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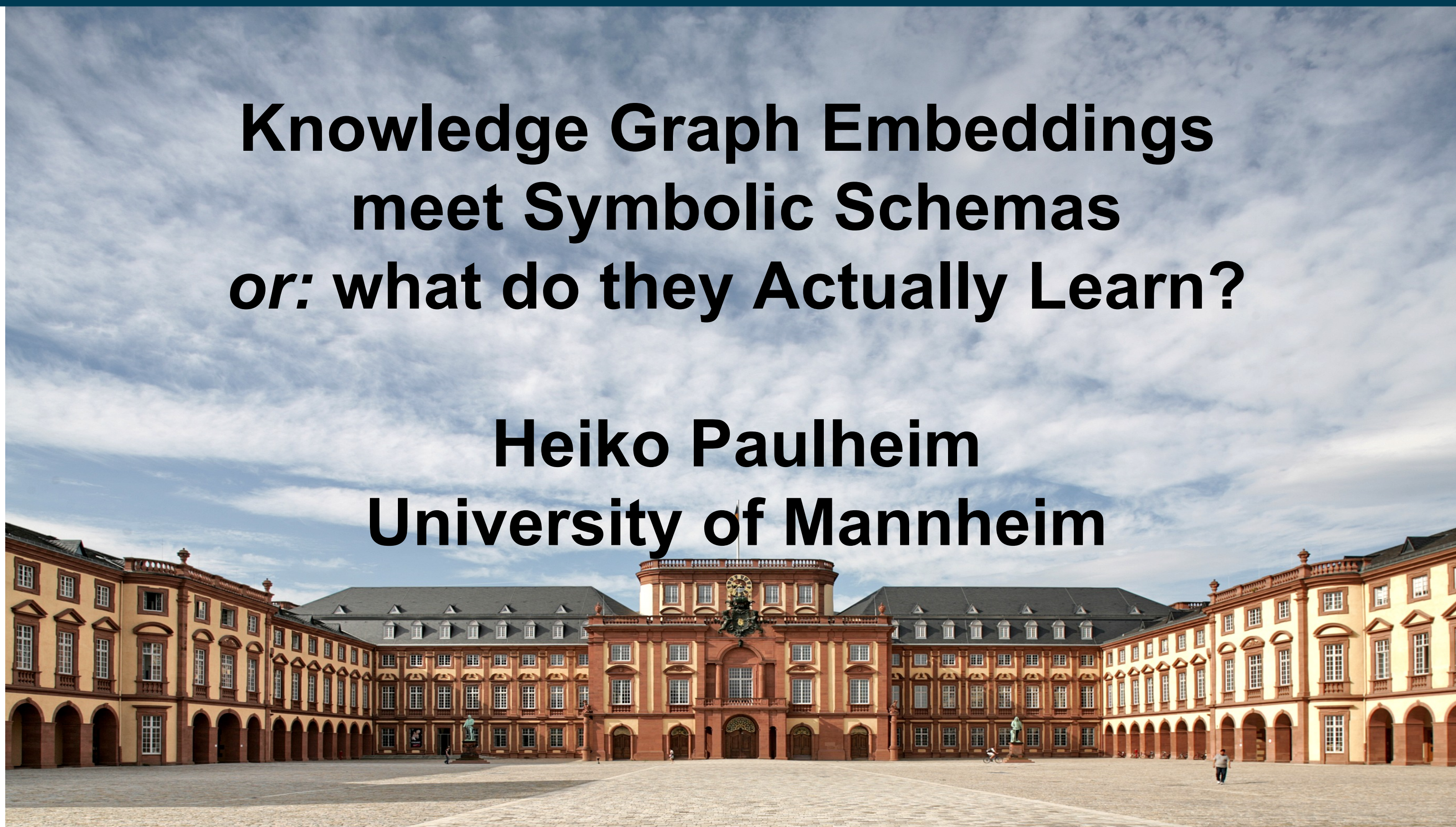


Knowledge Graph Embeddings meet Symbolic Schemas *or:* what do they Actually Learn?

Heiko Paulheim
University of Mannheim

Brief Introduction

Ontologies-Based Business Integration

SoKNOS

ADiWa.

Ontology-based Application Integration

FeGeLOD
Feature Generation from Linked Open Data

SDType

rdf2vec

Kare§KoKI

ReNewRS

teaming.ai

WebIsALOD

CaLiGraph

DBkWik

MELT

kgextension

Pre PhD Years | PhD Years | PostDoc Years | Assistant Professor | Full Professor

2006 2008 2011 2013 2014 2017

h_da
HOCHSCHULE DARMSTADT
UNIVERSITY OF APPLIED SCIENCES

TECHNISCHE UNIVERSITÄT DARMSTADT

UNIVERSITY OF MANNHEIM

SAP

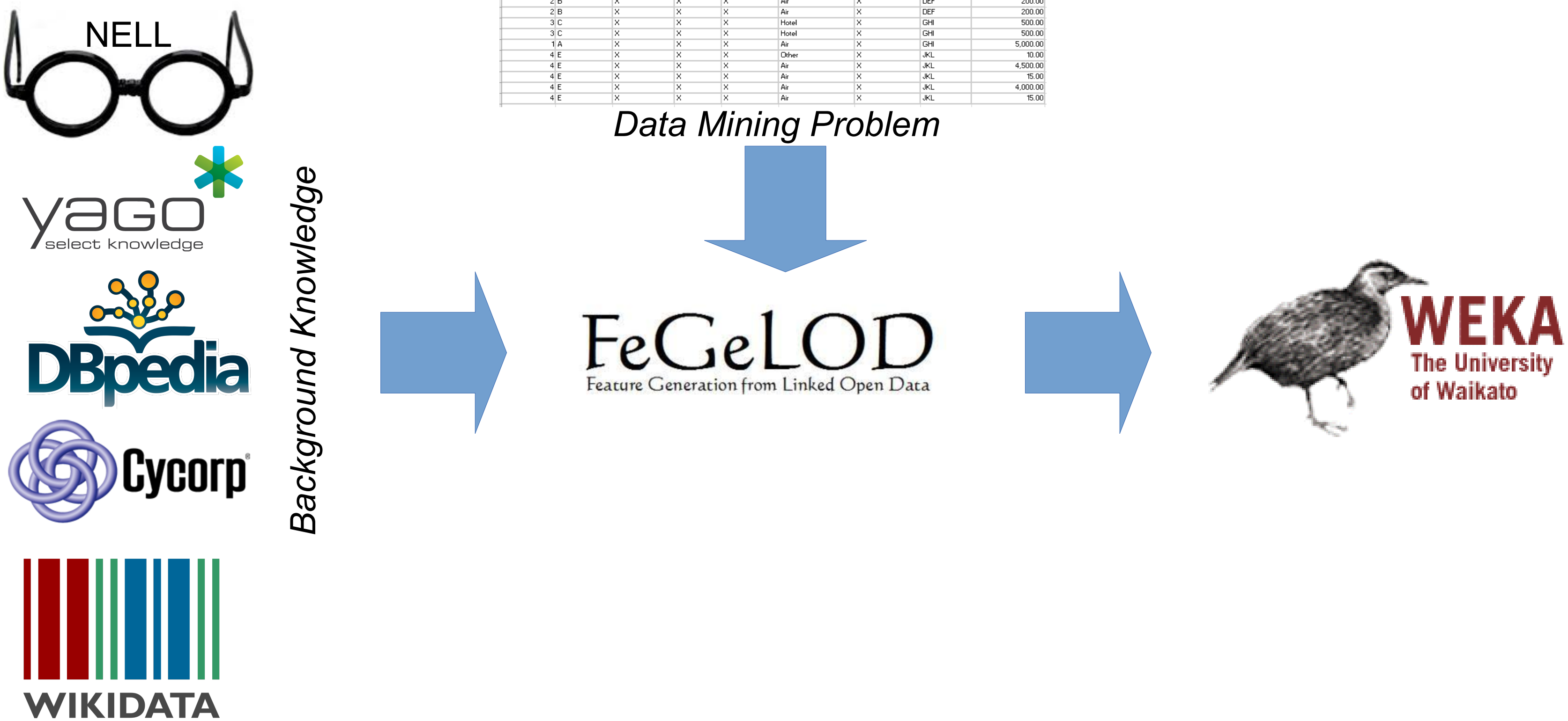
The Beginning of my KG Embedding Journey

- Using Open (RDF) Data for improving data mining

Source

Employee ID	Employee	HR cost center	Report Name	Approval Status	Expense Type	Vendor	Project	Expense Amount
1	A	X	X	X	Other	X	ABC	10.00
2	B	X	X	X	Transportation	X	ABC	100.00
2	B	X	X	X	Air	X	ABC	200.00
2	B	X	X	X	Air	X	ABC	200.00
2	B	X	X	X	Air	X	DEF	200.00
2	B	X	X	X	Air	X	DEF	200.00
3	C	X	X	X	Hotel	X	GHI	500.00
3	C	X	X	X	Hotel	X	GHI	500.00
1	A	X	X	X	Air	X	GHI	5,000.00
4	E	X	X	X	Other	X	JKL	10.00
4	E	X	X	X	Air	X	JKL	4,500.00
4	E	X	X	X	Air	X	JKL	15.00
4	E	X	X	X	Air	X	JKL	4,000.00
4	E	X	X	X	Air	X	JKL	15.00

Data Mining Problem

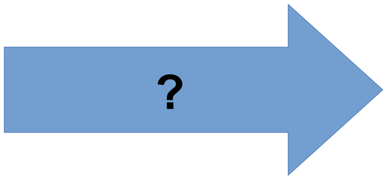


Graphs vs. Vectors

- Data Science tools for prediction etc.
  - Python, Weka, R, RapidMiner, …
  - Algorithms that work on vectors, not graphs
- Bridges built over the past years:
  - FeGeLOD (Weka, 2012), RapidMiner LOD Extension (2015) Python KG Extension (2021)

FeGeLOD
Feature Generation from Linked Open Data

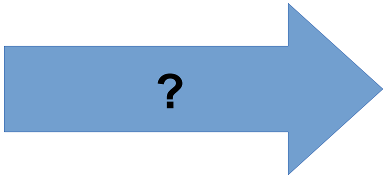
kgextension



Row No.	attribute_1	attribute_2	attribute_3	attribute_4	attribute_5	attribute_6	attribute_7	attribute_8	attribute_9	attribute_10	attribute_11
1	0.020	0.037	0.043	0.021	0.095	0.099	0.154	0.160	0.311	0.211	0.161
2	0.045	0.052	0.084	0.069	0.118	0.258	0.216	0.348	0.334	0.287	0.492
3	0.026	0.058	0.110	0.108	0.097	0.228	0.243	0.377	0.560	0.619	0.633
4	0.010	0.017	0.062	0.021	0.021	0.037	0.110	0.128	0.060	0.126	0.088
5	0.076	0.067	0.048	0.039	0.059	0.065	0.121	0.247	0.356	0.446	0.415
6	0.029	0.045	0.028	0.017	0.038	0.099	0.120	0.183	0.210	0.304	0.299
7	0.032	0.096	0.132	0.141	0.167	0.171	0.073	0.140	0.208	0.351	0.179
8	0.052	0.055	0.084	0.032	0.116	0.092	0.103	0.061	0.146	0.284	0.280
9	0.022	0.037	0.048	0.048	0.065	0.059	0.075	0.010	0.068	0.149	0.116
10	0.016	0.017	0.035	0.007	0.019	0.067	0.106	0.070	0.096	0.025	0.080
11	0.004	0.006	0.015	0.034	0.031	0.028	0.040	0.027	0.032	0.045	0.049
12	0.012	0.031	0.017	0.031	0.036	0.010	0.018	0.058	0.112	0.084	0.055
13	0.008	0.009	0.005	0.025	0.034	0.055	0.053	0.096	0.101	0.124	0.110
14	0.009	0.006	0.025	0.049	0.120	0.159	0.139	0.099	0.096	0.190	0.190
15	0.012	0.043	0.060	0.045	0.060	0.035	0.053	0.034	0.105	0.212	0.164
16	0.030	0.061	0.065	0.092	0.162	0.229	0.218	0.203	0.146	0.085	0.248
17	0.035	0.012	0.019	0.047	0.074	0.118	0.168	0.154	0.147	0.291	0.233
18	0.019	0.061	0.038	0.077	0.139	0.081	0.057	0.022	0.104	0.119	0.124
19	0.027	0.009	0.015	0.028	0.041	0.076	0.103	0.114	0.079	0.152	0.168
20	0.013	0.015	0.064	0.173	0.257	0.256	0.295	0.411	0.498	0.592	0.583
21	0.047	0.051	0.082	0.125	0.178	0.307	0.301	0.236	0.383	0.376	0.302
22	0.066	0.058	0.084	0.037	0.046	0.077	0.077	0.113	0.235	0.184	0.287
23	0.010	0.048	0.030	0.030	0.065	0.108	0.236	0.238	0.007	0.188	0.146
24	0.011	0.015	0.014	0.008	0.021	0.106	0.102	0.044	0.093	0.073	0.074

Graphs vs. Vectors

- Transformation strategies (aka *propositionalization*)
  - e.g., types: type_horror_movie=true
  - e.g., data values: year=2011
  - e.g., aggregates: nominations=7



