



TECHNISCHE  
UNIVERSITÄT  
DRESDEN



Fraunhofer  
Dresden  
IAIS

# Complex Question Answering

## over Knowledge Graphs



Mikhail Galkin  
PhD, Research Scientist  
TU Dresden & Fraunhofer IAIS  
**Dresden**



@migalkin



@michael\_galkin



@mgalkin

# Outline

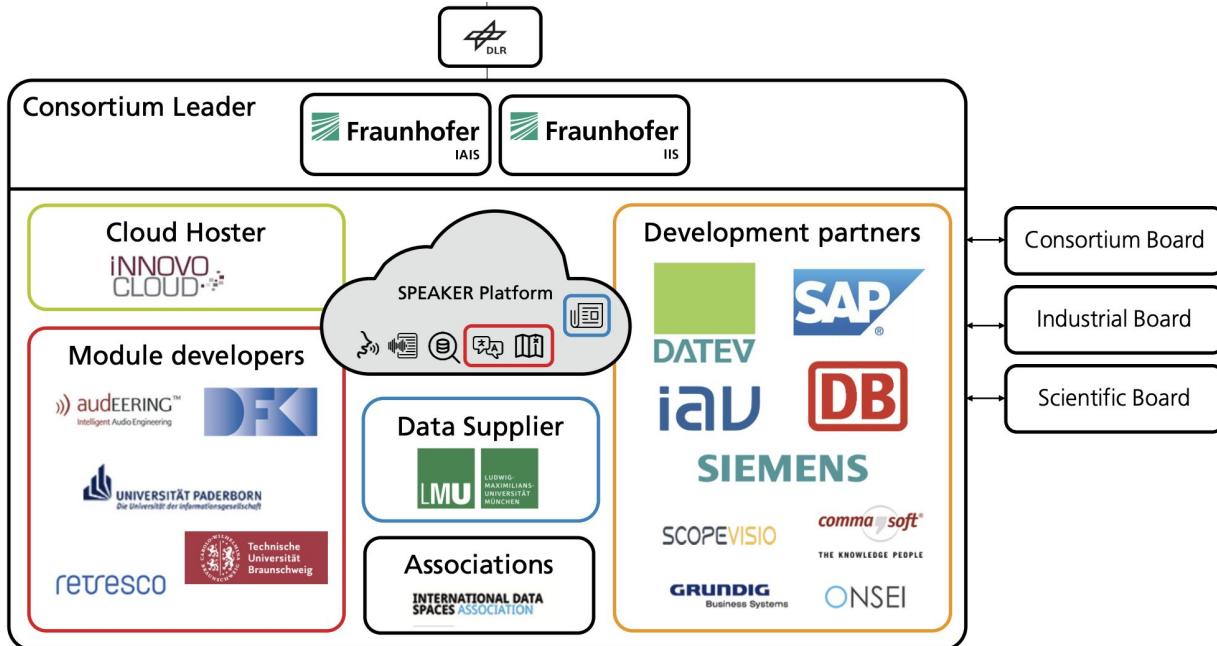
- Introduction: Knowledge Graphs
- Large KGs:
  - Template-based
  - Pipeline-based
- Smaller KGs: Neural Reasoning
  - Neural and Multi-Hop QA
  - Query Embedding

# About

## SPEAKER

Industrial Speech  
Assistance Platform

- ConvAI
- Question Answering
- Knowledge Graphs
- Speech
- Privacy
- Customizable & Domain-specific



# On the definition of a Knowledge Graph

Given entities E, relations R, KG is a directed multi-relational graph G that comprises triples (s, p, o)

$$\mathcal{G} \subseteq \mathcal{E} \times \mathcal{R} \times \mathcal{E}$$
$$(s, p, o) \in \mathcal{G}$$

“Abstract schema and instances”

- \* describes entities and relations
- \* defines a schema
- \* interrelating arbitrary entities
- \* various topical domains

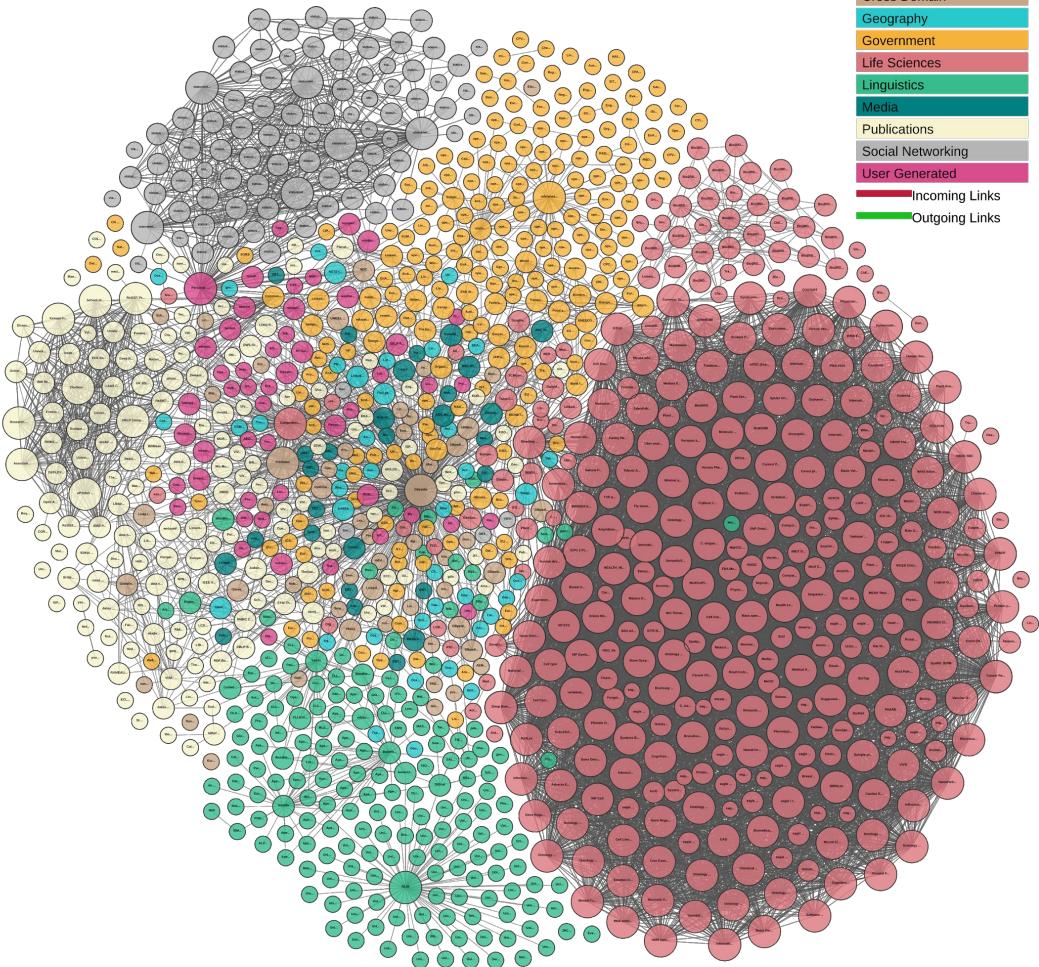
“Every RDF / LPG / RDF\* graph is a knowledge graph”

Graph-structured world model

# World models?

Entities and  
relations define our  
**domain of discourse**

How to encode it?



