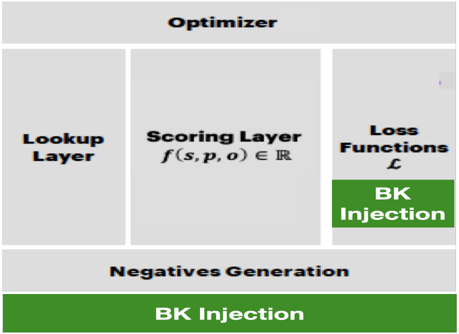
By two components:

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`.



A First Approach: TransOWL, TransROWL

[d'Amato *et al.*, 2021c]

- 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

$$
\begin{aligned}
L \; = \; & \overbrace{\sum_{\substack{\langle h,r,t\rangle\in\Delta \\ \langle h',r,t'\rangle\in\Delta'}} [\gamma + f_r(h,t) - f_r(h',t')]_+}^{\textbf{TransE}\ \textit{loss function}} + \sum_{\substack{\langle t,q,h\rangle\in\Delta_{\textbf{inverseOf}} \\ \langle t',q,h'\rangle\in\Delta'_{\textbf{inverseOf}}}} [\gamma + f_q(t,h) - f_q(t',h')]_+ \\
& + \sum_{\substack{\langle h,s,t\rangle\in\Delta_{\textbf{equivProperty}} \\ \langle h',s,t'\rangle\in\Delta'_{\textbf{equivProperty}}}} [\gamma + f_s(h,t) - f_s(h',t')]_+ + \sum_{\substack{\langle h,\textbf{typeOf},l\rangle\in\Delta\cup\in\Delta_{\textbf{equivClass}} \\ \langle h',\textbf{typeOf},l'\rangle\in\Delta'\cup\Delta'_{\textbf{equivClass}}}} [\gamma + f_{\textbf{typeOf}}(h,l) - f_{\textbf{typeOf}}(h',l')]_+ \\
& + \sum_{\substack{\langle h,\textbf{subClassOf},p\rangle\in\Delta_{\textbf{subClass}} \\ \langle h',\textbf{subClassOf},p'\rangle\in\Delta'_{\textbf{subClass}}}} [(\gamma - \beta) + f(h,p) - f(h',p')]_+
\end{aligned}
$$

where $q \equiv r^-$, $s \equiv r$ (properties), $l \equiv t$ and $t \sqsubseteq p$ (classes) and $f(h,p) = \|\mathbf{e}_h - \mathbf{e}_p\|$

An Alternative Approach: TransROWL^R

[d'Amato *et al.*, 2021c]

Adopting an axiom-based regularization of the loss function
as for TransE^R [Minervini *et al.*, 2017b]

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

Loss function

$$
\begin{aligned}
L \quad = & \sum_{\substack{\langle h,r,t\rangle \in \Delta \\ \langle h',r',t'\rangle \in \Delta'}} [\gamma + f'_r(h,t) - f'_r(h',t')]_+ \\
& +\lambda_{\mathbf{1}} \sum_{r \equiv q^- \in \mathcal{T}_{\mathbf{inverseOf}}} \|r + q\| \; + \lambda_{\mathbf{2}} \sum_{r \equiv q^- \in \mathcal{T}_{\mathbf{inverseOf}}} \|M_r - M_q\| \\
& +\lambda_{\mathbf{3}} \sum_{r \equiv p \in \mathcal{T}_{\mathbf{equivProp}}} \|r - p\| \; + \lambda_{\mathbf{4}} \sum_{r \equiv p \in \mathcal{T}_{\mathbf{equivProp}}} \|M_r - M_p\| \\
& +\lambda_{\mathbf{5}} \sum_{e' \equiv e'' \in \mathcal{T}_{\mathbf{equivClass}}} \|e' - e''\| \; + \lambda_{\mathbf{6}} \sum_{s' \subseteq s'' \in \mathcal{T}_{\mathbf{subClass}}} \|\mathbf{1} - \beta - (s' - s'')\|
\end{aligned}
$$

Main Outcome: TransROWL slightly outperforming TransROWL^R

Other KG Embedding Methods Leveraging BK

- Jointly embedding KGs and logical rules [Guo *et al.*, 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 *et al.*, 2017a]

