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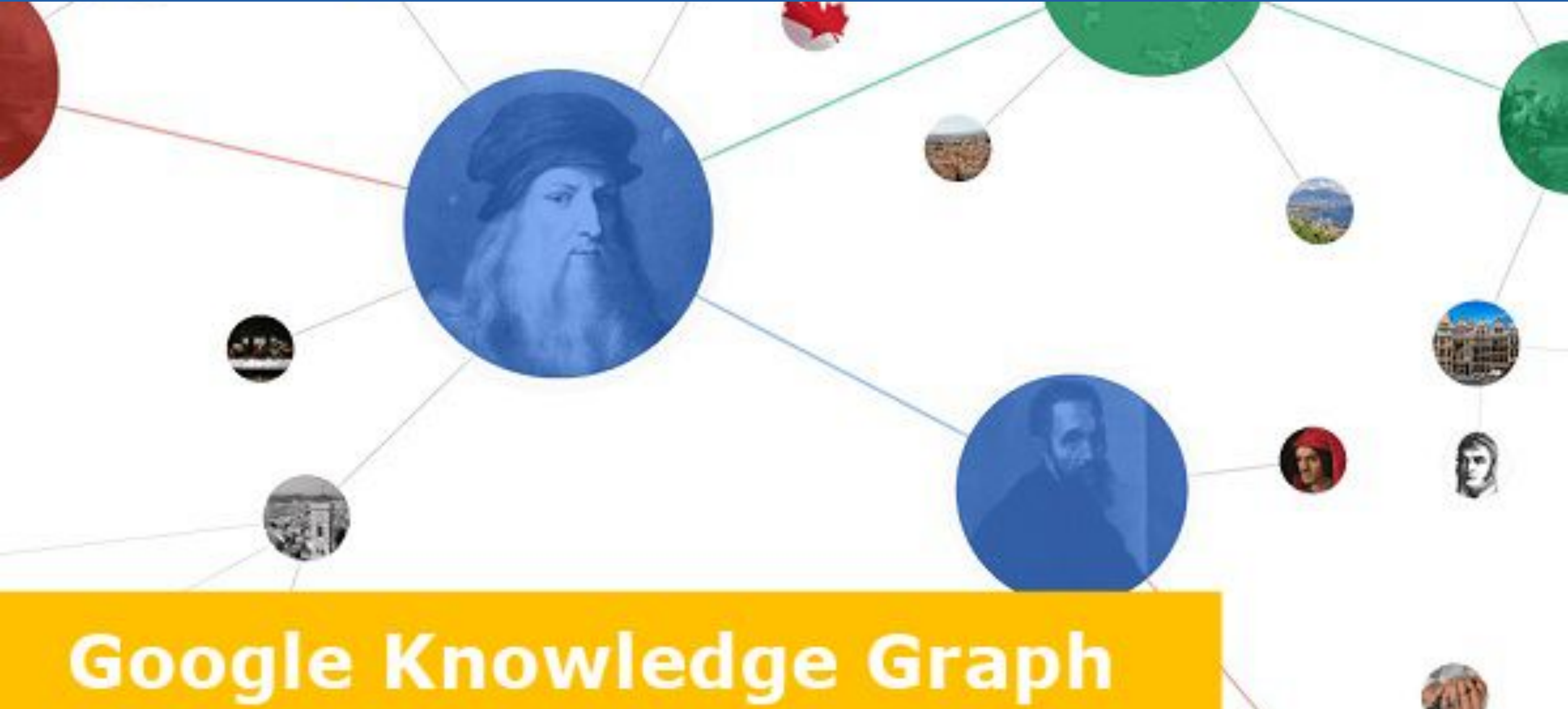
Deep Learning, Knowledge Graphs and their Applications

Dr. Mehwish Alam

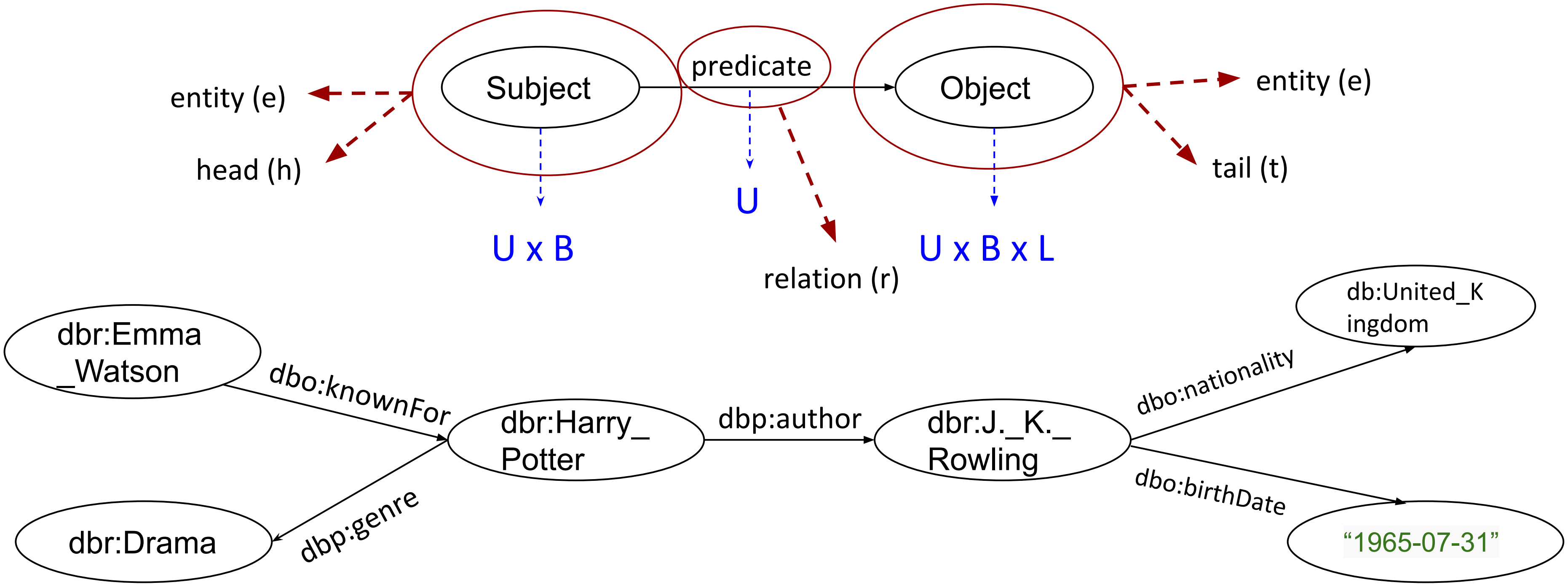
Workshop on Deep Learning meets Ontologies and Natural Language Processing co-located with FOIS 2020.
16. Sept. 2020

What is a Knowledge Graph?

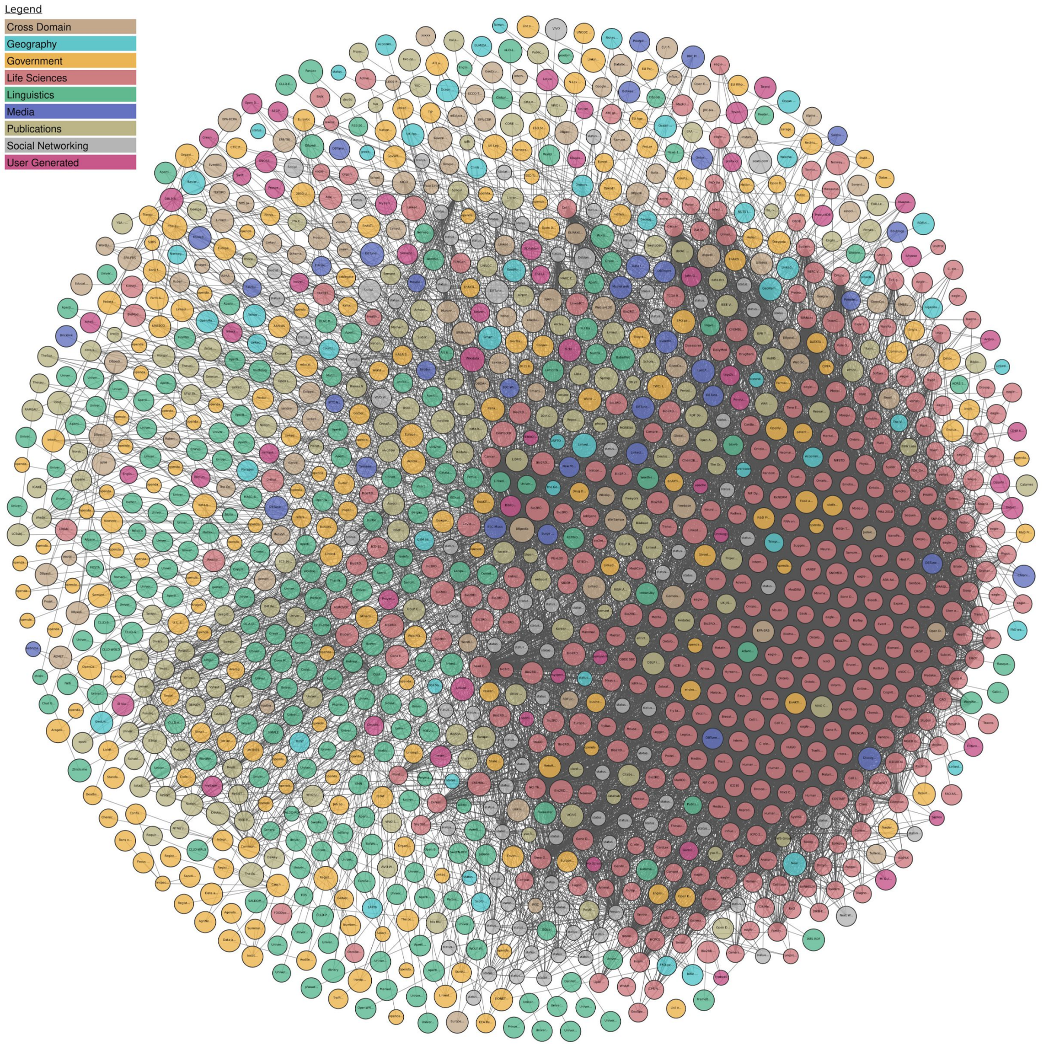


Amith Singhal, [Introducing the Knowledge Graph: things, not strings](), Google Blog, May 16, 2012

What is a Knowledge Graph?