Source: <https://lod-cloud.net/>

# On representation of Knowledge Graphs



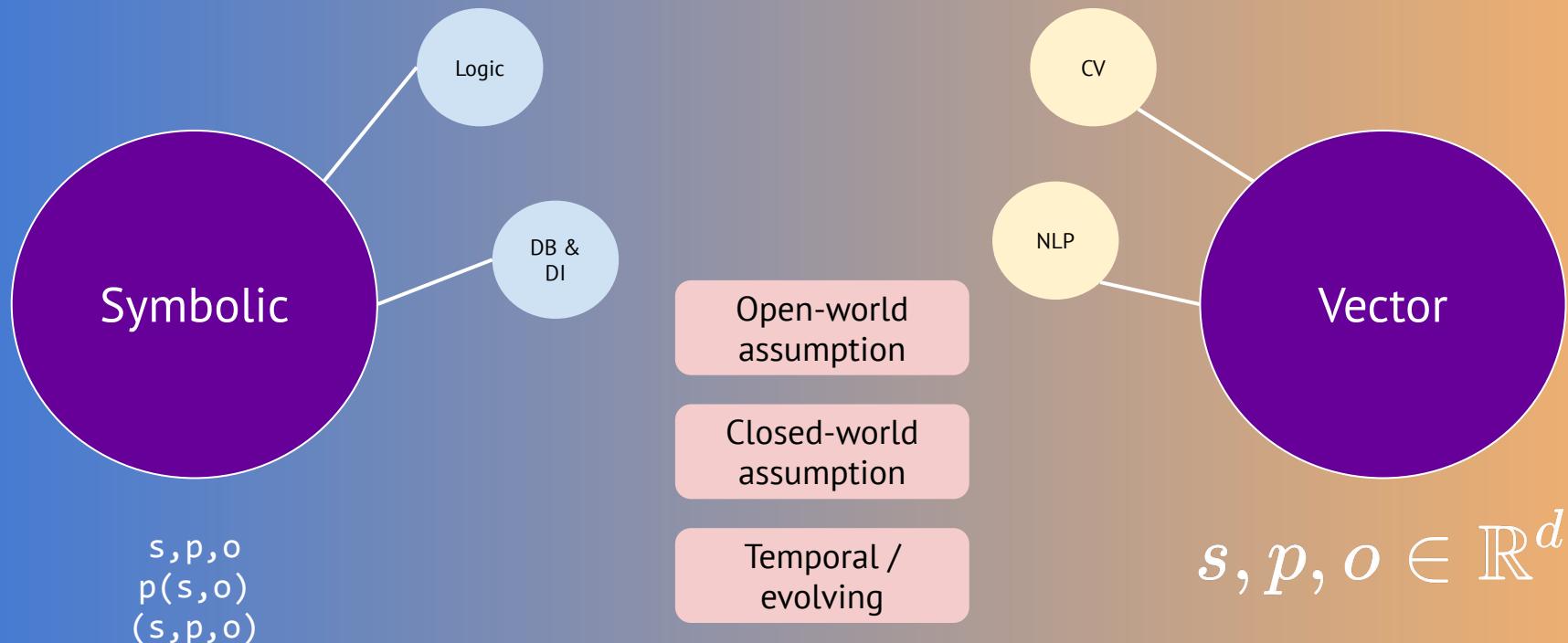
Symbolic

$s, p, o$   
 $p(s, o)$   
 $(s, p, o)$

Vector

$s, p, o \in \mathbb{R}^d$

# On representation of Knowledge Graphs



# Symbolic: Triples



RDJ

RDJ

Sherlock\_Holmes

Sherlock\_Holmes

dbp:resides

dbp:born

dbp:studio

dbp:starring

SF .

NY .

WB .

RDJ .

Avengers

Avengers

Iron\_Man

Iron\_Man

dbp:studio

dbp:starring

dbp:studio

dbp:starring

Marvel .

RDJ .

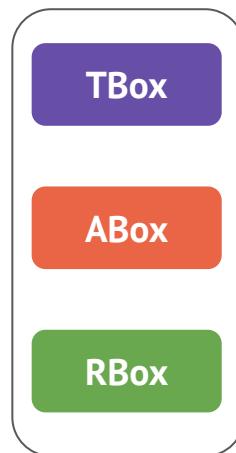
Marvel .

RDJ .

# Symbolic: Description Logics

Based on logical formalisms, e.g., Description Logics (DL), RDFS, OWL

schema, ontology,  
theory



instances, facts,  
assertions

restrictions,  
constraints

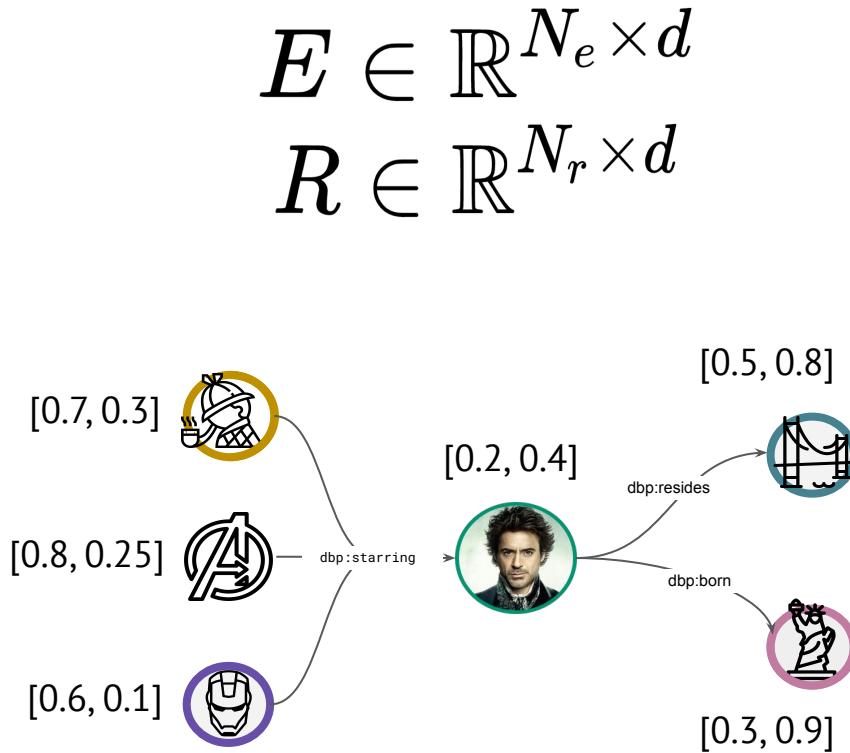
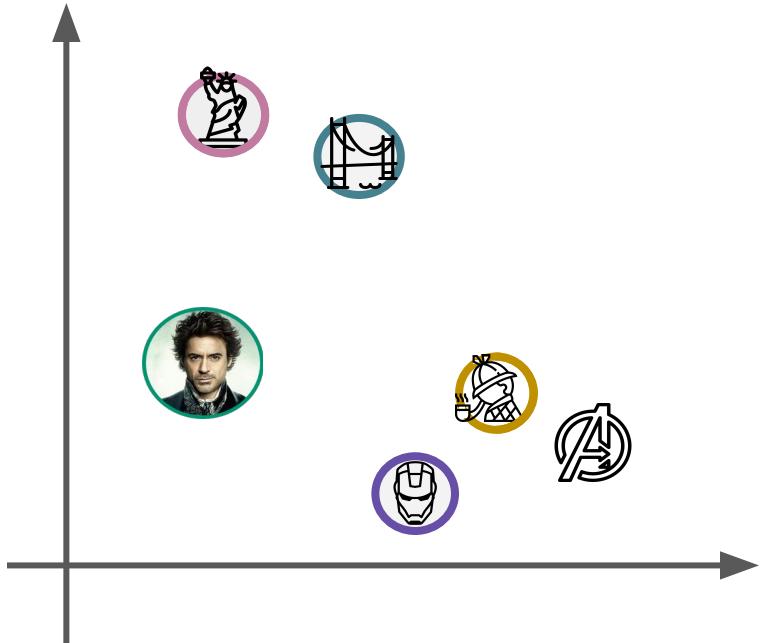
**SuccessfulArtist  $\sqsubseteq \geq 1 \text{ actedIn}.\text{Blockbuster}$**

**SuccessfulArtist(RobertDowneyJr)**

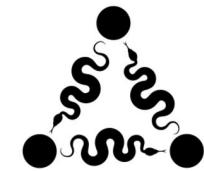
**actedIn  $\sqsubseteq \text{participated}$**

Logically consistent collection of axioms

# Vector: Embeddings



# KG Embeddings: PyKEEN 1.0



PyKEEN

- PyTorch 😍
- 13 datasets + your own graphs
- 23 KG embedding models and counting
  
