Ontology (Knowledge Graph) Embeddings

Ernesto Jiménez-Ruiz

Lecturer in Artificial Intelligence

Before we start...

Students' module evaluation

– Your feedback is very important.

– Evaluations are anonymous.

– Access via e-mail from `evaluations@city.ac.uk` or from MyMoodle

– More information: `https://studenthub.city.ac.uk/student-administration/online-module-evaluation-at-city`

Additional (potential) MSc Projects

DYAD: `https://www.dyad.net/`

– Helathcare domain.

– KG and graph machine learning.

Invited talks next week (15+5 min.)

- **Valentina Carapella**
  - Data Scientist at Perspectum (`https://perspectum.com/`)
  - *"KG Use Cases from Medical Imaging Science"*

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- **Vicenzo Cutrona**
  - PhD Student Università degli Studi di Milano - Bicocca.
  - R&D OpenLab @ Corvallis SRL (`https://corvallis.it/`)
  - *"Why semantic table understanding matters! Practical solutions to real-life problems"*

Where are we?

- ✓ Introduction.
- ✓ RDF-based knowledge graphs.
- ✓ SPARQL 1.0
- ✓ RDFS Semantics and RDF(S)-based knowledge graphs.
- ✓ OWL (2) ontology language. Focus on modelling.
- ✓ Application to Data Science.
- ✓ OWL 2 Profiles, SPARQL 1.1 and Entailment Regimes
- ✓ Ontology (Knowledge Graph) Alignment

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10. Graph Database Solutions and Invited Talks (March 31).

Hybrid Learning and Reasoning Systems

Motivation:

- Need of **richer AI** systems, *i.e.*, **semantically sound**, **explainable**, and **reliable**.

Gary Marcus. The Next Decade in AI: Four Steps Towards Robust Artificial Intelligence. CoRR abs/2002.06177 (2020)

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  - A `and` $($$R$ `some` $B$$)$ `subClassOf` C. $A(a)$, $B'(b)$, and $R(a, b)$.

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– **Solution?** Hybrid Learning and Reasoning Systems.

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Hybrid Learning and Reasoning Systems

- Unification of:
  - **statistical** (data-driven) and
  - **symbolic** (knowledge-driven) methods

† Michael van Bekkum et al. Modular Design Patterns for Hybrid Learning and Reasoning Systems: a taxonomy, patterns and use cases. CoRR abs/2102.11965. Under review (2021)

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  - **statistical** (data-driven) and
  - **symbolic** (knowledge-driven) methods
- Overview of **patterns** for hybrid systems. †
  - Focus on **Ontology** (knowledge graph) **embeddings** as a component for an hybrid system (*e.g.*, OWL2Vec*).

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Generic Patterns for Hybrid Systems

Focus on Knowledge Graph Embeddings

Introduction: Models

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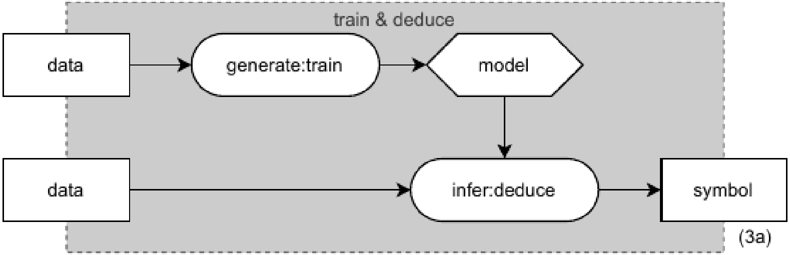
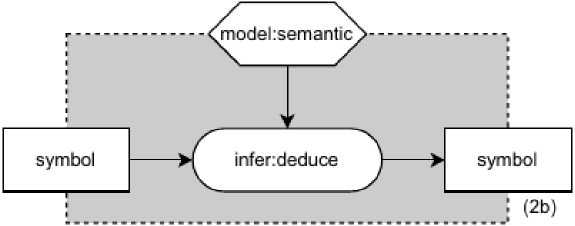
  - *e.g.*, Ontologies, Knowledge Graphs, Rule-based models.
- **Hybrid models** combine both.