eb of Data



The Linked Open Data Cloud from lod-cloud.net

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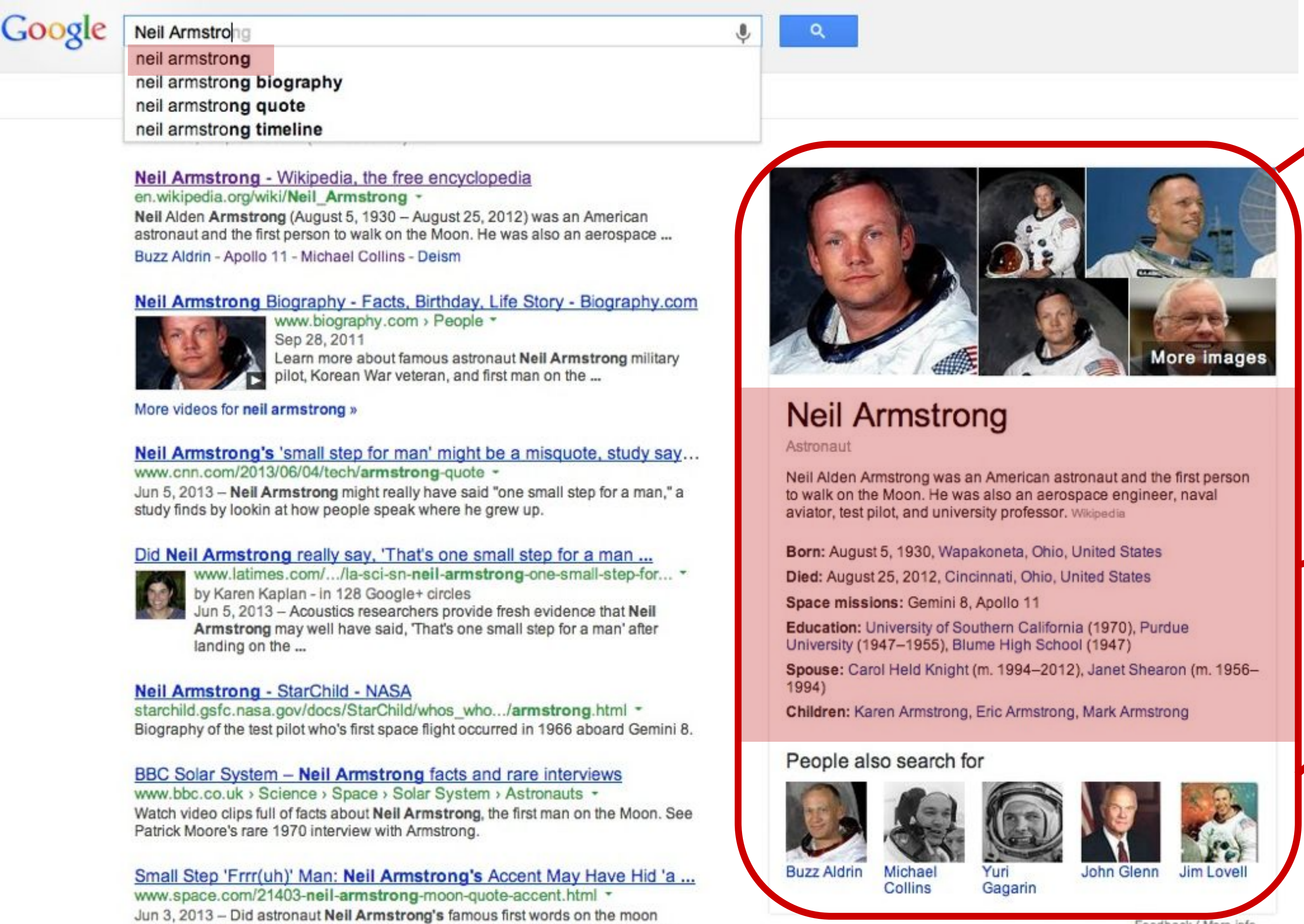

Google Knowledge Graph

70×10^9 facts
10^9 entities
(03/2017)

structured (meta)data

search recommendations

Tencent 腾讯

UniProt

USGS

Google

Bing

Alibaba.com

Bai du 百度

PubMed

Cochrane

UBER eats

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airbnb

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BBC

The New York Times

GETTY

NXP

NETFLIX

REUTERS

KUNGL. BIBLIOTEKET

National Library of Sweden

LIBRARY OF CONGRESS

Bloomberg

overheid.nl

EPA United States Environmental Protection Agency

BnF

RENAULT

legislation.gov.uk

kadaster

POLITIE

Wolters Kluwer

Bodleian Libraries UNIVERSITY OF OXFORD

SIEMENS

European Commission

IOS Press

Walmart

LEI. INFO

EUROMONEY

zalando

ebay

BEST BUY

Deloitte.

ELSEVIER

SPRINGER NATURE

amazon.com

accenture

Artificial Intelligence and Machine Learning

Artificial Intelligence

- Reasoning
- NLP
- Planning

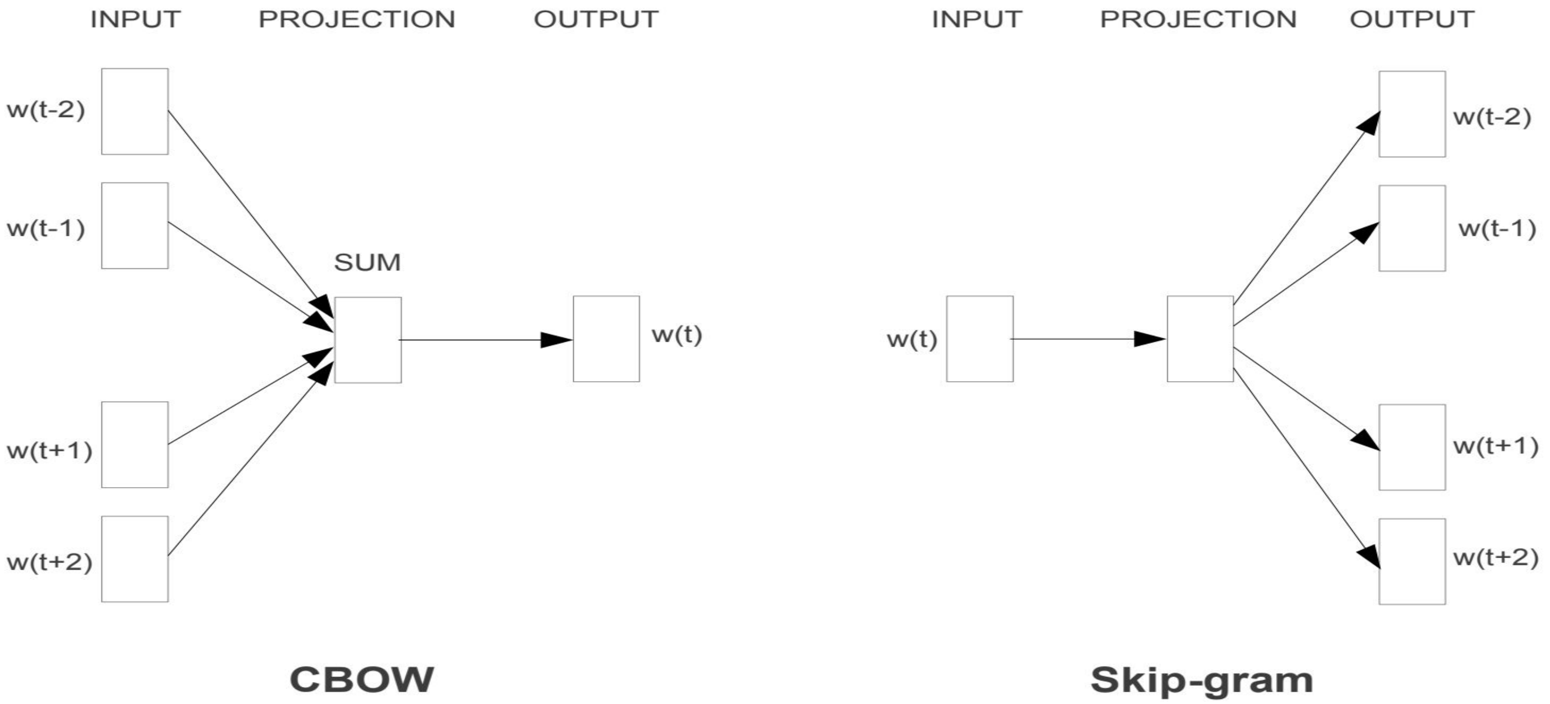
Machine Learning

- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning
- Deep Learning (Neural Networks)

"The Goal of AI is to develop machines that behave as though they were intelligent."

- John McCarthy (1955)

Word2Vec



T. Mikolov, I. Sutskever, K. Chen, G. S. Corrado, J. Dean. Distributed representations of words and phrases and their compositionality. NIPS, 2013

Limitations

- Out Of Vocabulary Exceptions (OOV)
- Reason:
  - **Internal structure** of the word is **ignored**
  - Problems for **morphologically rich languages** such as Turkish or French etc.
  - In French or Spanish more than 40 different inflections

fastText

- Considers internal structure of the word
- Good for morphologically rich languages
- Based on **skipgram** model with **bag of character n-gram representation** of the words.
- Uses **character n-grams** as well as the **actual words** in the **scoring function**.
- Computes **likelihood of each word given a context**.

<student>

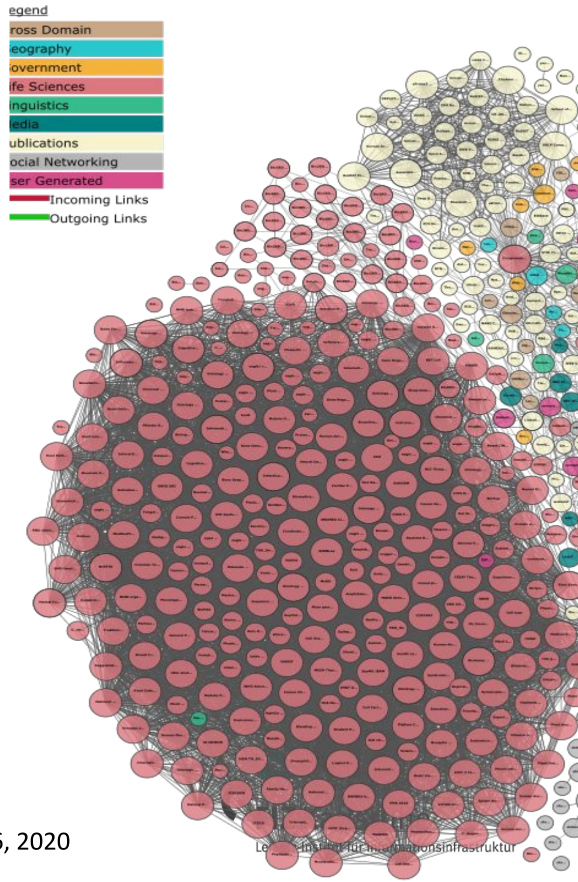
N = 2 : <st, tu, ud, de, en, nt>

N = 4 : <stud, tude, uden, dent>

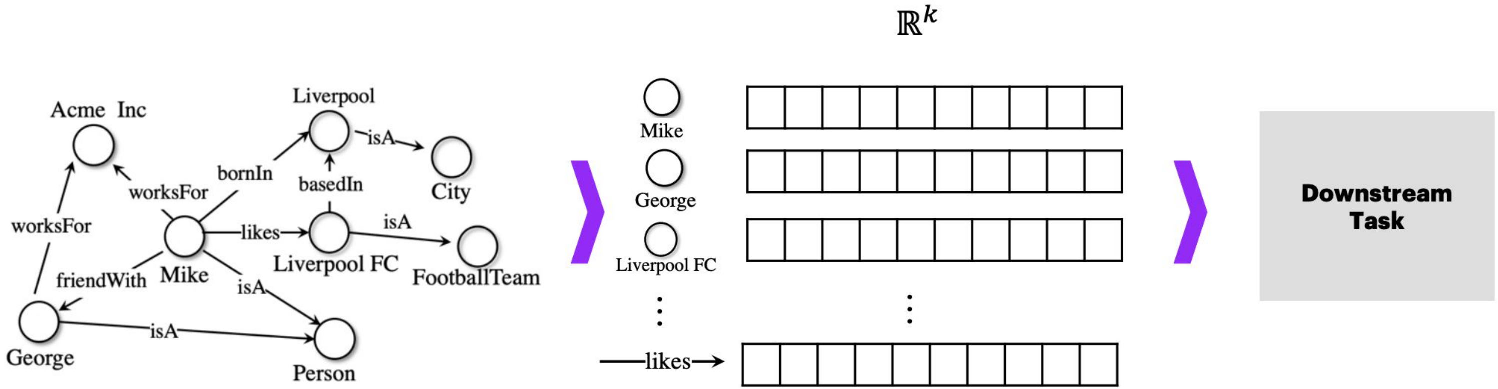
P. Bojanowski, E. Grave, A. Joulin, T. Mikolov. Enriching Word Vectors with Subword Information. Transactions of the Association for Computational Linguistics, 2017.