- 7 losses
- 6 optimizers
- 6 metrics
- 5 regularizers
- 2 training loops
- 2 negative samplers
- Tracking in MLFlow, WANDB

build passing License MIT DOI 10.5281/zenodo.3982977 Optuna integrated

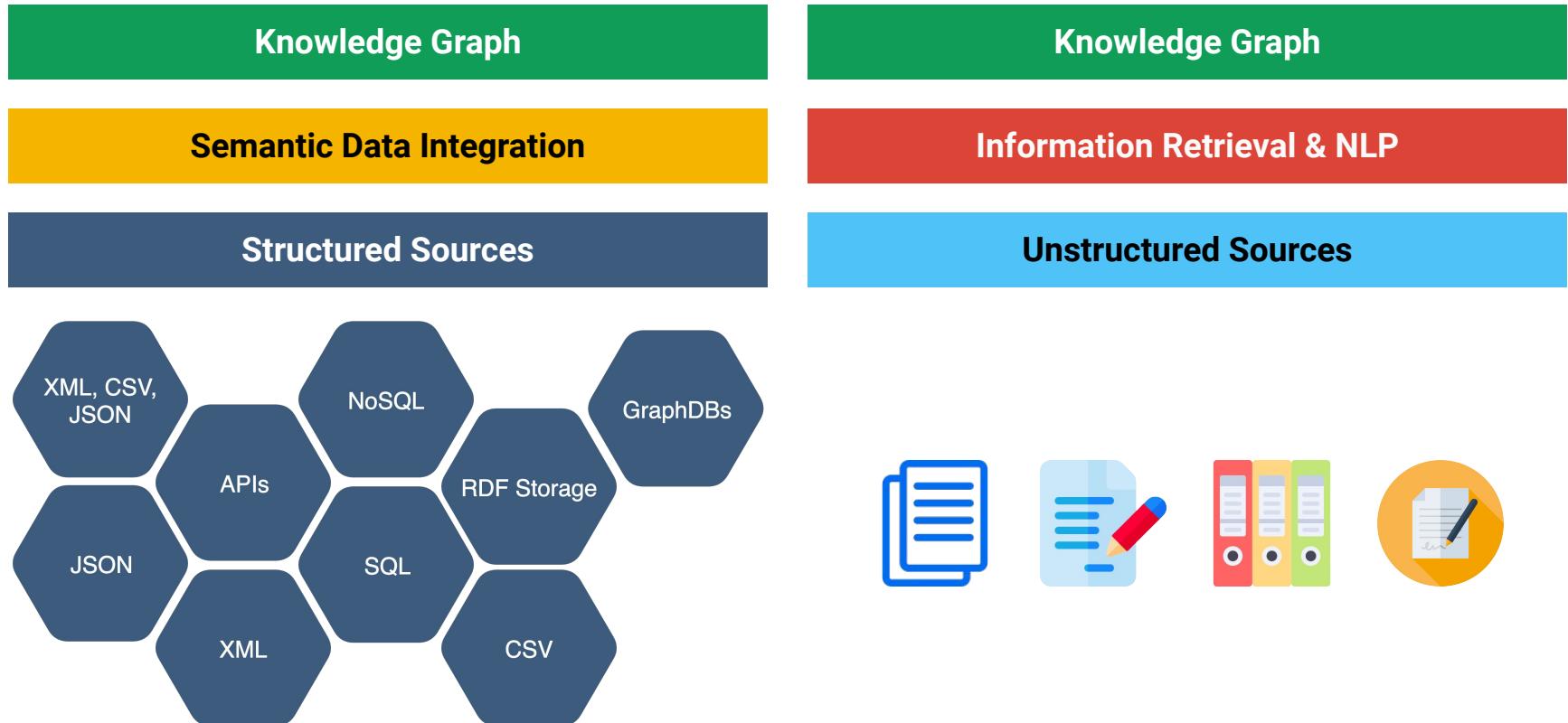
<https://github.com/pykeen/pykeen>



Benchmarked!

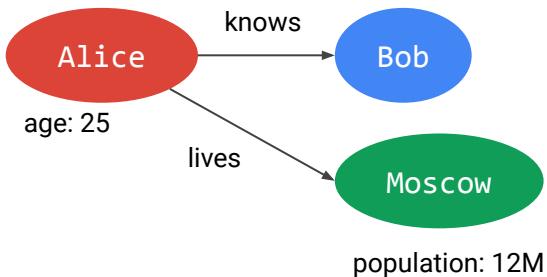
Ali et al. Bringing Light Into the Dark: A Large-scale Evaluation of Knowledge Graph Embedding Models Under a Unified Framework. arxiv:2006.13365

# Building KGs

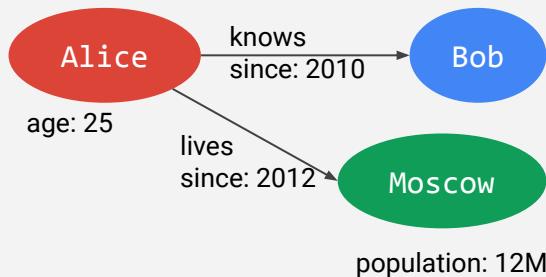


# Graph Databases

## RDF



## LPG (Labeled Property Graph)

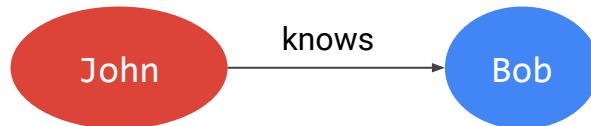


- Query language: SPARQL
- Predicate attributes only from RDFS/OWL
- Semantic schema
- Logical reasoning

- Query languages: Cypher, Gremlin, GraphQL
- Key-value predicate attributes
- Non-semantic schema
- No reasoning

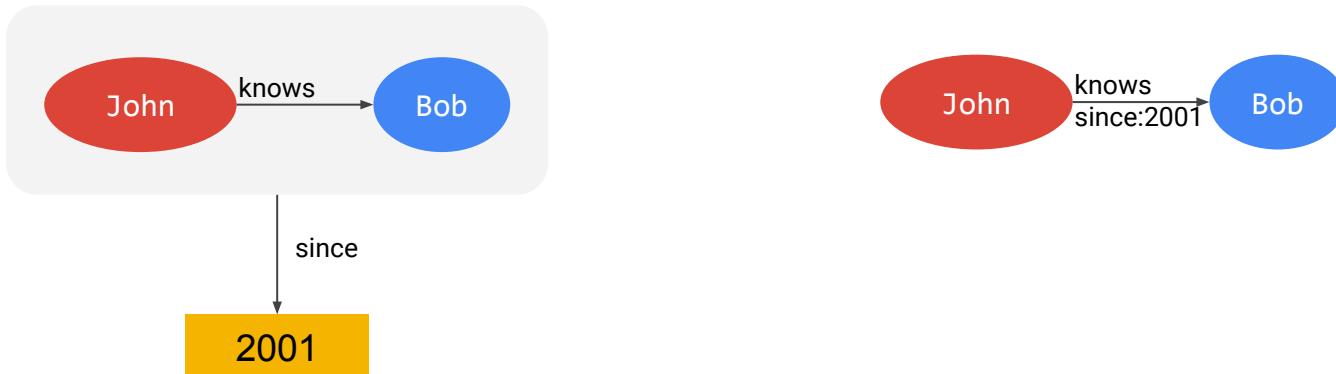
# Graph Databases - Queries

SPARQL	Cypher
<pre>SELECT ?s ?friend WHERE {     ?s a :Person;     :name "John" ;     :knows ?friend .}</pre>	<pre>MATCH (s:Person)-[:knows]-(friend) WHERE s.name = "John" RETURN s, friend ;</pre>



# Graph Databases - Queries

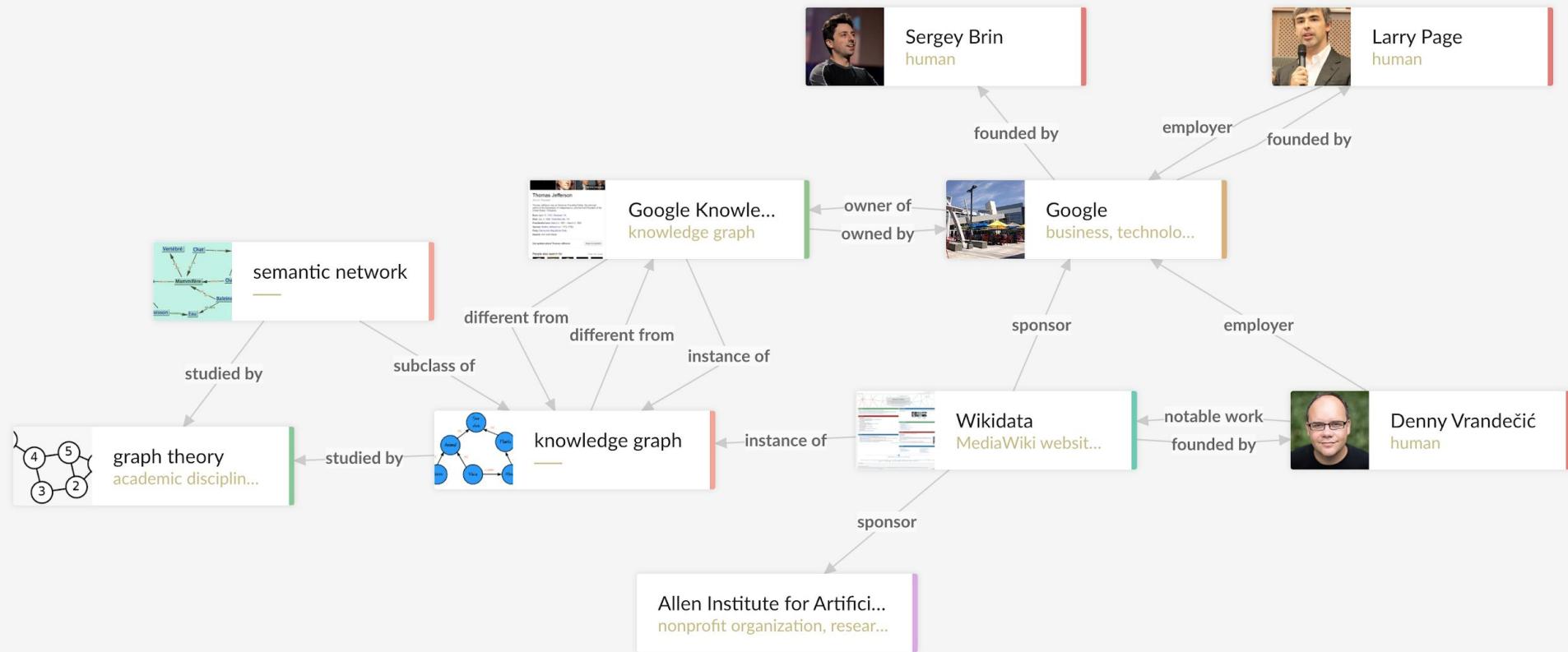
SPARQL* (Reification)	Cypher
<pre>SELECT ?s WHERE { &lt;&lt;?s :knows :js&gt;&gt; :since 2001 }</pre>	<pre>MATCH (s:Person)-[ :knows {since:2001}] -&gt; (js) RETURN s;</pre>



