Machine learning with ontologies

Robert Hoehndorf

Before the tutorial

See `https://github.com/bio-ontology-research-group/ontology-tutorial`:

- install Docker (e.g.: `apt-get install docker`)
- `docker pull coolmaksat/embeddings:latest`
- `docker pull leechuck/ontology-ml:latest`
- ```
  docker run -i -t -p 8888:8888
  leechuck/ontology-ml /bin/bash -c "jupyter
  notebook
  --notebook-dir=/home/borg/ontology-tutorial/
  --ip='0.0.0.0' --port=8888 --no-browser
  --allow-root"
  ```
  ```

Overview

Ontologies, axioms, and bioinformatics

- ontologies are ubiquitous
- rich formal characterization (axioms)
- how can they be used for (predictive) data analysis?
  - "fuzzy", similarity-based search
  - predictive analysis and machine learning
  - background knowledge

Learning goals

- machine learning with ontologies as *features* (or background knowledge)
- unsupervised or supervised:
  - here: mostly unsupervised *feature* learning
- focus on existing tools and methods
  - Jupyter Notebooks and code examples
- not covered:
  - learning ontologies (axioms, definitions) from data
  - natural language processing
  - reasoning with ontologies
  - learning on "knowledge graphs"
  - machine learning theory

Agenda

- Introduction: ontologies, axioms, reasoning, graphs
- Machine learning:
  - graph-based
  - syntactic
  - model-theoretic
- (Semantic similarity)
  - probably not

Preliminaries: ontologies

- Specific artifacts expressing the intended meaning of a vocabulary in terms of primitive categories and relations describing the nature and structure of a domain of discourse
  - in order to account for the competent use of vocabulary in real situations (such as annotations in databases, etc.)
- the intended meaning of *primitive* categories and relations is expressed through axioms (axiomatic method, Tarski)

Preliminaries: axioms

- *classes* represent kinds of things in the world
  - *Arm*, *Apoptosis*, *Influenza*, *Homo sapiens*, *Drinking behavior*, *Membrane*
- *instances* of classes are individuals satisfying the classes' intension
  - my arm, the influenza I had last year, one ethanol molecule, etc.
- *relations* between instances arise from interactions, configurations, etc., of individuals
  - my arm is **part of** me, the **duration of** my influenza was 10 days
- *axioms* specify the conditions that instances of a class must satisfy
  - every instance of *Hand* is a **part of** an instance of *Arm*

Description Logics: overview

- TBox: axioms pertaining to the terminology of the domain (classes)
- ABox: axioms stating facts (assertions) about the world
- RBox: axioms holding for relations
- Reasoning: derive implicitly represented knowledge (e.g., subsumption)
- a "knowledge graph" is an ABox + RBox

Manchester OWL Syntax

DL Syntax	Manchester Syntax	Example
$C \sqcap D$	C and D	Human and Male
$C \sqcup D$	C or D	Male or Female
$\neg C$	not C	not Male
$\exists R.C$	R some C	hasChild some Human
$\forall R.C$	R only C	hasChild only Human
$(\geq nR.C)$	R min n C	hasChild min 1 Human
$(\leq nR.C)$	R max n C	hasChild max 1 Human
$(= nR.C)$	R exactly n C	hasChild exactly 1 Human
$\{a\} \sqcup \{b\} \sqcup \ldots$	{a b ...}	{John Robert Mary}

Ontologies provide background knowledge

Annotation	Value
label	T cell aggregation
definition	The adhesion of one T cell to one or more other T cells via adhesion molecules.
class	http://purl.obolibrary.org/obo/GO_0070489
ontology	GO-PLUS
Equivalent	leukocyte aggregation and (has participant some T cell)
SubClassOf	lymphocyte aggregation, has participant some T cell
has_obo_namespace	biological_process
id	GO:0070489
synonyms	T-cell aggregation, T lymphocyte aggregation, T-lymphocyte aggregation

Ontologies provide background knowledge

Annotation	Value
label	T cell activation
definition	The change in morphology and behavior of a mature or immature T cell resulting from exposure to a mitogen, cytokine, chemokine, cellular ligand, or an antigen for which it is specific.
class	http://purl.obolibrary.org/obo/GO_0042110
ontology	GO-PLUS
Equivalent	cell activation and (has input some T cell)
SubClassOf	has input some T cell, lymphocyte activation
has_obo_namespace	biological_process
id	GO:0042110
synonyms	T-lymphocyte activation, T lymphocyte activation, T-cell activation

Ontologies provide background knowledge

MSN	Moesin	extracellular exosome		UniProt	Homo sapiens	HDA
MSN	Moesin	T cell aggregation		UniProt	Homo sapiens	IDA
MSN	Moesin	cellular response to testosterone stimulus	occurs in endothelial cell	UniProt	Homo sapiens	IDA
IL6	Interleukin-6	positive regulation of T cell proliferation		BHF-UCL	Homo sapiens	IDA
IL6	Interleukin-6	T-helper 17 cell lineage commitment		UniProt	Homo sapiens	ISS

Using background knowledge

Problem statement (first attempt):

Given a set of biological entities and their ontology-based annotations. Can we discover *new* relations between the biological entities, or between entities and classes in the ontology?

Using background knowledge

Problem statement (first attempt):

Given a set of biological entities and their ontology-based annotations. Can we discover *new* relations between the biological entities, or between entities and classes in the ontology?

- what relations, and when is a fact "new"?

Using background knowledge

Problem statement (first attempt):

Given a set of biological entities and their ontology-based annotations. Can we discover *new* relations between the biological entities, or between entities and classes in the ontology?

- what relations, and when is a fact "new"?
- what features are relevant?
  - depends on the relation!

Using background knowledge

Problem statement (first attempt):

Given a set of biological entities and their ontology-based annotations. Can we discover *new* relations between the biological entities, or between entities and classes in the ontology?

- what relations, and when is a fact "new"?
- what features are relevant?
  - depends on the relation!
- finding new facts is only one (minor?) use case
  - other uses: encode background knowledge for machine learning models (e.g., function prediction); add new classes; expand definition; etc.

Semantic similarity

semantic similarity measures:

- for words, terms, classes
- role of background knowledge:
  - statistical/distributional semantics, large corpora
  - ontologies: (graph) topology
- similarity measures: hand-crafted or data-driven?

Semantic similarity: some examples

- Are cyclin dependent kinases *functionally* more similar to lipid kinases or to riboflavin kinases? How about *phenotypically*?
- Which protein in the *mouse* is functionally most similar to the zebrafish *gustducin* protein?
- Which mouse knockout resembles *Bardet-Biedl Syndrome 8*?
- Are there mouse knockouts that resemble the side effects of diclofenac?
- Which genetic disease produces similar symptoms to ebola?
- Does functional similarity correlate with phenotypic similarity?

Semantic similarity or machine learning

- semantic similarity measures are mostly hand-crafted
  - capture certain intuition about what constitutes "similarity"
  - different measures for different kinds of similarity
  - usually interpretable (and explainable)

Semantic similarity or machine learning

- semantic similarity measures are mostly hand-crafted
  - capture certain intuition about what constitutes "similarity"
  - different measures for different kinds of similarity
  - usually interpretable (and explainable)
- machine learning methods are mostly data-driven
  - the architecture of the model is still hand-crafted
  - usually hard to interpret

Ontologies and graphs

- semantic similarity measures and machine learning models on ontologies can be graph-based, feature-based, or model-based

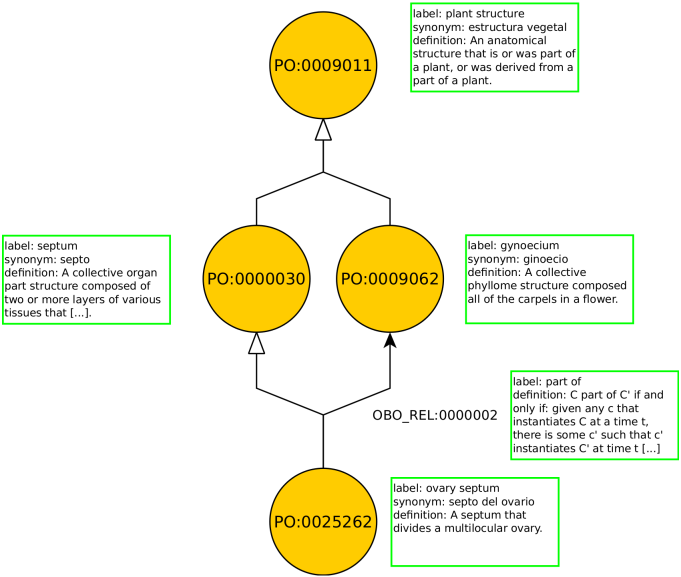
Ontologies and graphs

- semantic similarity measures and machine learning models on ontologies can be graph-based, feature-based, or model-based
- we may need to generate graphs from ontologies
  - *is-a* relations are easy (this is just `owl:subClassOf`)
  - how about *part-of*, *regulates*, *precedes*, etc.?
  - disjointness, universal vs. existential quantification, cardinality restrictions, intersection, union, negation?

Ontologies and graphs

- semantic similarity measures and machine learning models on ontologies can be graph-based, feature-based, or model-based
- we may need to generate graphs from ontologies
  - *is-a* relations are easy (this is just `owl:subClassOf`)
  - how about *part-of*, *regulates*, *precedes*, etc.?
  - disjointness, universal vs. existential quantification, cardinality restrictions, intersection, union, negation?
- relational patterns are implicit in OWL axioms
  - in first order logic
  - needs to translate them into OWL
  - defined in OBO Relation Ontology

Relations as patterns



Relations as patterns

- OBO Relation Ontology (RO):
  - `https://github.com/oborel/obo-relations`
- Basic Formal Ontology (BFO):
  - provides top-level classes
    - Continuant, Process, Function, Material object, etc.