Machine learning pattern (non hybrid)



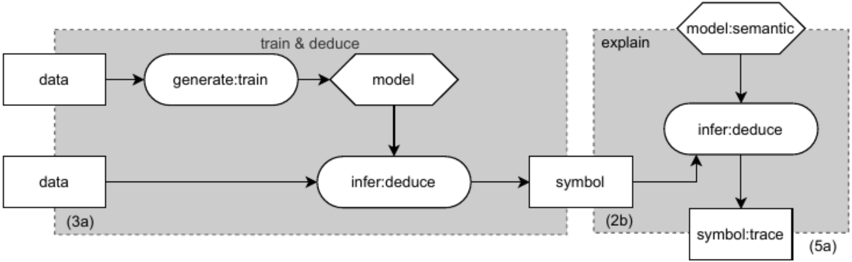
For example, image classification as in the `http://www.image-net.org/` challenge (symbol = label from WordNet).

Semantic model pattern (non hybrid)



- Standard reasoning (*e.g.*, classification, class membership).
- Rule-mining and ontoloy learning based on symbolic data (*i.e.*, ABox).

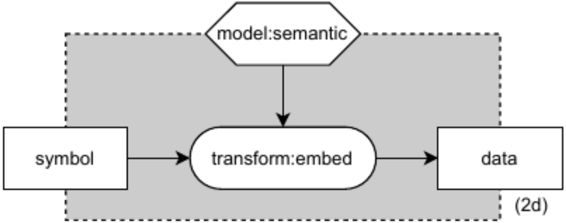
Explainability



The semantic model explains/interprets the prediction.

Explaining Trained Neural Networks with Semantic Web Technologies: First Steps. NeSy 2017.
Human-driven FOL explanations of deep learning. IJCAI 2020

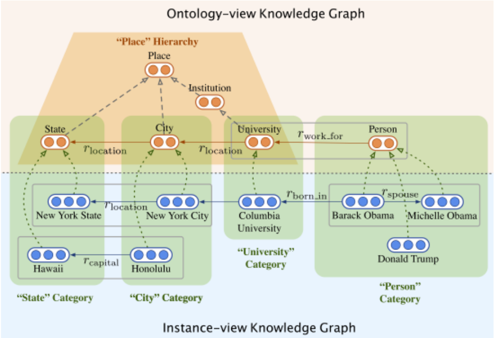
Knowledge graph embeddings

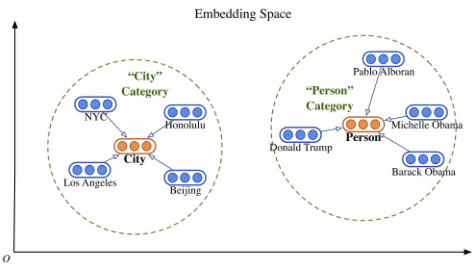


Symbols are transformed into vectors (*e.g.*, OWL2Vec)

Knowledge Graph Embedding: A Survey of Approaches and Applications. TKDE 2017
OWL2Vec*: Embedding of OWL Ontologies. CoRR abs/2009.14654 (2020)

Knowledge graph embeddings (example)

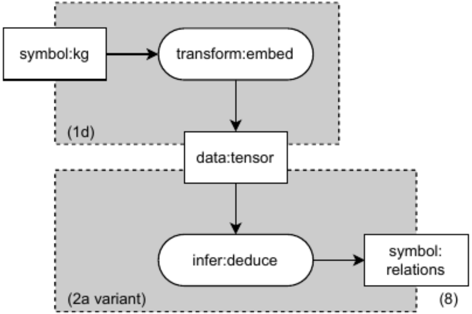




KG Embedding Systems exploit the neighbourhood of an entity to calculate its vector.

Example from: Universal Representation Learning of Knowledge Bases by Jointly Embedding Instances and Ontological Concepts. KDD 2019.

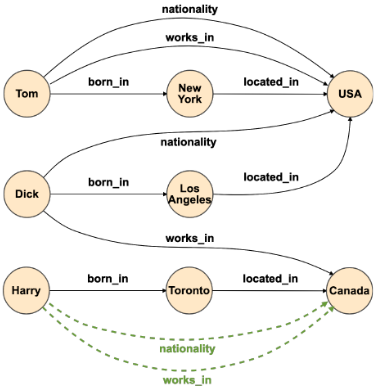
Knowledge Graph Embeddings: Link prediction



– Plausability of a triple `<subject predicate object>` given a scoring function.