Deep Learning for Knowledge Graphs

- NLP and Knowledge Extraction via Deep Learning to **populate and extend Knowledge Graphs**
- NLP and Knowledge Extraction via Deep Learning for **Ontology Learning** to **extend and refine Knowledge Graphs**
- NLP and Graph Analysis supported by Deep Learning for **Ontology Alignment** and **Link Discovery** to **combine and integrate Knowledge Graphs**



Graph Representation Learning



- Node Embeddings (Node2Vec, DeepWalk, LINE, etc.) [13]
- Graph Neural Networks: Graph Convolutional Networks [11], Graph Attention Networks, Neural Message Passing, …
- **Knowledge Graph Embeddings: TransE, DistMult, ...**

Knowledge Graph Embedding Techniques

Categories	Without literals	With literals
Translational Distance Models	TransE and its extensions: TransH, TransR, TransD, TranSparse, TransA, etc.	TransEA, DKRL, IKRL, Jointly(desp), Jointly, SSP, KDCoE, EAKGAE
Semantic Matching Models	RESCAL and Its Extensions: DistMult, HolE, ComplEx, etc. Semantic Matching with Neural Networks: SME, NTN, MLP, etc.	LiteralE, MKBE, MTKGNN, KGlove with literals, Extended RESCAL, LiteralE with blocking
Models using Relation Paths	PTransE, Traversing KGs in Vector Space, RTRANSE, Compositional vector space, Reasoning using RNN, Context-dependent KG embedding.	KBLRN
Models using Temporal Information	Time-Aware Link Prediction, co-evolution of event and KGs, Know-evolve.	
Models using Graph Structures	GAKE, Link Prediction in Multi-relational Graphs.	KBLRN

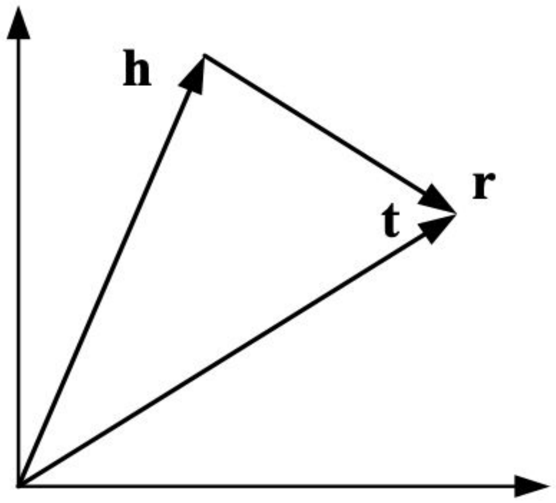
Translational Distance Model

- Exploit distance-based scoring functions
- Measure the **plausibility of a fact** as the **distance between the two entities**
- A translation carried out by the relation.
- Models: TransE, TransH, TransR, TransD, TransSparse, TransM, TransEdge

Q. Wang, Z. Mao, B. Wang, L. Guo. Knowledge graph embedding: A survey of approaches and applications. IEEE Transactions on Knowledge and Data Engineering (TKDE), 2017.

TransE

- Entities and relations are embedded into **same vector space**.
- Consider relation r as translation from entity h to entity t
- Learning Assumption **h+r=t**

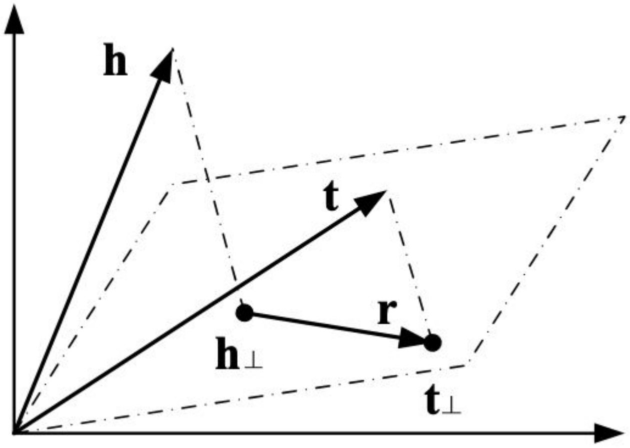


Entity and Relation Space

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

TransH

- From original space to Hyperplane
- TransH enables **different roles of an entity in different relations**.
- Entities h and t are projected into specific **hyperplane of relation r**.
- Then predict new links based on translation on hyperplane.

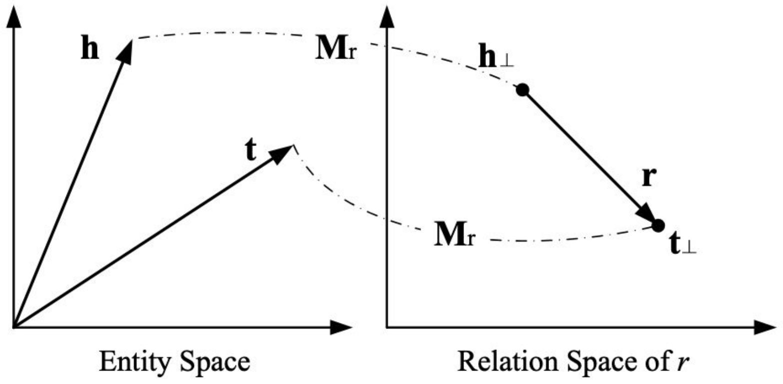


Entity and Relation Space

Z. Wang et al. "Knowledge graph embedding by translating on hyperplanes." *AAAI*, 2014.

TransR

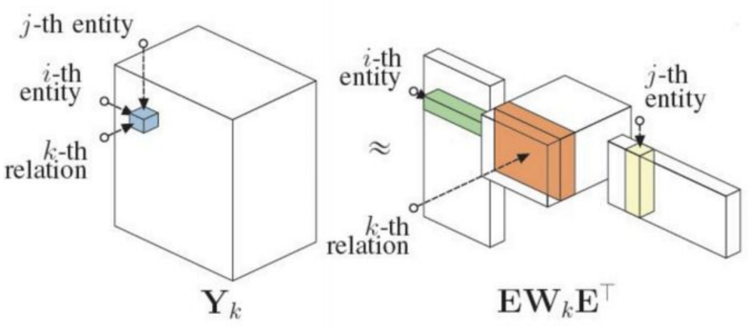
- TransR is similar to TransH.
- Entities h and t are projected into **specific subspace of relation r**.
- Predict new links based on translation in subspace.



Y. Lin et al. "Learning entity and relation embeddings for knowledge graph completion." AAAI, 2015.

Semantic Matching Models

- *Exploit similarity-based scoring functions*
- *Measures* ***plausibility of facts*** *by* ***matching latent semantics of entities and relations***
- Based on Matrix Operation
- Represent **relation as a matrix** and produce **score function by operation on matrix**.
- RESCAL, DistMult, HolE, etc.

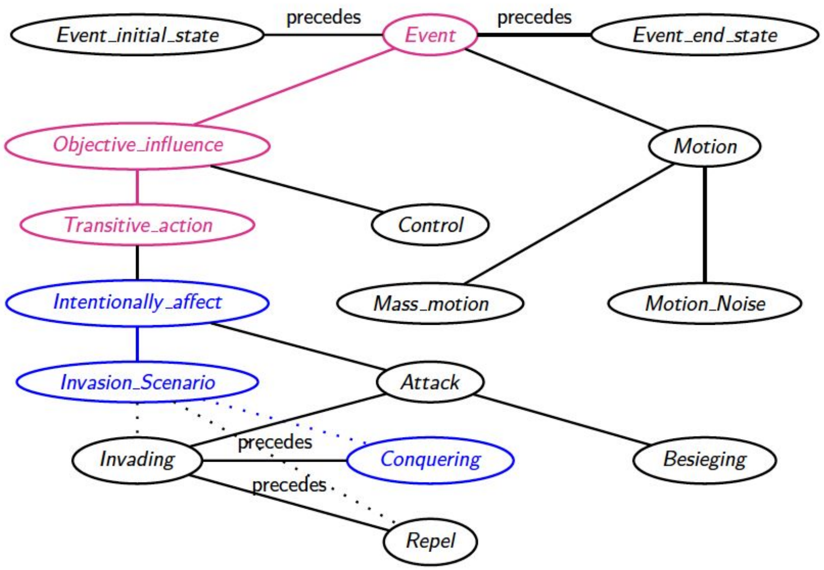


Methods Using Graph Structures

- Use Contextual information around an entity.
- Walk based methods
- RDF2Vec
  - Word2Vec converts raw text into vector representations
  - RDF2Vec converts a graph into a sequence of nodes and edges
  - Methods:
    - Graph Walks
    - Weisfeiler-Lehman Subtree RDF Graph Kernels

P. Ristoski, H. Paulheim. Rdf2vec: Rdf graph embeddings for data mining. *International Semantic Web Conference, 2016*.

Graph walks



Depth = 3

Generated Sequences:

- Event → inheritsFrom → Objective Inuence→ inheritsFrom → Transitive Action ...
- Intentionally act → inheritsFrom → Invasion Scenario → subFrameOf → Conquering ...

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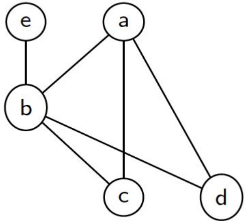
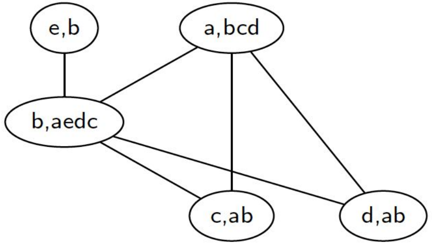
Weisfeiler-Lehman Subtree RDF Graph Kernels





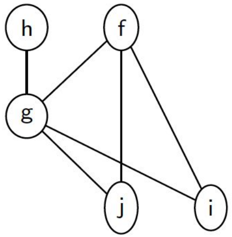
a,bcd $\longrightarrow$ f

e,b $\longrightarrow$ h

b,aedc $\longrightarrow$ g

d,ab $\longrightarrow$ i

c,ab $\longrightarrow$ j



Generated Sequences:

- b⟶ g⟶ j; b⟶ g⟶ i; b⟶ g⟶ f; b⟶ g⟶ h; b⟶ g⟶ j⟶ f
- a⟶ f⟶ g; a⟶ f⟶ j; a⟶ f⟶ i; a⟶ f⟶ g⟶ h

Applications

- In-KG Applications:
  - Link Prediction: *head, tail, relation prediction*
  - Triple Classification: *Whether unseen triple fact is true or not*
  - Entity Classification: *Classifying entities into different semantic categories*

- Out-KG Applications
  - Relation Extraction
  - Question Answering
  - Recommender System