  - used for some OBO Foundry ontologies
- RO and BFO provide a top-level system of classes and relations shared across many biomedical ontologies
- this system may define patterns used to generate graphs

Relations as patterns

- `X SubClassOf: Y`: $X \xrightarrow{\text{is-a}} Y$
- `X SubClassOf: part-of some Y`: $X \xrightarrow{\text{part-of}} Y$
- `X SubClassOf: regulates some Y`: $X \xrightarrow{\text{regulates}} Y$
- `X DisjointWith: Y`: $X \xleftrightarrow{\text{disjoint}} Y$
- `X EquivalentTo: Y`: $X \overset{\equiv}{\leftrightarrow} Y$, $\{X, Y\}$

Asserted and inferred

- relation patterns can be asserted or inferred
- `X SubClassOf: part-of some Y`
- `Y SubClassOf: part-of some Z`
- `part-of o part-of SubPropertyOf: part-of`
- $\vdash$ `X SubClassOf: part-of some Z`

Methods and tools

OBO Format represents ontologies as graphs:

- Protege/OWLAPI: OBO export
- OBO toolsets (e.g., ROBOT)
- `https://github.com/bio-ontology-research-group/Onto2Graph`

Methods and tools

OBO Format represents ontologies as graphs:

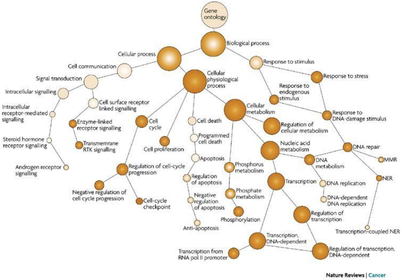
- Protege/OWLAPI: OBO export
- OBO toolsets (e.g., ROBOT)
- `https://github.com/bio-ontology-research-group/Onto2Graph`
- a conversion of an ontologies into a graph will almost always lead to a loss of information

Methods and tools

OBO Format represents ontologies as graphs:

- Protege/OWLAPI: OBO export
- OBO toolsets (e.g., ROBOT)
- `https://github.com/bio-ontology-research-group/Onto2Graph`
- a conversion of an ontologies into a graph will almost always lead to a loss of information
- edges should be "meaningful": not merely syntax
  - the RDF serialization of OWL is a graph and contains all information but is a bad idea for semantic similarity or machine learning (more later)

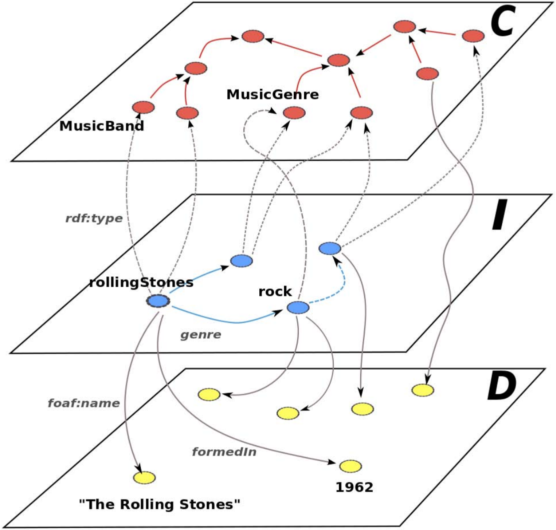
An example: protein–protein interactions and GO functions



Machine learning with ontologies: approaches

- graph-based
- syntactic
- model-theoretic

How to measure similarity?



From Harispe et al., Semantic Similarity From Natural Language And Ontology Analysis, 2015.

How to measure similarity?

- Shortest Path
  - applicable to arbitrary "knowledge graphs"
  - does not capture similarity well over all edge types, e.g., *disjointWith*, *differentFrom*, *opposite-of*, etc.
- Random Walk
  - with or without restart
  - iterated
  - does not consider edge labels $\Rightarrow$ captures only adjacency of nodes
  - scores whole graph with *probability* of being in a state
  - can take multiple seed nodes
    - can be used to find disease genes

Graph-based learning

- feature learning on graphs

Graph-based learning

- feature learning on graphs
- e.g., iterated, edge-labeled random walk
  - walks form *sentences*
  - sentences form a *corpus*
  - feature learning on corpus through Word2Vec (or factorization of co-occurrence matrix)
  - RDF2Vec: `http://data.dws.informatik.uni-mannheim.de/rdf2vec/`
  - with support for reasoning over ontologies: `https://github.com/bio-ontology-research-group/walking-rdf-and-owl`

Graph-based learning

- feature learning on graphs
- e.g., iterated, edge-labeled random walk
  - walks form *sentences*
  - sentences form a *corpus*
  - feature learning on corpus through Word2Vec (or factorization of co-occurrence matrix)
  - RDF2Vec: `http://data.dws.informatik.uni-mannheim.de/rdf2vec/`
  - with support for reasoning over ontologies: `https://github.com/bio-ontology-research-group/walking-rdf-and-owl`
- Translational knowledge graph embeddings: TransE, TransR, TransE, HolE, etc.
  - analogy- or translation-based
  - `https://github.com/SmartDataAnalytics/PyKEEN`

Graph-based learning

- feature learning on graphs
- e.g., iterated, edge-labeled random walk
  - walks form *sentences*
  - sentences form a *corpus*
  - feature learning on corpus through Word2Vec (or factorization of co-occurrence matrix)
  - RDF2Vec: `http://data.dws.informatik.uni-mannheim.de/rdf2vec/`
  - with support for reasoning over ontologies: `https://github.com/bio-ontology-research-group/walking-rdf-and-owl`
- Translational knowledge graph embeddings: TransE, TransR, TransE, HolE, etc.
  - analogy- or translation-based
  - `https://github.com/SmartDataAnalytics/PyKEEN`
- Graph Convolution Neural Networks (not discussed here)

Graph embeddings

Definition

Let $KG = (V, E, L; \vdash)$ be an ontology graph with a set of vertices V, a set of edges $E \subseteq V \times V$, a label function $L : V \cup E \mapsto Lab$ that assigns labels from a set of labels Lab to vertices and edges, and an inference relation $\vdash$. An ontology graph embedding is a function $f_\eta : L(V) \cup L(E) \mapsto \mathbf{R}^n$.

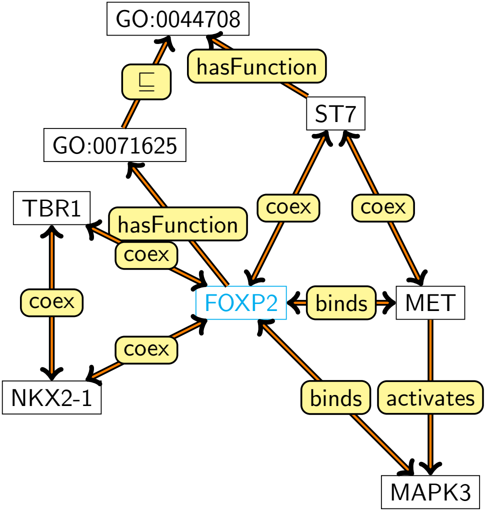
Graph embeddings

Definition

Let $KG = (V, E, L; \vdash)$ be an ontology graph with a set of vertices V, a set of edges $E \subseteq V \times V$, a label function $L : V \cup E \mapsto Lab$ that assigns labels from a set of labels Lab to vertices and edges, and an inference relation $\vdash$. An ontology graph embedding is a function $f_\eta : L(V) \cup L(E) \mapsto \mathbf{R}^n$.