Knowledge Graph Embedding for Link Prediction: A Comparative Analysis. TKDD 2021

Knowledge Graph Embeddings: Link prediction (example)



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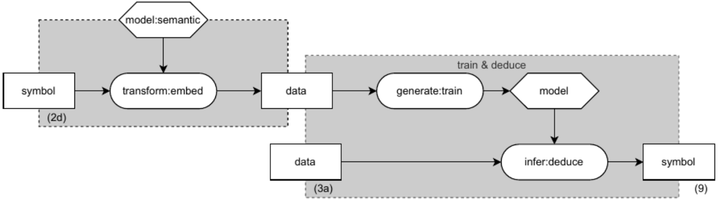
Learning with (knowledge) embeddings

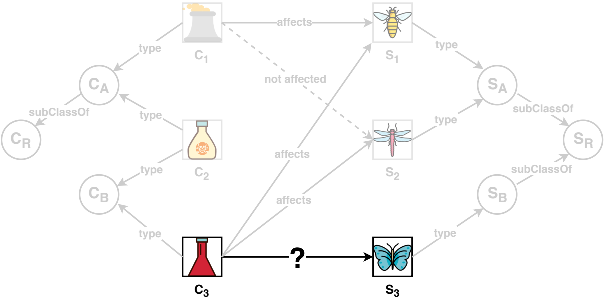


- Applying knowledge graph embeddings in a subsequent classification step.
- Graph Neural Networks over the KG structure.
- Key for zero-shot learning approaches

Prediction of Adverse Biological Effects of Chemicals Using Knowledge Graph Embeddings. Under review. 2021.
A Comprehensive Survey on Graph Neural Network. IEEE Transactions on Neural Networks and Learning Systems 2019.
Knowledge-aware Zero-Shot Learning: Survey and Perspective. arXiv:2103.00070. 2021

Learning with (knowledge) embeddings (example)

– **Prediction of adverse biological effects** of chemicals via KG embeddings.



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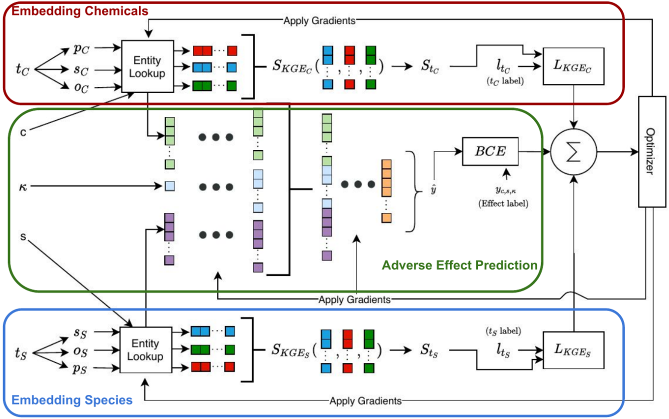
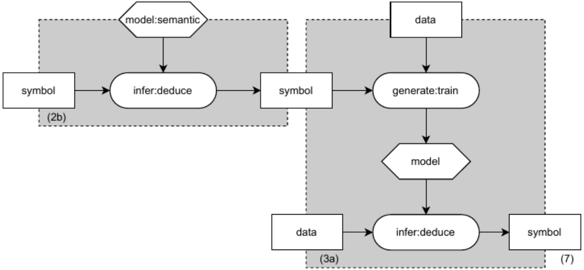


Prediction of Adverse Biological Effects of Chemicals Using Knowledge Graph Embeddings. Under review. 2021.

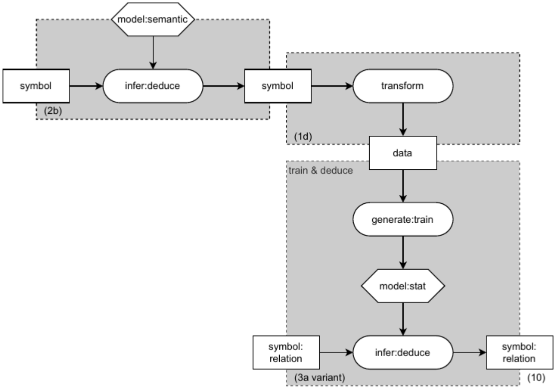
Learning with prior kowledge



- Domain knowledge (*e.g.*, a KG) used to constraint search space during training.
- **Semantic loss function**: impact of the violation of the symbolic knowledge.