Libraries for KG Embeddings

PyTorch BigGraph

https://github.com/facebookresearch/PyTorch-BigGraph

AmpliGraph

https://github.com/Accenture/AmpliGraph

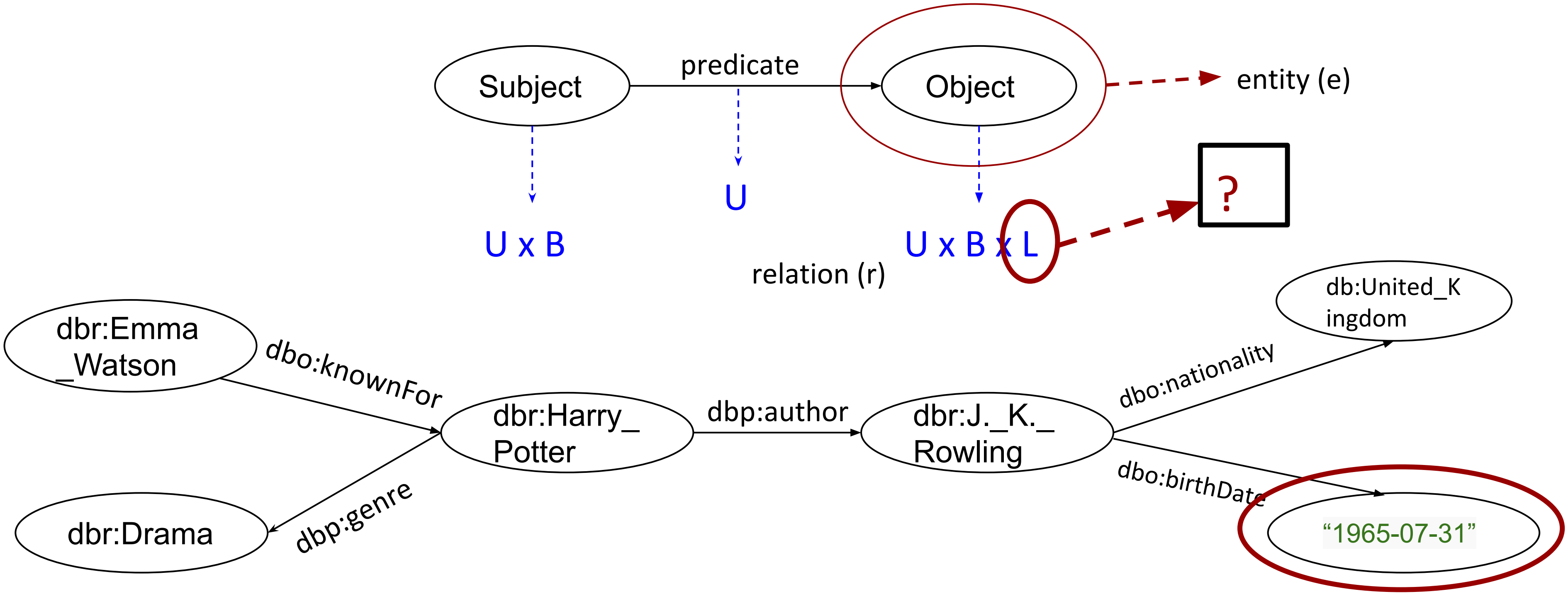
PyKeen

https://github.com/SmartDataAnalytics/PyKEEN

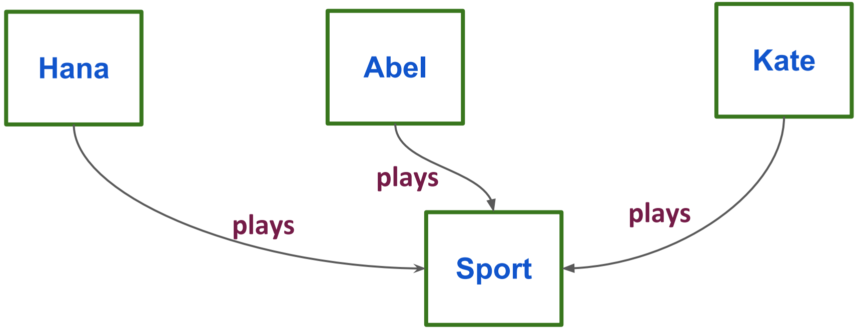
OpenKE

http://openke.thunlp.org/

What about literals?



Why Literals for KG Embedding?



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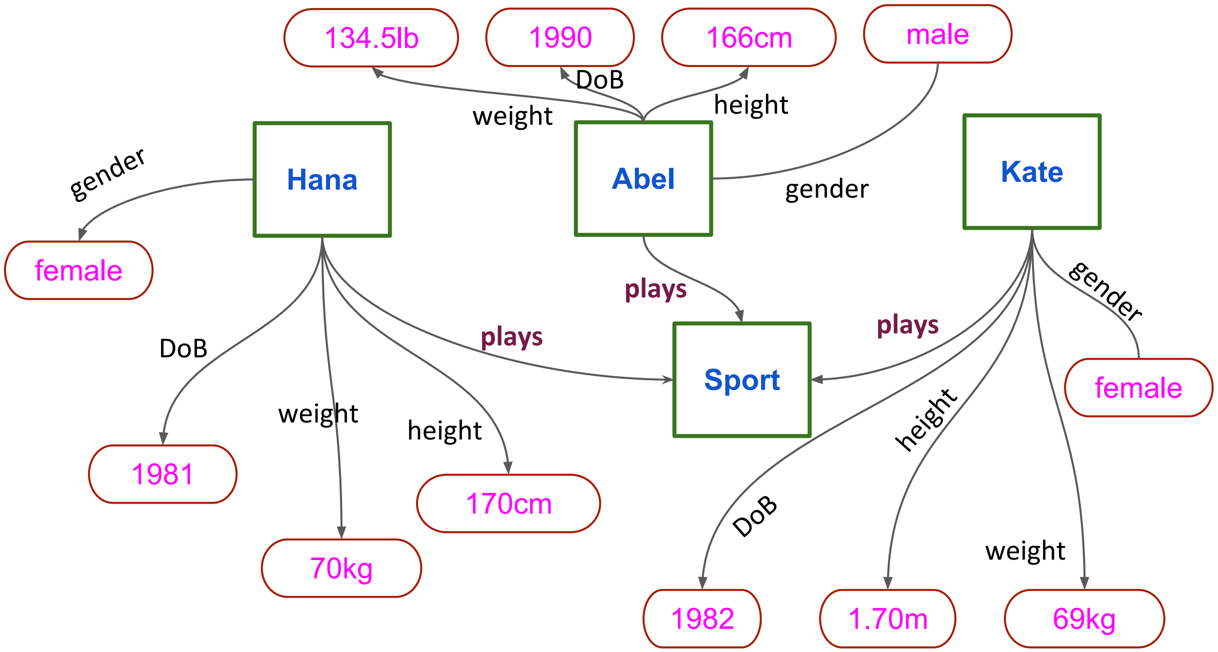

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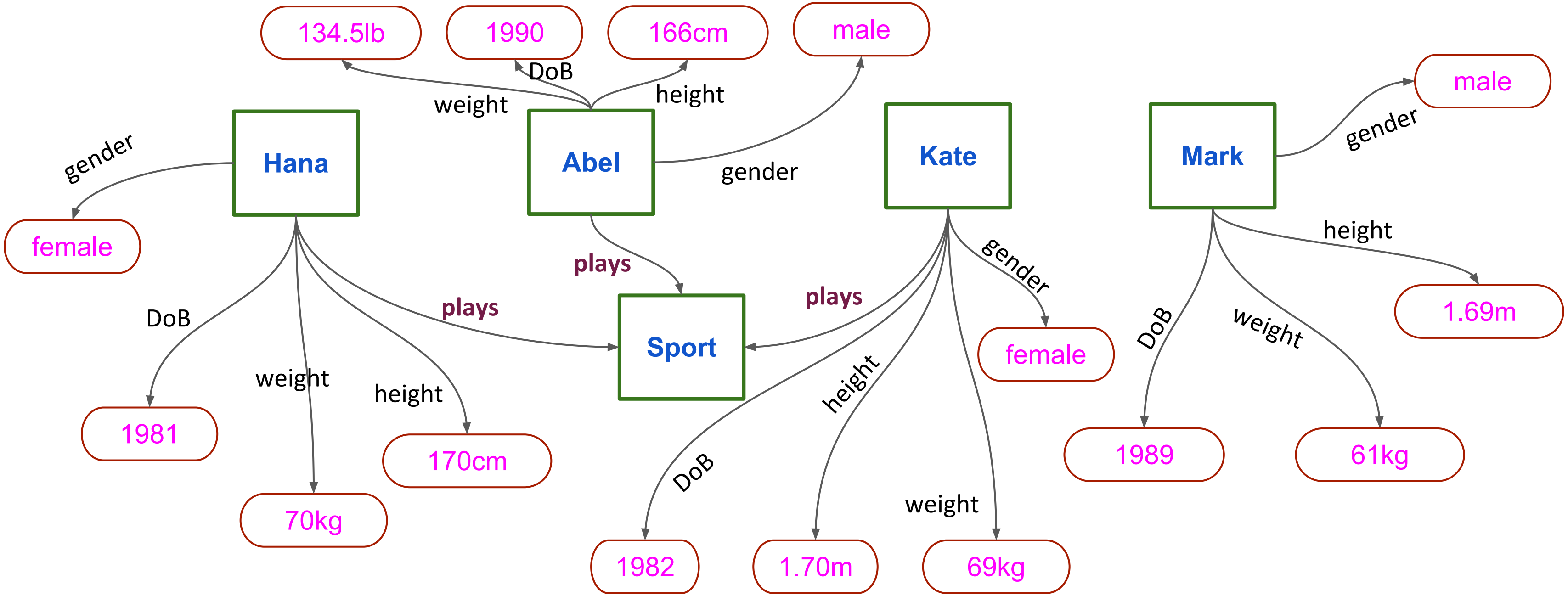

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Types of Literals

- **Text Literals**
  - Short text

    fb:m.03vdmh fb:type.object.name "Photo-essay"@en .
  - Long text:

    fb:m.03vdmh fb:common.topic.description "A photo-essay is a set or series of photographs that are intended to tell a story or …"@en .
- **Numerics Literals**

  fb:g.1269m_vlb fb:people.person.date_of_birth "1957"^^<http://www.w3.org/2001/XMLSchema#gYear> .

  fb:m.064r8g fb:people.person.weight_kg "102.0" .

- **Others:** Images, audio files, video files, and etc.

@prefix fb: <http://rdf.freebase.com/ns/>

KG Embedding Models with Text Literals

- Extended RESCAL
  Tensor factorization

- Description-Embodied Knowledge Representation Learning (DKRL)
  TransE + CBOW/CNN

- Multilingual KG Embeddings for cross-lingual KG alignment (KDCoE)
  TransE + AGRU for multilingual KGs

Drawback:
Don’t consider short text!!

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KG Embedding Models with Numeric Literals

- Multi-Task Knowledge Graph Neural Network (MT-KGNN)
  Regression, Binary Classification

- Knowledge Base Representations with Latent, Relational, and Numerical Features (KBLRN)
  TransE, Probabilistic Product of Experts

- LiteralE
  Learnable transformation function

- TransEA
  TransE, Linear Regression

Drawbacks:

- *Units and data types of literals are not interpreted*
- *Multi-valued literals are not treated.*