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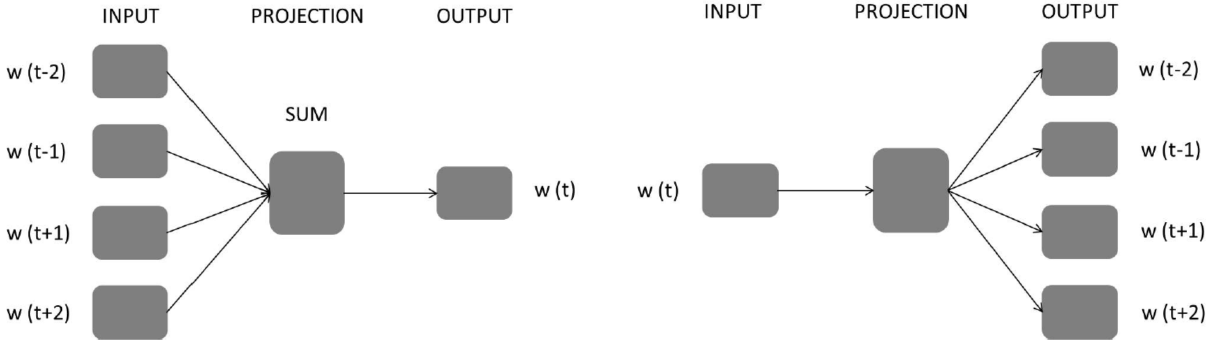
Graphs vs. Vectors

- Observations with simple propositionalization strategies
  - Even simple features (e.g., add all numbers and types) can help on many problems
  - More sophisticated features often bring additional improvements
    - Combinations of relations and individuals
      - e.g., movies directed by Steven Spielberg
    - Combinations of relations and types
      - e.g., movies directed by Oscar-winning directors
    - …
  - But
    - The search space is enormous!
    - *Generate first, filter later* does not scale well

Towards RDF2vec

- Excursion: word embeddings
  - word2vec proposed by Mikolov et al. (2013)
  - predict a word from its context or vice versa
    - Idea: similar words appear in similar contexts, like
      - Jobs, Wozniak, and Wayne founded **Apple** Computer Company in April 1976
      - **Google** was officially founded as a company in January 2006
  - usually trained on large text corpora
    - projection layer: embedding vectors



RDF2vec in a Nutshell

- Basic idea:
  - extract random walks from an RDF graph:

    Mulholland Dr. $\xrightarrow{\text{director}}$ David Lynch $\xrightarrow{\text{nationality}}$ US
  - feed walks into word2vec algorithm
- Order of magnitude (e.g., DBpedia)
  - ~6M entities ("words")
  - start up to 500 random walks per entity, length up to 8

    → corpus of >20B tokens
- Result:
  - entity embeddings
  - most often outperform other propositionalization techniques

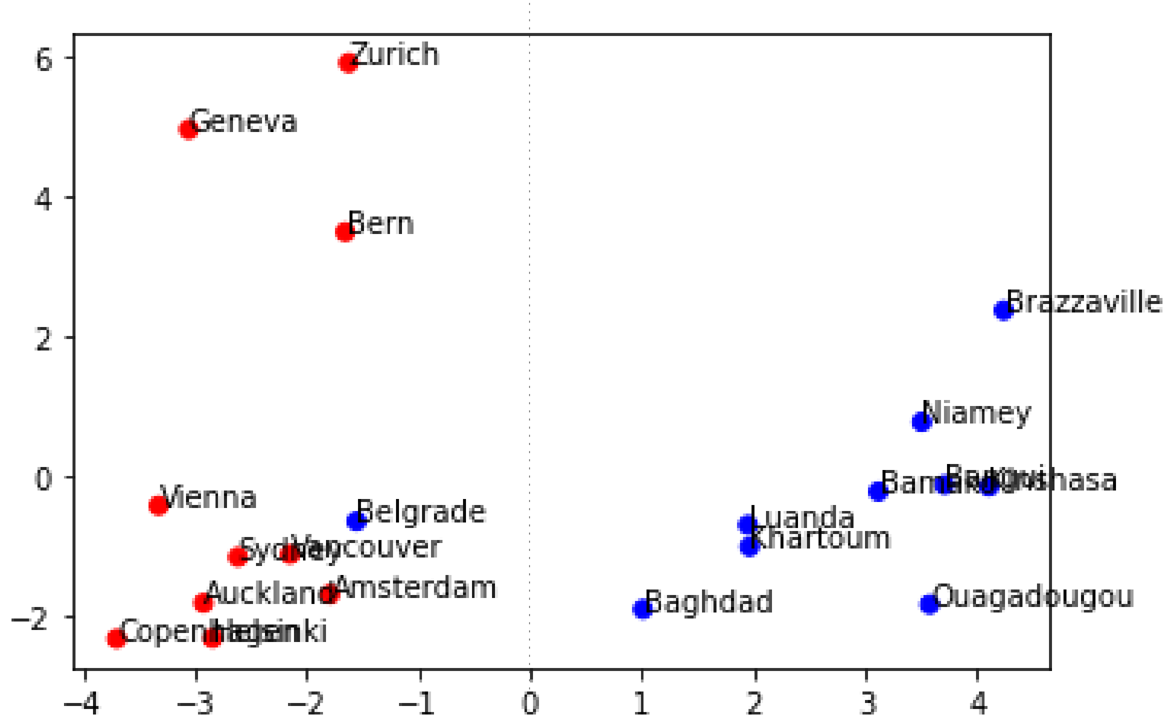
Ristoski and Paulheim (2016): RDF2vec: RDF graph embeddings for data mining

The End of Petar’s PhD Journey…

- ...and the beginning of the RDF2vec adventure

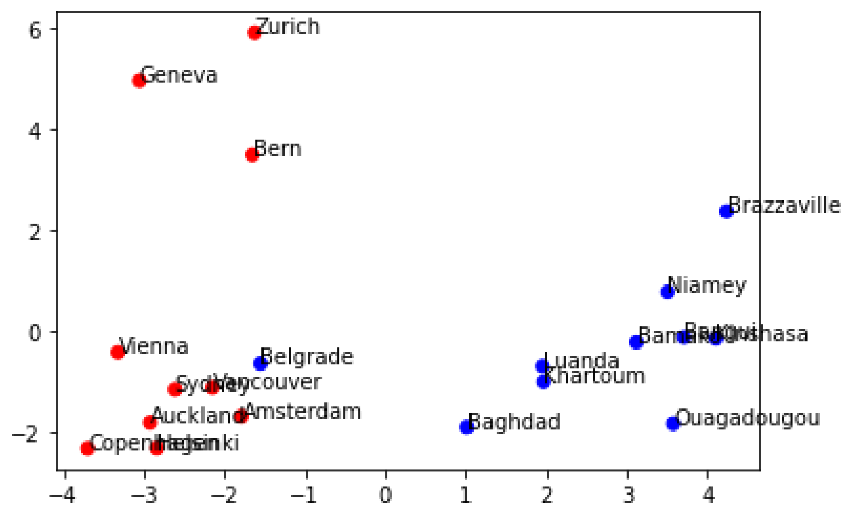
Why does RDF2vec Work?

- Example: PCA plot of an excerpt of a cities classification problem
  - From cities classification task in the embedding evaluation framework by Pellegrino et al.



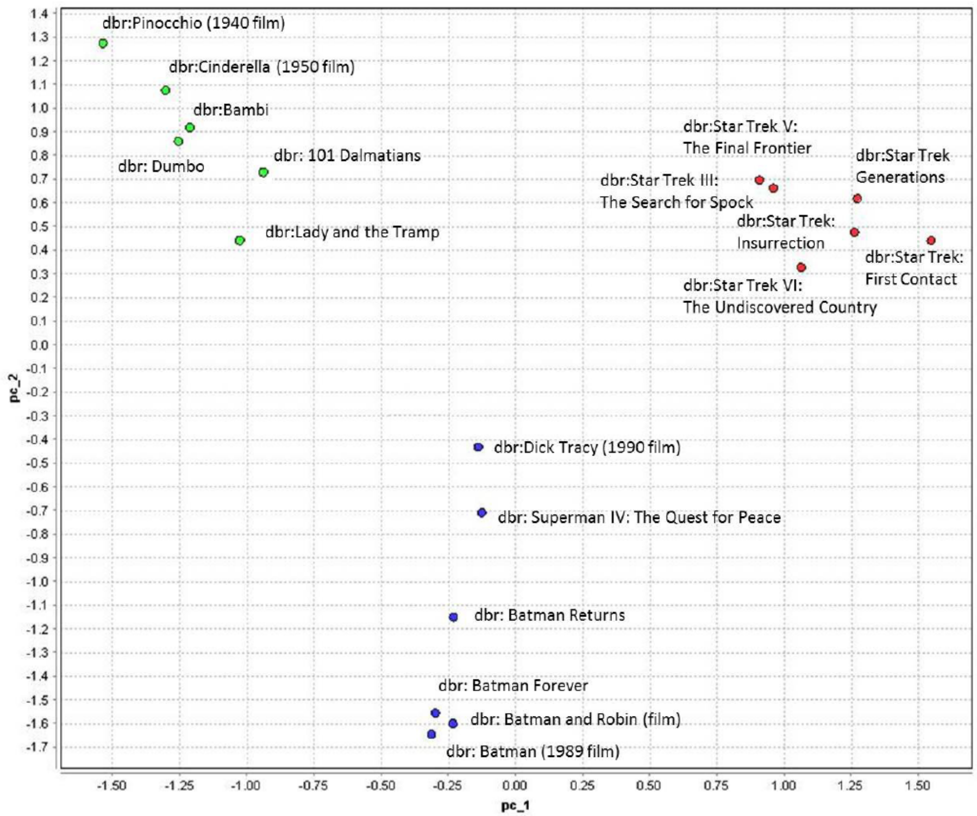
Why does RDF2vec Work?

- In downstream machine learning, we usually want *class separation*
  - to make the life of the classifier as easy as possible
- Class separation means
  - Similar entities (i.e., same class) are projected *closely* to each other
  - Dissimilar entities (i.e., different classes) are projected *far away* from each other



Why does RDF2vec Work?

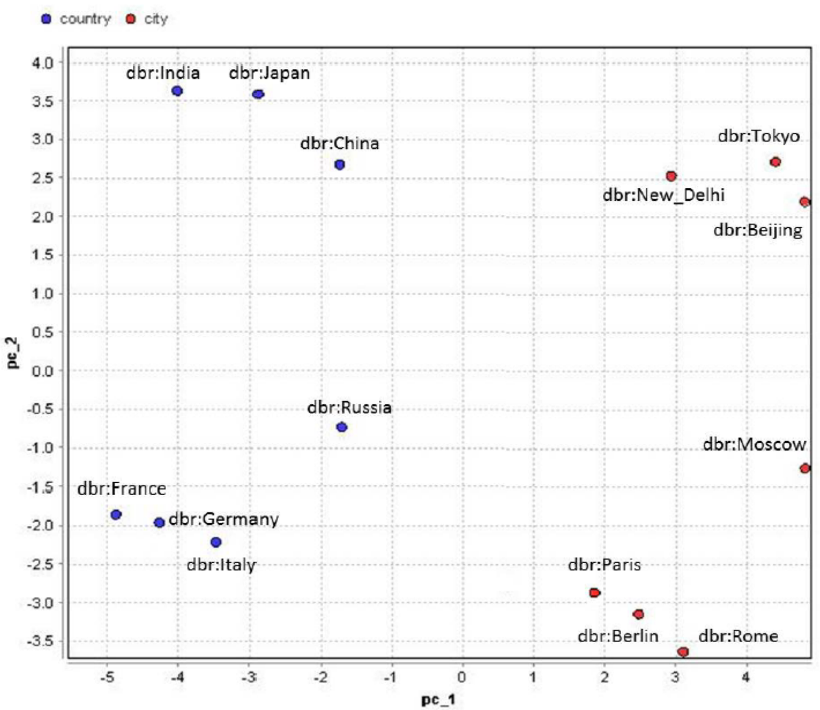
- Observation: close projection of similar entities
  - Usage example: content-based recommender system based on k-NN

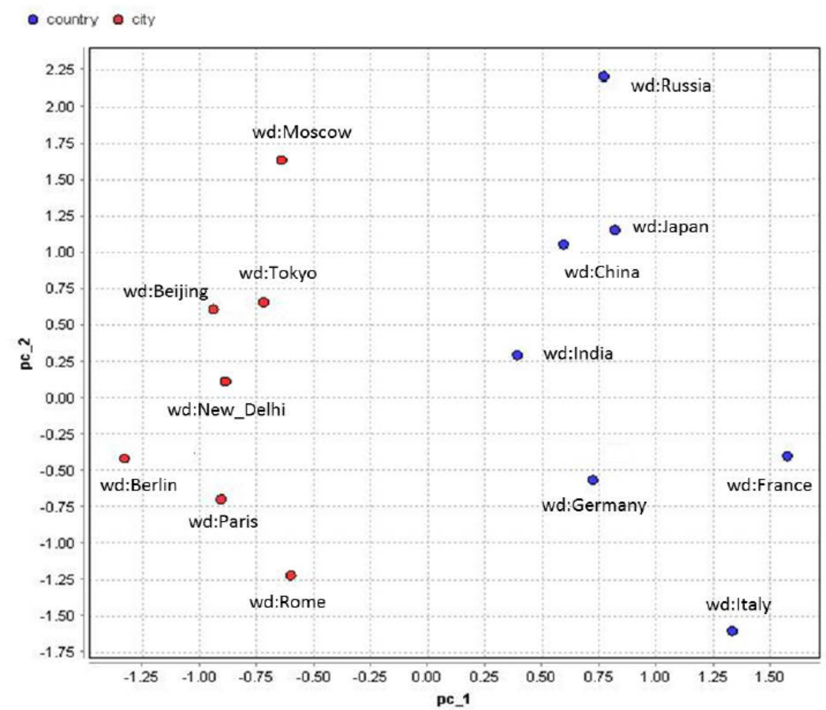


Ristoski and Paulheim (2016): RDF2vec: RDF graph embeddings for data mining

Embeddings for Link Prediction

- RDF2vec observations
  - similar instances form clusters, direction of relation is ~stable
  - link prediction by analogy reasoning (Japan – Tokyo ≈ China – Beijing)