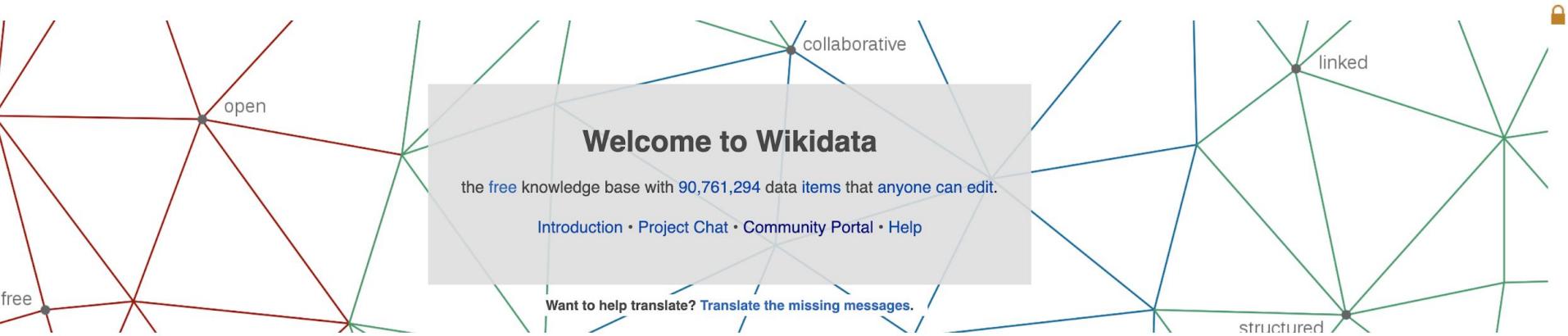
# Knowledge Graphs in the Wild



# Knowledge Graphs in the Wild



# www.wikidata.org



**90M+**

**1150M+**

**6K+**

entities

statements

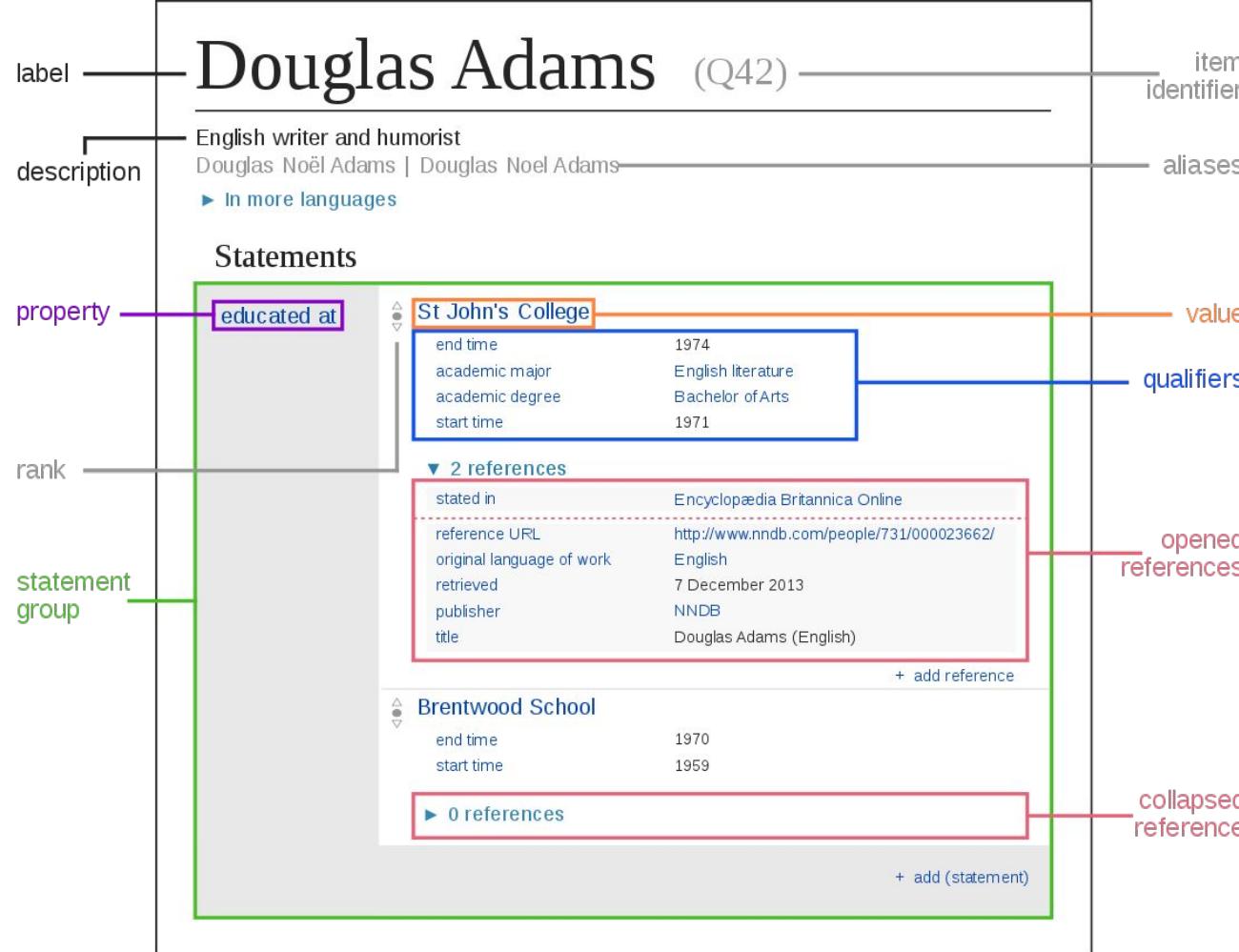
properties

**(nodes)**

**(edges)**

**(edge types)**

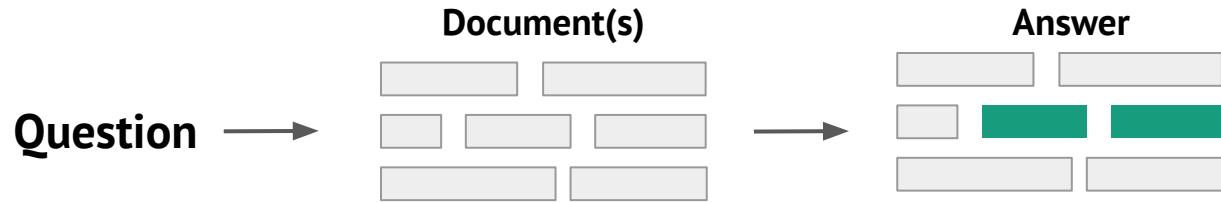
# Wikidata Data Model



# Question Answering



Machine Reading  
Comprehension



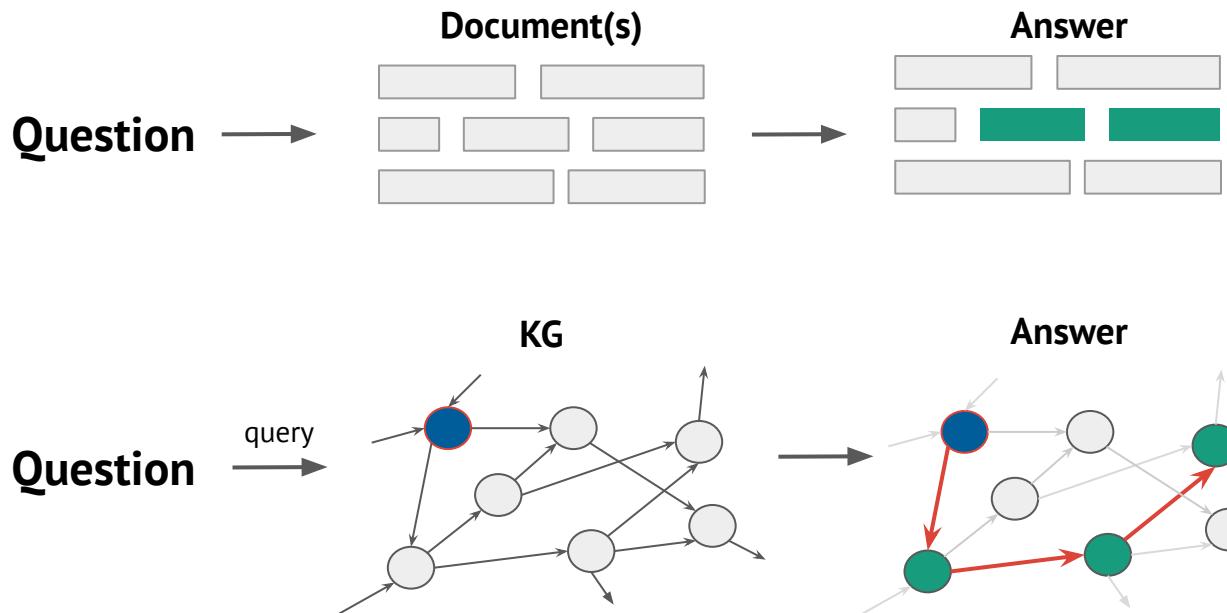
# Question Answering

MRC

Machine Reading  
Comprehension

KGQA

Knowledge Graph-based  
Question Answering

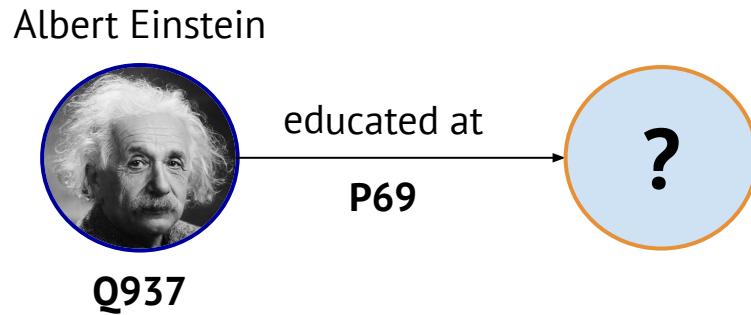


# ✓ Simple KGQA

Pretty much solved!

1-hop

Factoid  
questions



Where was Albert Einstein educated?

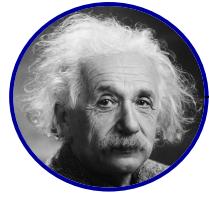
# ✓ Simple KGQA

Pretty much solved!

1-hop

Factoid  
questions

Albert Einstein



Q937

educated at  
P69

?

Where was Albert Einstein educated?

University  
of Zurich



ETH  
Zurich



	Entity Span Accuracy	Relation Avg. F1	Accuracy
BiLSTM	93.2	96.7	82.4
BERT	95.2	97.5	83.5