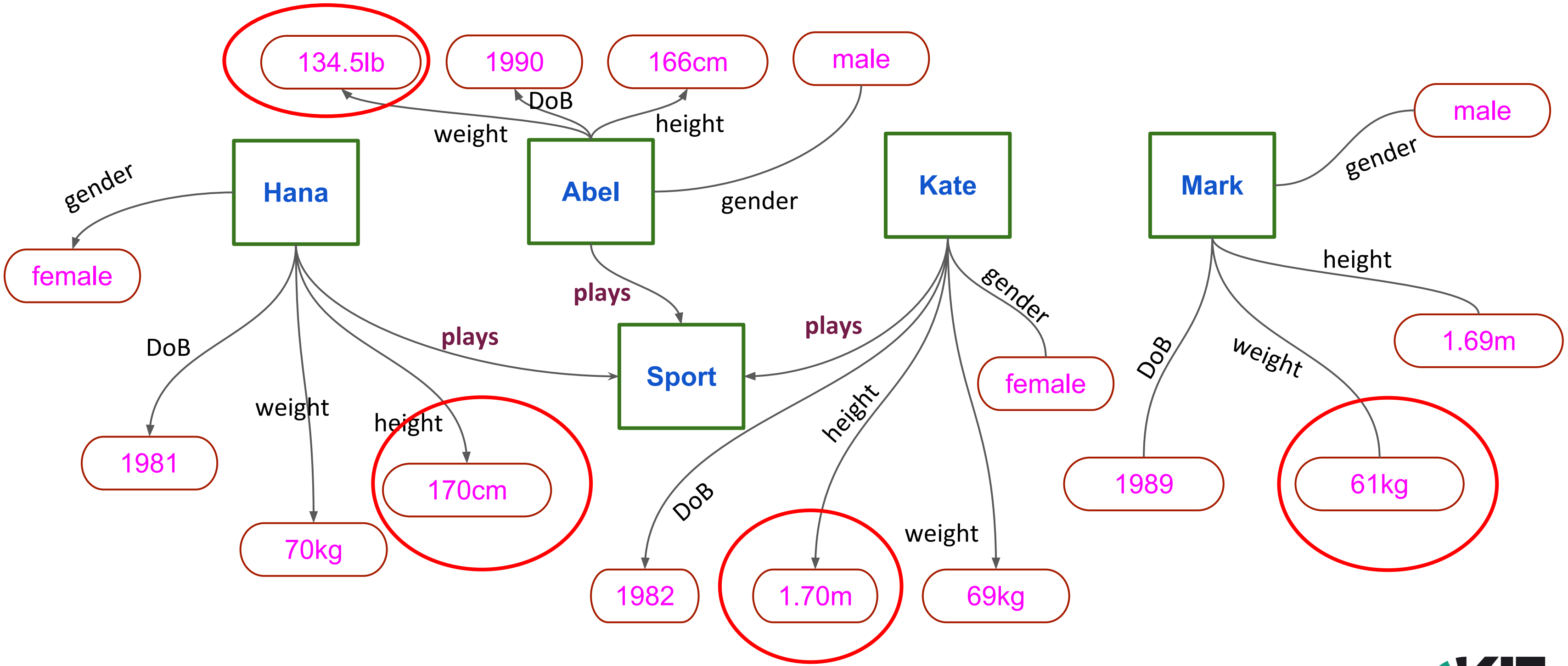
Other kind of literals

- Image Literals: IKRL, MTKGRL
- Multi-modal Liaterls:
  - Numeric & Text Literals: LiteralE with blocking, EAKGAE.
  - Numeric, Text & Image Literals: MKBE
- Evaluation Tasks:
  - Link Prediction: *head, tail, relation prediction*
  - Triple Classification: *Whether unseen triple fact is true or not*
  - Entity Classification: *Classifying entities into different semantic categories*

Applications

	Link prediction	Triple Classif.	Entity Classif.	Entity Alignment	Attribute Value Prediction	Nearest Neighbor Analysis	Data Linking	Document classification
Extended RESCAL	✓							
LiteralE	✓					✓		
TransEA	✓							
KBLRN	✓							
DKRL	✓		✓					
KDCoE	✓			✓				
KGlove with literals		✓						✓
IKRL	✓	✓						
EAKGE	✓			✓				
MKBE	✓				✓			
MT-KGNN		✓			✓			
LiteralE with blocking							✓	

Limitations



Results for Link Prediction on FB15K-237

	Datasets	
	FB15K	**FB15K-237**
Entities	14951	14541
Object Relations	1345	237
Data Relations	118	118
Relational Triplets	592213	310116
Train sets	483142	272115
Valid sets	50000	17535
Test sets	59071	20466

Tail Prediction

Models	MR	MRR	Hits@1	Hits@3	Hits@10
DistMult-LiteralE$_{glin}$	426	0.195	0.119	0.214	0.349
ComplEx-LiteralE$_{glin}$	575	0.17	0.104	0.185	0.306
ConvE-LiteralE$_{glin}$	362	0.187	0.112	0.204	0.338
DistMult-LiteralE$_{g}$	359	**0.215**	0.137	0.234	0.371
ComplEx-LiteralE$_{g}$	493	0.175	0.106	0.19	0.312
ConvE-LiteralE$_{g}$	459	0.131	0.07	0.137	0.256
KBLN	501	0.207	0.128	0.23	0.362
MTKGNN	580	0.191	0.12	0.208	0.338
TransEA	**203**	0.206	**0.25**	**0.409**	0.57

Head Prediction

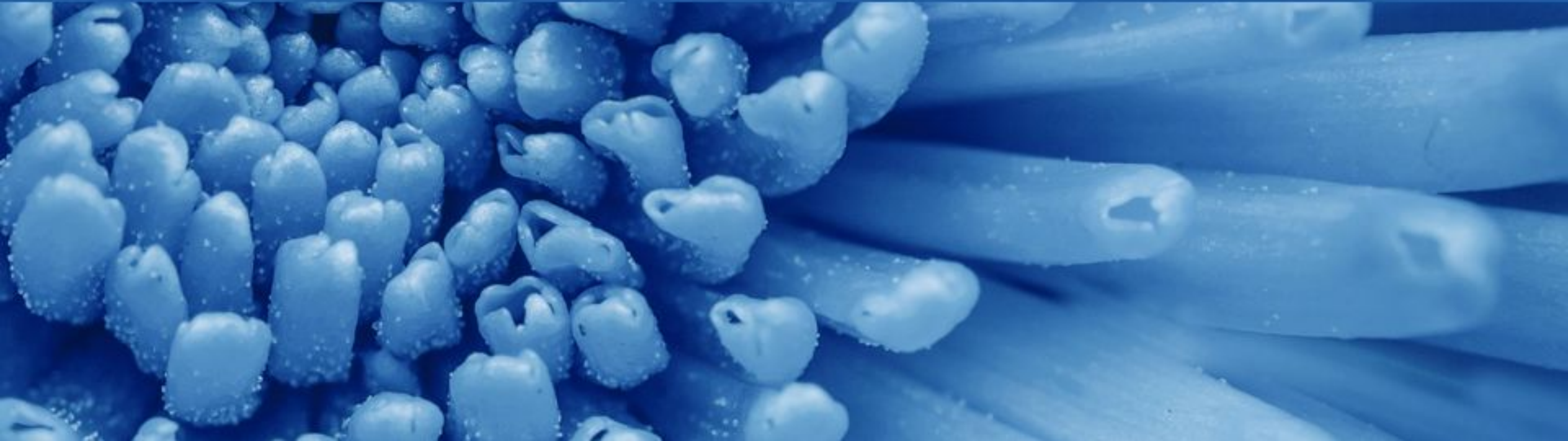
Models	MR	MRR	Hits@1	Hits@3	Hits@10
DistMult-LiteralE$_{glin}$	245	0.377	0.279	0.422	0.568
ComplEx-LiteralE$_{glin}$	371	0.36	0.271	0.4	0.538
ConvE-LiteralE$_{glin}$	**208**	0.388	0.296	0.427	0.572
DistMult-LiteralE$_{g}$	209	**0.413**	**0.320**	**0.456**	**0.591**
ComplEx-LiteralE$_{g}$	315	0.366	0.277	0.404	0.543
ConvE-LiteralE$_{g}$	236	0.317	0.229	0.345	0.501
KBLN	381	0.386	0.295	0.426	0.564
MTKGNN	437	0.383	0.295	0.423	0.559
TransEA	389	0.111	0.094	0.197	0.342

Both Head and Tail Prediction

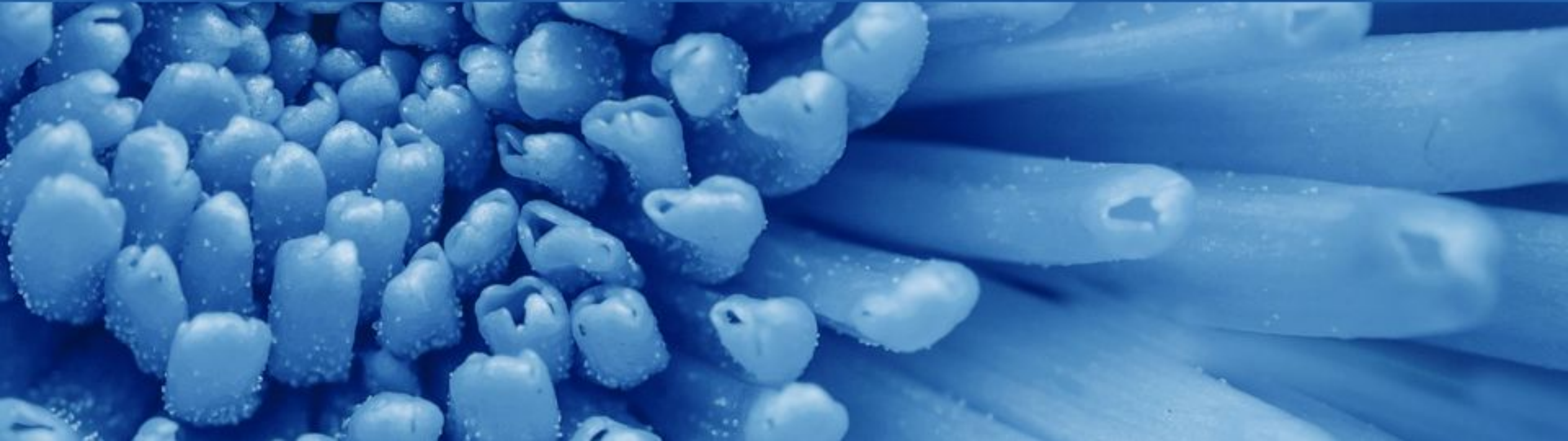
Models	MR	MRR	Hits@1	Hits@3	Hits@10
DistMult-LiteralE$_{glin}$	335	0.286	0.199	0.318	0.458
ComplEx-LiteralE$_{glin}$	473	0.265	0.187	0.292	0.422
ConvE-LiteralE$_{glin}$	285	0.287	0.204	0.315	0.455
DistMult-LiteralE$_{g}$	**284**	**0.314**	**0.228**	**0.345**	**0.481**
ComplEx-LiteralE$_{g}$	404	0.27	0.191	0.297	0.427
ConvE-LiteralE$_{g}$	347	0.224	0.149	0.241	0.378
KBLN	441	0.296	0.211	0.328	0.463
MTKGNN	508	0.287	0.207	0.315	0.448
TransEA	296	0.158	0.172	0.303	0.456

G. A. Gesese, R. Biswas, M. Alam, H. Sack. A Survey on Knowledge Graph Embeddings with Literals: Which model links better Literal-ly?. *Semantic Web Journal (Accepted), 2020.*

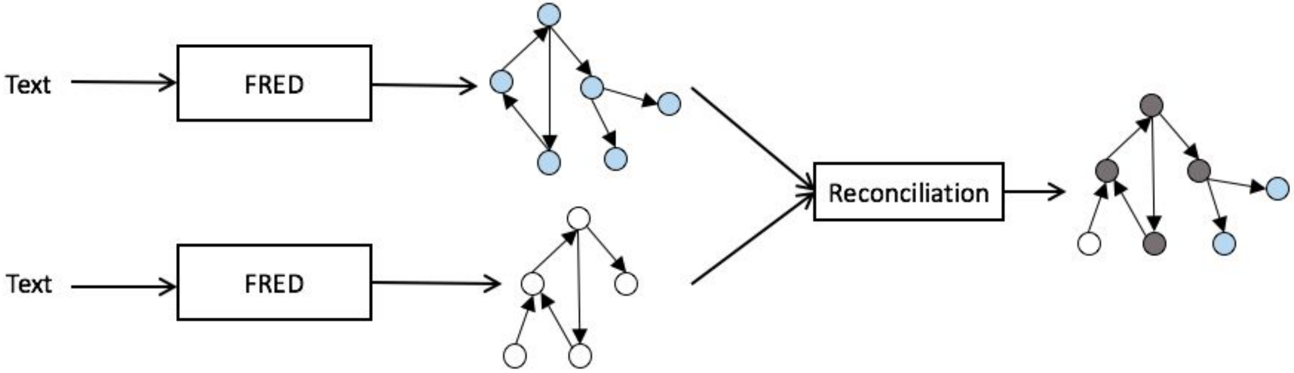
Knowledge Graph Embeddings for Downstream Tasks