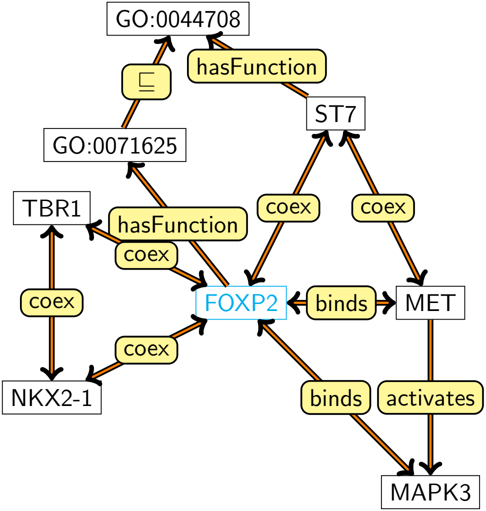
- key idea: preserve *some* structure of the graph in $\mathbb{R}^n$ (under operations in $\mathbb{R}^n$)
- $\mathbb{R}^n$ enables *new* operations (such as many similarity measures)
- useful as *feature* vectors

Random walks



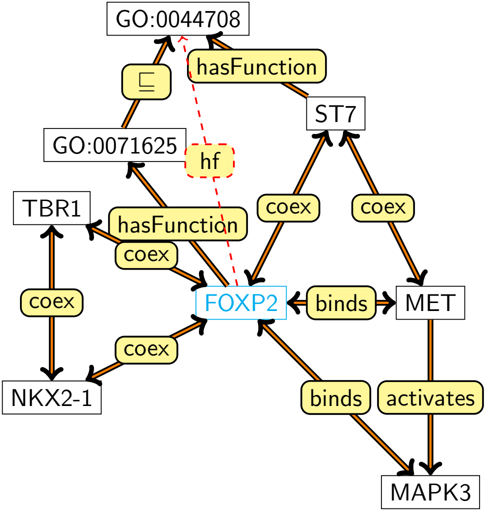
- FOXP2 is characterized by *adjacent* and close nodes and edges
- different edges may "transmit" information differently

Random walks



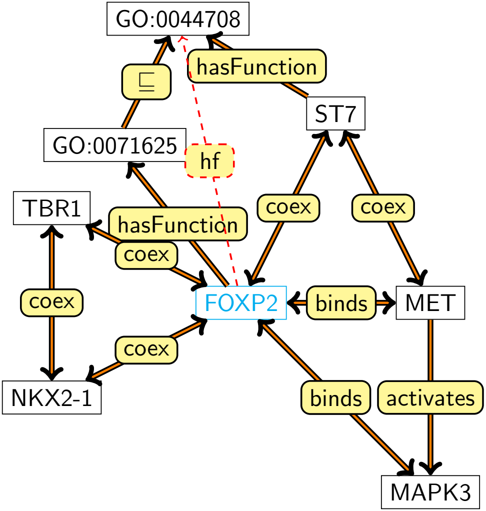
- precompute the deductive closure:
- for all ϕ: if $\mathcal{KG} \models \phi$, add ϕ to $\mathcal{KG}$

Random walks



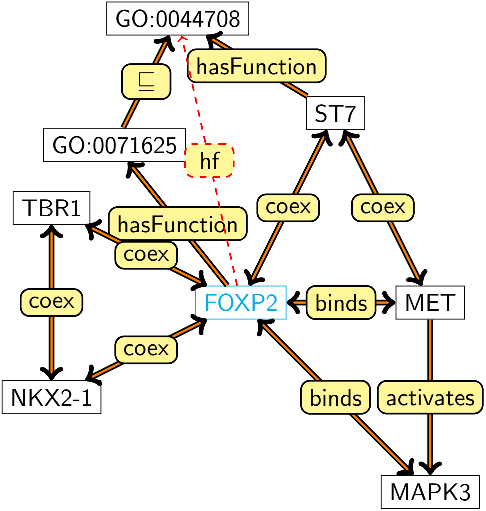
- precompute the deductive closure:
- for all ϕ: if $\mathcal{KG} \models \phi$, add ϕ to $\mathcal{KG}$

Random walks



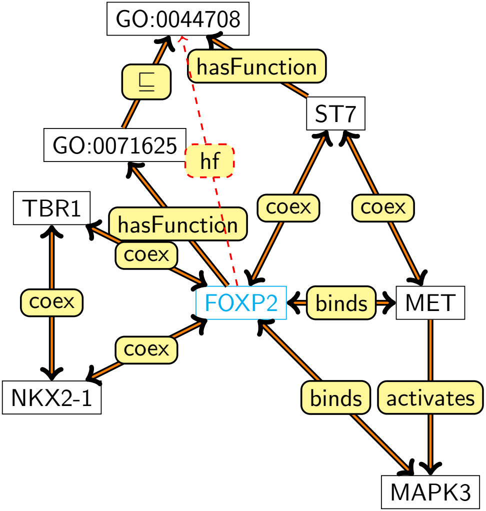
- Exploring the graph:

Random walks



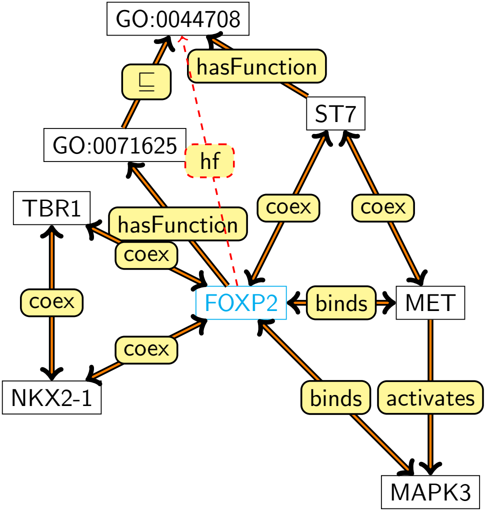
- Exploring the graph:
- :FOXP2 :binds :MET :coex :ST7 :hasFunction GO:0044708

Random walks



- Exploring the graph:
- :FOXP2 :binds :MET :coex :ST7 :hasFunction GO:0044708
- :FOXP2 :hasFunction GO:0071625 subClassOf GO:0044708

Random walks



- Exploring the graph:
- :FOXP2 :binds :MET :coex :ST7 :hasFunction GO:0044708
- :FOXP2 :hasFunction GO:0071625 subClassOf GO:0044708
- :FOXP2 :coex :TBR1 :coex :NKX2-1 :coex :TBR1 :coex ...

Word2Vec

Maximize:

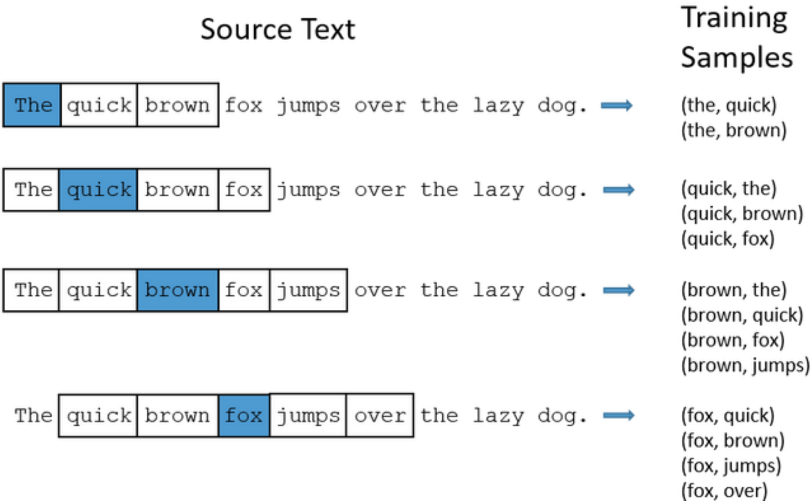
$$\frac{1}{N}\sum_{n=1}^{N}\sum_{-c\leq j\leq c, j\neq 0}\log p(w_{n+j}|w_n) \tag{1}$$

with

$$p(w_o|w_i) = \frac{\exp({v'_{w_o}}^T v_{w_i})}{\sum_{w=1}^{W}\exp({v'_w}^T v_{w_i})} \tag{2}$$

(at least conceptually; different strategies are used to approximate Eqn. 2)

Word2Vec


Source Text
Training Samples
The quick brown fox jumps over the lazy dog.
(the, quick)
(the, brown)
The quick brown fox jumps over the lazy dog.
(quick, the)
(quick, brown)
(quick, fox)
The quick brown fox jumps over the lazy dog.
(brown, the)
(brown, quick)
(brown, fox)
(brown, jumps)
The quick brown fox jumps over the lazy dog.
(fox, quick)
(fox, brown)
(fox, jumps)
(fox, over)

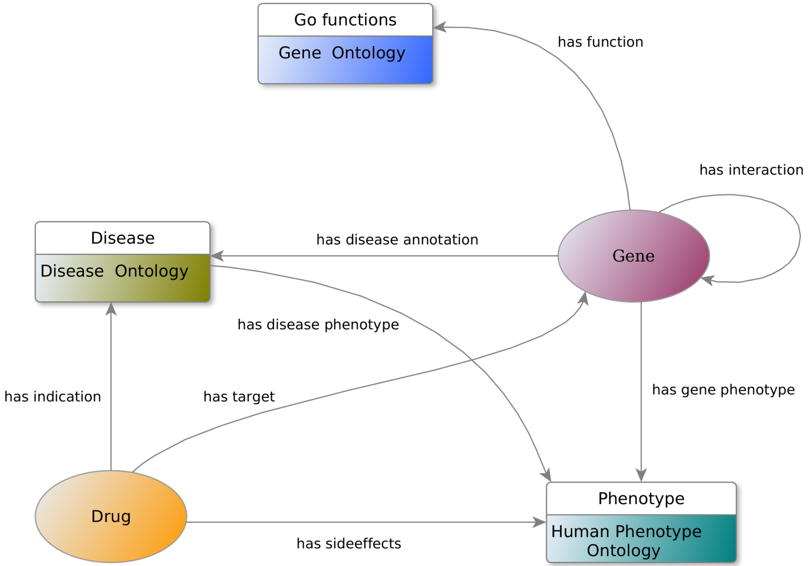
Word2Vec and Random Walks

- random walks "flatten" a graph
  - walks capture node neighborhood
  - and generate a "corpus"
- random walks capture graph "structure"
  - hub-nodes, communities, etc.
  - determine "importance" of nodes
- embeddings capture co-occurrence
  - similar graph neighborhood $\Rightarrow$ similar co-occurrence $\Rightarrow$ similar vector
- embeddings generate "feature" vectors
  - functions from symbols (words, labels) into $\mathbb{R}^n$

What to do with embeddings?

- useful for edge prediction, similarity, clustering, as feature vectors
  - supervised: edge prediction (e.g., SVM, ANN)
    - e.g.: find a function $f : \mathbb{R}^n \times \mathbb{R}^n \mapsto [0, 1]$ s.t. $\sqrt{\frac{\sum_{t=1}^{T}(\hat{y}_t - y_t)^2}{T}}$ (RMSE) is minimized for a set of true labels y_k
  - unsupervised: clustering, similarity, visualization
    - cosine similarity (for L2-normalized features)
    - Word2Vec embeddings capture similarity between co-occurrence vectors

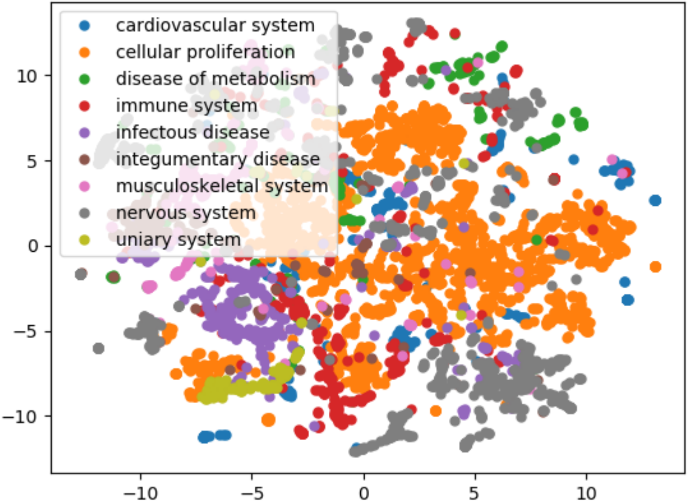
Random walks



Visualizing feature vectors: dimensionality reduction

- project n-dimensional vectors in 2D (or 3D) space
- and color with some known labels
  - high-level/general classes in an ontology work great
- PCA or t-SNE
- `https://lvdmaaten.github.io/tsne/`

Visualizing feature vectors



Features: supervised learning

- feature vectors represent graph neighborhood of nodes
  - adjacent nodes and edges
  - ontology classes (asserted & inferred)
- useful in supervised prediction tasks
- relation prediction:
  - input: two features vectors (from embedding function)
  - output: 0 or 1 (relation or not)
  - training data: positive and negative cases
    - $R(x, y)$ and $\neg R(x, y)$

Features: supervised learning

Object property	Source type	Target type	Without reasoning		With reasoning	
			F-measure	AUC	F-measure	AUC
has target	Drug	Gene/Protein	0.94	0.97	0.94	0.98
has disease annotation	Gene/Protein	Disease	0.89	0.95	0.89	0.95
has side-effect*	Drug	Phenotype	0.86	0.93	0.87	0.94
has interaction	Gene/Protein	Gene/Protein	0.82	0.88	0.82	0.88
has function*	Gene/Protein	Function	0.85	0.95	0.83	0.91
has gene phenotype*	Gene/Protein	Phenotype	0.84	0.91	0.82	0.90
has indication	Drug	Disease	0.72	0.79	0.76	0.83
has disease phenotype*	Disease	Phenotype	0.72	0.78	0.70	0.77

Ontologies, graphs, and text

The forkhead-box P2 (FOXP2) gene polymorphism has been reported to be involved in the susceptibility to schizophrenia; however, few studies have investigated the association between FOXP2 gene polymorphism and clinical symptoms in schizophrenia.