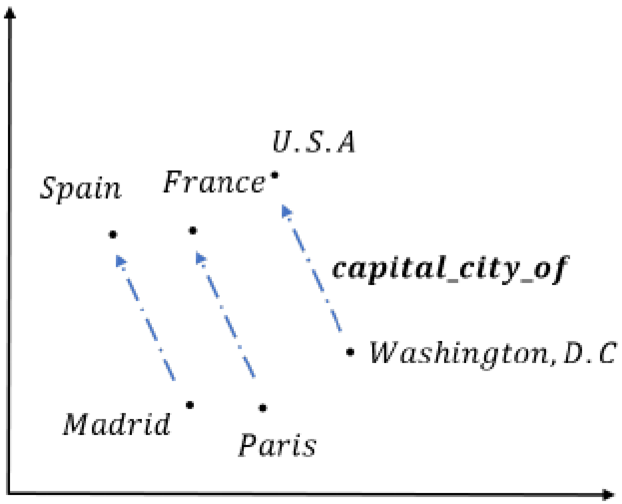


Ristoski & Paulheim: RDF2vec: RDF Graph Embeddings for Data Mining. ISWC, 2016

Embeddings for Link Prediction

- In RDF2vec, relation preservation is a by-product
- TransE (and its descendants): direct modeling
  - Formulates RDF embedding as an optimization problem
  - Find mapping of entities and relations to R^n so that
    - across all triples <s,p,o>

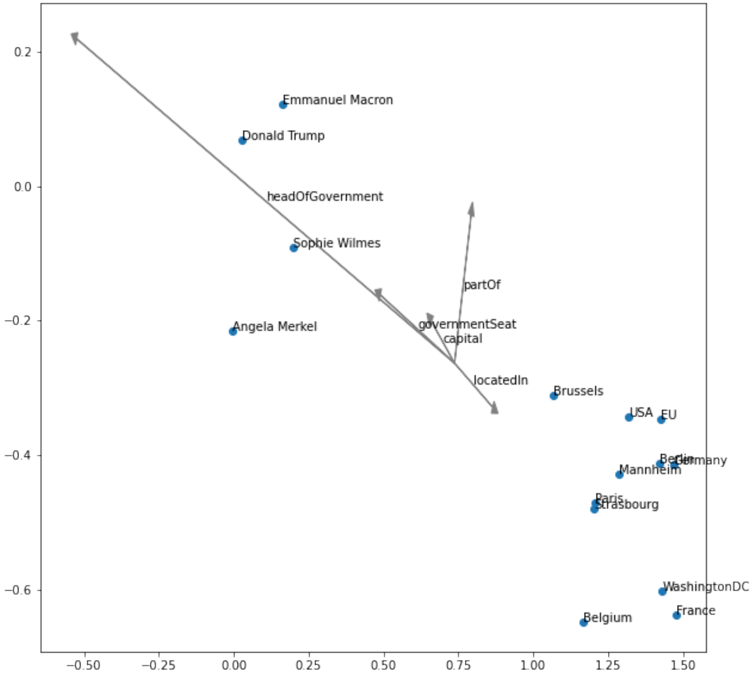
      Σ ||s+p-o|| is minimized
    - try to obtain a smaller error
      for *existing* triples
      than for *non-existing* ones

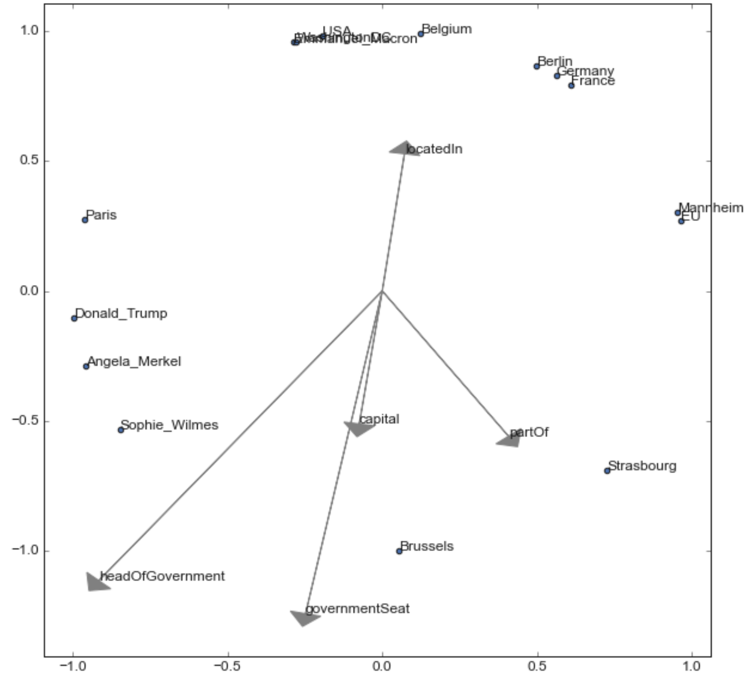


Bordes et al: Translating Embeddings for Modeling Multi-relational Data. NIPS 2013.
Fan et al.: Learning Embedding Representations for Knowledge Inference on Imperfect and Incomplete Repositories. WI 2016

Link Prediction vs. Node Embedding

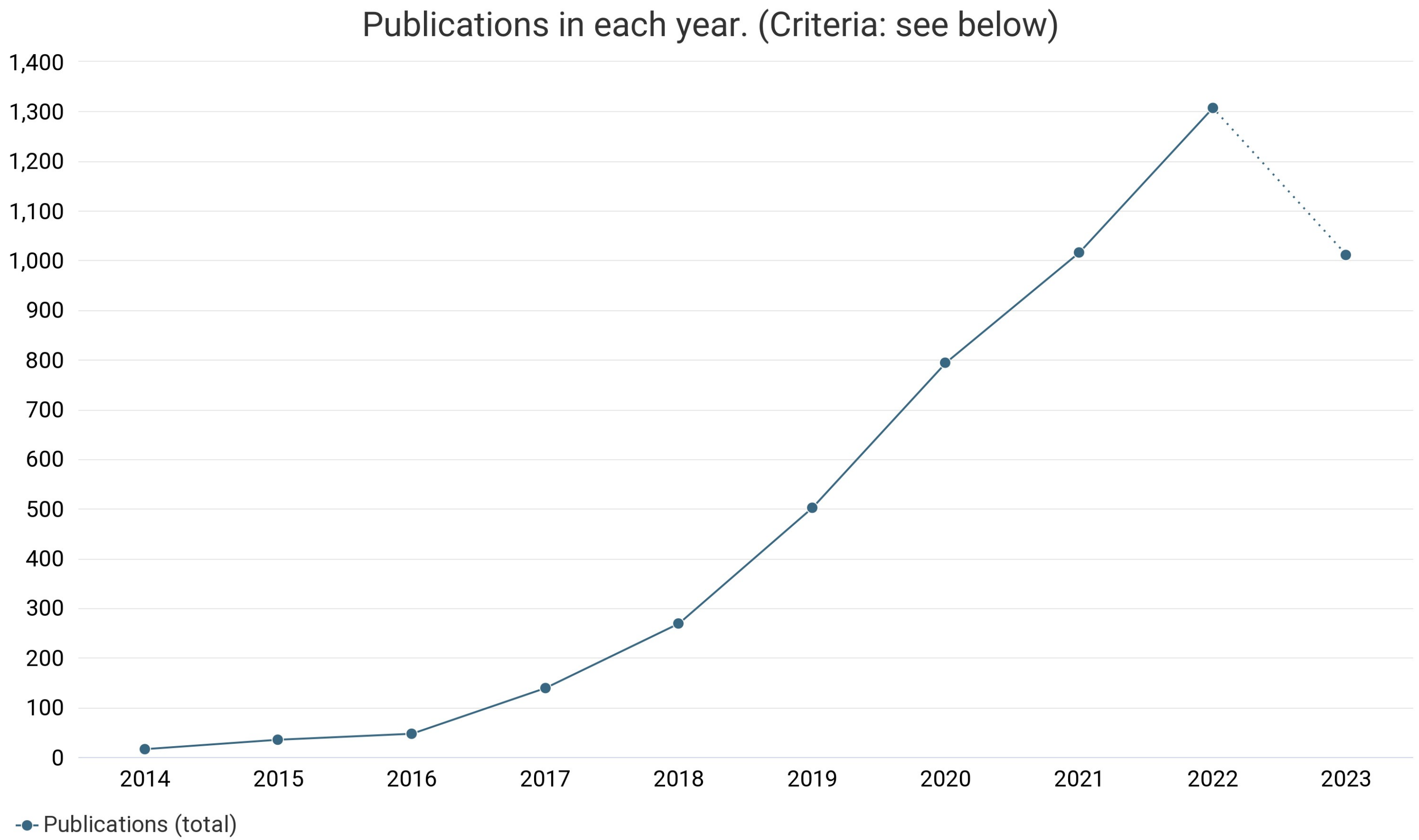
- Hypothesis:
  - Embeddings for link prediction also cluster similar entities
  - Node embeddings can also be used for link prediction





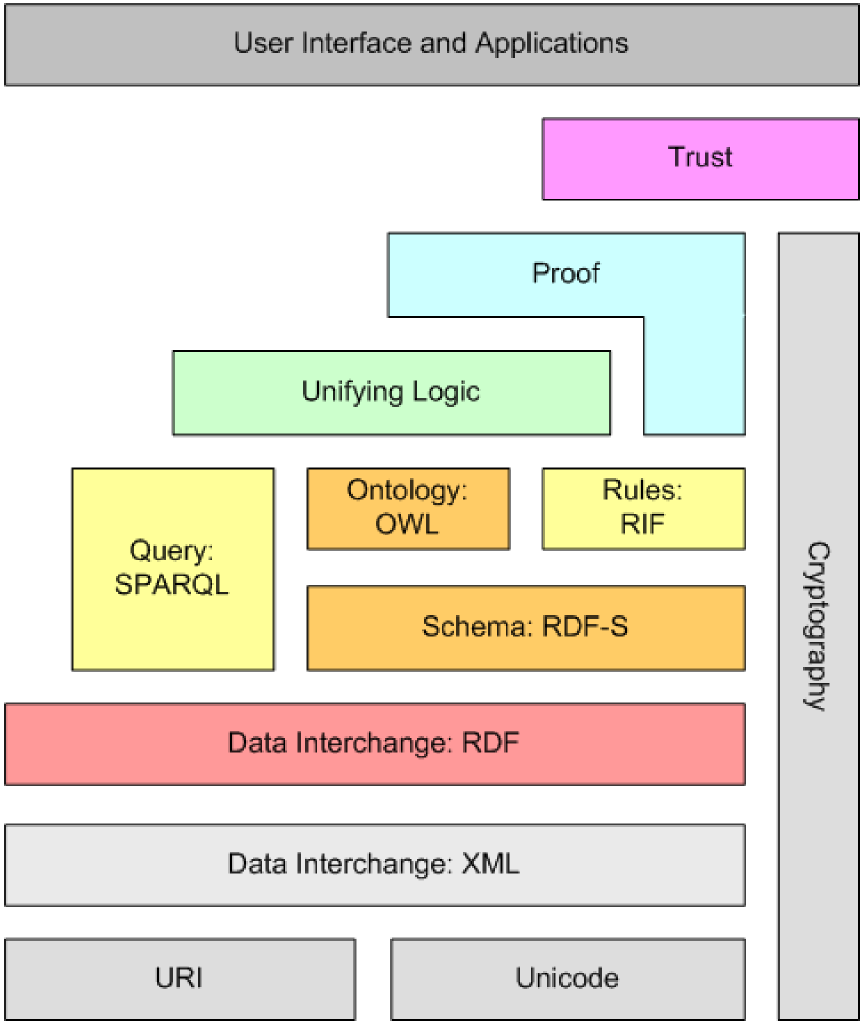
Portisch, Heist, Paulheim: Knowledge Graph Embedding for Data Mining vs. Knowledge Graph Embedding for Link Prediction - Two Sides of the Same Coin? Semantic Web Journal, 2022