Event-based Knowledge Reconciliation using Frame Embeddings and Frame Similarity



Knowledge Reconciliation



Why Knowledge Reconciliation:

- Text Summarization
- Document Similarity
- Generating Textual Analytics

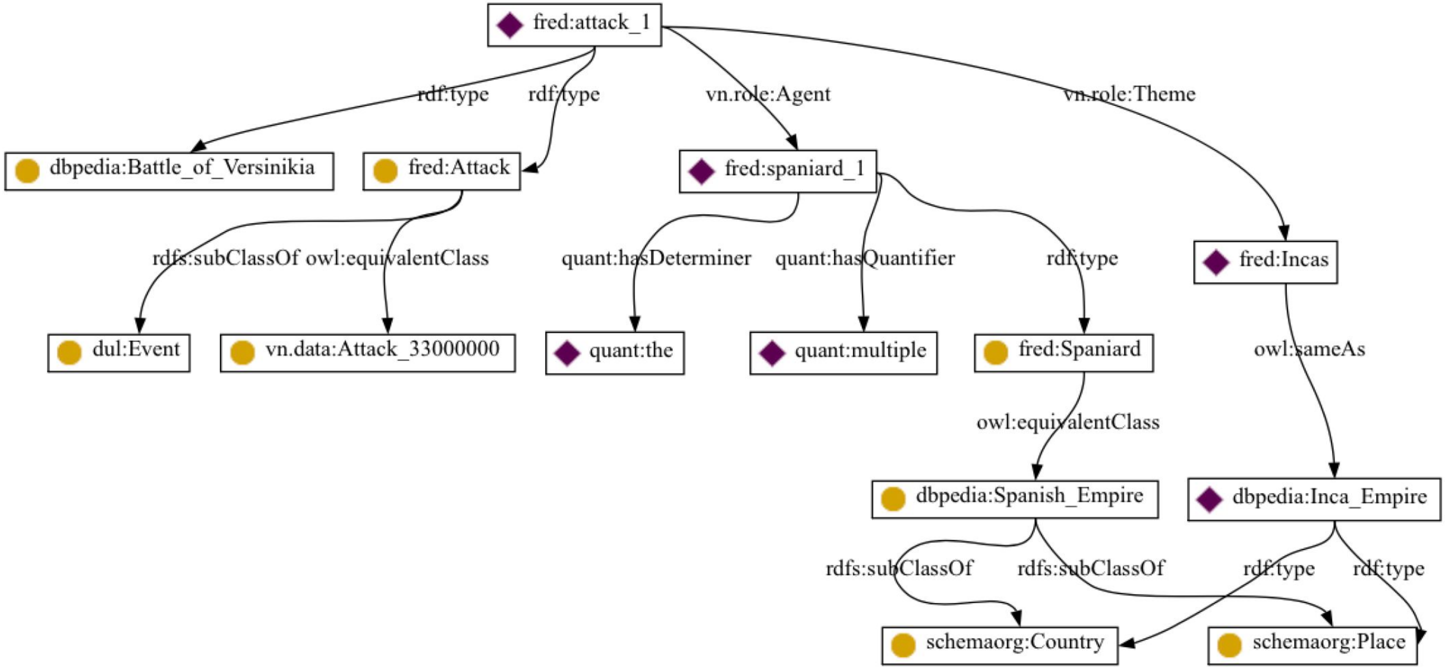
Existing Tool MERGILO

- Graph Compression
- Graph Alignment
- Uses String matching and Word Similarity

M. Alam, D. R. Recupero, M. Mongiovi, A. Gangemi, P. Ristoski. Event-based knowledge reconciliation using frame embeddings and frame similarity. *Knowledge-Based Systems*, 2017.

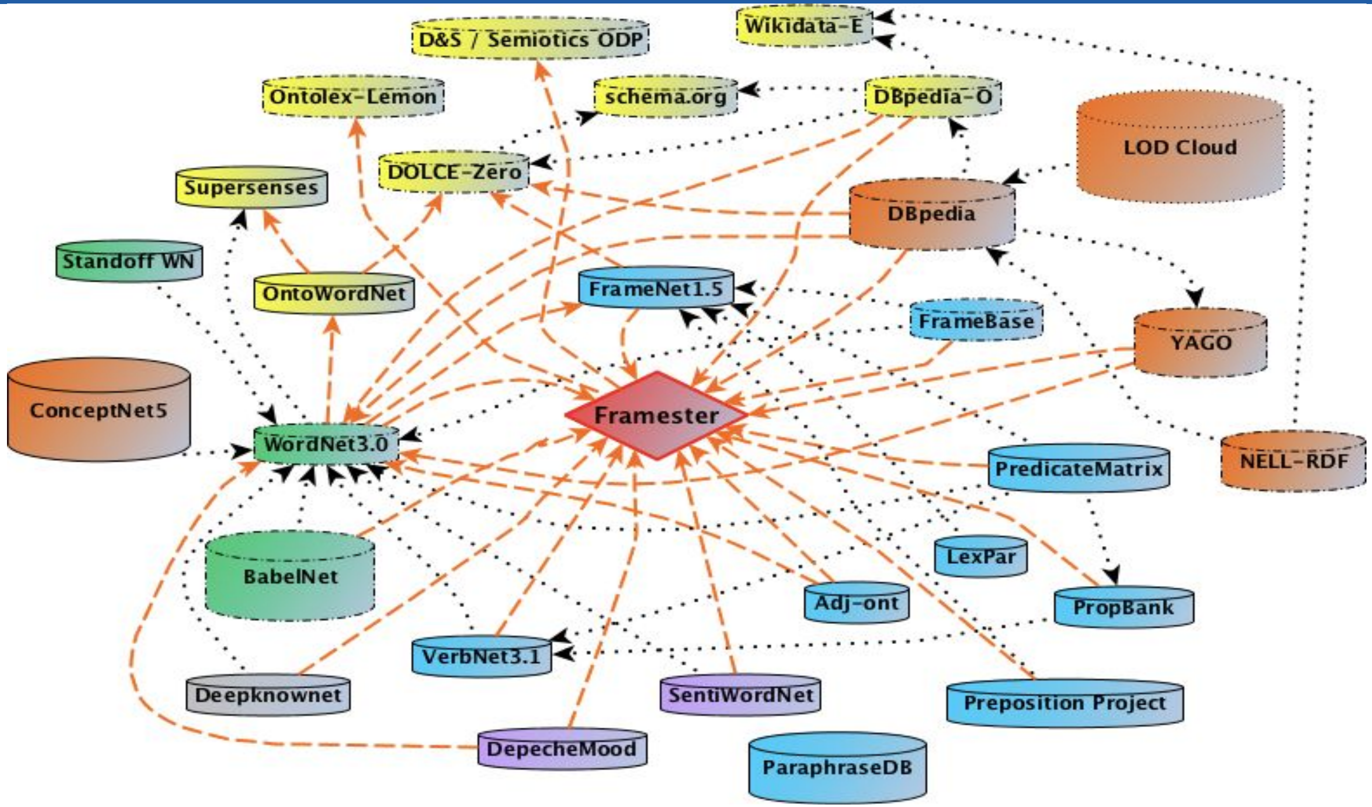
FRED - Event Oriented Knowledge Graphs from Text

Spaniards attacked the Incas



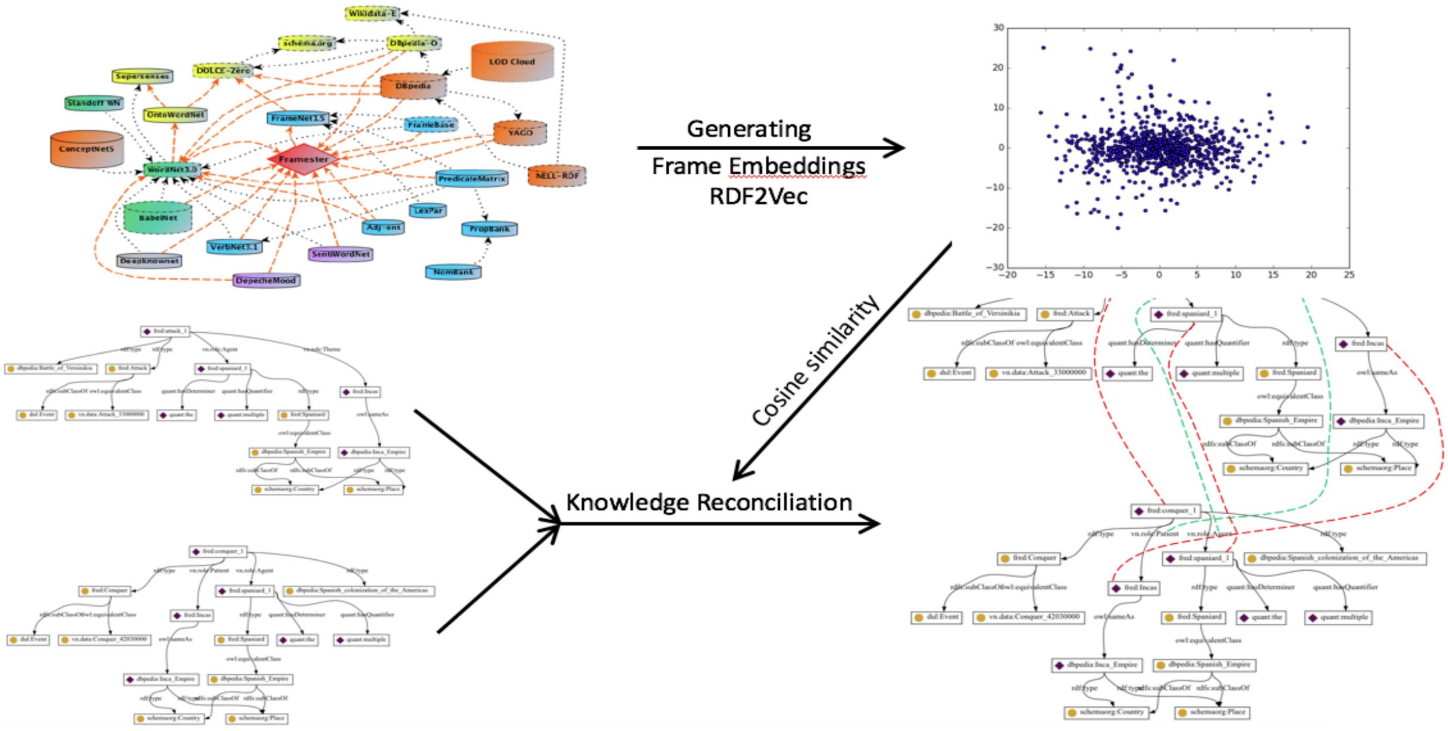
A. Gangemi, V. Presutti, D. R. Recupero, A. G. Nuzzolese, F. Draicchio, M. Mongiovì: Semantic Web Machine Reading with FRED. Semantic Web Journal, 2017.