Ontologies, graphs, and text

The forkhead-box P2 (FOXP2) gene polymorphism has been reported to be involved in the susceptibility to schizophrenia; however, few studies have investigated the association between FOXP2 gene polymorphism and clinical symptoms in schizophrenia.

- :FOXP2 :binds :MET :coex :ST7 :hasFunction GO:0044708
- :FOXP2 :hasFunction GO:0071625 subClassOf GO:0044708
- :FOXP2 :coex :TBR1 :coex :NKX2-1 :coex :TBR1 :coex ...

Ontologies, graphs, and text

The :FOXP2 gene polymorphism has been reported to be involved in the susceptibility to schizophrenia; however, few studies have investigated the association between :FOXP2 gene polymorphism and clinical symptoms in schizophrenia.

- :FOXP2 :binds :MET :coex :ST7 :hasFunction GO:0044708
- :FOXP2 :hasFunction GO:0071625 subClassOf GO:0044708
- :FOXP2 :coex :TBR1 :coex :NKX2-1 :coex :TBR1 :coex ...

Tools and resources

- RDF2Vec: random walks on RDF + Word2Vec
- RDF2Vec: Weisfeiler-Lehmann kernel on RDF
- `https://datalab.rwth-aachen.de/embedding/RDF2Vec/`

Tools and resources

- RDF2Vec: random walks on RDF + Word2Vec
- RDF2Vec: Weisfeiler-Lehmann kernel on RDF
- `https://datalab.rwth-aachen.de/embedding/RDF2Vec/`
- Walking RDF+OWL: random walks on RDF + Elk + Word2Vec
  - inference
- `https://github.com/bio-ontology-research-group/walking-rdf-and-owl`

Some limitations

- "word"-based (Word2Vec):
  - semantics is reduced to co-occurrence (in ABox/TBox statements)
  - "disjointWith" vs. "part-of" vs. "subClassOf"

Jupyter excercise

- Open the Jupyter notebook `graph.ipynb`
- Follow the examples in the first part of the notebook (random walks)
- If you don't have a powerful CPU in your laptop (with multiple cores), you may want to lower the number of iterations (`n_iter`) during TSNE
- some of the code will take a while to run
  - if things are too slow, you can keep it running while we continue or complete this after the tutorial

Translating embeddings

Definition

Let $KG = (V, E, L; \vdash)$ be a knowledge graph with a set of vertices V, a set of edges $E \subseteq V \times V$, a label function $L : V \cup E \mapsto Lab$ that assigns labels from a set of labels Lab to vertices and edges, and an inference relation $\vdash$. A knowledge graph embedding is a function $f_\eta : L(V) \cup L(E) \mapsto \mathbf{R}^n$.

Translating embeddings

Definition

Let $KG = (V, E, L; \vdash)$ be a knowledge graph with a set of vertices V, a set of edges $E \subseteq V \times V$, a label function $L : V \cup E \mapsto Lab$ that assigns labels from a set of labels Lab to vertices and edges, and an inference relation $\vdash$. A knowledge graph embedding is a function $f_\eta : L(V) \cup L(E) \mapsto \mathbf{R}^n$.

Graph as edgelist: set of (s, p, o) statements

Translating embeddings

Definition

Let $KG = (V, E, L; \vdash)$ be a knowledge graph with a set of vertices V, a set of edges $E \subseteq V \times V$, a label function $L : V \cup E \mapsto Lab$ that assigns labels from a set of labels Lab to vertices and edges, and an inference relation $\vdash$. A knowledge graph embedding is a function $f_\eta : L(V) \cup L(E) \mapsto \mathbf{R}^n$.

Graph as edgelist: set of (s, p, o) statements
Idea: $\mu(s) + \mu(p) \approx \mu(o)$

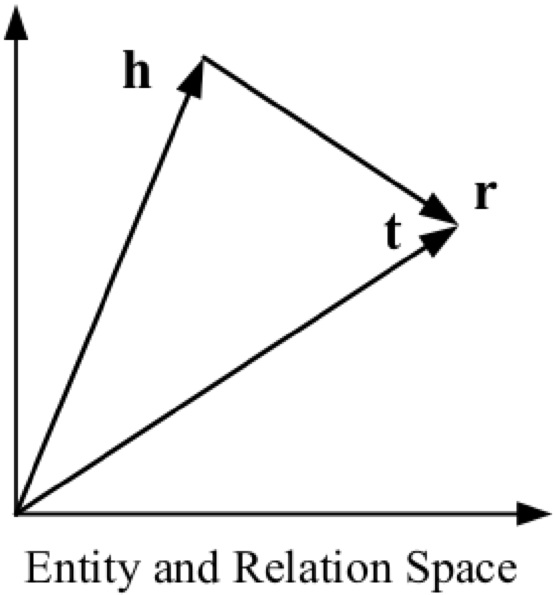
Translating embeddings

Definition

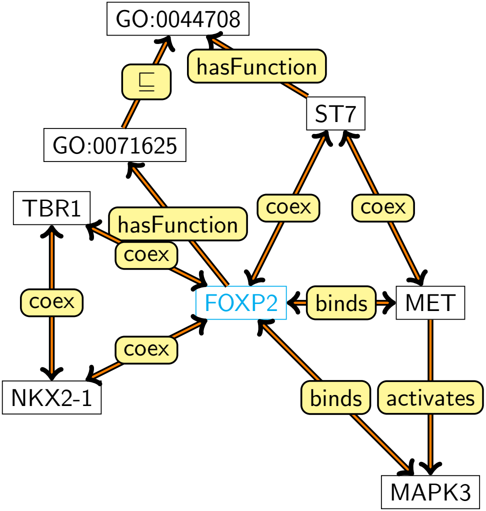
Let $KG = (V, E, L; \vdash)$ be a knowledge graph with a set of vertices V, a set of edges $E \subseteq V \times V$, a label function $L : V \cup E \mapsto Lab$ that assigns labels from a set of labels Lab to vertices and edges, and an inference relation $\vdash$. A knowledge graph embedding is a function $f_\eta : L(V) \cup L(E) \mapsto \mathbf{R}^n$.