Embeddings are Here to Stay

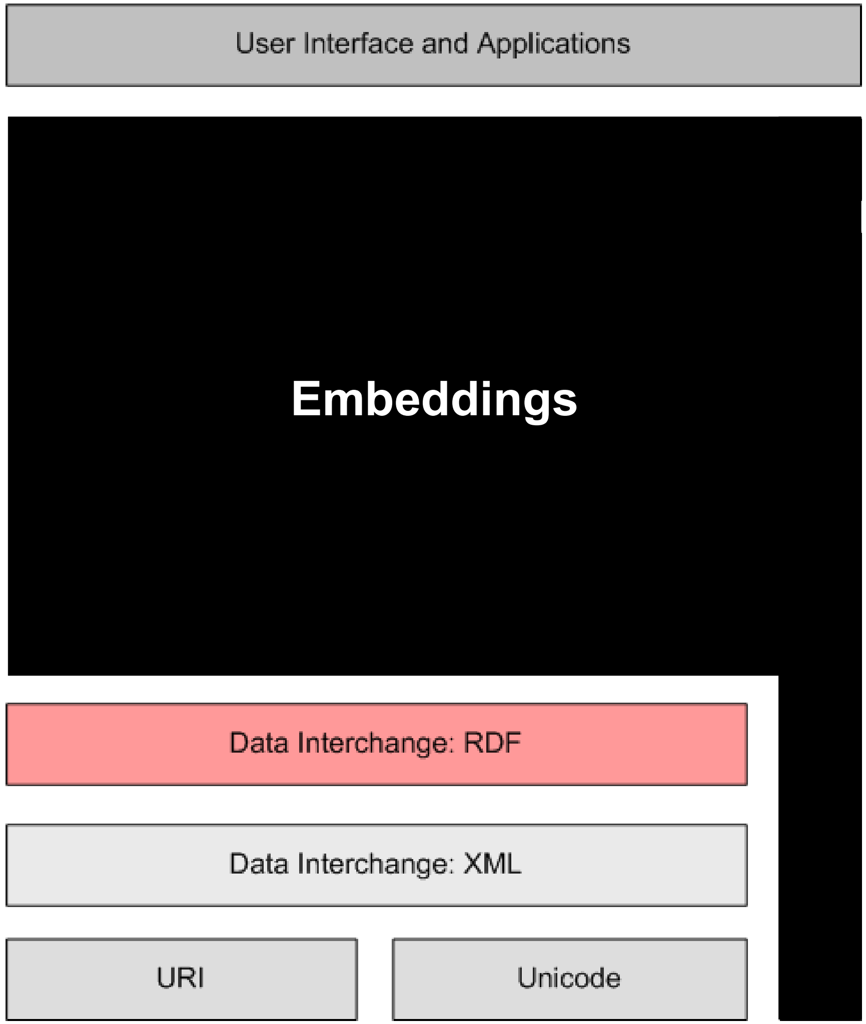


Source: https://app.dimensions.ai
Exported: September 11, 2023
Criteria: 'knowledge graph embedding' in title and abstract.

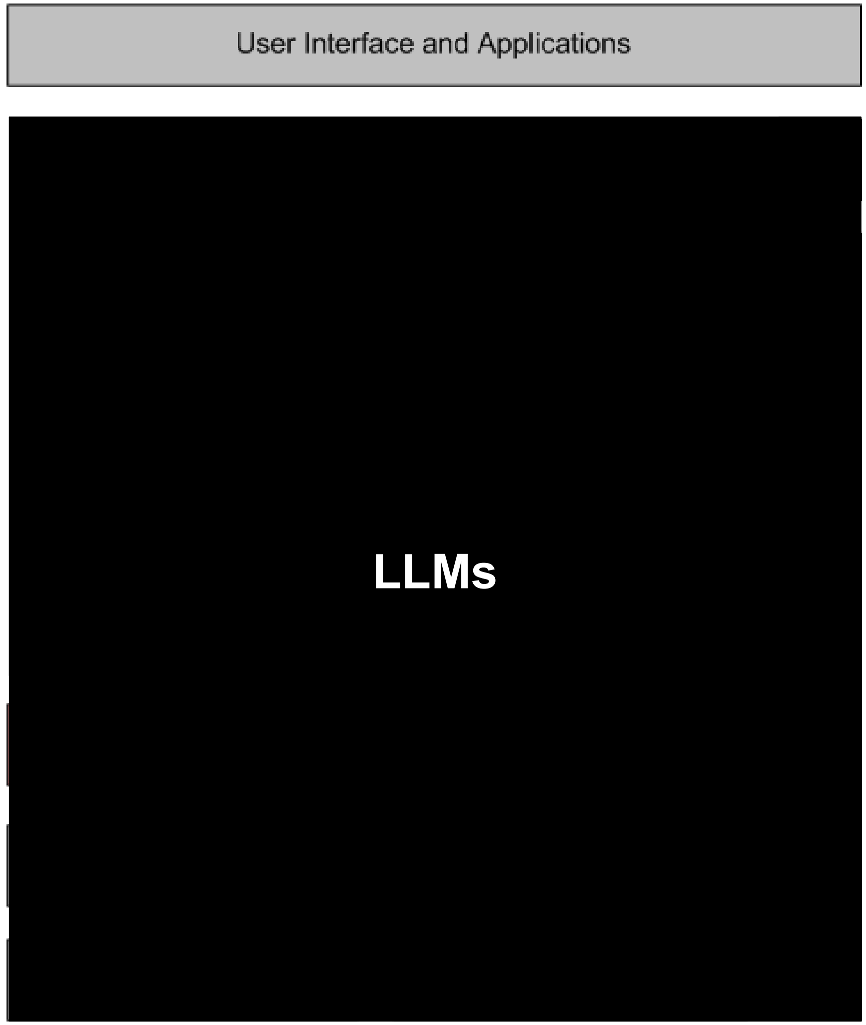
The 2009 Semantic Web Layer Cake



The 2018 Semantic Web Layer Cake

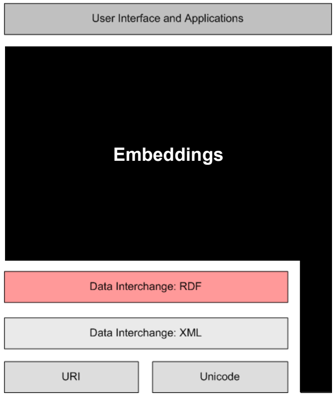


The 2023 Semantic Web Layer Cake



The People's Front of Embeddings Keeps Asking:

Do we no Longer Need Semantic Schemas?



- Schemas/ontologies are sometimes used for
  - injection in embedding creation process, e.g.
    - Graph preprocessing (inference)
    - Creation of non-trivial negatives
    - Ontological compliance as loss term
    - Pre-training on protograph
  - analysis of results
    - Measuring ontological compliance (e.g., Sem@k)
    - Quantifying representational capability
  - ...

To Materialize or Not to Materialize?

To Materialize or Not to Materialize?

To Materialize or Not to Materialize?

To Materialize or Not to Materialize?

To Materialize or Not to Materialize?

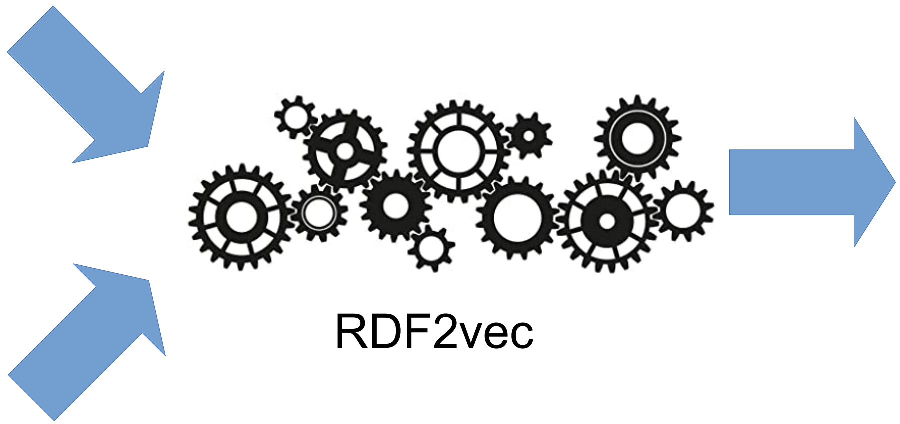
Back Home...

Experimental Setup

DBpedia

DBpedia
+ inferences

(a) DL-Learner (b) WIKIDATA



- Classification
- Regression
- Entity Similarity
- Entity Relatedness
- Document Similarity

Iana and Paulheim (2020): More is not always better: The negative impact of a-box materialization on RDF2vec knowledge graph embeddings

Experimental Results

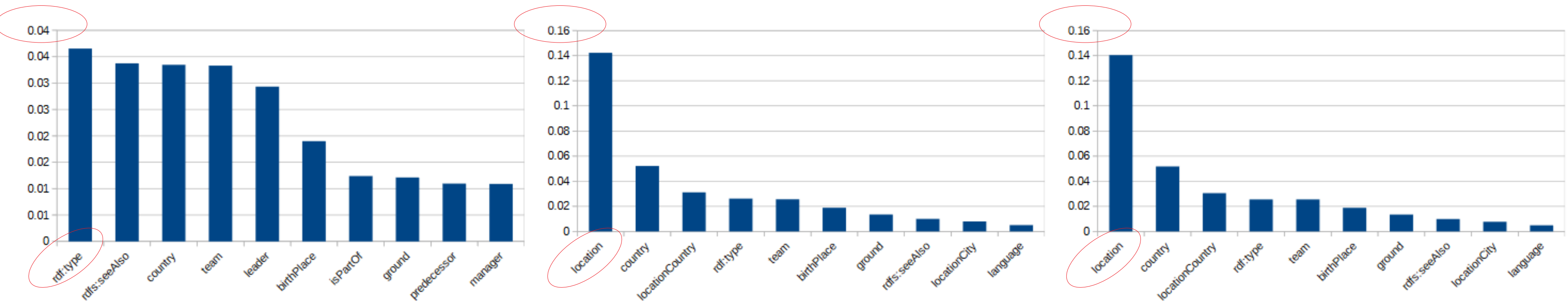
- Classification: unmaterialized is better in 60/80 cases
- Regression: unmaterialized is better in 39/60 cases
- Entity similarity: unmaterialized is better in 16/20 cases
- Entity relatedness: unmaterialized is better in 13/20 cases

- But: document similarity: materialized is always better
  - task has a very different nature
  - more heterogeneity

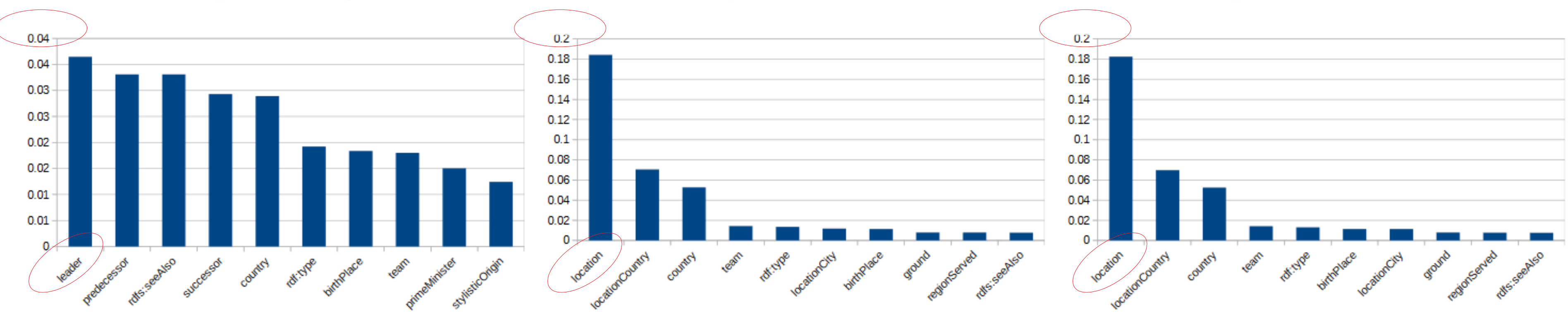
Iana and Paulheim (2020): More is not always better: The negative impact of a-box materialization on RDF2vec knowledge graph embeddings

To Materialize or not to Materialize?

- Explanation 1: materialization skews property distributions



(a) depth=4, original (b) depth=4, Wikidata (c) depth=4, DL-Learner



(d) depth=8, original (e) depth=8, Wikidata (f) depth=8, DL-Learner

Iana and Paulheim (2020): More is not always better: The negative impact of a-box materialization on RDF2vec knowledge graph embeddings

To Materialize or not to Materialize?

- Explanation 2 is a bit more complex...
- Thought experiment:
  - DBpedia mostly does not include persons' gender
  - learn classifier for gender
- Spouse is a symmetric property, but…
  - distribution is highly uneven
  - 80% of all subjects of *spouse* are women

`Ayda_Field spouse Robbie_Williams .`

Table 3: Proportion of men and women who have the specified attributes in their infoboxes. Proportions were tested with a chi-square test, with effect size estimated using Cohen's w.

	% Men	% Women	χ^2	w
birthName	4.01	11.46	4.84*	0.81
careerStation	8.95	1.13	6.84**	0.94
deathDate	32.82	19.35	5.53*	0.64
deathYear	44.68	25.45	8.28**	0.66
formerTeam	4.40	0.24	3.94*	0.97
numberOfMatches	8.60	1.06	6.61*	0.94
occupation	12.52	23.28	4.97*	0.68
position	13.62	1.68	10.46**	0.94
spouse	1.56	6.86	4.10*	0.88
team	14.06	1.97	10.39**	0.93
title	9.17	19.65	5.59*	0.73
years	8.95	1.12	6.84**	0.94

Graells-Garrido et al: (2012): First Women, Second Sex: Gender Bias in Wikipedia

To Materialize or not to Materialize?