A semantic loss function for deep learning with symbolic knowledge. ICML 2018
Logic Tensor Networks. `https://github.com/logictensornetworks/logictensornetworks`

Learning to reason

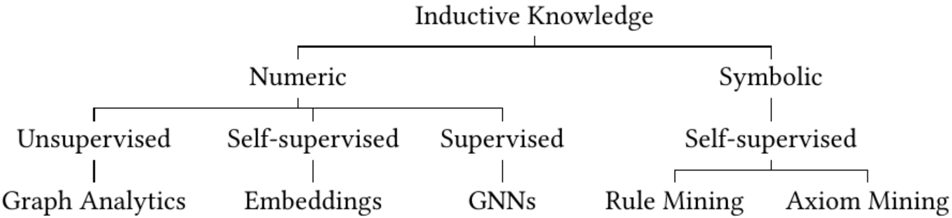


Ontology Reasoning with Deep Neural Networks. JAIR 2021

Inductive Techniques for Knowledge Graphs

Focus on Knowledge Graph Embeddings

Inductive techniques for knowledge graphs



- Input: A Knowledge Graph (symbolic)
- Output: Numeric or Symbolic

Knowledge Graphs. arXiv:2003.02320. 2021

Graph analytics (unsupervised)

Exploit techniques from **graph theory** and **network analysis**. *e.g.*,:

- **Centrality**: the most important nodes (*i.e.*, concepts, instances) or edges (*i.e.*, properties) of a graph.
- **Community detection**: subgraphs that are densely connected.
- **Connectivity**: how well-connected are the nodes of a graph to identify isolated nodes or subgraphs.

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- **Community detection**: subgraphs that are densely connected.
- **Connectivity**: how well-connected are the nodes of a graph to identify isolated nodes or subgraphs.
- **Path finding**: all possible paths between two nodes.
- **Node similarity**: based on their connection to other nodes (*e.g.*,random-walks techniques).

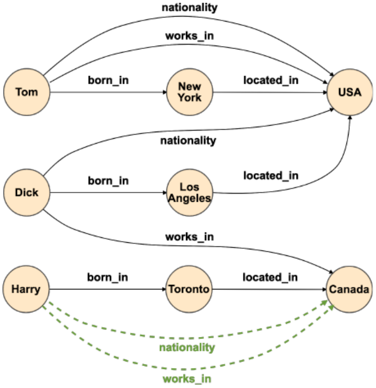
Graph Neural Networks (supervised)

- Machine learning models for **graph-structured data**.
- The **neural network** is **based on the shape and connections** of the (knowledge) graph
- **End-to-end supervised learning** (*e.g.*, classification).
- Can be used to classify nodes or the graph itself.

A Comprehensive Survey on Graph Neural Network. IEEE Transactions on Neural Networks and Learning Systems 2019.

Symbolic learning (self-supervised)

– Identifies patterns in the data



Symbolic learning (self-supervised)

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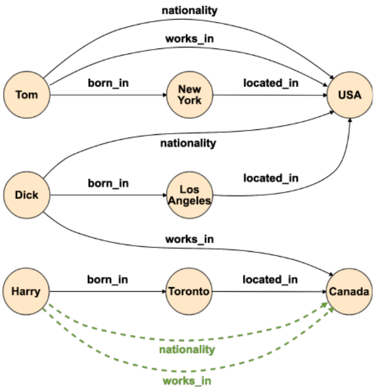
– Learn hypotheses in a symbolic (logical) language. For example:

  – As a rule: `nationality(x,z) :- born_in(x,y) ∧ located_in(y,z)`

  – As an OWL 2 axioms: `born_in ∘ located_in SubPropertyOf: nationality`



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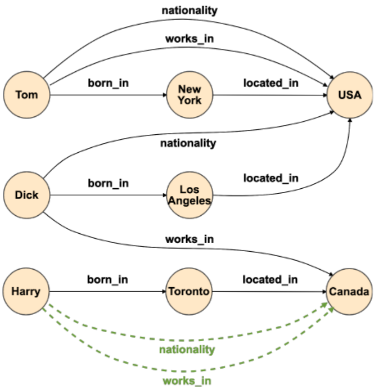
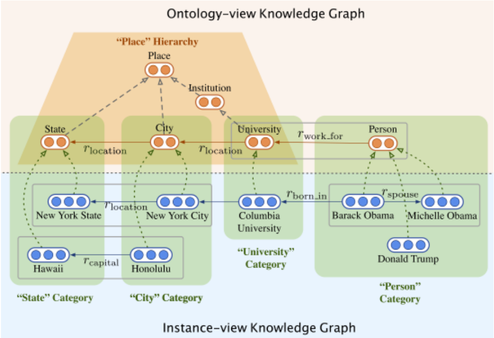
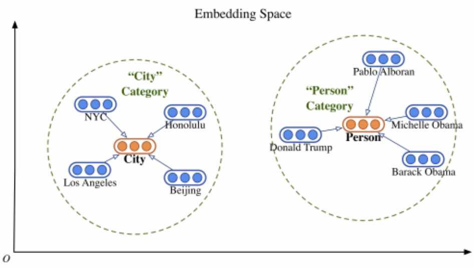
- Can help explaining/interpret (link) predictions: *e.g.*, why `nationality(Hernry, Canada)`?



Knowledge graph embeddings (self-supervised)





Example from: Universal Representation Learning of Knowledge Bases by Jointly Embedding Instances and Ontological Concepts. KDD 2019.

Knowledge graph embeddings (self-supervised)

KGE approaches (excluding those based on language models) typically:

- Receive as input a set of **positive** (the ones in the KG) and **negative triples**.
- Include a **scoring function** that accepts as input the embedding of the elements of a triple (there is an initialization step).

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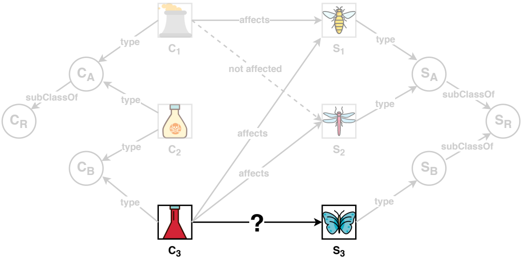
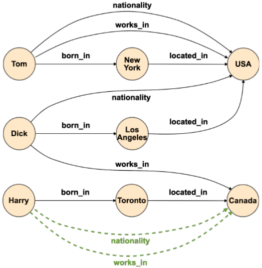
- Receive as input a set of **positive** (the ones in the KG) and **negative triples**.
- Include a **scoring function** that accepts as input the embedding of the elements of a triple (there is an initialization step).
- Learn embedding so that the score for positive triples is maximized while the score for negative triples is minimized (*i.e.*, **loss function**).
- Compute **similar vectors** for similar nodes (*i.e.*, concepts/instances) and edges (*i.e.*, properties).

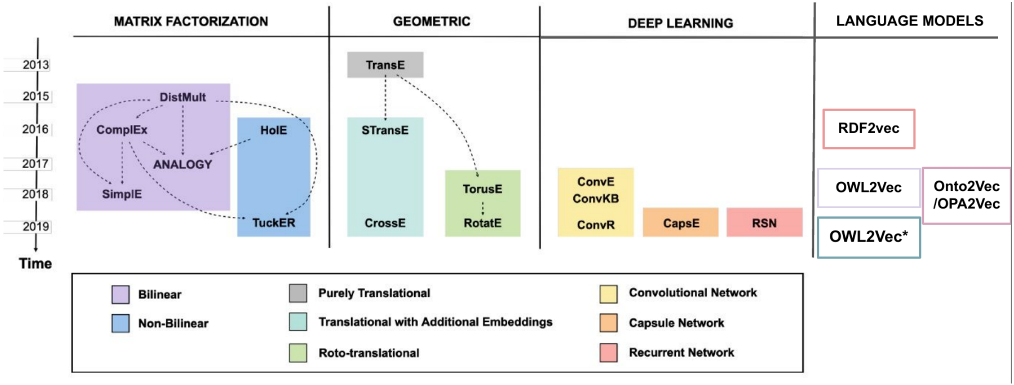
Knowledge graph embeddings (applications)

- The computed embedding can be used in a **downstream machine learning task** (*e.g.*, prediction of adverse effect chemical-species).
- The scoring function can be used to evaluate the plausibility of a triple for **link prediction** or **KG completion**.