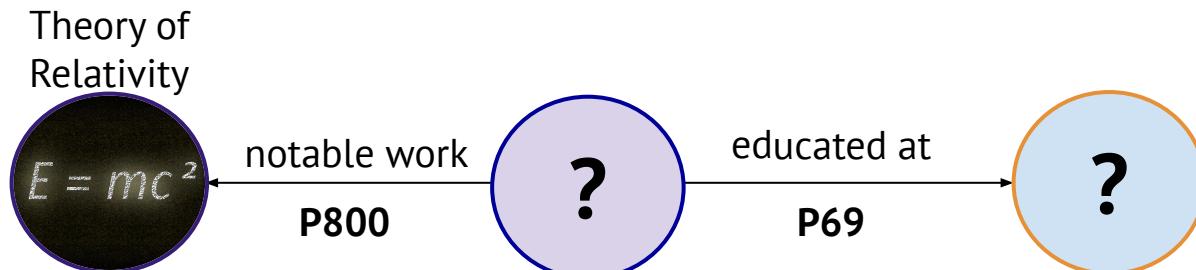
# Complex KGQA

Where was the author of the theory of relativity educated?

Multi-hop

Complex

FOL / EPFO  
queries



$Q = y, \exists x: \text{notableWork}(x, \text{Theory of Relativity}) \wedge \text{educatedAt}(x, y)$

# Complex Question Answering

Large KGs (Wikidata-scale)

>1M triples

Build SPARQL queries  
Execute against a graph database

Supervised ML methods as certain  
pipeline components

Smaller KGs

< 1M triples

In-memory neural reasoning  
Graph embeddings

End-to-end or mostly neural

# Complex Question Answering

Large KGs (Wikidata-scale)

Smaller KGs

Pre-defined SPARQL templates

Neural Multi-Hop Reasoning

NL -> SPARQL pipelines

Query Embedding

# Complex Question Answering

Large KGs (Wikidata-scale)

Smaller KGs

Pre-defined SPARQL templates

Neural Multi-Hop Reasoning

NL -> SPARQL pipelines

Query Embedding

# Template-based QA

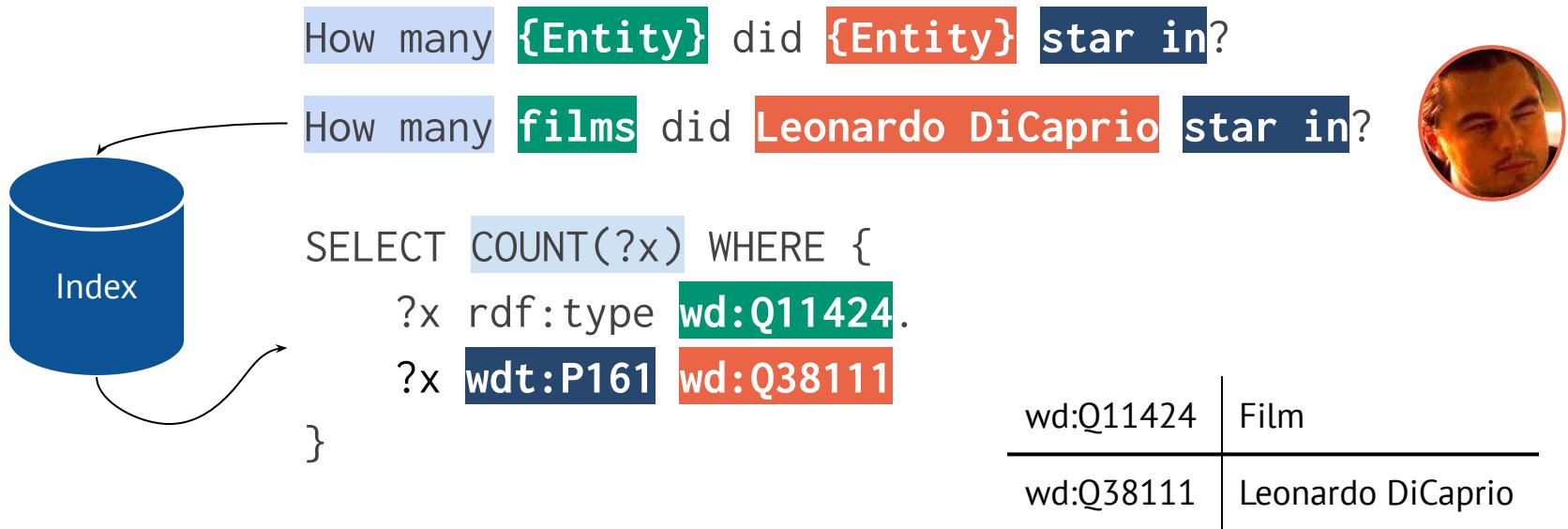
Natural  
language

How many {Entity} did {Entity} star in?