Graph as edgelist: set of (s, p, o) statements
Idea: $\mu(s) + \mu(p) \approx \mu(o)$
Minimize: $\sum_t \|\mu(s) + \mu(p) - \mu(o)\|$ (chose your norm, usually L2)

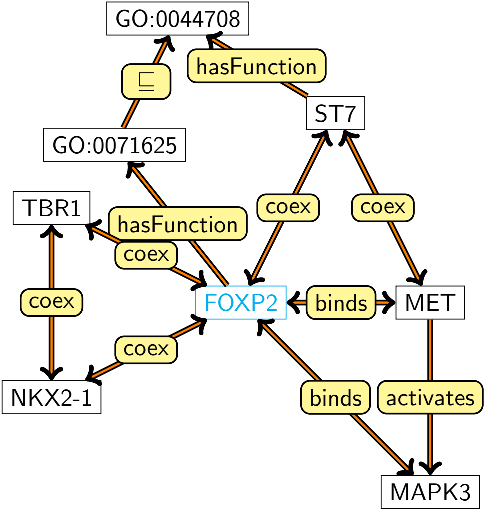
Translating embeddings



Translating embeddings

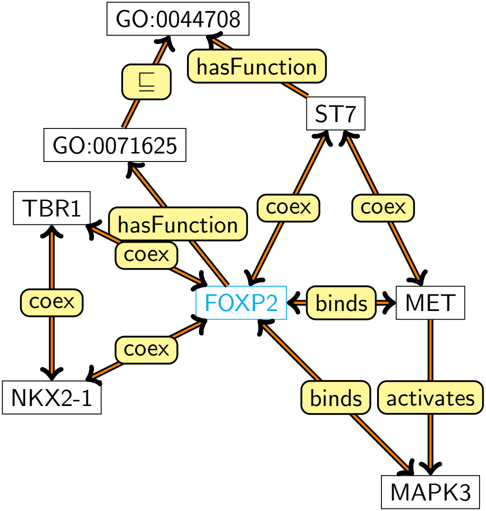


Translating embeddings



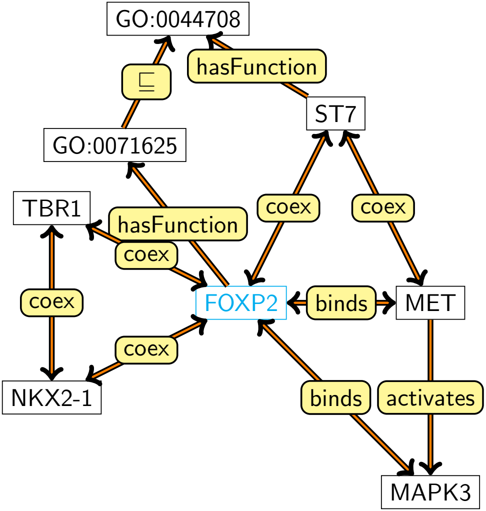
- FOXP2 + binds = MET

Translating embeddings



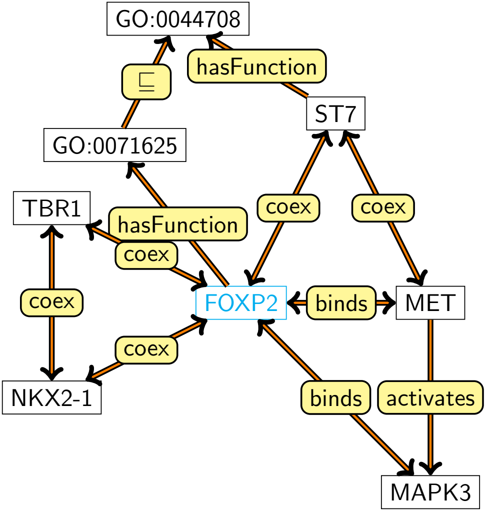
- FOXP2 + binds = MET
- MAP + activates = MAPK3

Translating embeddings



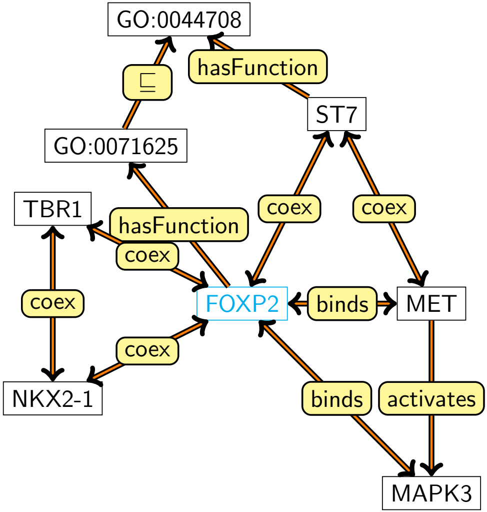
- FOXP2 + binds = MET
- MAP + activates = MAPK3
- MET + binds = FOXP2

Translating embeddings



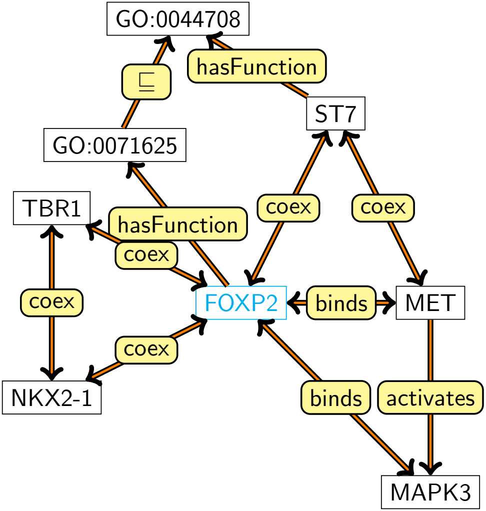
- FOXP2 + binds = MET
- MAP + activates = MAPK3
- MET + binds = FOXP2
- ST7 + hasFunction = `GO:0044708`

Translating embeddings



- FOXP2 + binds = MET
- MAP + activates = MAPK3
- MET + binds = FOXP2
- ST7 + hasFunction = `GO:0044708`
- ...

Translating embeddings



- FOXP2 + binds - MET = 0
- MAP + activates - MAPK3 = 0
- MET + binds - FOXP2 = 0
- ST7 + hasFunction - `GO:0044708` = 0
- ...

Translating embeddings

Algorithm 1 Learning TransE

input Training set $S = \{(h, \ell, t)\}$, entities and rel. sets E and L, margin γ, embeddings dim. k.

initialize $\boldsymbol{\ell} \leftarrow \text{uniform}(-\frac{6}{\sqrt{k}}, \frac{6}{\sqrt{k}})$ for each $\ell \in L$

    $\boldsymbol{\ell} \leftarrow \boldsymbol{\ell} / \|\boldsymbol{\ell}\|$ for each $\ell \in L$

    $\mathbf{e} \leftarrow \text{uniform}(-\frac{6}{\sqrt{k}}, \frac{6}{\sqrt{k}})$ for each entity $e \in E$

loop

  $\mathbf{e} \leftarrow \mathbf{e} / \|\mathbf{e}\|$ for each entity $e \in E$

  $S_{batch} \leftarrow \text{sample}(S, b)$ // sample a minibatch of size b

  $T_{batch} \leftarrow \emptyset$ // initialize the set of pairs of triplets

  for $(h, \ell, t) \in S_{batch}$ **do**

    $(h', \ell, t') \leftarrow \text{sample}(S'_{(h,\ell,t)})$ // sample a corrupted triplet

    $T_{batch} \leftarrow T_{batch} \cup \left\{\left((h, \ell, t), (h', \ell, t')\right)\right\}$

  end for

  Update embeddings w.r.t. $$\sum_{\left((h,\ell,t),(h',\ell,t')\right) \in T_{batch}} \nabla \left[\gamma + d(\boldsymbol{h} + \boldsymbol{\ell}, \boldsymbol{t}) - d(\boldsymbol{h'} + \boldsymbol{\ell}, \boldsymbol{t'})\right]_+$$

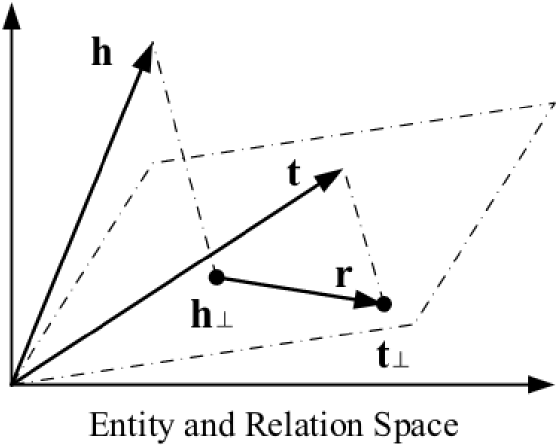
end loop

Bordes et al. (2013). Translating Embeddings for ModelingMulti-relational Data.

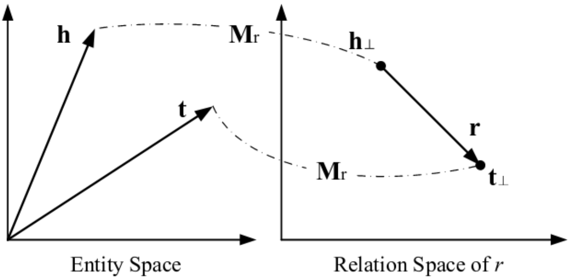
Some properties of TransE

- graph-based
  - works well on RDF graphs
  - and ontology graphs
- 1:1 relations only
  - not suitable for hierarchies (1-N relations)
  - not suitable for N-N relations
  - no transitive, symmetric, reflexive relations

Translating embeddings



Translating embeddings



(c) TransR.

