Neural-symbolic Knowledge Representation with Ontology and Knowledge Graph Embeddings

Jiaoyan Chen

Lecturer in Department of Computer Science, University of Manchester

Senior Researcher in University of Oxford

AMS NSAI-Med/DSI Event, 5th July 2024, Zurich

What is an ontology?

Knowledge representation of a domain (e.g., concepts/classes, instances/entities, properties, and logical relationships)

$$\begin{aligned}\mathcal{T} = \{&\text{Father} \sqsubseteq \text{Parent} \sqcap \text{Male},\ \text{Mother} \sqsubseteq \text{Parent} \sqcap \text{Female},\\ &\text{Child} \sqsubseteq \exists \text{hasParent.Father},\ \text{Child} \sqsubseteq \exists \text{hasParent.Mother},\\ &\text{hasParent} \sqsubseteq \text{relatedTo}\}\\ \mathcal{A} = \{&\text{Father(Alex)}, \text{Child(Bob)}, \text{hasParent(Bob, Alex)}\}\end{aligned}$$

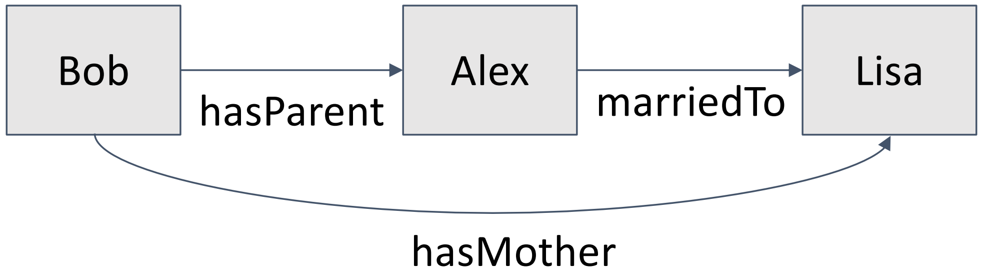
A toy ontology on a family

- Formal
- Explicit
- Shared

How to define formal, explicit and shared ontologies?

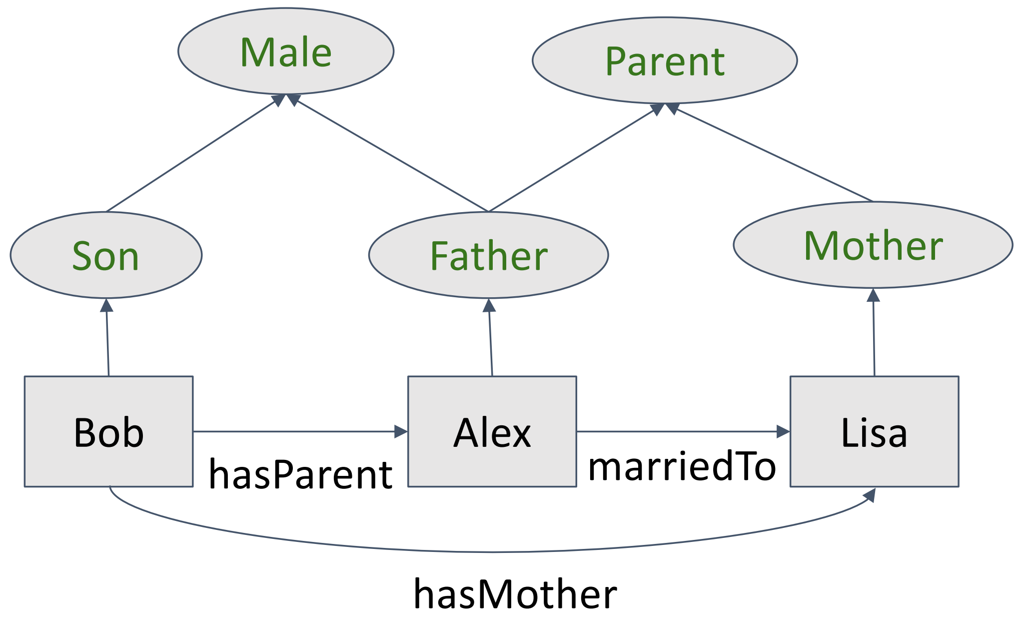
Ontology Languages

- **RDF** (Resource Description Framework)
  - Triple: <Subject, Predicate, Object>
  - Representing facts:
    - E.g., <Bob, hasParent, Alex>