Framester

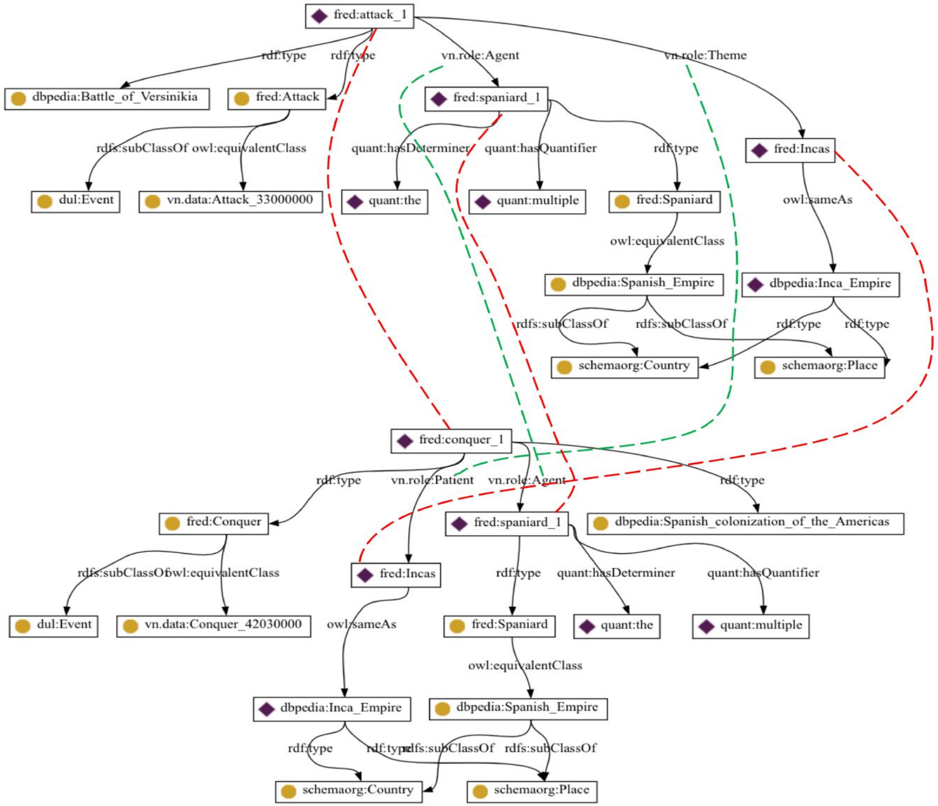


A. Gangemi, M. Alam, L. Asprino, V. Presutti, D.R. Recupero. Framester: A Wide Coverage Linguistic Linked Data Hub. *EKAW, 2020.*

Applications Using Knowledge Graph Embeddings



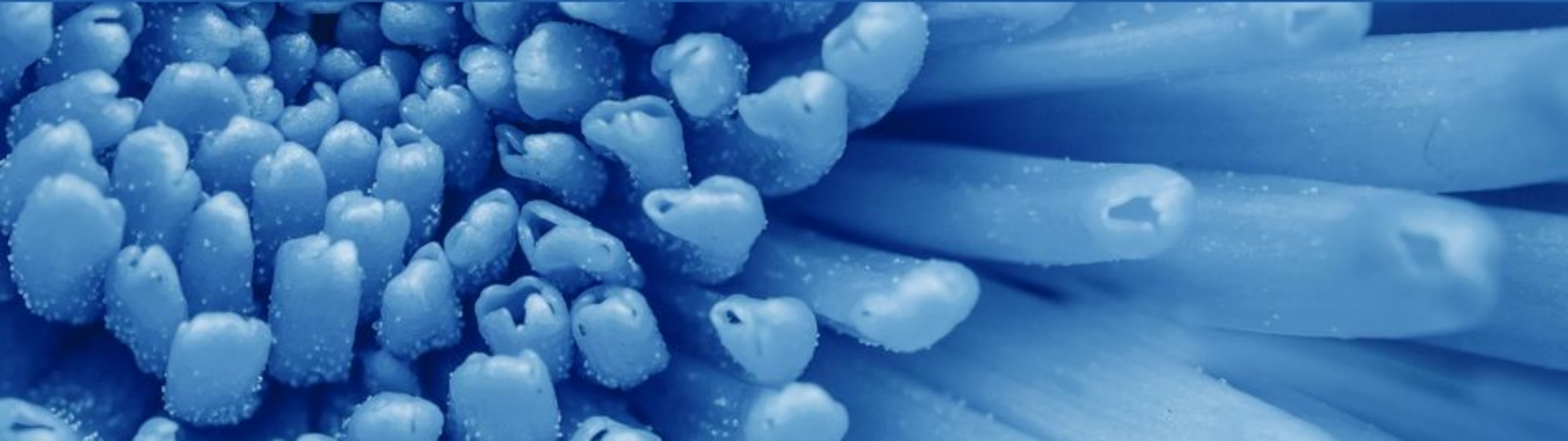
Reconciled Knowledge Graph



Cross-document Coreference Resolution (CCR) on RDF

		muc	bcub	ceafm	blanc	ceafe
MERGILO Baseline		24.05	17.36	28.61	10.70	26.20
FrameNet Inheritance Similarity Measures						
Wu-Palmer		27.14	19.91	31.91	**12.81**	29.41
Path		27.16	19.93	31.85	12.73	29.38
Leacock Chodorow		27.04	19.80	31.74	12.77	29.21
Graph walks (full frame and role graphs)						
Frame2Vec	**Role2Vec**	**muc**	**bcub**	**ceafm**	**blanc**	**ceafe**
CBOW_200	CBOW_200	27.34	**19.99**	32.15	12.66	29.82
CBOW_200	SG_800	**27.38**	19.97	**32.29**	12.69	**29.98**
CBOW_200	SG_500	27.28	19.95	31.99	12.69	29.54
Graph kernels (full frame and role graphs)						
Frame2Vec	**Role2Vec**	**muc**	**bcub**	**ceafm**	**blanc**	**ceafe**
CBOW_200	SG_200	26.70	19.52	31.45	12.40	28.99
CBOW_200	SG_500	26.70	19.52	31.45	12.40	28.99
SG_200	CBOW_200	26.86	19.62	31.67	12.48	29.18
SG_500	CBOW_200	26.90	19.68	31.58	12.60	29.08

Weakly Supervised Short Text Categorization Using World Knowledge



Where do we find short-text?

Social Media | **News Articles** | **Chatbot**

Why short-text classification is challenging?

"Floyd revolutionized rock with the Wall."

Ambiguity!
Lack of contextual information!

Humans transfer knowledge from other similar situations or external resources.

Contextual Information is required for understanding.

Explicit Representation

Explicit representation refers to the conceptualization [1].

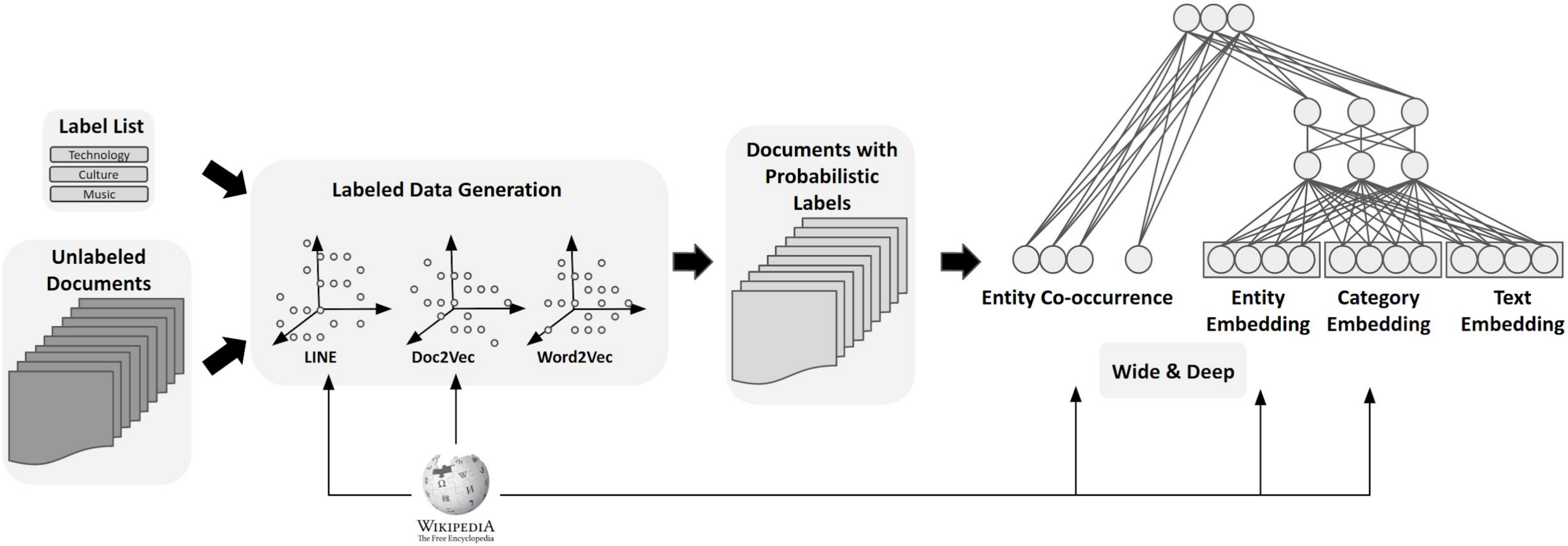
Floyd revolutionized **rock** with the **Wall**.

https://en.wikipedia.org/wiki/Pink_Floyd

https://en.wikipedia.org/wiki/Defensive_wall
https://en.wikipedia.org/wiki/Berlin_Wall
https://en.wikipedia.org/wiki/The_Wall

https://en.wikipedia.org/wiki/Rock_(geology)
https://en.wikipedia.org/wiki/Rock_music
https://en.wikipedia.org/wiki/Dwayne_Johnson

Wide & Deep Model for Short Text Classification

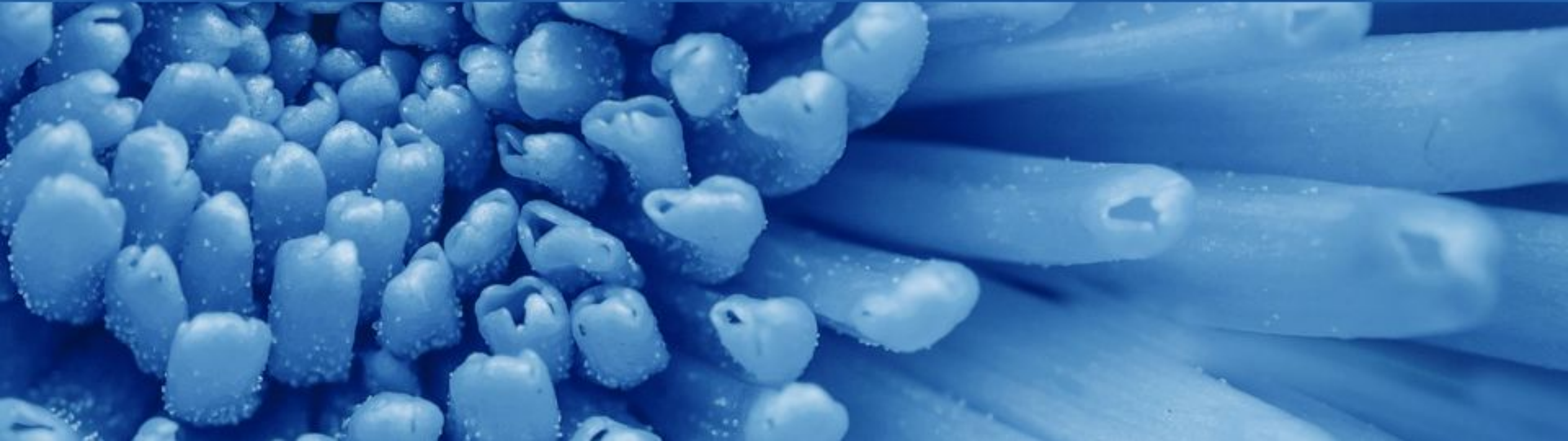


R. Türker, L. Zhang, M. Alam, H. Sack. Weakly Supervised Short Text Categorization Using World Knowledge. *International Semantic Web Conference, 2020.*

Classification Accuracy

Model	Feature	AG News	Snippets	DBpedia	Twitter
Wide	Entity Co-occurance (Ent Co)	0.561	0.447	0.499	0.278
Deep	Text	0.802	0.795	0.786	0.555
	Entity	0.790	0.764	0.775	0.521
	Category	0.773	0.698	0.754	0.444
	Text+Entity	0.793	0.785	0.779	0.524
	Text+Category	0.801	0.794	0.786	0.554
	Entity+Category	0.792	0.771	0.771	0.534
	Text+Entity+Category	0.792	0.786	0.785	0.529
Wide & Deep	Ent Co+Text	0.807	0.792	0.786	0.556
	Ent Co+Entity	0.791	0.774	0.768	0.520
	Ent Co+Category	0.792	0.693	0.774	0.446
	Ent Co+Text+Entity	0.787	0.802	0.776	0.53
	Ent Co+Text+Category	**0.814**	0.803	**0.792**	**0.581**
	Ent Co+Entity+Category	0.791	0.770	0.766	0.544
	Ent Co+Text+Entity+Category	0.790	**0.805**	0.778	0.572

Knowledge Graph Embeddings based Type Prediction



Motivation

What are the types of the following entities?