Translating embeddings

Method	Ent. embedding	Rel. embedding	Scoring function $f_r(h,t)$	Constraints/Regularization
TransE [14]	$\mathbf{h},\mathbf{t} \in \mathbb{R}^d$	$\mathbf{r} \in \mathbb{R}^d$	$-\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|_{1/2}$	$\|\mathbf{h}\|_2 = 1, \|\mathbf{t}\|_2 = 1$
TransH [15]	$\mathbf{h},\mathbf{t} \in \mathbb{R}^d$	$\mathbf{r},\mathbf{w}_r \in \mathbb{R}^d$	$-\|(\mathbf{h}-\mathbf{w}_r^\top\mathbf{h}\mathbf{w}_r)+\mathbf{r}-(\mathbf{t}-\mathbf{w}_r^\top\mathbf{t}\mathbf{w}_r)\|_2^2$	$\|\mathbf{h}\|_2 \le 1, \|\mathbf{t}\|_2 \le 1$ $\lvert\mathbf{w}_r^\top\mathbf{r}\rvert/\|\mathbf{r}\|_2 \le \epsilon, \|\mathbf{w}_r\|_2 = 1$
TransR [16]	$\mathbf{h},\mathbf{t} \in \mathbb{R}^d$	$\mathbf{r} \in \mathbb{R}^k, \mathbf{M}_r \in \mathbb{R}^{k\times d}$	$-\|\mathbf{M}_r\mathbf{h}+\mathbf{r}-\mathbf{M}_r\mathbf{t}\|_2^2$	$\|\mathbf{h}\|_2 \le 1, \|\mathbf{t}\|_2 \le 1, \|\mathbf{r}\|_2 \le 1$ $\|\mathbf{M}_r\mathbf{h}\|_2 \le 1, \|\mathbf{M}_r\mathbf{t}\|_2 \le 1$
TransD [50]	$\mathbf{h},\mathbf{w}_h \in \mathbb{R}^d$ $\mathbf{t},\mathbf{w}_t \in \mathbb{R}^d$	$\mathbf{r},\mathbf{w}_r \in \mathbb{R}^k$	$-\|(\mathbf{w}_r\mathbf{w}_h^\top+\mathbf{I})\mathbf{h}+\mathbf{r}-(\mathbf{w}_r\mathbf{w}_t^\top+\mathbf{I})\mathbf{t}\|_2^2$	$\|\mathbf{h}\|_2 \le 1, \|\mathbf{t}\|_2 \le 1, \|\mathbf{r}\|_2 \le 1$ $\|(\mathbf{w}_r\mathbf{w}_h^\top+\mathbf{I})\mathbf{h}\|_2 \le 1$ $\|(\mathbf{w}_r\mathbf{w}_t^\top+\mathbf{I})\mathbf{t}\|_2 \le 1$
TranSparse [51]	$\mathbf{h},\mathbf{t} \in \mathbb{R}^d$	$\mathbf{r} \in \mathbb{R}^k, \mathbf{M}_r(\theta_r) \in \mathbb{R}^{k\times d}$ $\mathbf{M}_r^1(\theta_r^1), \mathbf{M}_r^2(\theta_r^2) \in \mathbb{R}^{k\times d}$	$-\|\mathbf{M}_r(\theta_r)\mathbf{h}+\mathbf{r}-\mathbf{M}_r(\theta_r)\mathbf{t}\|_{1/2}^2$ $-\|\mathbf{M}_r^1(\theta_r^1)\mathbf{h}+\mathbf{r}-\mathbf{M}_r^2(\theta_r^2)\mathbf{t}\|_{1/2}^2$	$\|\mathbf{h}\|_2 \le 1, \|\mathbf{t}\|_2 \le 1, \|\mathbf{r}\|_2 \le 1$ $\|\mathbf{M}_r(\theta_r)\mathbf{h}\|_2 \le 1, \|\mathbf{M}_r(\theta_r)\mathbf{t}\|_2 \le 1$ $\|\mathbf{M}_r^1(\theta_r^1)\mathbf{h}\|_2 \le 1, \|\mathbf{M}_r^2(\theta_r^2)\mathbf{t}\|_2 \le 1$
TransM [52]	$\mathbf{h},\mathbf{t} \in \mathbb{R}^d$	$\mathbf{r} \in \mathbb{R}^d$	$-\theta_r\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|_{1/2}$	$\|\mathbf{h}\|_2 = 1, \|\mathbf{t}\|_2 = 1$
ManifoldE [53]	$\mathbf{h},\mathbf{t} \in \mathbb{R}^d$	$\mathbf{r} \in \mathbb{R}^d$	$-(\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|_2^2-\theta_r^2)^2$	$\|\mathbf{h}\|_2 \le 1, \|\mathbf{t}\|_2 \le 1, \|\mathbf{r}\|_2 \le 1$
TransF [54]	$\mathbf{h},\mathbf{t} \in \mathbb{R}^d$	$\mathbf{r} \in \mathbb{R}^d$	$(\mathbf{h}+\mathbf{r})^\top\mathbf{t}+(\mathbf{t}-\mathbf{r})^\top\mathbf{h}$	$\|\mathbf{h}\|_2 \le 1, \|\mathbf{t}\|_2 \le 1, \|\mathbf{r}\|_2 \le 1$
TransA [55]	$\mathbf{h},\mathbf{t} \in \mathbb{R}^d$	$\mathbf{r} \in \mathbb{R}^d, \mathbf{M}_r \in \mathbb{R}^{d\times d}$	$-(\lvert\mathbf{h}+\mathbf{r}-\mathbf{t}\rvert)^\top\mathbf{M}_r(\lvert\mathbf{h}+\mathbf{r}-\mathbf{t}\rvert)$	$\|\mathbf{h}\|_2 \le 1, \|\mathbf{t}\|_2 \le 1, \|\mathbf{r}\|_2 \le 1$ $\|\mathbf{M}_r\|_F \le 1, [\mathbf{M}_r]_{ij} = [\mathbf{M}_r]_{ji} \ge 0$
KG2E [45]	$\mathbf{h}\sim\mathcal{N}(\boldsymbol{\mu}_h,\boldsymbol{\Sigma}_h)$ $\mathbf{t}\sim\mathcal{N}(\boldsymbol{\mu}_t,\boldsymbol{\Sigma}_t)$ $\boldsymbol{\mu}_h,\boldsymbol{\mu}_t \in \mathbb{R}^d$ $\boldsymbol{\Sigma}_h,\boldsymbol{\Sigma}_t \in \mathbb{R}^{d\times d}$	$\mathbf{r}\sim\mathcal{N}(\boldsymbol{\mu}_r,\boldsymbol{\Sigma}_r)$ $\boldsymbol{\mu}_r \in \mathbb{R}^d, \boldsymbol{\Sigma}_r \in \mathbb{R}^{d\times d}$	$-\mathrm{tr}(\boldsymbol{\Sigma}_r^{-1}(\boldsymbol{\Sigma}_h+\boldsymbol{\Sigma}_t))-\boldsymbol{\mu}^\top\boldsymbol{\Sigma}_r^{-1}\boldsymbol{\mu}-\ln\frac{\det(\boldsymbol{\Sigma}_r)}{\det(\boldsymbol{\Sigma}_h+\boldsymbol{\Sigma}_t)}$ $-\boldsymbol{\mu}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}-\ln(\det(\boldsymbol{\Sigma}))$ $\boldsymbol{\mu}=\boldsymbol{\mu}_h+\boldsymbol{\mu}_r-\boldsymbol{\mu}_t$ $\boldsymbol{\Sigma}=\boldsymbol{\Sigma}_h+\boldsymbol{\Sigma}_r+\boldsymbol{\Sigma}_t$	$\|\boldsymbol{\mu}_h\|_2 \le 1, \|\boldsymbol{\mu}_t\|_2 \le 1, \|\boldsymbol{\mu}_r\|_2 \le 1$ $c_{min}\mathbf{I} \le \boldsymbol{\Sigma}_h \le c_{max}\mathbf{I}$ $c_{min}\mathbf{I} \le \boldsymbol{\Sigma}_t \le c_{max}\mathbf{I}$ $c_{min}\mathbf{I} \le \boldsymbol{\Sigma}_r \le c_{max}\mathbf{I}$
TransG [46]	$\mathbf{h}\sim\mathcal{N}(\boldsymbol{\mu}_h,\sigma_h^2\mathbf{I})$ $\mathbf{t}\sim\mathcal{N}(\boldsymbol{\mu}_t,\sigma_t^2\mathbf{I})$ $\boldsymbol{\mu}_h,\boldsymbol{\mu}_t \in \mathbb{R}^d$	$\boldsymbol{\mu}_r^i\sim\mathcal{N}(\boldsymbol{\mu}_t-\boldsymbol{\mu}_h,(\sigma_h^2+\sigma_t^2)\mathbf{I})$ $\mathbf{r}=\sum_i \pi_r^i\boldsymbol{\mu}_r^i \in \mathbb{R}^d$	$\sum_i \pi_r^i \exp\left(-\frac{\|\boldsymbol{\mu}_h+\boldsymbol{\mu}_r^i-\boldsymbol{\mu}_t\|_2^2}{\sigma_h^2+\sigma_t^2}\right)$	$\|\boldsymbol{\mu}_h\|_2 \le 1, \|\boldsymbol{\mu}_t\|_2 \le 1, \|\boldsymbol{\mu}_r^i\|_2 \le 1$
UM [56]	$\mathbf{h},\mathbf{t} \in \mathbb{R}^d$	——	$-\|\mathbf{h}-\mathbf{t}\|_2^2$	$\|\mathbf{h}\|_2 = 1, \|\mathbf{t}\|_2 = 1$
SE [57]	$\mathbf{h},\mathbf{t} \in \mathbb{R}^d$	$\mathbf{M}_r^1, \mathbf{M}_r^2 \in \mathbb{R}^{d\times d}$	$-\|\mathbf{M}_r^1\mathbf{h}-\mathbf{M}_r^2\mathbf{t}\|_1$	$\|\mathbf{h}\|_2 = 1, \|\mathbf{t}\|_2 = 1$

Wang et al. Knowledge Graph Embedding: A Survey ofApproaches and Applications.

PyKEEN

- Python package to generate knowledge graph embeddings
- supports many different graph embedding types: TransE, TransR, TransD, RESCAL, etc.
- hyperparameter optimization ("HPO") and evaluation included
- `https://github.com/SmartDataAnalytics/PyKEEN`

Some limitations

- graph-based (same as random walks):
  - ontologies are not graphs!
  - converting ontologies to graphs loses information
  - no axioms, no definitions

Jupyter excercise

- run the PyKEEN part of `graph.ipynb`
- again: this may take a while
- you can also explore `https://github.com/SmartDataAnalytics/PyKEEN`
- try to expand the notebook to predict “new” relations
  - using numpy directly, or PyKEEN’s predictions methods

Ontologies: axioms, not graphs!

Overview | Browse | DLQuery | Download

Annotation	Value
label	B cell apoptotic process
definition	Any apoptotic process in a B cell, a lymphocyte of B lineage with the phenotype CD19-positive and capable of B cell mediated immunity.
class	http://purl.obolibrary.org/obo/GO_0001783
ontology	GO-PLUS
Equivalent	apoptotic process and (occurs in some B cell)
SubClassOf	occurs in some B cell, lymphocyte apoptotic process
id	GO:0001783
has_obo_namespace	biological_process

Ontologies: axioms, not graphs!

Gene Ontology:

- `behavior DisjointWith: 'developmental process'`
- `behavior SubclassOf: only-in-taxon some metazoa`
- `'cell proliferation' DisjointWith: in-taxon some fungi`
- `'cell growth' EquivalentTo: growth and ('results in growth of' some cell)`
- ...

Ontology embeddings

Definition

Let $O = (\Sigma = (C, R, I); ax; \vdash)$ be an ontology with a set of classes C, a set of relations R, a set of instances I, a set of axioms ax and an inference relation $\vdash$. An ontology embedding is a function $f_\eta : C \cup R \cup I \mapsto \mathbb{R}^n$ (or $\Sigma(O) \mapsto \mathbb{R}^n$.

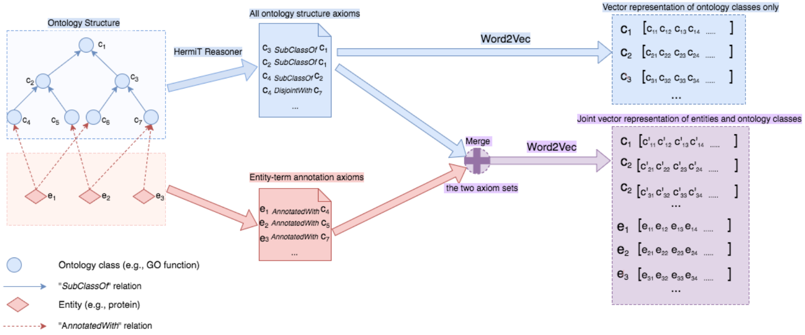
Ontology embeddings

Definition

Let $O = (\Sigma = (C, R, I); ax; \vdash)$ be an ontology with a set of classes C, a set of relations R, a set of instances I, a set of axioms ax and an inference relation $\vdash$. An ontology embedding is a function $f_\eta : C \cup R \cup I \mapsto \mathbb{R}^n$ (or $\Sigma(O) \mapsto \mathbb{R}^n$.