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

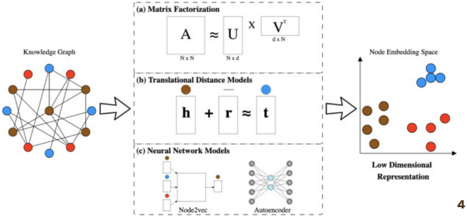
ML as input to KG

(KG Refinement: Link Prediction)

(**Explanation of Link Predictions on KGs**)

(KG Refinement at Schema Level)

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

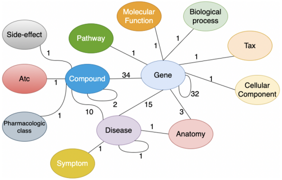


[4]

This may affects:

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

DRKG – Drug Repurposing Knowledge Graph



[5]

[4] Picture 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

[5] Picture from https://github.com/topics/knowledge-graph-embeddings

A-Posteriori Explanations of Link Predictions

A-posteriori methods: find suitable explanation(s) based on the observed output and the model input, independently on the KGE adopted - Developed solutions

KELPIE [Rossi *et al.*, 2022]: generates necessary and sufficient (path) conditions and an articulated new evaluation protocol

CrossE [Zhang *et al.*, 2019]: embedding model for link predictions providing explanations

- the search for a path linking the subject h and object t of a predicted triple $\langle h, r, t \rangle$
  - **Max lenght 2** $\rightarrow$ six types of paths possible:
    Length 1: $P_1 = \{\langle h, r_s, t \rangle\}$, $P_2 = \{\langle t, r_s, h \rangle\}$
    Length 2: $P_3 = \{\langle e', r_s, h \rangle, \langle e', r', t \rangle\}$, $P_4 = \{\langle e', r_s, h \rangle, \langle t, r', e' \rangle\}$,
    $P_5 = \{\langle h, r_s, e' \rangle, \langle e', r', t \rangle\}$, $P_6 = \{\langle h, r_s, e' \rangle, \langle t, r', e' \rangle\}$,
    where r_s similar to r, r' any other relationship, e' any other entity;
- search driven by similarities between relation/entity embeddings by Euclidean distance
- structural comparisons with other paths in the KG to reinforce the reliability of the explanation found (referred to as support)

Explaining Link Predictions with CrossE

Given the predicted triple: ⟨`NickMason`, `recordLabel`, `CapitolRecords`⟩

why is it provided?

User is able to understand motivations, and trust (or not) the prediction

Example of exmplanation

⟨`NickMason`, `associatedBand`, `PinkFloyd`⟩,
⟨`PinkFloyd`, `recordLabel`, `CapitolRecords`⟩

Ideally supported by analogous situations to be found in the KG e.g.

⟨`RingoStarr`, `recordLabel`, `Parlophone`⟩

for which the computed explanation is:
⟨`RingoStarr`, `associatedBand`, `TheBeatles`⟩,
⟨`TheBeatles`, `recordLabel`, `Parlophone`⟩.

Exploiting Semantics for Providing Explanations to Link Predictions on KGs

Idea: SemanticCrossE provide semantic-based explanations for link predictions on KGs

[d'Amato *et al.*, 2021a]

Extends CrossE by adopting a Semantic Cosine similarity that leads the explanation process

- exploits the underlying KG semantics → Domain, Range and Classes considered
- increases the cosine similarity of two (entities / relationships) vector embeddings on the ground of available additional semantic information which is captured by a semantic Score function

Definition (semantic Cosine)

Given KG $\mathcal{K}(\mathcal{E}, \mathbb{R})$, the semantic Cosine measure for two entities $e, e' \in \mathcal{E}$ is defined by:

$$\mathrm{semCos}_{\alpha,\beta}(e, e') = \alpha \cdot \mathrm{sScore}(e, e') + \beta \cdot \mathrm{sim}_{\mathsf{cos}}(\mathsf{e}, \mathsf{e}')$$

where e the respective entity embedding vector; $\alpha, \beta \in [0, 1]$ chosen s.t. $\alpha + \beta = 1$.

In the case of relations $r, r' \in \mathbb{R}$ the measure is defined analogously.