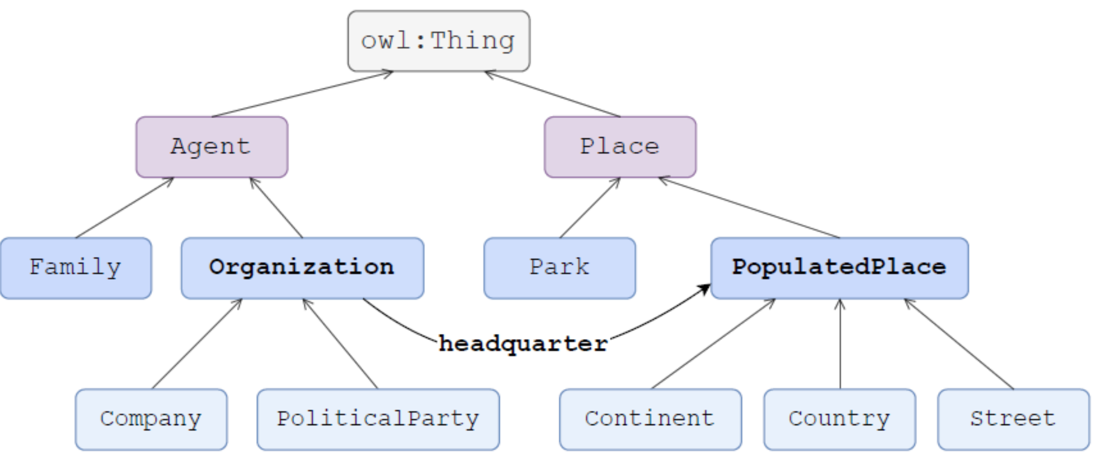
- Thought experiment: learn classifier for gender
- Spouse is a symmetric property, but…
  - 80% of all subjects of *spouse* are women
- Assume that an embedding captures that information

  → a downstream classifier can reach >80% accuracy
- On the other hand
  - Materialization completely erases that information
- Bottom line: missing information can be a signal
  - Machine learning terminology: MAR vs. MNAR

Iana and Paulheim (2021): More is not Always Better: The Negative Impact of A-box Materialization on RDF2vec Knowledge Graph Embeddings

Protographs

- Schema of a graph
  - Can be seen as a “prototype” for the actual instances
  - Allows for instantiation of a smaller KG prototype
    - Very fast training



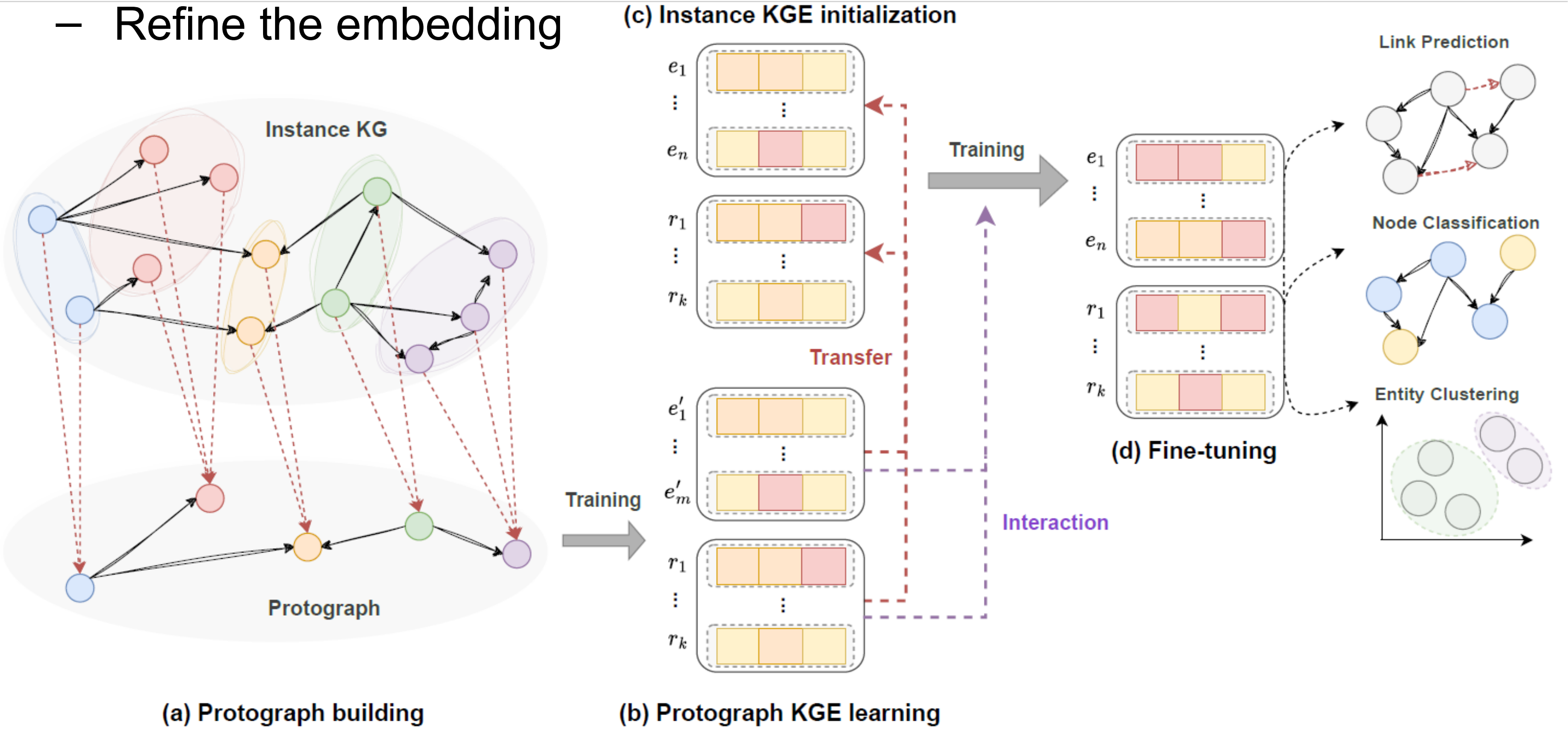
h	r	t
Organization	headquarter	PopulatedPlace
Organization	headquarter	Continent
Organization	headquarter	Country
Organization	headquarter	Street
Company	headquarter	PopulatedPlace
SportsClub	headquarter	PopulatedPlace
PoliticalParty	headquarter	PopulatedPlace

Prototriples

Nicolas Hubert, Heiko Paulheim, Pierre Monnin, Armelle Brun and Davy Monticolo: Schema First! Learn Versatile Knowledge Graph Embeddings by Capturing Semantics with MASCHInE. Under Review.

Protographs

- After initialization:
  - Transfer prototype embeddings to actual instances
  - Refine the embedding



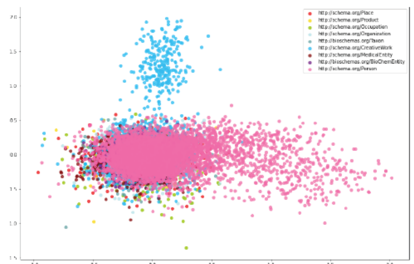
Nicolas Hubert, Heiko Paulheim, Pierre Monnin, Armelle Brun and Davy Monticolo: Schema First! Learn Versatile Knowledge Graph Embeddings by Capturing Semantics with MASCHInE. Under Review.

Protographs

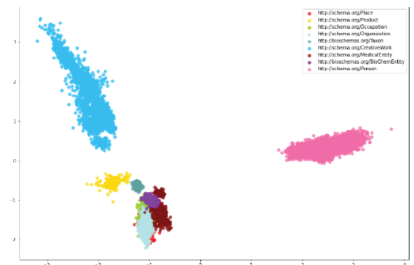
- Results
  - Class separation gets better
  - Gains on node clustering & classification, slight degradation on LP

(a) TransE (V)

(b) TransE (P2)



(c) DistMult (V)

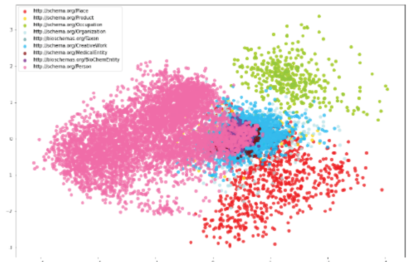


(d) DistMult (P2)

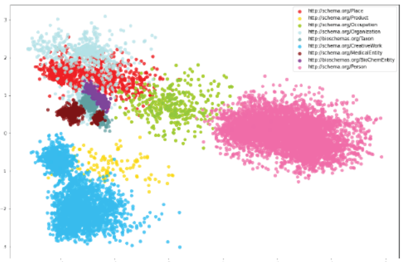
Nicolas Hubert, Heiko Paulheim, Pierre Monnin, Armelle Brun and Davy Monticolo: Schema First! Learn Versatile Knowledge Graph Embeddings by Capturing Semantics with MASCHInE. Under Review.

Class Separation, Clustering, etc.

- What do Knowledge Graph Embeddings actually learn?

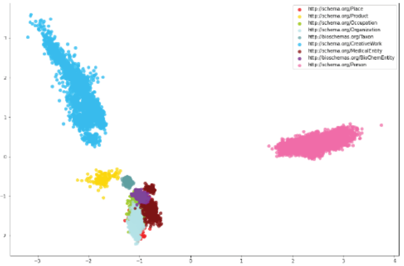


(a) TransE (V)



(b) TransE (P2)

(c) DistMult (V)



(d) DistMult (P2)

Nicolas Hubert, Heiko Paulheim, Pierre Monnin, Armelle Brun and Davy Monticolo: Schema First! Learn Versatile Knowledge Graph Embeddings by Capturing Semantics with MASCHInE. Under Review.

Close Projection of Similar Entities

- What does *similar* mean?

Similarity vs. Relatedness

- Closest 10 entities to *Angela Merkel* in different vector spaces

RDF2vec	TransE-L1	TransE-L2	TransR
Joachim Gauck	Gerhard Schröder	Gerhard Schröder	Sigmar Gabriel
Norbert Lammert	James Buchanan	Helmut Kohl	Frank-Walter Steinmeier
Stanislaw Tillich	Neil Kinnock	Konrad Adenauer	Philipp Rösler
Andreas Voßkuhle	Nicolas Sarkozy	Helmut Schmidt	Gerhard Schröder
Berlin	Joachim Gauck	Werner Faymann	Joachim Gauck
German language	Jacques Chirac	Alfred Gusenbauer	Christian Wulff
Germany	Jürgen Trittin	Kurt Georg Kiesinger	Guido Westerwelle
federalState	Sigmar Gabriel	Philipp Scheidemann	Helmut Kohl
Social Democratic Party	Guido Westerwelle	Ludwig Erhard	Jürgen Trittin
deputy	Christian Wulff	Wilhelm Marx	Jens Böhrnsen

RotatE	DistMult	RESCAL	ComplEx
Pontine raphe nucleus	Gerhard Schröder	Gerhard Schröder	Gerhard Schröder
Jonathan W. Bailey	Milan Truban	Kurt Georg Kiesinger	Diána Mészáros
Zokwang Trading	Maud Cuney Hare	Helmut Kohl	Francis M. Bator
Steven Hill	Tristan Matthiae	Annemarie Huber-Hotz	William B. Bridges
Chad Kreuter	Gerda Hasselfeldt	Wang Zhaoguo	Mette Vestergaard
Fred Hibbard	Faustino Sainz Muñoz	Franz Vranitzky	Ivan Rosenqvist
Mallory Ervin	Joachim Gauck	Bogdan Klich	Edward Clouston
Paulinho Kobayashi	Carsten Linnemann	İrsen Küçük	Antonio Capuzzi
Fullmetal Alchemist and the Broken Angel	Norbert Blüm	Helmut Schmidt	Steven J. McAuliffe
Archbishop Dorotheus of Athens	Neil Hood	Mao Zedong	Jenkin Coles

Portisch et al. (2022): Knowledge Graph Embedding for Data Mining vs. Knowledge Graph Embedding for Link Prediction - Two Sides of the Same Coin?