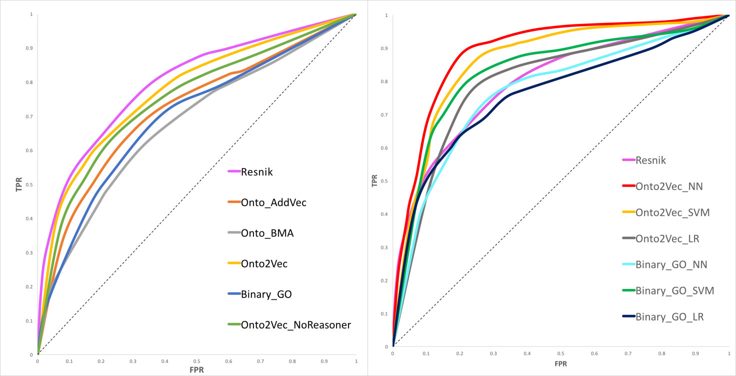
For example, we can use co-occurrence within $ax^\vdash$ to constrain the embedding function, where the constraints on co-occurrence are formulated using the Word2Vec skipgram model.

Onto2Vec



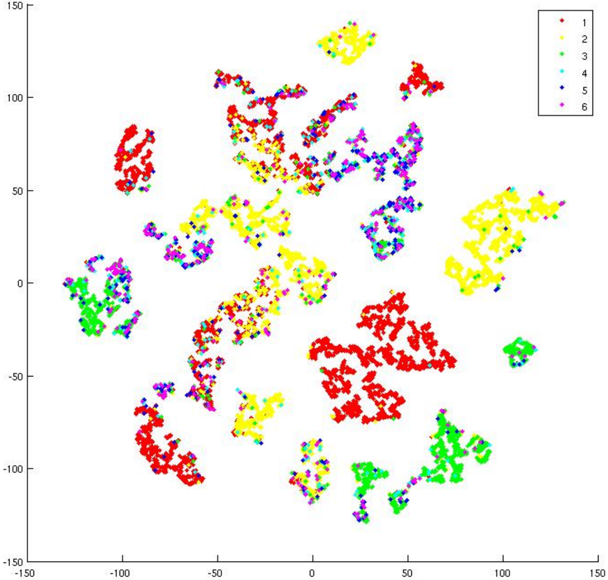
Ontology Structure
HermiT Reasoner
All ontology structure axioms
c_3 SubClassOf c_1
c_2 SubClassOf c_1
c_4 SubClassOf c_2
c_4 DisjointWith c_7
...
Word2Vec
Vector representation of ontology classes only
c_1 $[c_{11}\ c_{12}\ c_{13}\ c_{14}\ \ldots\ ]$
c_2 $[c_{21}\ c_{22}\ c_{23}\ c_{24}\ \ldots\ ]$
c_3 $[c_{31}\ c_{32}\ c_{33}\ c_{34}\ \ldots\ ]$
...
Entity-term annotation axioms
e_1 AnnotatedWith c_4
e_2 AnnotatedWith c_5
e_3 AnnotatedWith c_7
...
Merge
the two axiom sets
Word2Vec
Joint vector representation of entities and ontology classes
c_1 $[c'_{11}\ c'_{12}\ c'_{13}\ c'_{14}\ \ldots\ ]$
c_2 $[c'_{21}\ c'_{22}\ c'_{23}\ c'_{24}\ \ldots\ ]$
c_2 $[c'_{31}\ c'_{32}\ c'_{33}\ c'_{34}\ \ldots\ ]$
...
e_1 $[e_{11}\ e_{12}\ e_{13}\ e_{14}\ \ldots\ ]$
e_2 $[e_{21}\ e_{22}\ e_{23}\ e_{24}\ \ldots\ ]$
e_3 $[e_{31}\ e_{32}\ e_{33}\ e_{34}\ \ldots\ ]$
...
Ontology class (e.g., GO function)
"SubClassOf" relation
Entity (e.g., protein)
"AnnotatedWith" relation

Predicting PPIs: trainable similarity measures



Smaili et al. Onto2Vec: joint vector-based representation of biological entities and their ontology-based annotations.

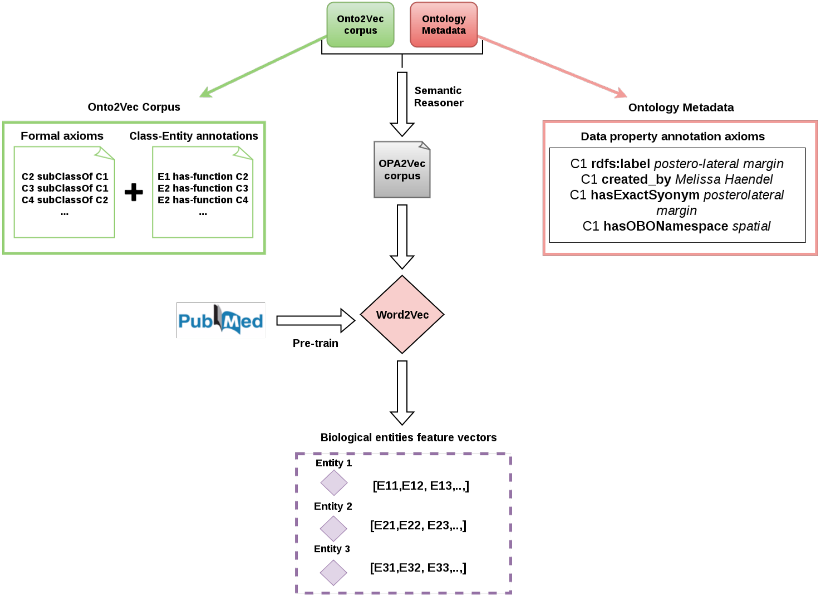
Visualizing embeddings



Combination with text

- ontologies contain more than axioms:
  - labels, synonyms, definitions, authors, etc.
- Description Logic axioms != natural language
- transfer learning: learn on one domain/task, apply to another
  - e.g.: learn on literature, apply to ontologies
  - words have "meaning" in literature, Description Logic symbols have "meaning" in ontology axioms
- Ontologies Plus Annotations 2 Vec (OPA2Vec) combines both

Ontologies Plus Annotations 2 Vec



Axioms contribute to prediction tasks: GO and GO-PLUS

	Human	Yeast	Arabidopsis
GO_Onto2Vec	0.7660	0.7701	0.7559
GO_Onto2Vec_NN	0.8779	0.8711	0.8364
GO_plus_Onto2Vec	0.7880	0.7943	0.7889
GO_plus_Onto2Vec_NN	**0.9021**	**0.8937**	**0.8834**

Evaluating individual axioms

Testing how much each ontologies' axioms contribute to predictions:

	Human		Arabidopsis	
	Onto2Vec	**Onto2Vec_NN**	**Onto2Vec**	**Onto2Vec_NN**
GO (Baseline)	0.7660	0.8779	0.7559	0.8364
ChEBI	0.7899(+0.0239)	0.8914(+0.0135)	0.7703(+0.0144)	0.8518(+0.0154)
PO	0.7752(+0.0092)	0.8776(-0.0003)	0.7671(+0.0112)	0.8469(+0.0105)
CL	0.7743(+0.0083)	0.8810(+0.0031)	0.7612(+0.0053)	0.8371(+0.0007)
PATO	0.7657(-0.0003)	0.8768(-0.0011)	0.7563(+0.0004)	0.8380(+0.0016)

Evaluating definitions

Testing how much each ontologies' annotation properties contribute to predictions:

	Human		Arabidopsis	
	Onto2Vec	**Onto2Vec_NN**	**Onto2Vec**	**Onto2Vec_NN**
GO (Baseline)	0.8727	0.9033	0.8613	0.8903
ChEBI	0.8571(-0.0156)	0.8801(-0.0232)	0.8601(-0.0012)	0.8880(-0.0023)
PO	0.8680(-0.0047)	0.8824(-0.0209)	0.8632(+0.0019)	0.8908(+0.0005)
CL	0.8811(+0.0084)	0.9037(+0.0004)	0.8614(+0.0001)	0.8899(-0.0004)
PATO	0.8562(-0.0165)	0.8711(-0.0322)	0.8544(-0.0069)	0.8860(-0.0043)

OPA2Vec

- `https://github.com/bio-ontology-research-group/opa2vec`
- command line tool
  - input: OWL ontology, set of entities with annotations/associations
  - output: vectors for each class and entity
- includes Elk and HermiT
- limitations: word-based
  - still ignores semantics!

OPA2Vec Jupyter excercise

- open the notebook `OPA2Vec.ipynb`
- run the whole notebook
  - this should be relatively fast and not take too much time on a modern laptop
- play with the prediction methods (cosine similarity)

How to overcome the semantic gap?

- none of the models discussed above are truly “semantic”
  - all syntactic
  - graph-based or based on axioms

How to overcome the semantic gap?

- none of the models discussed above are truly "semantic"
  - all syntactic
  - graph-based or based on axioms
- what do we actually mean by "semantics"?

How to overcome the semantic gap?

- none of the models discussed above are truly "semantic"
  - all syntactic
  - graph-based or based on axioms
- what do we actually mean by "semantics"?
  - formal definition of "truth" relies on "models"

How to overcome the semantic gap?

- none of the models discussed above are truly "semantic"
  - all syntactic
  - graph-based or based on axioms
- what do we actually mean by "semantics"?