Definition (semantic Score)

Given $\mathcal{C}$ set of the classes occurring in $\mathcal{K}(\mathcal{E}, \mathbb{R})$, and the functions $Cl \colon \mathcal{E} \to \mathcal{C}$, $Do \colon \mathbb{R} \to \mathcal{C}$, and $Ra \colon \mathbb{R} \to \mathcal{C}$ that return, resp., the conjunction of the classes an entity belongs to, and the domain and range of a relation, the semantic Score function for pairs of entities $e, e' \in \mathcal{E}$ is defined by:

$$\mathrm{sScore}(e, e') = \frac{|\mathrm{ret}[Cl(e) \sqcap Cl(e')]|}{|\mathrm{ret}[Cl(e) \sqcup Cl(e')]|}$$

where $\mathrm{ret}_{\mathcal{K}}(C)$ returns the entities that can be proven to belong to a given class C

Analogously, given any two relationships $r, r' \in \mathbb{R}$, it is defined:

$$\mathrm{sScore}(r, r') = \frac{|\mathrm{ret}[Do(r) \sqcap Do(r')]|}{|\mathrm{ret}[Do(r) \sqcup Do(r')]|} + \frac{|\mathrm{ret}[Ra(r) \sqcap Ra(r')]|}{|\mathrm{ret}[Ra(r) \sqcup Ra(r')]|}$$

- Approximated form of semantic Cosine measure (specifically of the semantic Score function) employed [d'Amato *et al.*, 2021a]
- Efficient computation obtained by a preliminary clustering phase [d'Amato *et al.*, 2023]

Main Outcome:

- ApproxSemanticCrossE showed improved results both in terms of recall and support
- ApproxSemanticCrossE not affected by noisy (irrelevant) explanations as for CrossE and partially cosineCrossE → qualitative evaluation conducted

A more efficient solution developed with **KELPIE++** [Barile *et al.*, 2024]

ML as input to KG

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(**KG Refinement at Schema Level**)

Learning Disjointness Axioms

Missing Disjointness Axioms: Issues

Disjointness axioms often missing [Wang *et al.*, 2006]

Problems:

- introduction of noise

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

- counterintuitive inferences

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

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

- **hard collecting negative examples when adopting numeric approaches**

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 mining disjointness axioms

[Rizzo *et al.*, 2021]

Definition (Problem Definition)

Given

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

Find

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

Learning Disjointness Axioms: Developed Methods

Statistical-based approach

- NAR - exploiting negative association rules [Fleischhacker and Völker, 2011]
- PCC - exploiting Pearson's correlation coeff. [Völker *et al.*, 2015]

do not exploit any background knowledge and reasoning capabilities

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

Terminological Cluster Tree

Defined a method [6] for eliciting disjointness axioms [Rizzo *et al.*, 2021]

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

Definition (Terminological cluster tree (TCT))

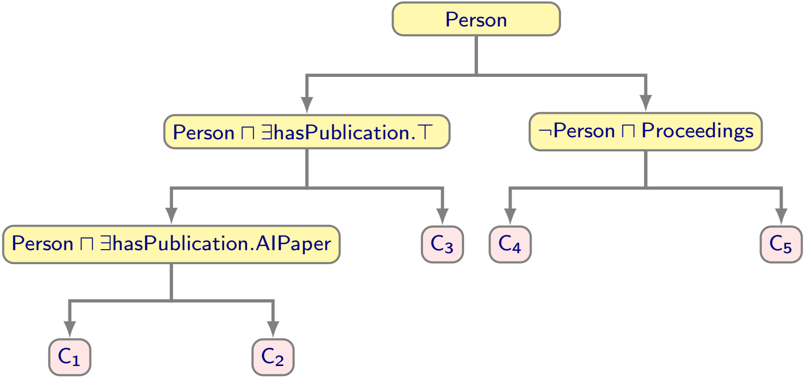
A binary logical tree where

- 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

[6] Implemented system publicly available at https://github.com/Giuseppe-Rizzo/TCTnew

Example of TCT

Given $\mathsf{I} \subseteq \mathrm{Ind}(\mathcal{A})$, 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

Conclusions

Conclusions:

- Injecting semantics and exploiting reasoning capabilities may improve the effectiveness of ML solutions for KG
    - Framework for injecting BK into KGE models
    - Solution for injecting semantics when computing a-posteriori explanations to link predictions
- Supplementing schema level information (disjointness axioms) needed

Next Research Challenges:

- Extend the framework for injecting BK to more complex KGE models
- Learning disjointness axioms from KGE
- Develop a standardized evaluation protocol for evaluating explanations
- New solutions required for enhancing LLMs with KG semantics

Thank you

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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 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
    - reasoner employed for collecting P and N

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

Distance measure between individuals adopted for TCT

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

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

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

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

Projection Function:

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