Back to Class Separation

- What is a class?
  - e.g., cities per se
  - e.g., cities in Norway
  - e.g., cities in Norway above 500k inhabitants
- Or something different, such as
  - e.g., everything located in Oslo
  - e.g., everything Oslo is known for

Back to Class Separation

- Observation: there are different kinds of classes:
  - Classes of objects of the same category (e.g., cities)

    → those are *similar*
  - Classes of objects of different categories (e.g., buildings, dishes, organizations, persons)

    → those are *related*

Intermediate Observation

- In most vector spaces of link prediction embeddings (TransE etc.): proximity ~ similarity
- In RDF2vec embedding space:
  proximity ~ a mix of similarity and relatedness

RDF2vec	TransE-L1	TransE-L2	TransR
Joachim Gauck	Gerhard Schröder	Gerhard Schröder	Sigmar Gabriel
Norbert Lammert	James Buchanan	Helmut Kohl	Frank-Walter Steinmeier
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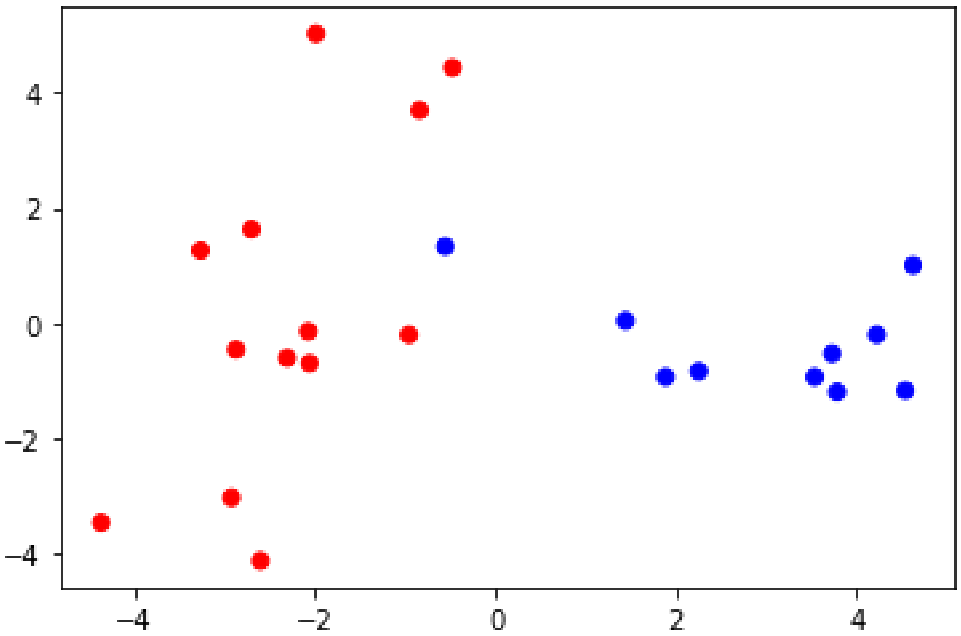
Archbishop Dorotheus of Athens	Neil Hood	Mao Zedong	Jenkin Coles

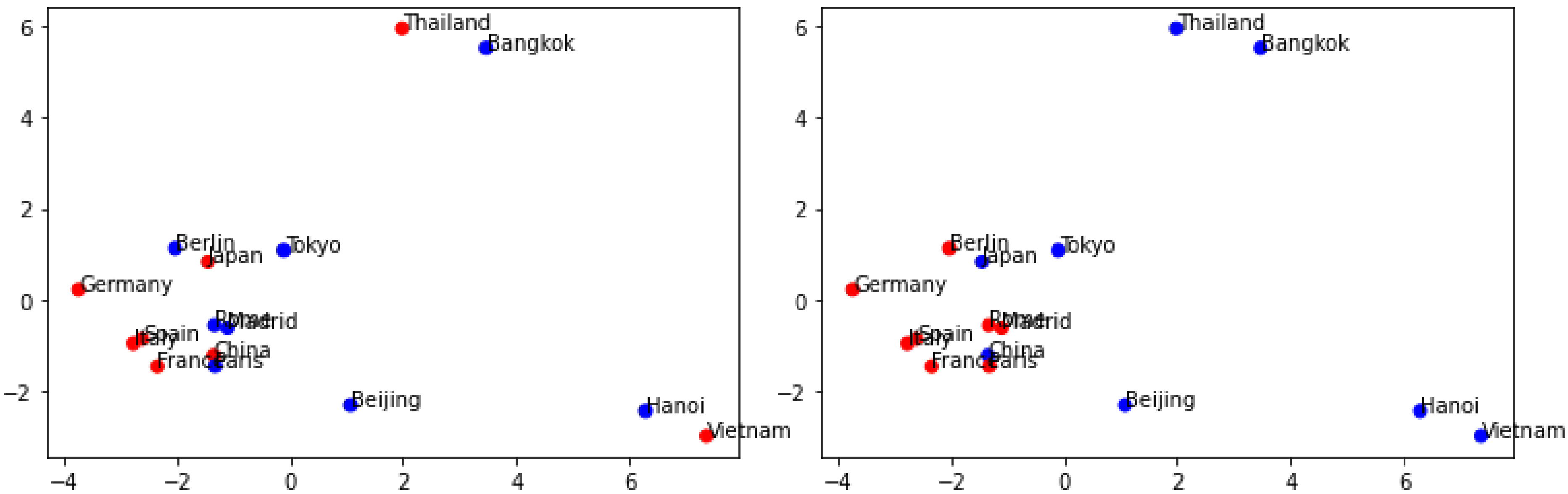
So… why does RDF2vec Work Then?

- Recap: downstream ML algorithms need class separation
  - but RDF2vec groups items by similarity *and relatedness*
- Why is RDF2vec still so good at classification?



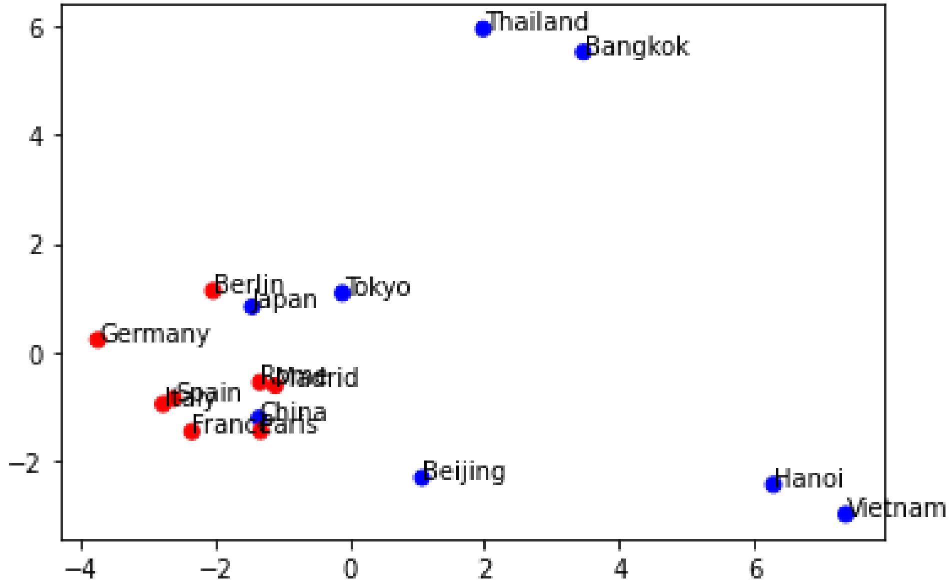
Example

- It depends on the classification problem at hand!
  - Cities vs. countries
  - Places in Europe vs. places in Asia



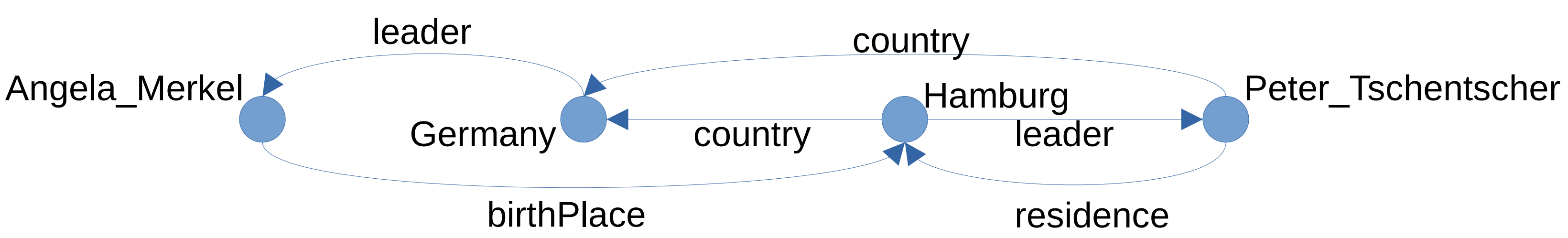
So… why does RDF2vec Work Then?

- Many downstream classification tasks are *homogeneous*
  - e.g., classifying cities in different subclasses
- For homogeneous entities:
  - relatedness provides finer-grained distinctions



Variants of RDF2vec

- Observation: order matters!
- Recap word embeddings:
  - Jobs, Wozniak, and Wayne founded **Apple** Computer Company in April 1976
  - **Google** was officially founded as a company in January 2006
- Graph walks:
  - Hamburg → country → **Germany** → leader → Angela_Merkel
  - Germany → leader → **Angela_Merkel** → birthPlace → Hamburg
  - Hamburg → leader → **Peter_Tschentscher** → residence → Hamburg



Portisch and Paulheim: Putting RDF2vec in Order. ISWC, 2021

Variants of RDF2vec

- Which parts of a walk denote what?
  - *Hamburg → country → **Germany** → leader → Angela_Merkel*
  - *Germany → leader → **Angela_Merkel** → birthPlace → Hamburg*
  - *Hamburg → leader → **Peter_Tschentscher** → residence → Hamburg*
  - *California → leader → **Gavin_Newsom** → birthPlace → San_Francisco*

- Common predicates (leader, birthPlace)
  - Similar entities
- Common entities (Hamburg)
  - Related entities
  - For same-class entities: *similar* entities!
- Approach: entity walks (e-walks) and property walks (p-walks)

Portisch and Paulheim (ESWC 2022): Walk this Way! Entity Walks and Property Walks for RDF2vec.

The RDF2vec Zoo

- We now have an entire zoo of RDF2vec variants
  - SG vs. CBOW
  - Order-aware vs. unordered (“classic”)
  - Walk variants

Which Classes can be Learned with RDF2vec?

- We already saw that there are different notions of *classes*
- Idea: compile a list of class definitions as a benchmark
  - Classes are expressed as DL formulae, e.g.
  - $\exists r.\top$, e.g. Class *person with children*
  - $\exists r.\{e\}$, e.g.: Class *person born in New York City*
  - $\exists R.\{e\}$, e.g., Class *person with any relation to New York City*
  - $\exists r.C$, e.g., Class *person playing in a basketball team*
  - *…*

Which Classes can be Learned with RDF2vec?

- Formulating hypotheses
  - e.g., $\exists r.T$, cannot be learned when using e-walks
- Testing hypotheses
  - using queries against DBpedia
- ...

The DLCC DBpedia Gold Standard

- Six classes (person, book, city, movie, album, species)
- Twelve test cases
  - Sometimes also with “harder” negatives
- Three sizes per test case (50, 500, 5,000 examples)
  - Each is a balanced binary classification problem

- >200 hand written SPARQL queries
- Dataset and code available online

Hypotheses (Overview)

- Different patterns require different signals, e.g.,
  - Specific relations (visible to classic and p-walks)
  - Specific entities (visible to classic and e-walks)
  - Distinguishing subject and object (only possible for oa variants)
  - ...and mixes of those

	Test Case	DL Expression	$RDF2vec$	$RDF2vec_{oa}$	$p-RDF2vec$	$p-RDF2vec_{oa}$	$e-RDF2vec$	$e-RDF2vec_{oa}$
H1a	tc01	$r.\top$		✓		✓		
H1a'	tc02	$r^{-1}.\top$		✓		✓		
H1b	tc03	$\exists r.\top \sqcup \exists r^{-1}.\top$	✓	✓	✓	✓		
H2a	tc04	$\exists R.\{e\} \sqcup \exists R^{-1}.\{e\}$	✓	✓			✓	✓
H2b	tc05	$\exists R_1.(\exists R_2.\{e\}) \sqcup \exists R_1^{-1}.(\exists R_2^{-1}\{e\})$	✓	✓			✓	✓
H3	tc06	$r.\{e\}$		✓				
H4a	tc07	$\exists r.T$		✓		(✓)		
H4b	tc08	$\exists r^{-1}.T$						
H5	tc09	$\geq 2r.\top$		(✓)		(✓)		
H5'	tc10	$\geq 2r^{-1}.\top$		(✓)		(✓)		
H6a	tc11	$\geq 2r.T$		(✓)				
H6b	tc12	$\geq 2r^{-1}.T$						

Which Classes can be Learned with RDF2vec?

- Formulating hypotheses
  - e.g., $\exists r.T$, cannot be learned when using e-walks
- Testing hypotheses
  - using queries against DBpedia
- Seeing surprises
  - e.g., models trained on e-walks can reach ~90% accuracy in that case

Experiments on DBpedia Gold Standard

- Most hypotheses could **not** be confirmed
- All problems are learnable with an accuracy >75%
  - i.e., significantly better than guessing
- Also LP embeddings such as TransE work surprisingly well