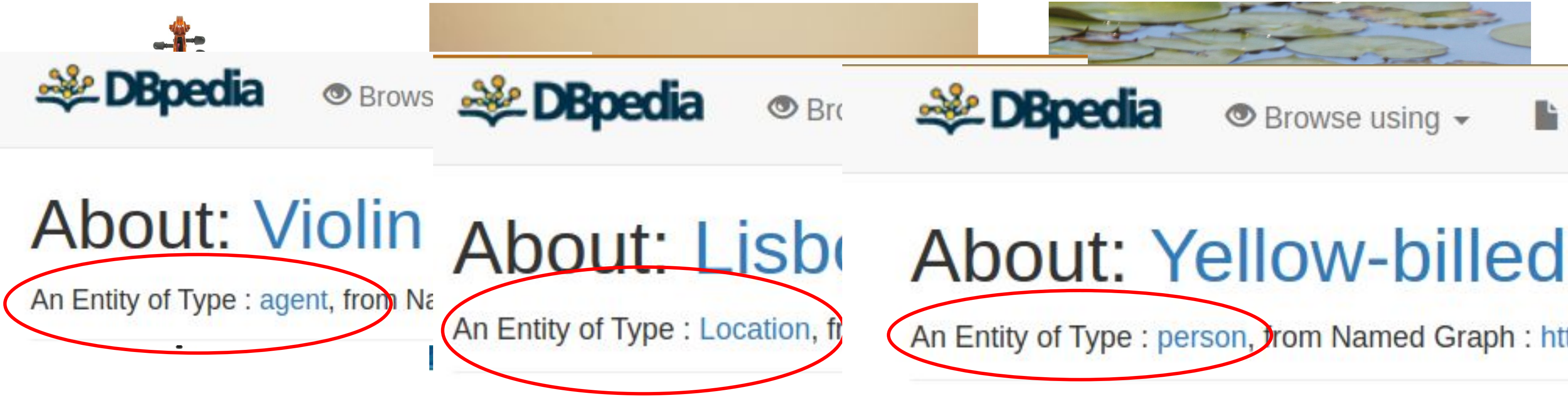
Violin	Lisbon	Yellow billed duck
		
Instrument	City	Bird

R. Biswas, R. Soforonova, M. Alam, H. Sack. Entity Type Prediction in Knowledge Graphs using Embeddings. *DL4KG@ESWC, 2020*.

Motivation

What are the types of the following entities?

Violin | Lisbon | Yellow billed duck

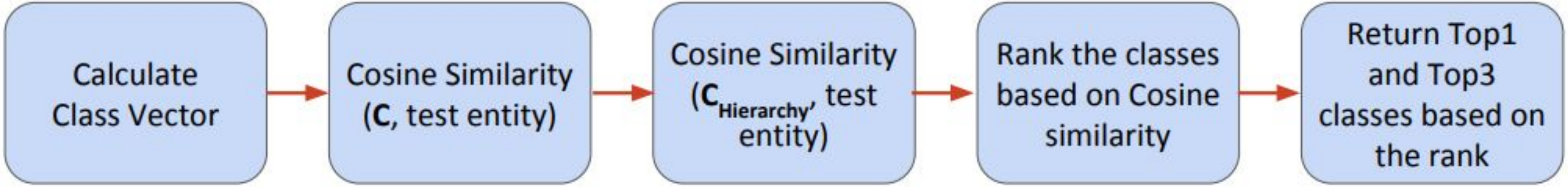


Instrument | City | Bird

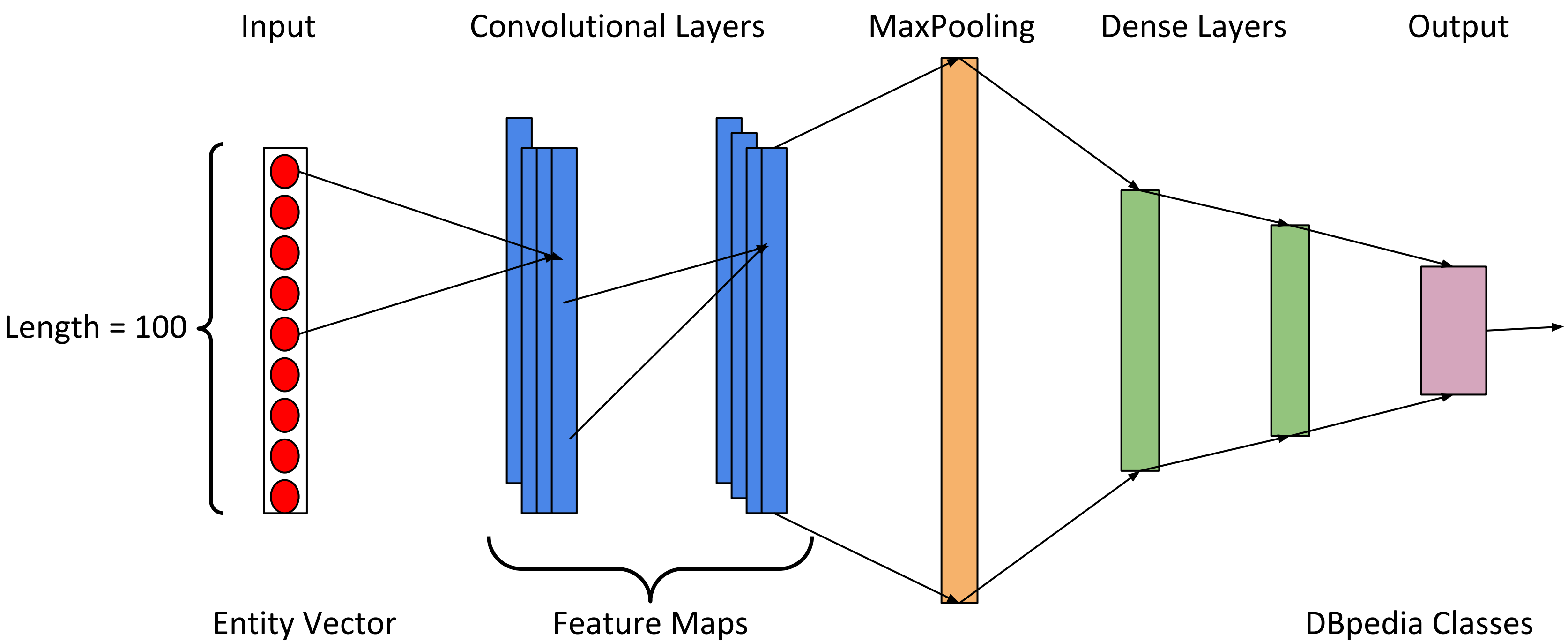
Karlsruher Institut für Technologie
FIZ Karlsruhe
Leibniz-Institut für Informationsinfrastruktur

Pipeline of the Unsupervised Approach

Unsupervised approach is based on the vector similarity between the class vector and entity vector



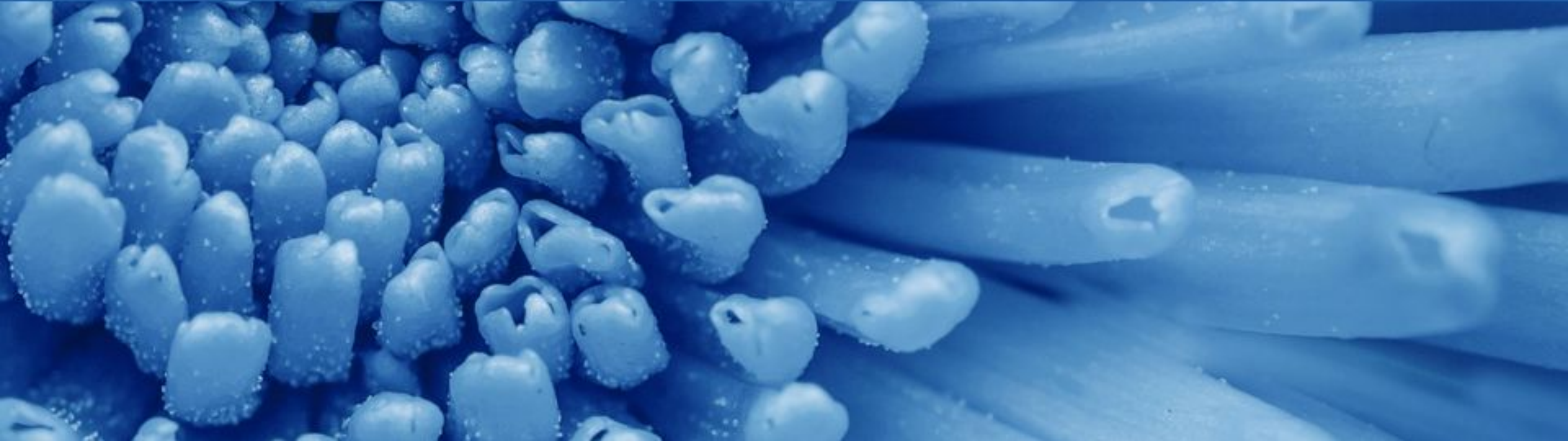
Supervised Approach - 1D CNN



Wrapping Up

- What did we see so far:
  - Knowledge Graphs
  - Graph Neural Networks
  - Knowledge Graph Embeddings with or without Literals
  - Downstream tasks using Knowledge Graph Embeddings
- What next?
  - Temporal Knowledge Graph Embeddings
  - More expressivity
  - Explainability in Knowledge Graph Embeddings

Some Advertisements



Special Issue in Deep Learning and Knowledge Graphs

Call for papers: Special Issue on Deep Learning and Knowledge Graphs

Submitted by Pascal Hitzler on 07/04/2020 - 05:29

Call for papers: Special Issue on

Deep Learning and Knowledge Graphs

Over the past years there has been a rapid growth in the use and the importance of Knowledge Graphs (KGs) along with their application to many important tasks. KGs are large networks of real-world entities described in terms of their semantic types and their relationships to each other. On the other hand, Deep Learning has also become an important area of research, achieving important breakthroughs in various research fields, especially Natural Language Processing (NLP) and Image Processing. Moreover, in recent years Deep Learning methods have been combined with KGs. For example: 1) knowledge representation learning techniques aimed at embedding entities and relations in a KG into a dense and low-dimensional semantic space, 2) relation extraction techniques, aimed at extracting facts and relations from text and needed to construct KGs, 3) entity linking techniques, aimed at completing KGs, 4) using KGs as an additional prior for image recognition, etc.

In order to pursue more advanced methodologies, it has become critical that the communities related to Deep Learning, Knowledge Graphs, and NLP join their forces in order to develop more effective algorithms and applications. This special issue aims to reinforce the relationships between these communities and foster interdisciplinary research in the areas of KG, Deep Learning, and Natural Language Processing.

Topics of Interest

- New approaches for the combination of Deep Learning and Knowledge Graphs
  - Methods for generating Knowledge Graph (node) embeddings
  - Scalability issues
  - Temporal Knowledge Graph Embeddings
  - Novel approaches

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Several PhD and Post Doc positions.

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