Ontology Languages

- **RDF Schema (RDFS)**
  - Meta data (schema) of instances and facts
    - E.g., hierarchical concepts and properties, property domain and range,



Ontology Languages

- **Web Ontology Language** (OWL)
  - Schema and logical relationships (domain knowledge)
  - Taxonomies and vocabularies

$$\mathcal{T} = \{\text{Father} \sqsubseteq \text{Parent} \sqcap \text{Male},\ \ \text{Mother} \sqsubseteq \text{Parent} \sqcap \text{Female},$$
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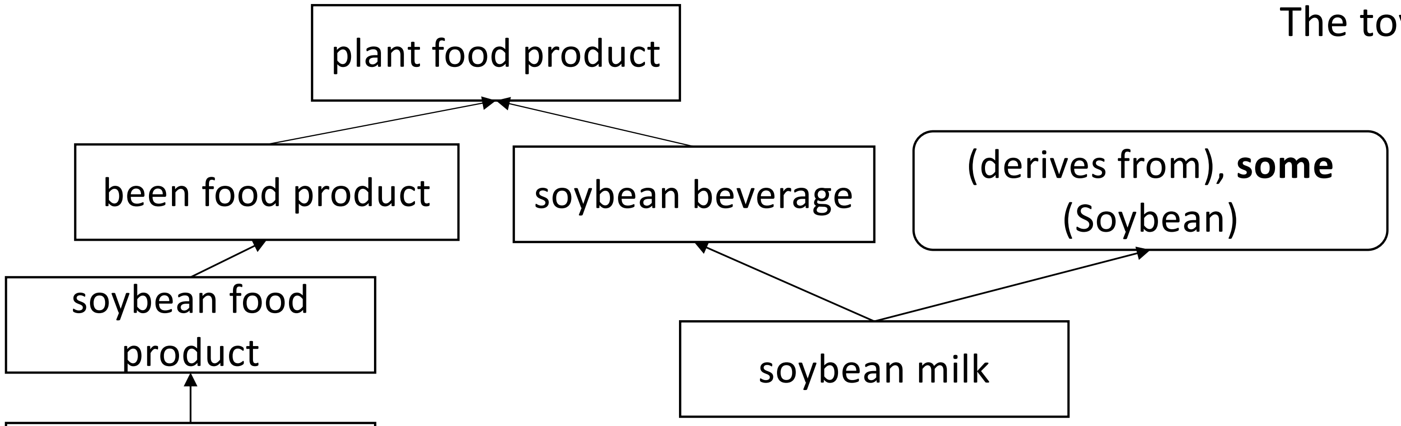
The toy ontology on a family



An example from the food ontology FoodOn

Why do we use RDF, RDFS and OWL?

Reason #1: Provide widely used vocabularies for defining all kinds of explicit, formal and shared knowledge

Reason #2: OWL supports Description Logics for representing complex knowledge

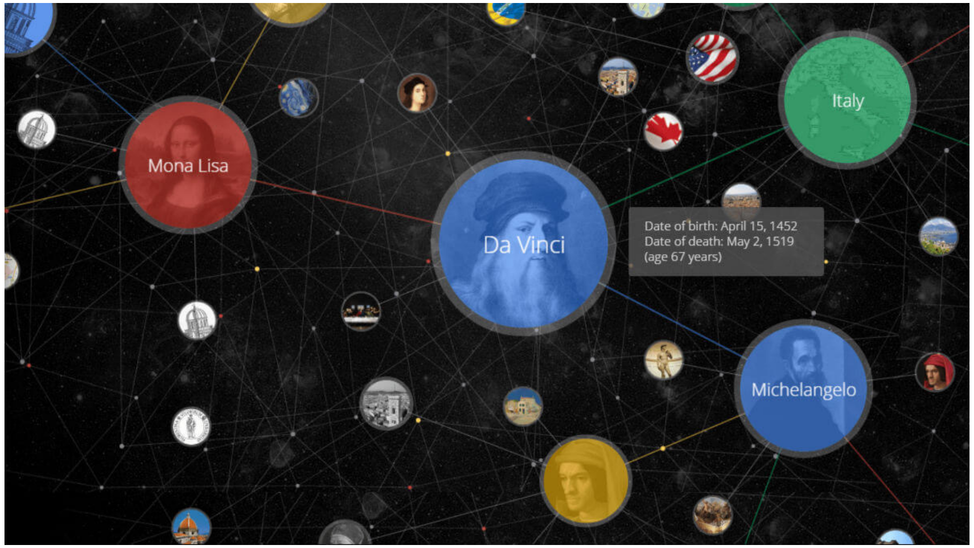
Reason #3: already have been widely deployed