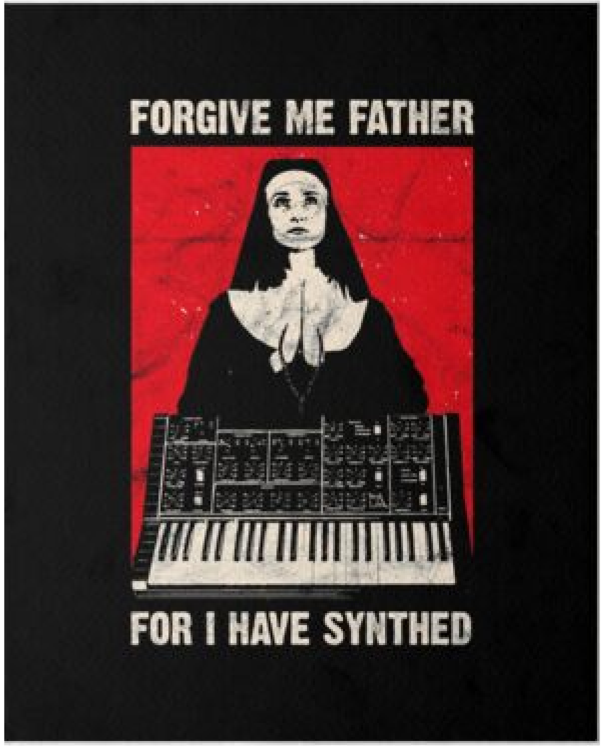
TC	SG	SG_{oa}	CBOW	$CBOW_{oa}$	s-SG	s-SG_{oa}	s-CBOW	s-$CBOW_{oa}$	e-SG	e-SG_{oa}	e-$CBOW_{oa}$	e-$CBOW_{oa}$	TransE-L1	TransE-L2	TransR	DistMult	ComplEx	RESCAL	RotatE
tc01	0.915	0.937	0.778	0.870	0.907	0.933	0.780	0.924	0.845	0.860	0.840	0.840	0.842	0.947	0.858	0.874	0.862	**0.966**	0.768
tc01 hard	0.681	0.891	0.637	0.891	0.627	0.903	0.576	0.894	0.644	0.651	0.659	0.659	0.799	**0.916**	0.744	0.646	0.651	0.830	0.618
tc02	0.953	0.961	0.865	0.956	0.930	0.972	0.901	**0.974**	0.883	0.895	0.906	0.906	0.852	0.970	0.832	0.859	0.853	0.908	0.737
tc02 hard	0.637	0.780	0.618	0.774	0.628	0.828	0.583	0.838	0.623	0.628	0.607	0.607	0.780	**0.849**	0.693	0.622	0.608	0.729	0.649
tc03	0.949	**0.958**	0.846	0.905	0.913	0.956	0.800	0.938	0.883	0.900	0.886	0.886	0.821	0.933	0.856	0.894	0.874	0.943	0.780
tc04	0.960	0.968	0.705	0.872	0.877	0.908	0.659	0.873	0.965	0.969	0.915	0.915	0.934	0.966	0.973	0.984	**0.990**	0.990	0.862
tc04 hard	0.963	0.984	0.674	**0.992**	0.725	0.828	0.583	0.782	0.938	0.990	0.983	0.983	0.814	0.912	0.855	0.917	0.935	0.918	0.789
tc05	0.986	0.992	0.772	0.906	0.869	0.899	0.719	0.870	0.990	**0.995**	0.931	0.931	0.867	0.948	0.881	0.907	0.905	0.908	0.802
tc06	0.957	0.963	0.698	0.850	0.876	0.903	0.641	0.857	0.960	0.969	0.928	0.928	0.929	0.965	0.976	0.985	**0.998**	0.990	0.846
tc06 hard	0.863	0.936	0.604	0.908	0.708	0.770	0.559	0.745	0.699	0.708	0.650	0.650	0.823	0.779	**0.964**	0.882	0.933	0.964	0.819
tc07	0.938	0.955	0.742	0.785	0.895	0.924	0.726	0.863	0.946	0.946	0.859	0.859	0.930	**0.987**	0.978	0.929	0.966	0.945	0.847
tc08	0.961	0.966	0.891	0.896	0.911	**0.968**	0.841	0.951	0.904	0.914	0.925	0.925	0.898	0.964	0.870	0.856	0.888	0.875	0.831
tc09	0.902	0.901	0.773	0.858	0.819	0.858	0.726	0.832	0.874	0.884	0.840	0.840	0.884	**0.928**	0.879	0.877	0.883	0.929	0.780
tc09 hard	0.785	0.793	0.659	0.751	0.698	0.741	0.600	0.712	0.777	0.782	0.744	0.744	0.749	**0.848**	0.758	0.774	0.776	0.820	0.676
tc10	0.947	0.958	0.918	0.905	0.924	0.975	0.852	0.969	0.911	0.912	0.925	0.925	0.957	**0.984**	0.898	0.918	0.931	0.927	0.878
tc10 hard	0.740	0.737	0.716	0.711	0.610	0.679	0.569	0.652	0.715	0.718	0.729	0.729	**0.775**	0.774	0.656	0.743	0.739	0.713	0.665
tc11	0.932	0.897	0.865	0.780	0.884	**0.991**	0.808	0.954	0.928	0.972	0.921	0.921	0.917	0.960	0.930	0.889	0.946	0.954	0.838
tc11 hard	0.725	0.737	0.687	0.676	0.684	0.707	0.631	0.707	0.763	0.734	0.641	0.641	0.712	**0.806**	0.753	0.666	0.723	0.726	0.638
tc12	0.955	0.938	0.888	0.909	0.900	0.971	0.830	0.965	0.893	0.905	0.904	0.904	0.961	**0.984**	0.879	0.912	0.894	0.927	0.834
tc12 hard	0.714	0.717	0.712	0.699	0.628	0.637	0.545	0.628	0.690	0.713	0.715	0.715	0.762	**0.765**	0.659	0.714	0.710	0.701	0.652

Experiments on DBpedia Gold Standard

- Challenge: isolating effects
  - Let's consider, ∃r.T: e.g. ∃almaMater.T
  - In theory, we should not be able to learn this with e-walks
  - Frequent entities in the neighborhoods of positive examples:
    - Politician (3k examples)
    - Bachelor of Arts (3k examples)
    - Harvard Law School (2k examples)
    - Lawyer (2k examples)
    - Northwestern University (2k examples)
    - Harvard University (2k examples)
    - Doctor of Philosophy (2k examples)
    - …
  - Those signals are visible to e-walks!

Which Classes can be Learned with RDF2vec?

- Maybe, DBpedia is not such a great testbed
  - Hidden patterns, e.g., for relation cooccurence
  - Many inter-pattern dependencies
  - Information not missing at random
- Possible solution:
  - Synthetic knowledge graphs!
  - First experiments show better visibility of expected effects



The DLCC Synthetic Gold Standard

- Same twelve test cases as before
- Synthesize a knowledge graph for each test case
  - Create an ontology
  - Create positive examples
  - Create negative examples (double check for accidental positives)
- Test bed
  - 12 different classification problems, 1k positives/negatives each
  - Ontology and graph structure are similar to DBpedia

Experiments on DLCC Synthetic Gold Standard

- Same twelve test cases as before
- Synthesize a knowledge graph for each test case
  - Create an ontology
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- Test bed
  - 12 different classification problems, 1k positives/negatives each
  - Ontology and graph structure are similar to DBpedia

Experiments on DLCC Synthetic Gold Standard

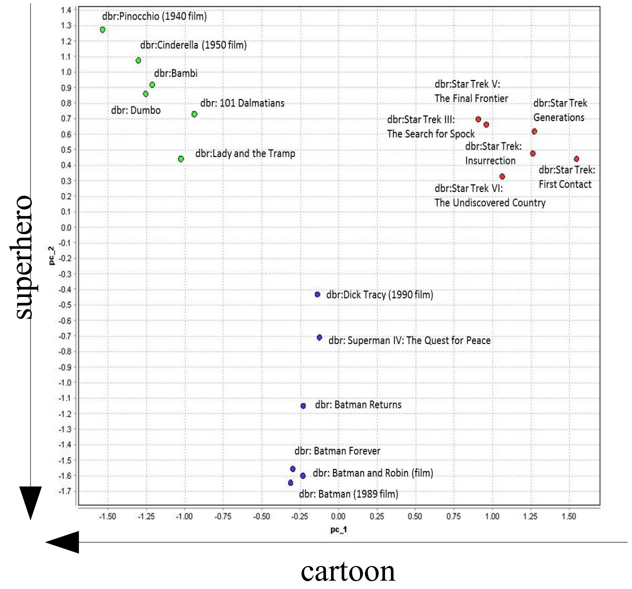
- Hypotheses can be mostly confirmed
  - Quantified restrictions (tc09-tc12) are very badly learned by all approaches (as expected)
  - tc06 is extremely well learned by LP embeddings
    - Classifying r.{e} is, in fact, classic link prediction/triple scoring
  - RDF2vec$_{oa}$ variant is not superior on synthetic data

TC	SG	SG$_{oa}$	CBOW	CBOW$_{oa}$	s-SG	s-SG$_{oa}$	s-CBOW	s-CBOW$_{oa}$	e-SG	e-SG$_{oa}$	e-CBOW	e-CBOW$_{oa}$	TransE-L1	TransE-L2	TransR	DistMult	ComplEx	RESCAL	RotatE
tc01	0.882	0.867	0.566	0.877	0.870	0.842	0.802	0.847	0.774	0.757	0.752	0.727	0.767	0.752	0.712	0.837	0.789	**0.895**	0.769
tc02	0.742	0.737	0.769	0.732	**0.822**	0.734	0.769	0.754	0.536	0.529	0.536	0.529	0.677	0.677	0.531	0.584	0.549	0.689	0.546
tc03	0.797	0.812	**0.927**	0.774	0.794	0.709	0.784	0.742	0.526	0.526	0.561	0.519	0.531	0.581	0.554	0.556	0.536	0.634	0.541
tc04	**1.000**	0.998	0.990	0.998	0.568	0.588	0.608	0.628	**1.000**	0.995	**1.000**	0.998	0.790	0.898	0.685	0.588	0.553	0.528	0.728
tc05	**0.892**	0.819	0.889	0.819	0.631	0.648	0.681	0.648	0.832	0.819	0.882	0.791	0.691	0.774	0.631	0.658	0.726	0.608	0.646
tc06	0.978	0.963	0.898	0.965	0.800	0.828	0.748	0.820	0.970	0.968	0.905	0.965	0.898	0.978	0.888	**1.000**	**1.000**	**1.000**	0.955
tc07	0.583	0.583	0.575	0.555	0.553	0.553	0.535	0.540	0.543	0.525	0.498	0.518	0.540	0.615	**0.673**	0.565	0.518	0.550	0.508
tc08	0.563	0.585	0.555	0.583	0.635	**0.628**	0.568	0.618	0.525	0.533	0.553	0.540	0.585	0.613	0.540	0.535	0.523	0.533	0.535
tc09	0.610	0.628	**0.648**	0.605	0.563	0.550	0.605	0.590	0.550	0.535	0.508	0.528	0.598	0.543	0.525	0.525	0.545	0.638	0.538
tc10	0.638	0.623	**0.665**	0.600	0.548	0.560	0.633	0.565	0.593	0.565	0.548	0.515	0.598	0.573	0.518	0.525	0.510	0.580	0.533
tc11	0.633	0.580	**0.668**	0.575	0.573	0.555	0.580	0.553	0.550	0.545	0.540	0.545	0.583	0.590	0.573	0.518	0.590	0.625	0.538
tc12	0.644	0.614	**0.657**	0.638	0.563	0.565	0.590	0.640	0.541	0.568	0.560	0.524	0.618	0.550	0.513	0.553	0.540	0.578	0.533

Portisch&Paulheim: The DLCC Node Classification Benchmark for Analyzing Knowledge Graph Embeddings. ISWC 2022.

Alternatives to Understand KG Embeddings

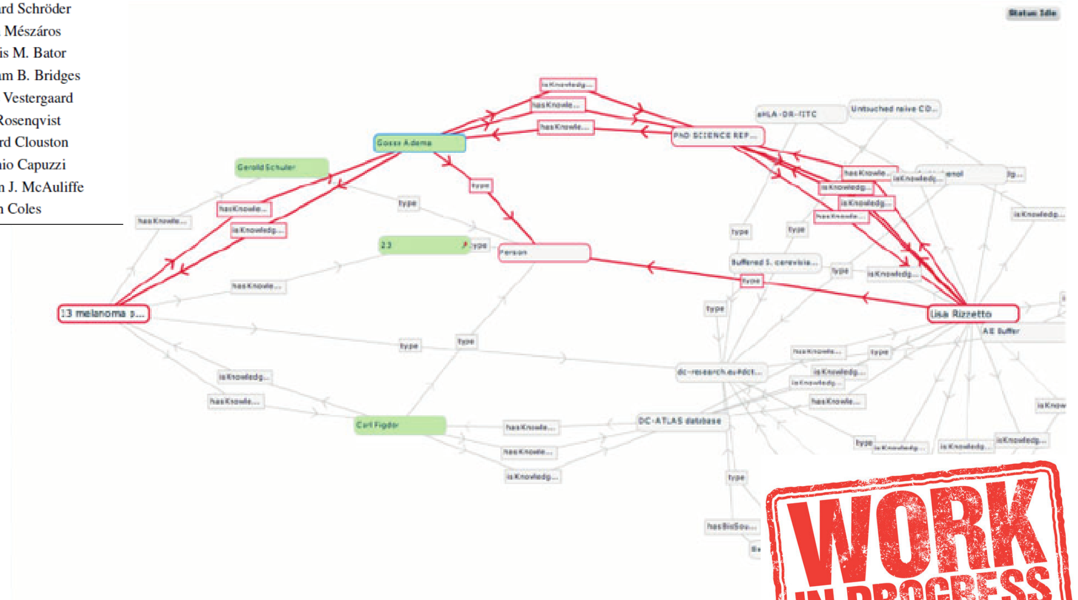
- Approach 1: learn symbolic interpretation function for dimensions
- Each dimension of the embedding model is a target for a separate *learning problem*
- Learn a function to explain the dimension
- E.g.: $y \approx -|\exists character.Superhero|$
- Just an approximation used for explanations and justifications