Knowledge graph embeddings (overview of approaches)



Incomplete list of approaches, adapted from: Knowledge Graph Embedding for Link Prediction: A Comparative Analysis. TKDD 2021

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- **Neural models**: unlike previous models they learn embeddings with non-linear scoring functions via a neural model.
- **Language models**: perform random walks over the KG to create a document of sentences and leverage existing language models (*e.g.*, word embedding) to learn vectors for each KG entity.

Knowledge graph embeddings (implementations)

- PyKEEN (Python KnowlEdge EmbeddiNgs) with PyTorch: `https://pykeen.github.io/`
- Open Knowledge Embedding implemented with PyTorch: `https://github.com/thunlp/OpenKE`
- Knowledge Embedding implemented with Keras: `https://github.com/NIVA-Knowledge-Graph/KGE-Keras`
- jRDF2Vec: `https://github.com/dwslab/jRDF2Vec`
- pyRDF2Vec: `https://github.com/IBCNServices/pyRDF2Vec`
- OWL2Vec* (python): `https://github.com/KRR-Oxford/OWL2Vec-Star`

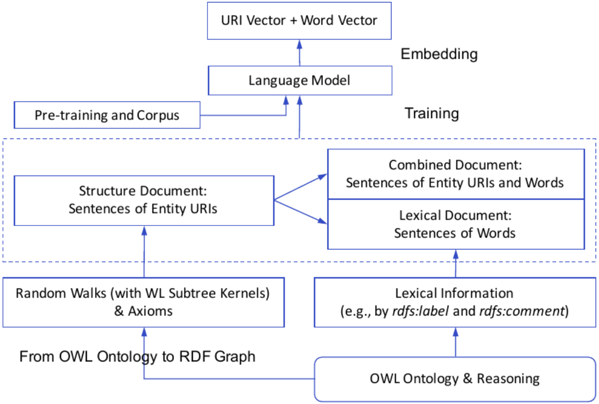
Knowledge graph embeddings (pre-trained)

- OpenKE:
  `http://139.129.163.161/index/toolkits#pretrained-embeddings`
- KGvec2go: `http://www.kgvec2go.org/`
- Drug-drug interaction:
  `https://github.com/rcelebi/GraphEmbedding4DDI/`

Embedding ontologies with OWL2Vec*

OWL2Vec* Overview

- **projects** the ontology into a graph,
- **walks** the graph,
- creates a**corpus of sentences** according to the walking strategies, and
- generates **embeddings** from that corpus.



OWL2Vec*: Embedding of OWL Ontologies. CoRR abs/2009.14654 (2020)

OWL2Vec*: ontology projection

Approximation of an OWL 2 ontology into an RDF graph.

<table>
<tr><th>Axiom of Condition 1</th><th>Axiom or Triple(s) of Condition 2</th><th>Projected Triple(s)</th></tr>
<tr><td>$A \sqsubseteq \square r.D$
or
$\square r.D \sqsubseteq A$</td><td>$D \equiv B \mid B_1 \sqcup \ldots \sqcup B_n \mid B_1 \sqcap \ldots \sqcap B_n$</td><td rowspan="6">$\langle A, r, B \rangle$ or
$\langle A, r, B_i \rangle$ for $i \in 1, \ldots, n$</td></tr>
<tr><td>$\exists r.\top \sqsubseteq A$ (domain)</td><td>$\top \sqsubseteq \forall r.B$ (range)</td></tr>
<tr><td>$A \sqsubseteq \exists r.\{b\}$</td><td>$B(b)$</td></tr>
<tr><td>$r \sqsubseteq r'$</td><td>$\langle A, r', B \rangle$ has been projected</td></tr>
<tr><td>$r' \equiv r^-$</td><td>$\langle B, r', A \rangle$ has been projected</td></tr>
<tr><td>$s_1 \circ \ldots \circ s_n \sqsubseteq r$</td><td>$\langle A, s_1, C_1 \rangle \ldots \langle C_n, s_n, B \rangle$ have been projected</td></tr>
<tr><td>$B \sqsubseteq A$</td><td>–</td><td>$\langle B, rdfs{:}subClassOf, A \rangle$
$\langle A, rdfs{:}subClassOf^-, B \rangle$</td></tr>
<tr><td>$A(a)$</td><td>–</td><td>$\langle a, rdf{:}type, A \rangle$
$\langle A, rdf{:}type^-, a \rangle$</td></tr>
<tr><td>$r(a, b)$</td><td>–</td><td>$\langle a, r, b \rangle$</td></tr>
</table>

$\square$ is one of: $\geq$, $\leq$, $=$, $\exists$, $\forall$. A, B, B_i and C_i are atomic concepts (classes), s_i, r and r' are roles (object properties), r^- is the inverse of a relation r, a and b are individuals, $\top$ is the top concept.