E.g., in Life Sciences: SNOMED Clinical Terms, The Gene Ontology (GO), FoodOn, Human Disease Ontology (DOID), The Orphanet Rare Disease ontology (ORDO)

Chen, J., et al. "Knowledge Graphs for the Life Sciences: Recent Developments, Challenges and Opportunities." *Transactions on Graph Data and Knowledge (TGDK)* (2023).

What is Knowledge Graph?

- “Knowledge Graph” was proposed by Google in 2012, referring to its services to enhance its search engine’s results with knowledge gathered from a variety of sources



- Knowledge ≈ Instances + Facts, represented as RDF triples e.g., <Box, hasParent, Alex>
- Linked and graph structured data

Ontology and Knowledge Graph Embedding

- To represent symbols (e.g., entities and relations) in a vector space with their relationships concerned, mainly for being consumed by statistical analysis and machine learning

$$v_{Bob} + v_{hasParent} \approx v_{Alex}$$

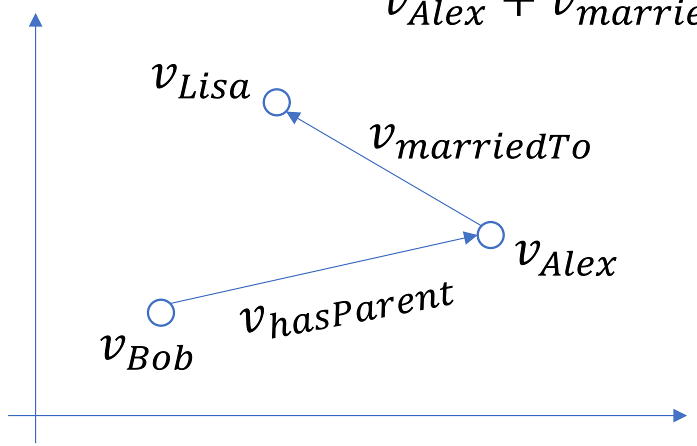
$$v_{Alex} + v_{marriedTo} \approx v_{Lisa}$$

$v_i \in R^n$

Example: **TransE for RDF triples**

<Bob, hasParent, Alex>
<Alex, marriedTo, Lisa>
…

Learning algorithm

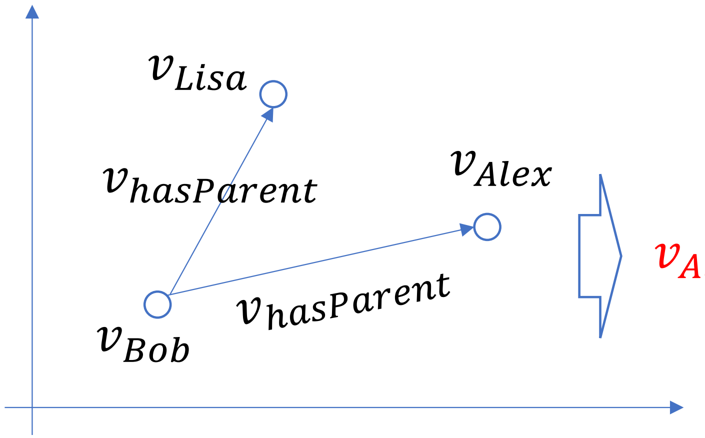


Bordes, A., et al. "Translating embeddings for modeling multi-relational data." *Advances in neural information processing systems* 26 (2013).

Ontology and Knowledge Graph Embedding

Limitations of the simple translation-based relation modeling

Cannot deal with **one-to-many, many-to-one and many-to-many relations**



$v_{Alex} = v_{Lisa}$!!