Alternatives to Understand KG Embeddings

- Approach 2: learn symbolic substitute function for similarity function

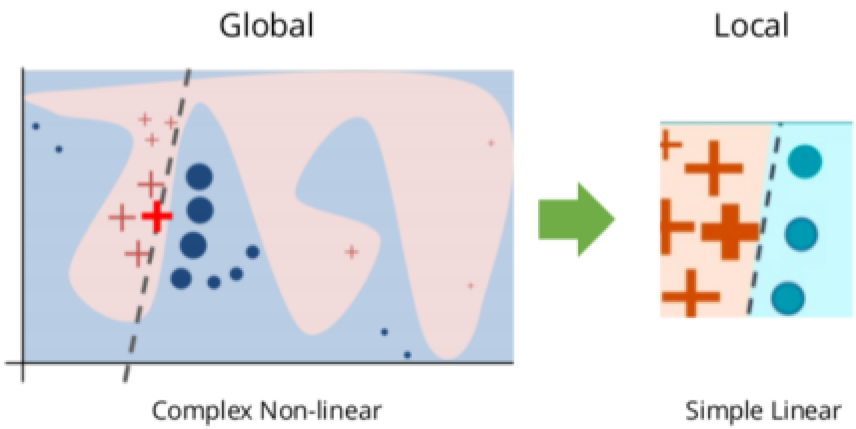
RDF2vec	TransE-L1	TransE-L2	TransR
Joachim Gauck	Gerhard Schröder	Gerhard Schröder	Sigmar Gabriel
Norbert Lammert	James Buchanan	Helmut Kohl	Frank-Walter Steinmeier
Stanislaw Tillich	Neil Kinnock	Konrad Adenauer	Philipp Rösler
Andreas Voßkuhle	Nicolas Sarkozy	Helmut Schmidt	Gerhard Schröder
Berlin	Joachim Gauck	Werner Faymann	Joachim Gauck
German language	Jacques Chirac	Alfred Gusenbauer	Christian Wulff
Germany	Jürgen Trittin	Kurt Georg Kiesinger	Guido Westerwelle
federalState	Sigmar Gabriel	Philipp Scheidemann	Helmut Kohl
Social Democratic Party	Guido Westerwelle	Ludwig Erhard	Jürgen Trittin
deputy	Christian Wulff	Wilhelm Marx	Jens Böhrnsen
RotatE	DistMult	RESCAL	ComplEx
Pontine raphe nucleus	Gerhard Schröder	Gerhard Schröder	Gerhard Schröder
Jonathan W. Bailey	Milan Truban	Kurt Georg Kiesinger	Diána Mészáros
Zokwang Trading	Maud Cuney Hare	Helmut Kohl	Francis M. Bator
Steven Hill	Tristan Matthiae	Annemarie Huber-Hotz	William B. Bridges
Chad Kreuter	Gerda Hasselfeldt	Wang Zhaoguo	Mette Vestergaard
Fred Hibbard	Faustino Sainz Muñoz	Franz Vranitzky	Ivan Rosenqvist
Mallory Ervin	Joachim Gauck	Bogdan Klich	Edward Clouston
Paulinho Kobayashi	Carsten Linnemann	İrsen Küçük	Antonio Capuzzi
Fullmetal Alchemist and the Broken Angel	Norbert Blüm	Helmut Schmidt	Steven J. McAuliffe
Archbishop Dorotheus of Athens	Neil Hood	Mao Zedong	Jenkin Coles



Right hand side picture: RelFinder (https://interactivesystems.info/developments/relfinder)

Alternatives to Understand KG Embeddings

- Approach 3: generate symbolic interpretations for individual predictions
  - Inspired by LIME:
    - Generate perturbed examples
    - Label them using embedding+downstream classifier
    - Learn symbolic model on this labeled set
  - Good news:
    - RDF2vec can, in principle, create embeddings for unseen entities
    - Those can be used to classify perturbed examples



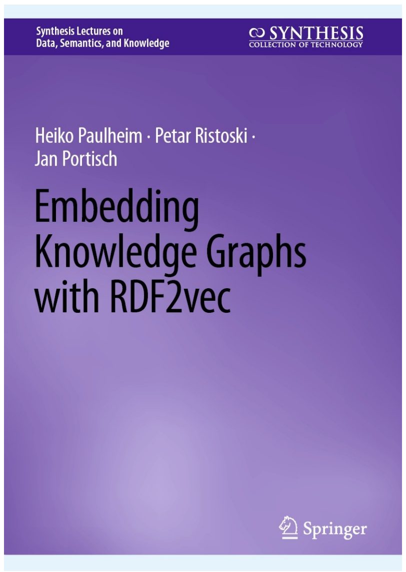
https://c3.ai/glossary/data-science/lime-local-interpretable-model-agnostic-explanations/

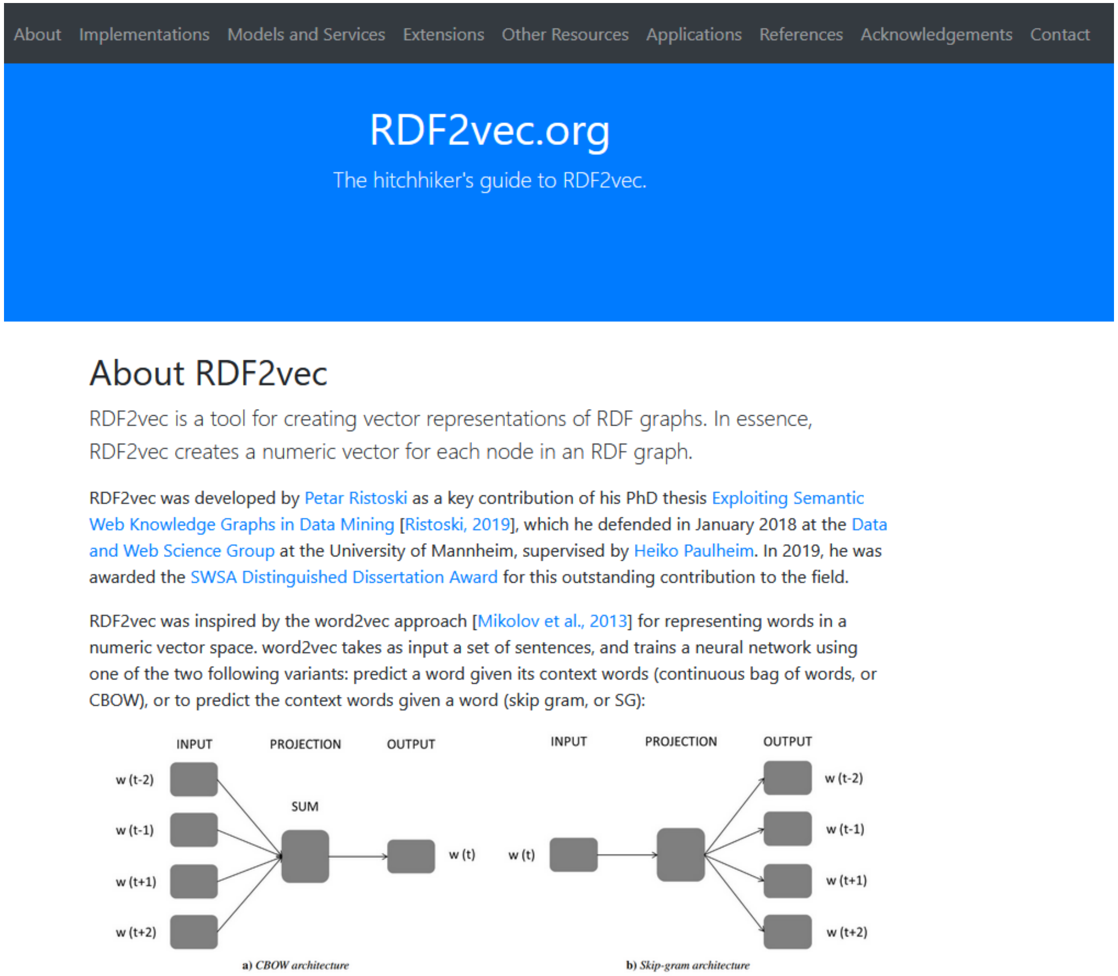
Summary

- Knowledge Graph Embeddings & Semantic Schemas
- We have seen today
  - How materialization and inference do (not) help
  - How schemas can be used for efficient initialization of KGE models
  - How to explore what embedding models can actually learn

More on RDF2vec

- Collection of
  - Implementations
  - Pre-trained models
  - >75 use cases in various domains





Credits

Thank you!

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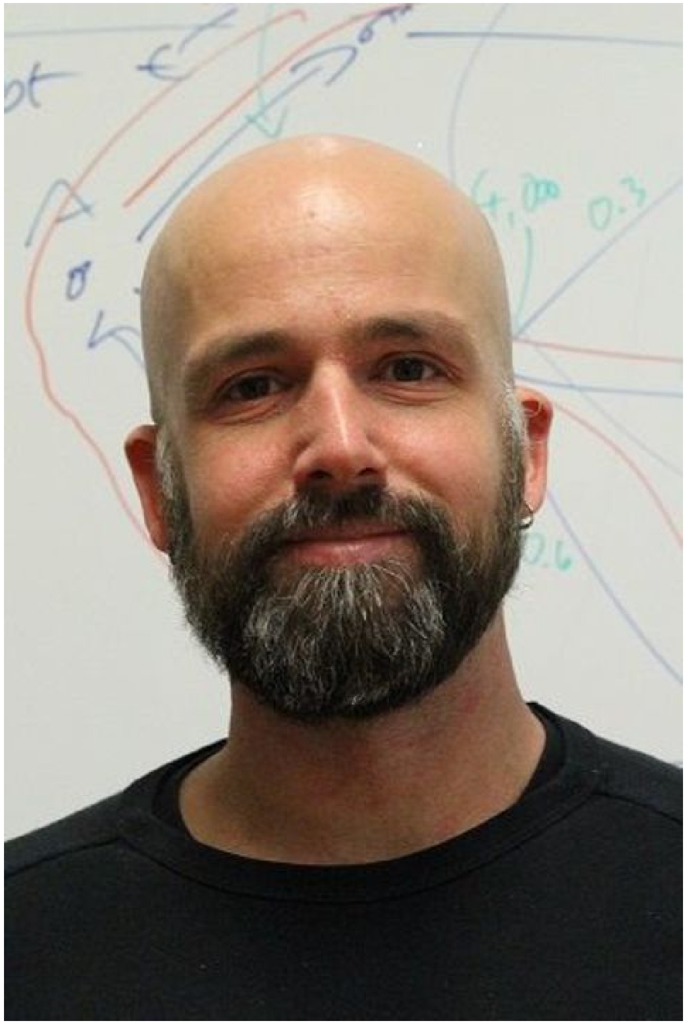

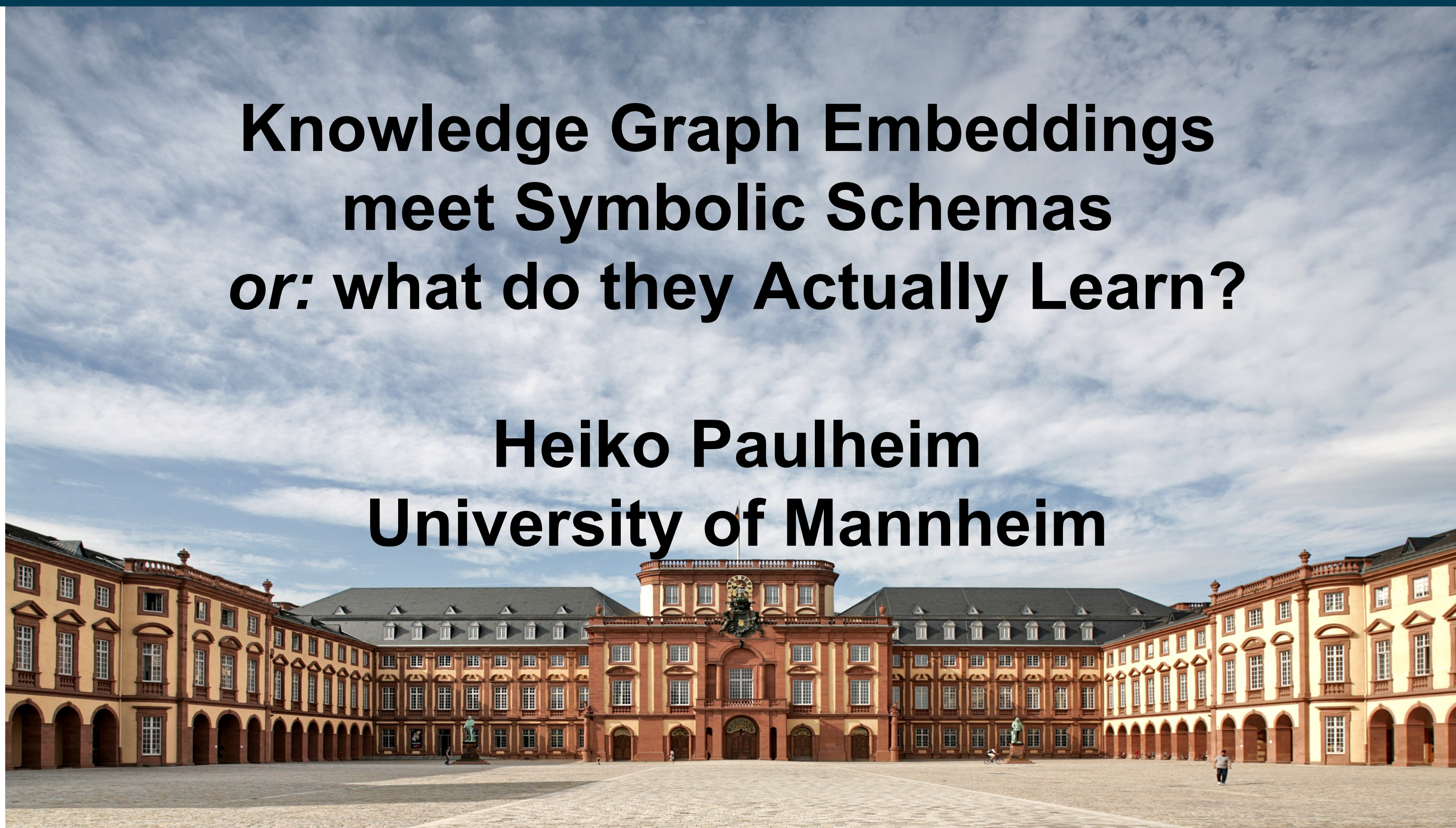

Knowledge Graph Embeddings meet Symbolic Schemas *or:* what do they Actually Learn?

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University of Mannheim