Pre-defined  
template

```
SELECT COUNT(?x) WHERE {  
    ?x rdf:type ?c.  
    ?x wdt:P161 ?y  
}
```

# Template-based QA



# Template-based QA

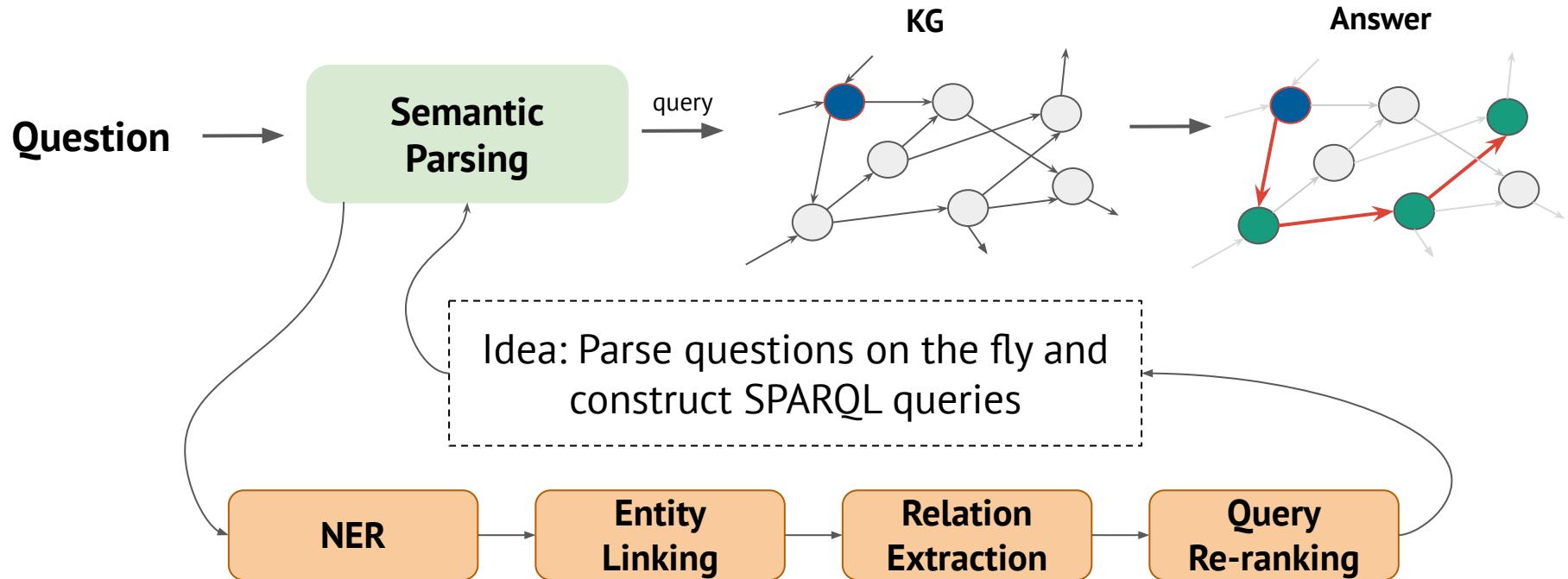
## Pros

- Independent of the KG size
- Fast & parallelizable
- Explainable query results

## Cons

- **Manual** curation of templates  
(100+ is already hard to sustain)
- Each new question formulation  
will require a **new** template
- **Hard-coded** to the KG schema  
(ontology)

# Pipelines: Semantic Parsing





# Pipelines: QAmp

2nd hop	1st hop					
(a) Q: Which <u>company</u>	<u>assembles</u>	its	<u>hardtop</u>	<u>style</u>	<u>cars</u>	in <u>Broadmeadows, Victoria</u> ?
$P_1^2$	$P_1^1$		$E_1^1$	$P_2^1$	$C_1^1$	$E_2^1$
dbo:company 1	dbo:assembly 0.9		<b>dbr:Hardtop 1</b>	<b>dbo:Automobile 1</b>	<b>dbr:Broadmeadows,_Victoria 0.9</b>	
dbp:companyLogo 0.8	<b>dbp:assembly 0.9</b>			dbr:Car 1		dbr:Victoria 0.2
<b>dbo:parentCompany 0.8</b>			<b>dbo:bodyStyle 0.5</b>			

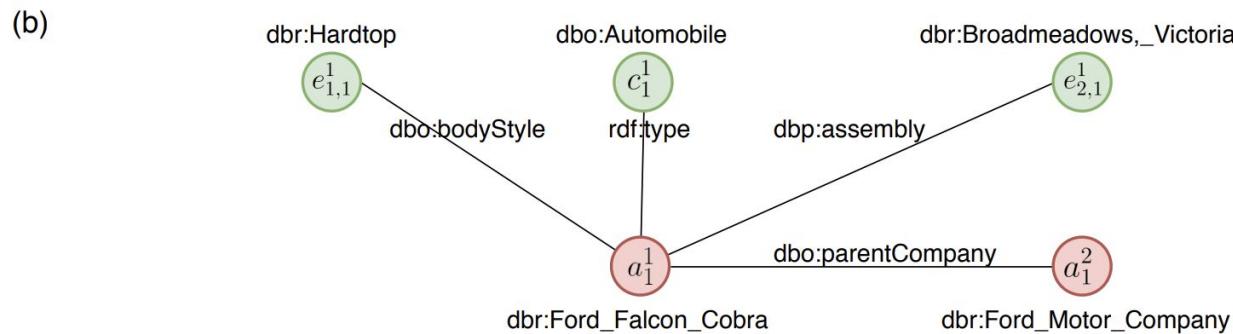


Figure 1: (a) A sample question  $Q$  highlighting different components of the question interpretation model: references and matched URIs with the corresponding confidence scores, along with (b) the illustration of a sample KG subgraph relevant to this question. The URIs in bold are the correct matches corresponding to the KG subgraph.

# Pipelines: QAmp

- Storage & Querying & subgraph retrieval: [HDT](#)
- Entity Linking: ElasticSearch + FastText

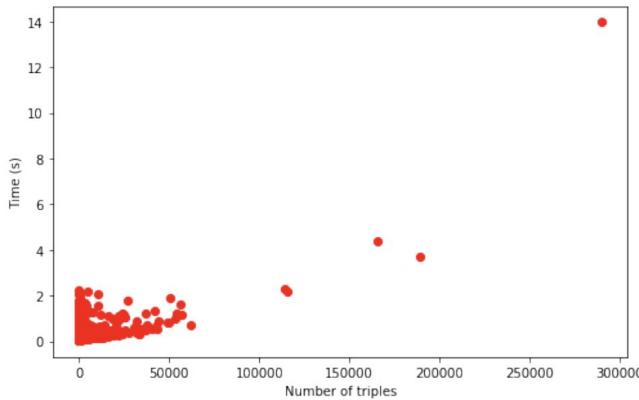


Figure 5: Processing times per question from the LC-QuAD test split (Min: 0.01s Median: 0.68s Mean: 0.72s Max: 13.97s)

Approach	P	R	F	Runtime
WDAqua	0.22*	0.38	0.28	1.50 s/q
QAmp (our approach)	0.25	0.50	0.33	0.72 s/q

# Pipelines: Krantikari

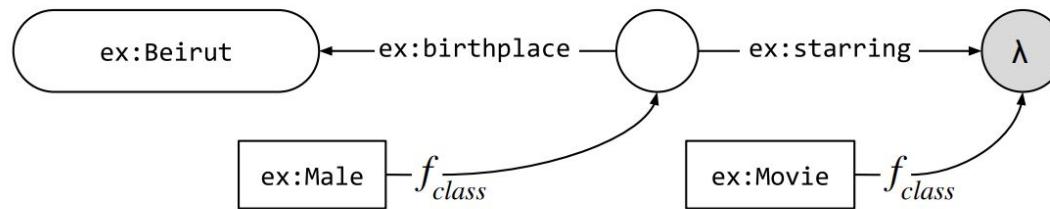


Idea: (1) mine core chains (relation paths) from a KG;  
 (2) re-rank the chains using slot attention

Name some movies starring Beirut born male actors?