How to embed an OWL (or RDFS) ontology like the family example? Cannot model **concepts and their logical relationships**

$$\mathcal{T} = \{\text{Father} \sqsubseteq \text{Parent} \sqcap \text{Male},\ \text{Mother} \sqsubseteq \text{Parent} \sqcap \text{Female},$$
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Wide research for modeling complex relations and graph patterns for embedding KGs: TransR, ComplEx, DistMult, ConvE, RDF2Vec …

Embedding OWL Ontologies

$\mathcal{T} = \{\text{Father} \sqsubseteq \text{Parent} \sqcap \text{Male},\ \text{Mother} \sqsubseteq \text{Parent} \sqcap \text{Female},$
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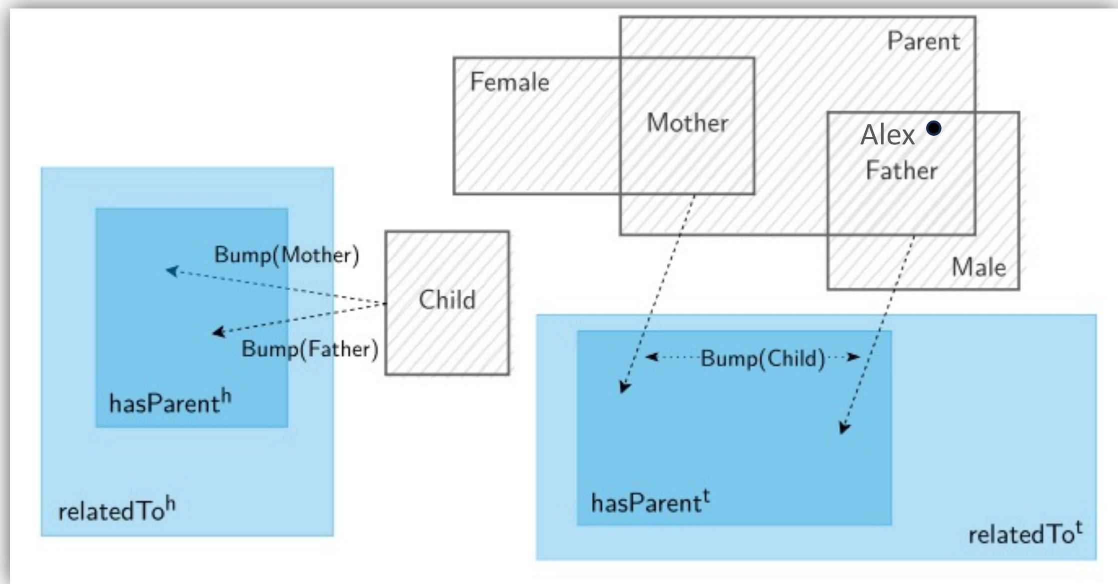
Learning Algorithms



Box²EL for OWL ontologies of Description Logic $\mathcal{EL}^{++}$ (like the family example)

Entity/instance: Point
Concept: Box (center vector & offset vector)
Relation/role: a head box & a tail box
Concept interaction: bump vector

Concept subsumption
Instance membership
Concept intersection
Role inclusion and composition

Existential quantification
$C \sqsubseteq \exists r.D$: Box(C) ⊗ Bump(D) ⊆ Head(r)
Box(D) ⊗ Bump(C) ⊆ Tail(r)