OWL2Vec*: sentence generation via random walks

Strategies:

- Random walks
- Weisfeiler Lehman (WL) kernel, which assign identifiers to subgraphs and includes them into the walk.

Structure Document Sentences

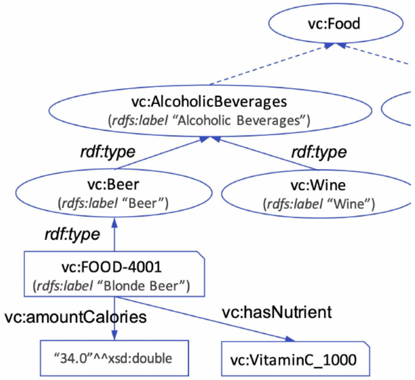
(vc:Beer, rdf:type, vc:FOOD-4001, vc:hasNutrient, vc:VitaminC_1000)

Lexical Document Sentences

("beer", "type", "blonde", "beer", "has", "nutrient", "vitamin", "c")

Combined Document Sentences

(vc:FOOD-4001, "has", "nutrient", "vitamin", "c")
OR
("blonde", "beer", "has", "nutrient", vc:VitaminC_1000)



OWL2Vec*: language model and embeddings

- OWL2Vec relies on the **Word2vec** as neural **language model**.
- Word2vec learns **embeddings** for all the elements in the documents (*i.e.*, both **words** and **URIs**)

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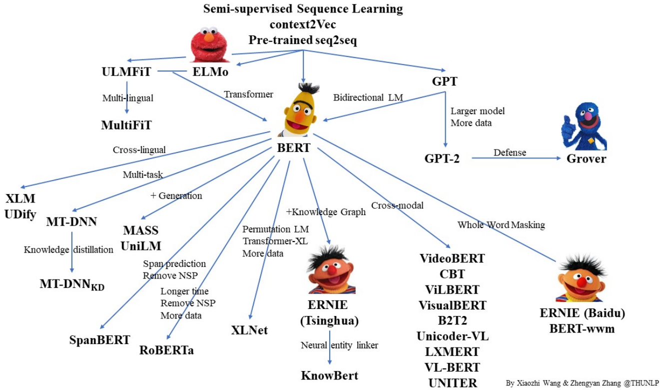
- Word2vec learns **embeddings** for all the elements in the documents (*i.e.*, both **words** and **URIs**)
- The embeddings of the ontology entities can be calculated via their **URI embedding** or via the **word embeddings** of their labels.
  - The URI `vc:FOOD-4001` (Blonde Beer) has a vector.
  - As well as the words `‘‘blonde’’` and `‘‘beer’’`.

OWL2Vec*: language model (future)

Other language models could be used in OWL2Vec*:

`https://github.com/thunlp/PLMpapers`



OWL2Vec*: applications

- **Class subsumption** and **class membership predictions** (as in OWl2Vec* paper)
- Embedding of chemicals and species to **predict adverse effects**.
- **Ontology alignment** (Samsung UK project with food ontologies) †
- **Ontology clustering** in life sciences ontologies to be applied in an Information Retrieval task. ‡

† J. Chen et al. Augmenting Ontology Alignment by Semantic Embedding and Distant Supervision. ESWC 2021
‡ A. Ritchie. Ontology Clustering with OWL2Vec*. Submitted 2021.

OWl2Vec*: clustering

Embedding of the Gene Ontology and its 3 branches: biological process, cellular component, and molecular function

A. Ritchie. Ontology Clustering with OWL2Vec*. Submitted 2021.

Acknowledgements

– OWL2Vec* developers and collaborators.

– Specially **Jiaoyan Chen**, University of Oxford

Laboratory Session

OWL2Vec* in practice

- Execute OWL2Vec* over the `Pizza` and `FoodOn` ontologies.
- Compute similarity among words and entities.
- Perform clustering and visualize results.