- birthplace + starring

type	$\lambda$ , ex:Movie
type	$\exists$ , ex:Male



(a) *Question, and corresponding Query Graph*

# Pipelines: Krantikari

LSTM

	LC-QuAD					QALD-7				
	CCA	MRR	P	R	F1	CCA	MRR	P	R	F1
BiLSTM [9]	0.61	0.70	0.63	0.75	0.68	0.28	0.41	0.20	0.36	0.26
CNN [11]	0.44	0.55	0.49	0.61	0.54	0.31	<b>0.45</b>	0.20	0.33	0.25
DAM [16]	0.57	0.66	0.59	0.72	0.65	0.28	0.40	0.20	0.36	0.26
HRM [24]	0.62	0.71	0.64	0.77	0.70	0.28	0.40	0.15	0.31	0.20
<b>Slot-Matching (LSTM)</b>	<b>0.63</b>	<b>0.72</b>	<b>0.65</b>	<b>0.78</b>	<b>0.71</b>	<b>0.31</b>	0.44	<b>0.28</b>	<b>0.44</b>	<b>0.34</b>

Table 1: Performance on LC-Quad and QALD-7. The reported metrics are core chain accuracy (CCA), mean reciprocal rank (MRR) of the core chain rankings, as well as precision (P), recall (R), and the F1 of the execution results of the whole system.

BERT

	QALD-7		LC-QuAD
	BERT	Slot Matching (BERT)	
BERT	<b>0.23</b>	0.18	0.67
Slot Matching (BERT)			<b>0.68</b>

Table 3: CCA for slot matching model, as proposed in Sec 4.2 initialized with the weights of BERT-Small, compared with regular transformers initialized with the same weights.

# NL 2 SPARQL

## Pros

- Some supervised ML can be applied
- Transfer learning works
- Component ↑ -> Performance ↑
- Explainable query results

## Cons

- **Fast** retrieval & communication to the KG is **essential**
- A **Snowball effect** of components error propagation
- **Brute-force** heuristics, e.g., extract a 2-hop subgraph & rank; extract all k-long relation paths and rank



Play around  
today with  
**DeepPavlov!**

## Template-based KGQA

```
from deeppavlov import configs, build_model

kbqa_model = build_model(configs.kbqa.kbqa_cq, download=True)
kbqa_model(['Magnus Carlsen is a part of what sport?'])
>>> ["chess"]

kbqa_model = build_model(configs.kbqa.kbqa_cq_rus, download=True)
kbqa_model(['Когда родился Пушкин?'])
>>> ["1799-05-26"]
```

# Complex Question Answering

Large KGs (Wikidata-scale)

Smaller KGs

Pre-defined SPARQL templates

Neural Multi-Hop Reasoning

NL -> SPARQL pipelines

Query Embedding

Where did Canadian citizens with Turing Award graduate?

```
SELECT ?y WHERE {  
    ?x :win      :TuringAward .  
    ?x :citizen   :Canada .  
    ?x :graduate  ?y . }
```

query

## Structured Sources



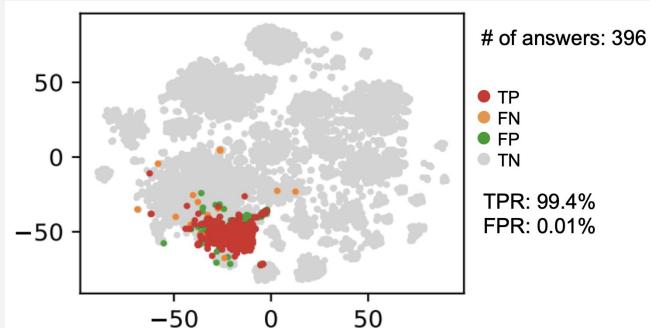
KGs are sparse and incomplete



Where did Canadian citizens with Turing Award graduate?

```
SELECT ?y WHERE {  
    ?x :win      :TuringAward .  
    ?x :citizen   :Canada .  
    ?x :graduate   ?y . }
```

embed



## Execution in a vector space

Ren et al. Query2box: Reasoning over Knowledge Graphs in Vector Space Using Box Embeddings. ICLR 2020

Daza et al. Message Passing Query Embedding. GRL @ ICML 2020  
cs224w.snap.stanford.edu

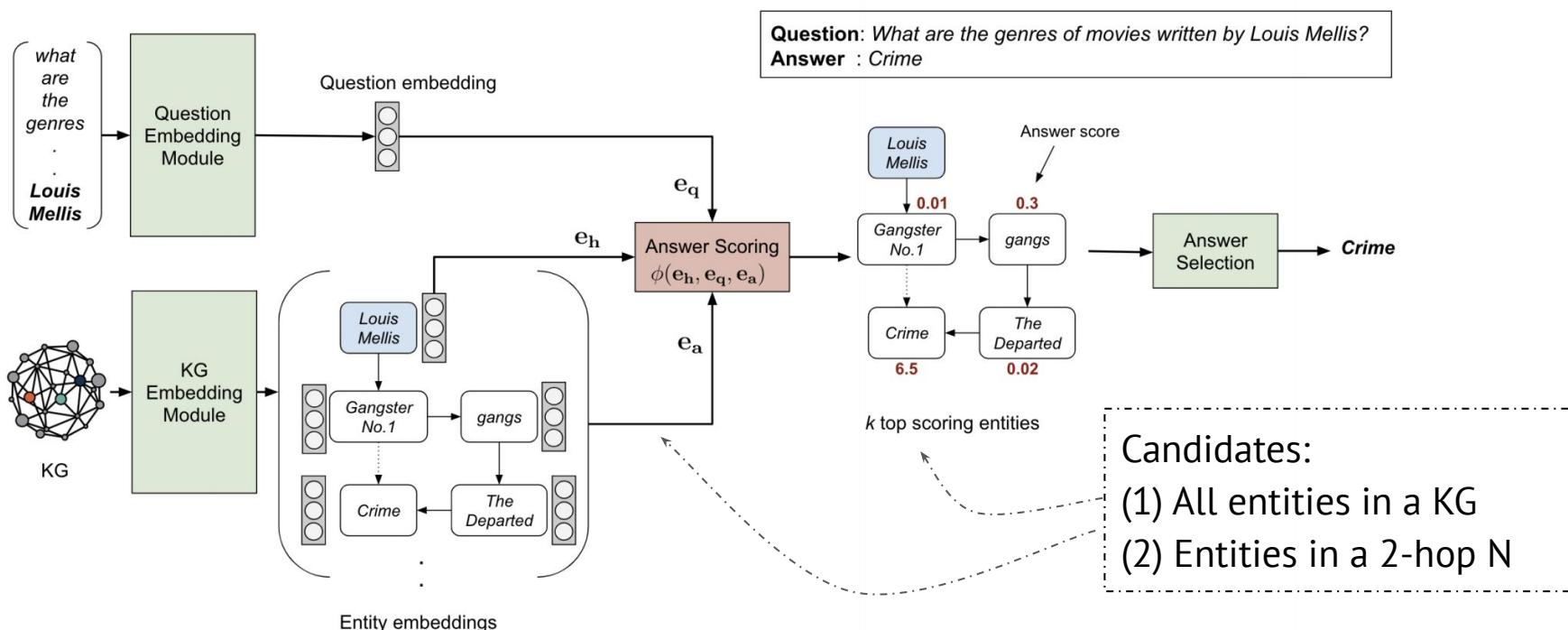


# EmbedKGQA

## Neural Multi-Hop Reasoning



Idea: score a triple (entity, question, answer)



# EmbedKGQA

## Neural Multi-Hop Reasoning

Additional training task: 1-hop link prediction

Model	MetaQA KG-Full			MetaQA KG-50		
	1-hop	2-hop	3-hop	1-hop	2-hop	3-hop
VRN	<b>97.5</b>	89.9	62.5	-	-	-
GraftNet	97.0	94.8	77.7	64.0 (91.5)	52.6 (69.5)	59.2 (66.4)
PullNet	97.0	<b>99.9</b>	91.4	65.1 (92.4)	52.1 (90.4)	59.7 (85.2)
KV-Mem	96.2	82.7	48.9	63.6 (75.7)	41.8 (48.4)	37.6 (35.2)
EmbedKGQA (Ours)	<b>97.5</b>	98.8	<b>94.8</b>	<b>83.9</b>	<b>91.8</b>	<b>70.3</b>

Model	WebQSP KG-Full	WebQSP KG-50
KV-Mem	46.7	32.7 (31.6)
GraftNet	66.4	48.2 (49.7)
PullNet	<b>68.1</b>	50.1 (51.9)
EmbedKGQA	66.6	<b>53.2</b>