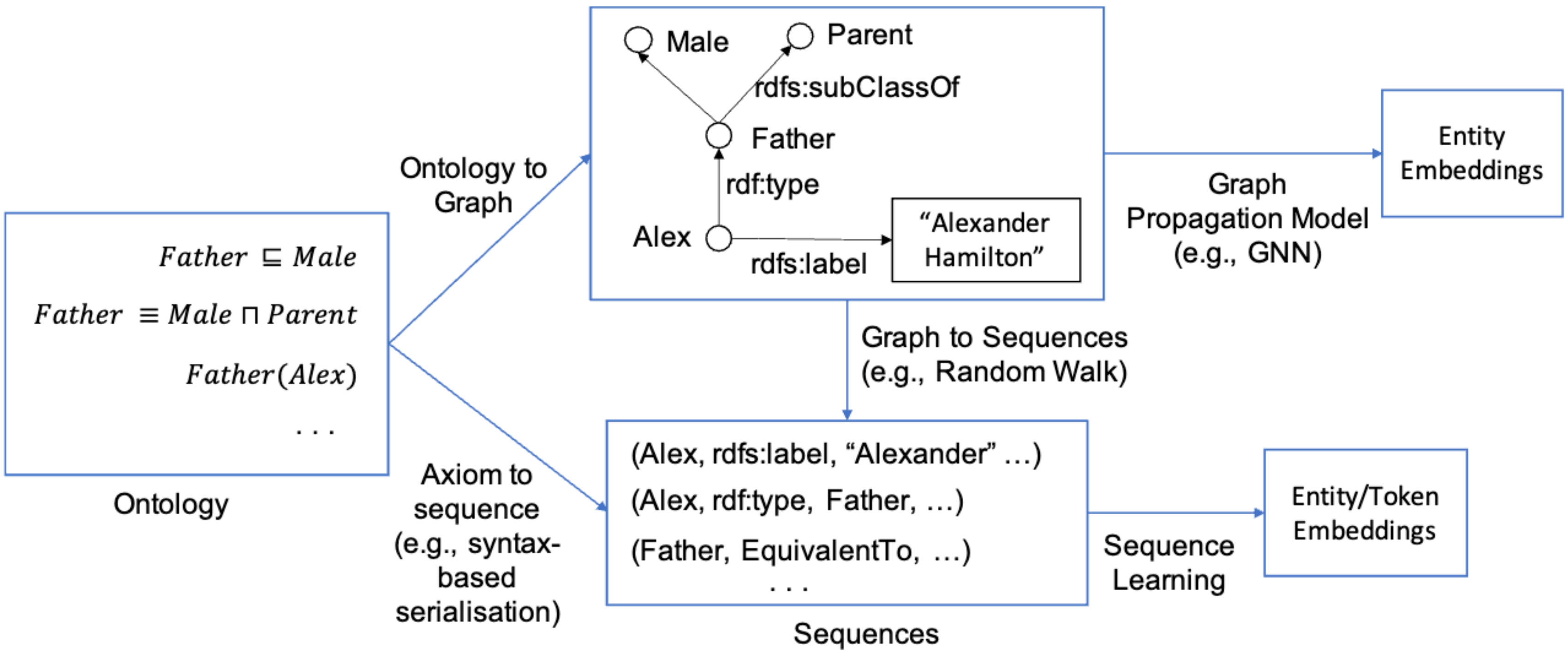
Jackermeier, M., Chen, J., Horrocks, I.,"Dual Box Embeddings for the Description Logics EL++." The Web Conference 2024.

Paradigms for Ontology Embedding

- Geometric modeling (like Box^{2}EL)
  - Pros: interpretable; sound representation of formal semantics
  - Cons: hard to incorporate informal semantics like textual literals; hard to deal with all the features of OWL
- Sequence modeling
  - Transform axioms and literals into sentences;
  - Train word embedding (sequence learning) models
- Graph propagation
  - Transform axioms into a graph

Chen, J., et al.,"Ontology Embedding: A Survey of Methods, Applications and Resources." https://arxiv.org/abs/2406.10964.