  - formal definition of "truth" relies on "models"
  - universal algebra over formal languages (with signature Σ)

Description Logic EL++

Name	Syntax	Semantics
top	$\top$	$\Delta^{\mathcal{I}}$
bottom	$\bot$	$\emptyset$
nominal	$\{a\}$	$\{a^{\mathcal{I}}\}$
conjunction	$C \sqcap D$	$C^{\mathcal{I}} \cap D^{\mathcal{I}}$
existential restriction	$\exists r.C$	$\{x \in \Delta^{\mathcal{I}} \mid \exists y \in \Delta^{\mathcal{I}} : (x, y) \in r^{\mathcal{I}} \wedge y \in C^{\mathcal{I}}\}$
generalized concept inclusion	$C \sqsubseteq D$	$C^{\mathcal{I}} \subseteq D^{\mathcal{I}}$
role inclusion	$r_1 \circ \ldots \circ r_n \sqsubseteq r$	$r_1^{\mathcal{I}} \circ \ldots \circ r_n^{\mathcal{I}} \subseteq r^{\mathcal{I}}$

Models

- Interpretations and Σ-structures
- Model $\mathfrak{A}$ of a formula ϕ: ϕ is true in $\mathfrak{A}$ ($\mathfrak{A} \models \phi$)
- Theory T: set of formulas
- $\mathfrak{A}$ is a model of T if $\mathfrak{A}$ is a model of all formulas in T
- Ontologies are (special kinds of) theories

EL Embeddings

- given a theory/ontology T with signature $\Sigma(T)$
- aim: find $f_e : \Sigma(T) \mapsto \mathbb{R}^n$ s.t. $f_e(\Sigma(T))$ is a model of T ($f_e(\Sigma(T)) \models T$)

EL Embeddings

- given a theory/ontology T with signature $\Sigma(T)$
- aim: find $f_e : \Sigma(T) \mapsto \mathbb{R}^n$ s.t. $f_e(\Sigma(T))$ is a model of T ($f_e(\Sigma(T)) \models T$)
- more general: find an algorithm that maps symbols (signatures) into $\mathbb{R}^n$ so that the *semantics* of the symbol (expressed through axioms and explicit in model structures) is preserved

EL Embeddings

- given a theory/ontology T with signature $\Sigma(T)$
- aim: find $f_e : \Sigma(T) \mapsto \mathbb{R}^n$ s.t. $f_e(\Sigma(T))$ is a model of T $(f_e(\Sigma(T)) \models T)$
- more general: find an algorithm that maps symbols (signatures) into $\mathbb{R}^n$ so that the *semantics* of the symbol (expressed through axioms and explicit in model structures) is preserved
- any consistent $\mathcal{EL}^{++}$theory has infinite models

EL Embeddings

- given a theory/ontology T with signature $\Sigma(T)$
- aim: find $f_e : \Sigma(T) \mapsto \mathbb{R}^n$ s.t. $f_e(\Sigma(T))$ is a model of T ($f_e(\Sigma(T)) \models T$)
- more general: find an algorithm that maps symbols (signatures) into $\mathbb{R}^n$ so that the *semantics* of the symbol (expressed through axioms and explicit in model structures) is preserved
- any consistent $\mathcal{EL}^{++}$theory has infinite models
- any consistent EL++ theory has models in $\mathbb{R}^n$ (Loewenheim-Skolem, upwards)

Key idea

- for all $r \in \Sigma(T)$ and $C \in \Sigma(T)$, define $f_e(r)$ and $f_e(C)$
- $f_e(C)$ maps to points in an open n-ball such that $f_e(C) = C^{\mathcal{I}}$: $C^{\mathcal{I}} = \{x \in \mathbb{R}^n | \, \|f_e(C) - x\| < r_e(C)\}$
  - these are the *extension* of a class in $\mathbb{R}^n$
- $f_e(r)$ maps a binary relation r to a vector such that $r^{\mathcal{I}} = \{(x, y) | x + f_e(r) = y\}$
  - that's the TransE property for *individuals*
- use the axioms in T as constraints

Algorithm

- normalize the theory:
  - every $\mathcal{EL}^{++}$theory can be expressed using four normal forms (Baader et al., 2005)
- eliminate the ABox: replace each individual symbol with a singleton class: a becomes $\{a\}$
- rewrite relation assertions $r(a, b)$ and class assertions $C(a)$ as $\{a\} \sqsubseteq \exists r.\{b\}$ and $\{a\} \sqsubseteq C$
  - something to remember for the next class-vs-instance discussion?
- normalization rules to generate:
  - $C \sqsubseteq D$
  - $C \sqcap D \sqsubseteq E$
  - $C \sqsubseteq \exists R.D$
  - $\exists R.C \sqsubseteq D$

Algorithm: loss functions

$$\begin{aligned} & loss_{C \sqsubseteq D}(c, d) = \\ & \max(0, \|f_\eta(c) - f_\eta(d)\| + r_\eta(c) - r_\eta(d) - \gamma) \\ & + |\, \|f_\eta(c)\| - 1| + |\, \|f_\eta(d)\| - 1| \end{aligned} \tag{3}$$

Algorithm: loss functions

Let $h = \frac{r_\eta(c)^2 - r_\eta(d)^2 + \|f_\eta(c) - f_\eta(d)\|^2}{2\|f_\eta(c) - f_\eta(d)\|}$, then the center and radius of the smallest n-ball containing the intersection of $\eta(C)$ and $\eta(D)$ are $f_\eta(c) + \frac{h}{\|f_\eta(c) - f_\eta(d)\|}(f_\eta(d) - f_\eta(c))$ and $\sqrt{r_\eta(c)^2 - h^2}$.

Algorithm: loss functions

$$loss_{C \sqsubseteq \exists R.D}(c, d, r) =$$
$$\max(0, \|f_\eta(c) + f_\eta(r) - f_\eta(d)\| + r_\eta(c) - r_\eta(d) - \gamma) \quad (4)$$
$$+ |\,\|f_\eta(c)\| - 1| + |\,\|f_\eta(d)\| - 1|$$

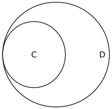
Algorithm: loss functions

$$loss_{\exists R.C \sqsubseteq D}(c, d, r) =$$
$$\max(0, \|f_\eta(c) - f_\eta(r) - f_\eta(d)\| - r_\eta(c) - r_\eta(d) - \gamma) \qquad (5)$$
$$+ | \, \|f_\eta(c)\| - 1| + | \, \|f_\eta(d)\| - 1|$$

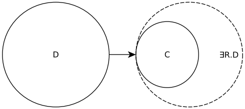
Algorithm: loss functions

$$\begin{aligned}&loss_{C \sqcap D \sqsubseteq \bot}(c, d, e) = \\ &\max(0, r_\eta(c) + r_\eta(d) - \|f_\eta(c) - f_\eta(d)\| + \gamma) \\ &+ |\,\|f_\eta(c)\| - 1| + |\,\|f_\eta(d)\| - 1|\end{aligned} \tag{6}$$

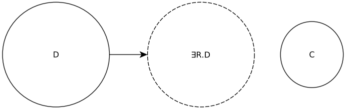
Algorithm: loss functions



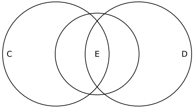
$C \sqsubseteq D$



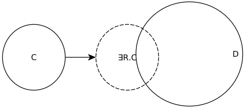
$C \sqsubseteq \exists R.D$



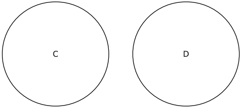
$C \not\sqsubseteq \exists R.D$



$C \sqcap D \sqsubseteq E$



$\exists R.C \sqsubseteq D$

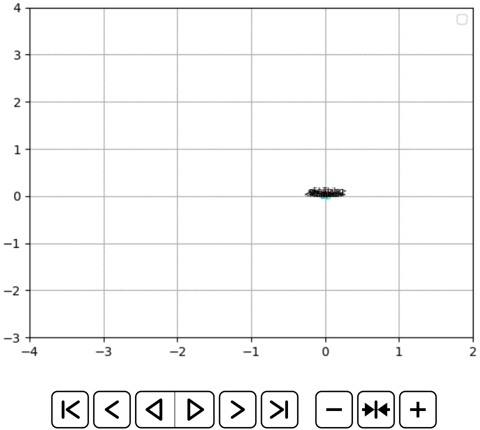


$C \sqcap D \sqsubseteq \bot$

EL Embeddings

$$
\begin{align}
Male &\sqsubseteq Person \tag{7}\\
Female &\sqsubseteq Person \tag{8}\\
Father &\sqsubseteq Male \tag{9}\\
Mother &\sqsubseteq Female \tag{10}\\
Father &\sqsubseteq Parent \tag{11}\\
Mother &\sqsubseteq Parent \tag{12}\\
Female \sqcap Male &\sqsubseteq \bot \tag{13}\\
Female \sqcap Parent &\sqsubseteq Mother \tag{14}\\
Male \sqcap Parent &\sqsubseteq Father \tag{15}\\
\exists hasChild.Person &\sqsubseteq Parent \tag{16}\\
Parent &\sqsubseteq Person \tag{17}\\
Parent &\sqsubseteq \exists hasChild.\top \tag{18}
\end{align}
$$

EL Embeddings



- model with $\Delta = R^n$
- support quantifiers, negation, conjunction,...

Jupyter excercise

- Run the new Docker image `coolmaksat/embeddings:latest`
- `docker run -i -t -p 8888:8888 coolmaksat/embeddings /bin/bash -c "jupyter notebook --notebook-dir=/usr/src/app/ --ip='0.0.0.0' --port=8888 --no-browser --allow-root"`

Summary

- ontologies contain background knowledge that is useful as background knowledge:
  - axioms
  - natural language (definitions, labels, synonyms)

Summary

- ontologies contain background knowledge that is useful as background knowledge:
  - axioms
  - natural language (definitions, labels, synonyms)
- feature learning (deep learning) on ontologies encodes this background knowledge
  - using ontology graphs, axioms, or model structures

Open research questions

Where is our semantics, in the machine learning model or the axioms?

- implicit or explicit?
- example: transitive relations
- ...