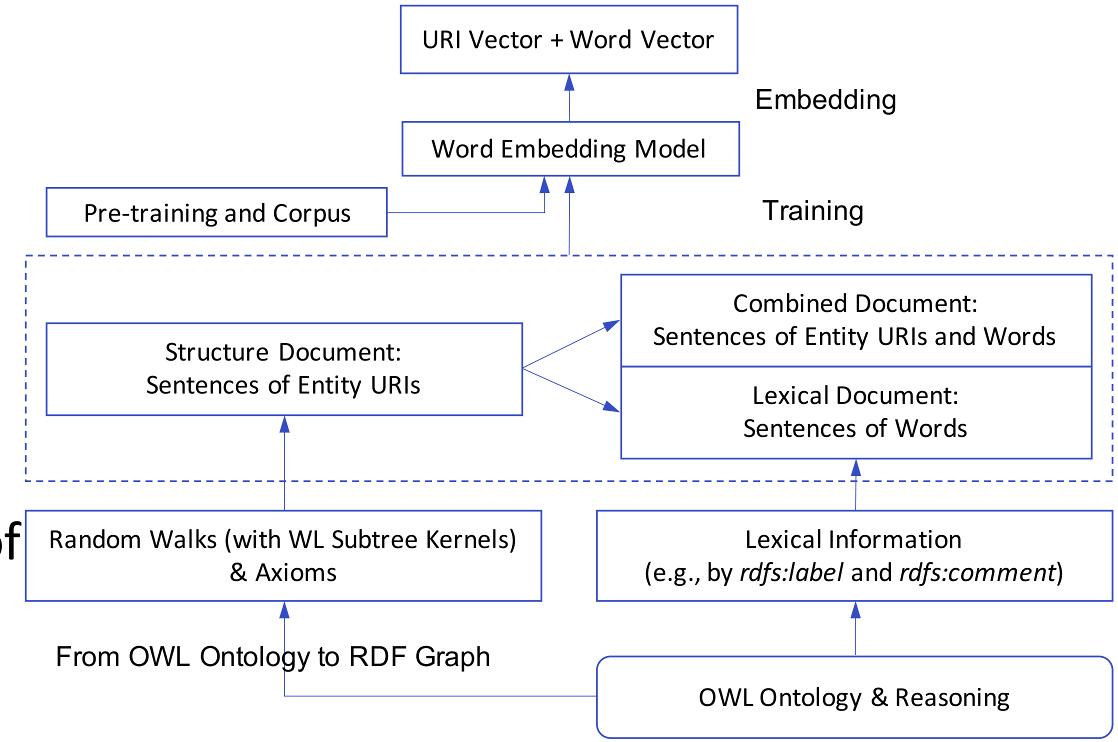
Paradigms for Ontology Embedding



Paradigms of Sequence Learning & Graph Propagation

A General Ontology Embedding Tool **OWL2Vec***

- **Pipeline & Sequence Modeling**
  - Extract sequences
    - Random walks on RDF graph
    - Literals
    - Axiom serialization in Manchester syntax
  - Train Word2Vec embeddings
- Pros & Cons
  - Consider literals and other kinds of ontology semantics
  - Embed correlations; miss some formal semantics (faithfulness)



Chen J., et al. "OWL2Vec*: Embedding of OWL ontologies." *Machine Learning* 110.7 (2021): 1813-1845.

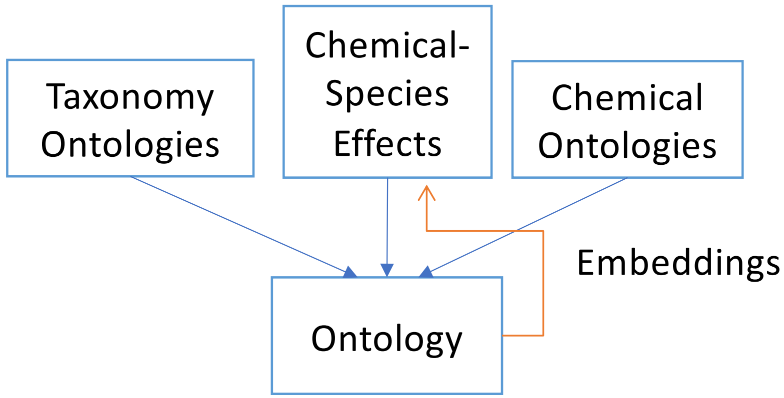
Application/Evaluation of Ontology Embeddings

- Link Prediction
  - E.g., protein-protein interaction prediction

	Model	H@10	H@10 (F)	H@100	H@100 (F)	MR	MR (F)	AUC	AUC (F)
Yeast	ELEm	0.10	0.23	0.50	0.75	247	187	0.96	0.97
	EmEL^{++}	0.08	0.17	0.48	0.65	336	291	0.94	0.95
	BoxEL	0.09	0.20	0.52	0.73	423	379	0.93	0.94
	ELBE	**0.11**	0.26	0.57	0.77	201	154	0.96	0.97
	$\mathrm{Box}^2\mathrm{EL}$	**0.11**	**0.33**	**0.64**	**0.87**	**168**	**118**	**0.97**	**0.98**
Human	ELEm	**0.09**	0.22	0.43	0.70	658	572	0.96	0.96
	EmEL^{++}	0.04	0.13	0.38	0.56	772	700	0.95	0.95
	BoxEL	0.07	0.10	0.42	0.63	1574	1530	0.93	0.93
	ELBE	**0.09**	0.22	0.49	0.72	434	362	0.97	**0.98**
	$\mathrm{Box}^2\mathrm{EL}$	**0.09**	**0.28**	**0.55**	**0.83**	**343**	**269**	**0.98**	**0.98**

Results of $\mathrm{Box}^2\mathrm{EL}$ on protein-protein interaction prediction.
the STRING database (ABox) + the Gene ontology (TBox)

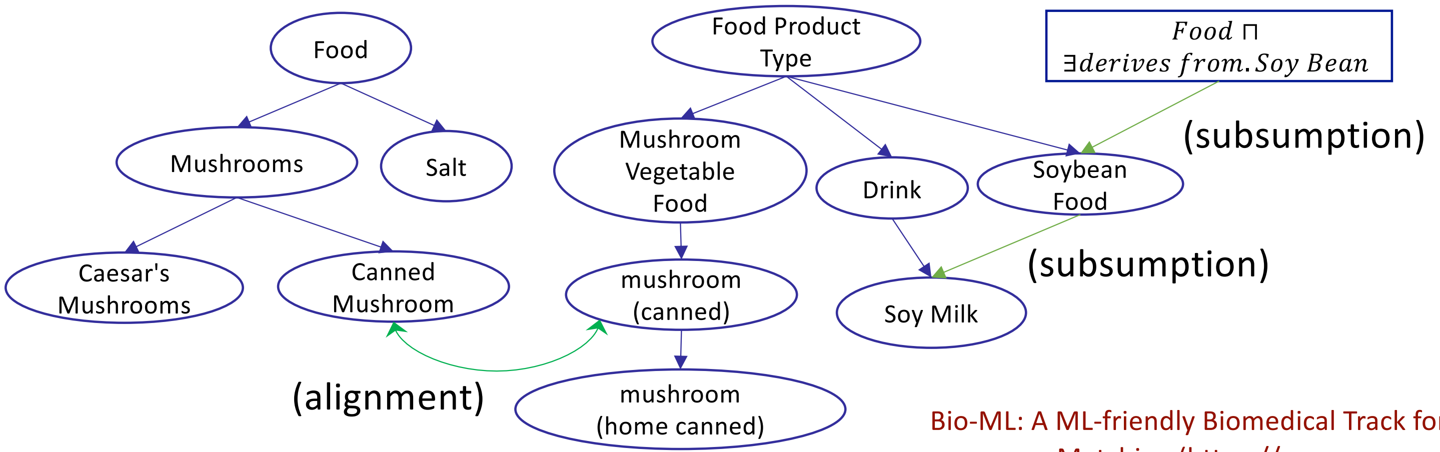
E.g., ecotoxicological effect prediction



Myklebust, Erik B., et al. "Prediction of adverse biological effects of chemicals using knowledge graph embeddings." *Semantic Web* 13.3 (2022): 299-338.

Applications and Evaluation of Ontology Embeddings

- Link Prediction
  - E.g., protein-protein interaction prediction, ecotoxicological effect prediction
- Knowledge Engineering
  - E.g., entity alignment, subsumption completion, ontology learning



Bio-ML: A ML-friendly Biomedical Track for Equivalence and Subsumption Matching (https://www.cs.ox.ac.uk/isg/projects/ConCur/oaei/)

Applications and Evaluation of Ontology Embeddings

- Link Prediction
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- Knowledge Engineering
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- Augmenting Machine Learning
  - E.g., injecting external knowledge of classes for zero-shot learning

Chen, J, et al. "Zero-Shot and Few-Shot Learning With Knowledge Graphs: A Comprehensive Survey." Proceedings of the IEEE (2023).

Applications and Evaluation of Ontology Embeddings

- Link Prediction
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- Augmenting Machine Learning
  - E.g., injecting external knowledge of classes for zero-shot learning
- Knowledge Retrieval
  - E.g., Embedding for Retrieval Augmented Generation (RAG)

https://www.deeplearning.ai/short-courses/knowledge-graphs-rag/

Challenges and Opportunities from (Large) Language Models

- Language models for neural knowledge representation, and for augmenting knowledge engineering

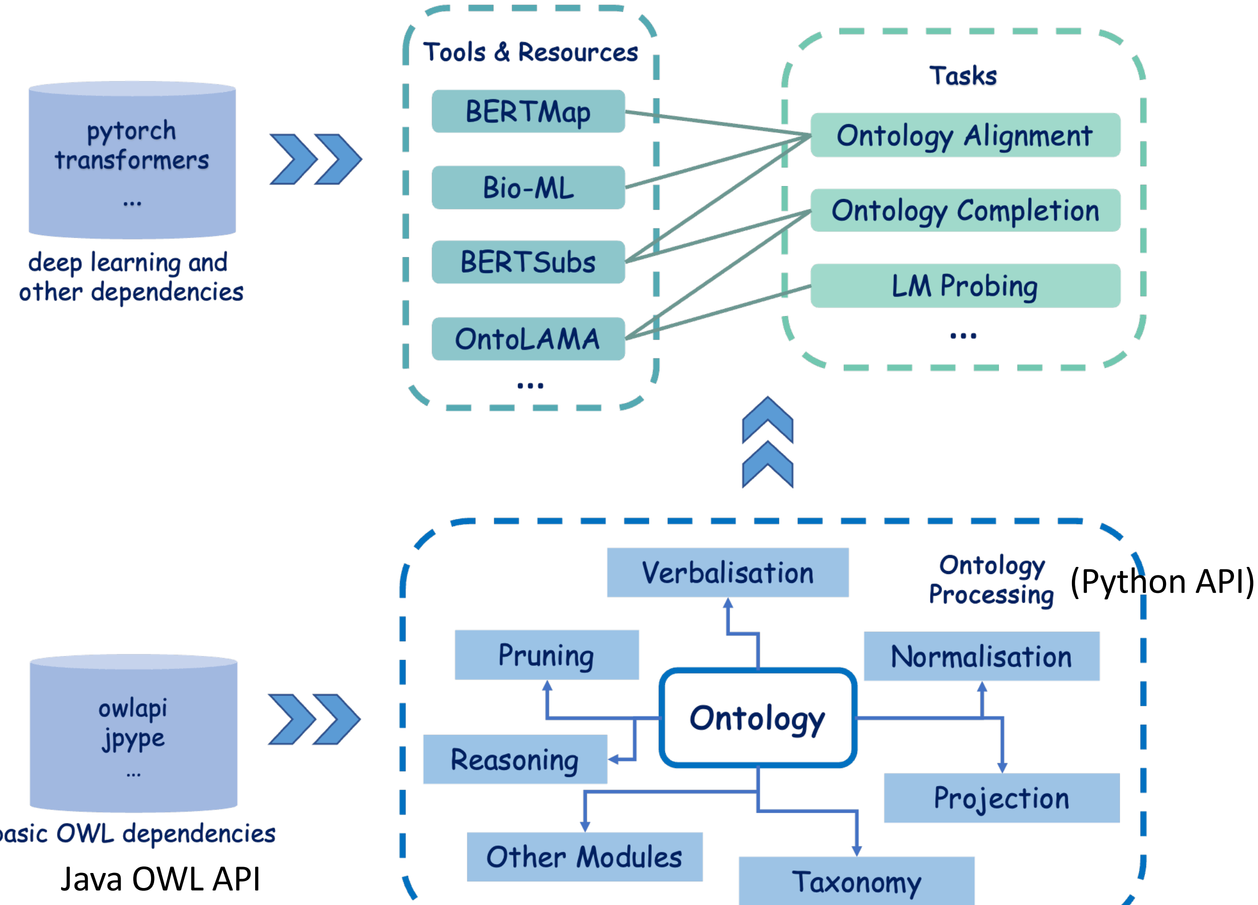
- Knowledge graph & ontology for LLMs

Pan, J., et al. "Large Language Models and Knowledge Graphs: Opportunities and Challenges." *Transactions on Graph Data and Knowledge* (2023).

An LM-based Ontology Engineering Library

DeepOnto

https://github.com/KRR-Oxford/DeepOnto



He, Y., et al. "DeepOnto: A Python package for ontology engineering with deep learning." *Semantic Web Journal* (2024).

How to augment Large Language Models?

- Knowledge Graphs
- Ontologies
- Tables / Data Lakes
- …
- (Kinds of) Embeddings

Symbolic and neural knowledge representations

LM Pre-train / Fine-tune for retrieval →

Retrieval Augmented Generation (RAG) →

Reasoning and generation

- Capture domain knowledge
- Reason with private knowledge
- Deal with evolving knowledge
- Add explanations / citations
- Rely on less samples / training
- …

Thanks for your attention