**43k** entities  
**9** relations  
**135k** triples

**1.8M** entities  
**5.7M** triples  
**8** GPUs ;)

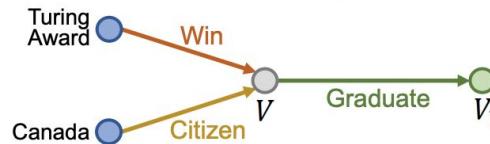
# Query2Box

## Query Embedding

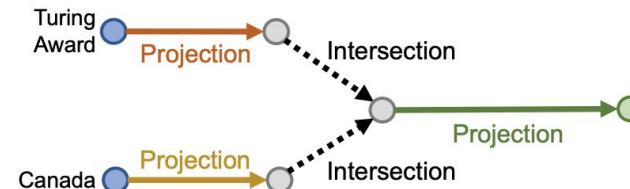
Subset of SPARQL - EPFO queries: Conjunctive + disjunction

**(A) Query  $q$  and Its Dependency Graph**

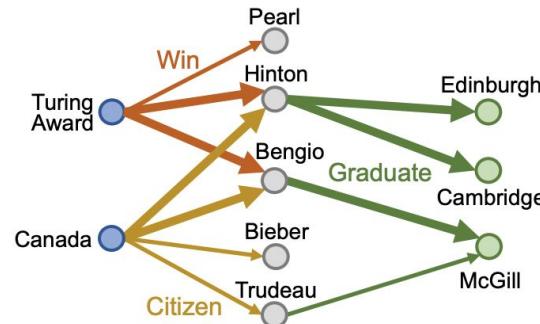
$$q = V_? . \exists V : \text{Win}(\text{TuringAward}, V) \wedge \text{Citizen}(\text{Canada}, V) \wedge \text{Graduate}(V, V_?)$$



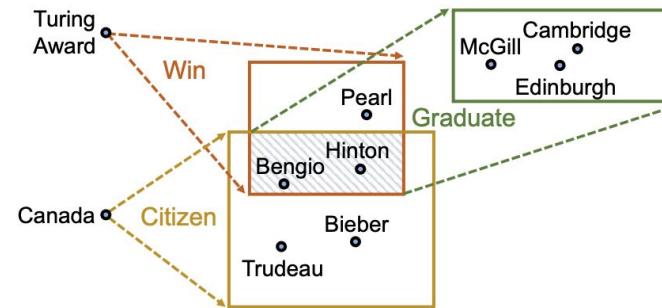
**(B) Computation Graph**



**(C) Knowledge Graph Space**



**(D) Vector Space**



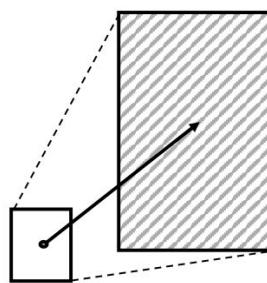
# Query2Box

Query Embedding

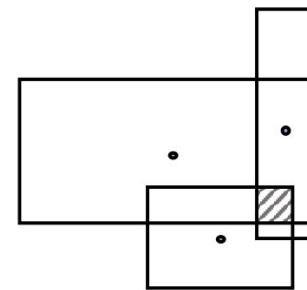


Idea: represent entities as d-dimensional boxes!

(A) Projection



(B) Intersection



(C) Distance

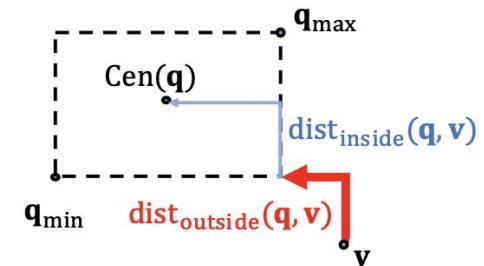


Figure 2: The geometric intuition of the two operations and distance function in QUERY2BOX. **(A)** Projection generates a larger box with a translated center. **(B)** Intersection generates a smaller box lying inside the given set of boxes. **(C)** Distance  $\text{dist}_{\text{box}}$  is the weighted sum of  $\text{dist}_{\text{outside}}$  and  $\text{dist}_{\text{inside}}$ , where the latter is weighted less.

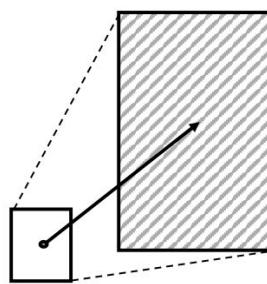
# Query2Box



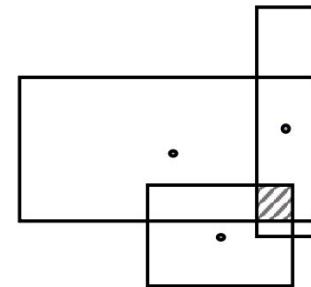
Query Embedding

Idea: represent entities as d-dimensional boxes!

(A) Projection



(B) Intersection



(C) Distance

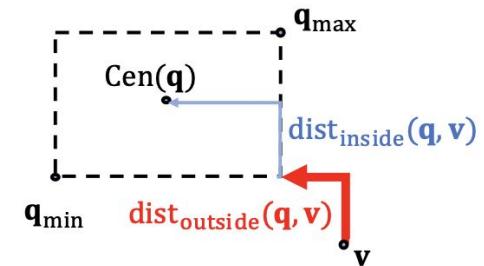


Figure 2: The geometric intuition of the two operations and distance function in QUERY2BOX. **(A)** Projection generates a larger box with a translated center. **(B)** Intersection generates a smaller box lying inside the given set of boxes. **(C)** Distance  $\text{dist}_{\text{box}}$  is the weighted sum of  $\text{dist}_{\text{outside}}$  and  $\text{dist}_{\text{inside}}$ , where the latter is weighted less.

Intersection  
operator

$$\text{Cen}(\mathbf{p}_{\text{inter}}) = \sum_i \mathbf{a}_i \odot \text{Cen}(\mathbf{p}_i), \quad \mathbf{a}_i = \frac{\exp(\text{MLP}(\mathbf{p}_i))}{\sum_j \exp(\text{MLP}(\mathbf{p}_j))},$$

$$\text{Off}(\mathbf{p}_{\text{inter}}) = \text{Min}(\{\text{Off}(\mathbf{p}_1), \dots, \text{Off}(\mathbf{p}_n)\}) \odot \sigma(\text{DeepSets}(\{\mathbf{p}_1, \dots, \mathbf{p}_n\})),$$

# Query2Box

Query Embedding

Theorem

Modeling any EPFO query needs  $O(|E|)$  params

# Query2Box

## Query Embedding

Theorem

Modeling any EPFO query needs  $O(|E|)$  params

Approach

Convert all queries to the DNF (union as the last step)

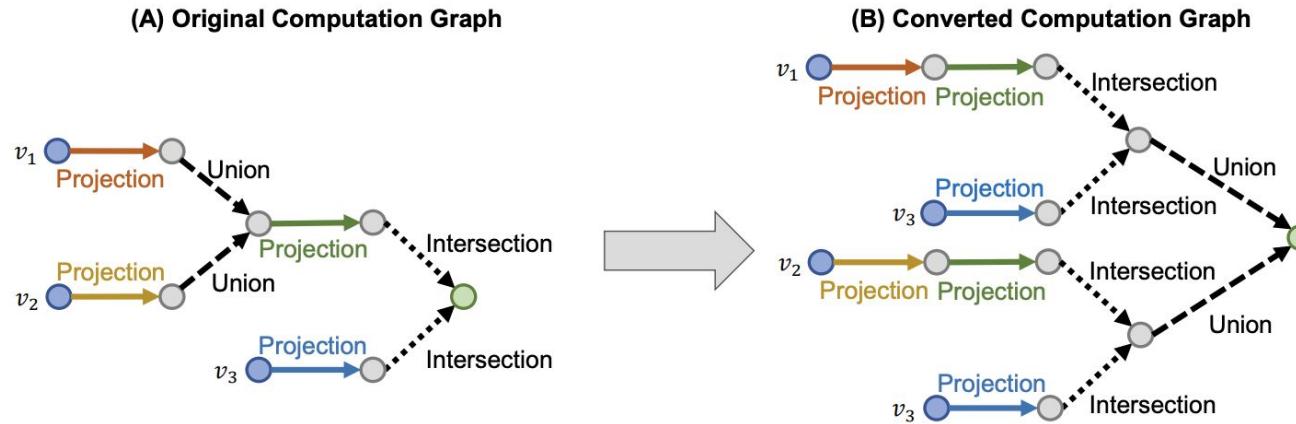


Figure 3: Illustration of converting a computation graph of an EPFO query into an equivalent computation graph of the Disjunctive Normal Form.

# Query2Box

## Query Embedding

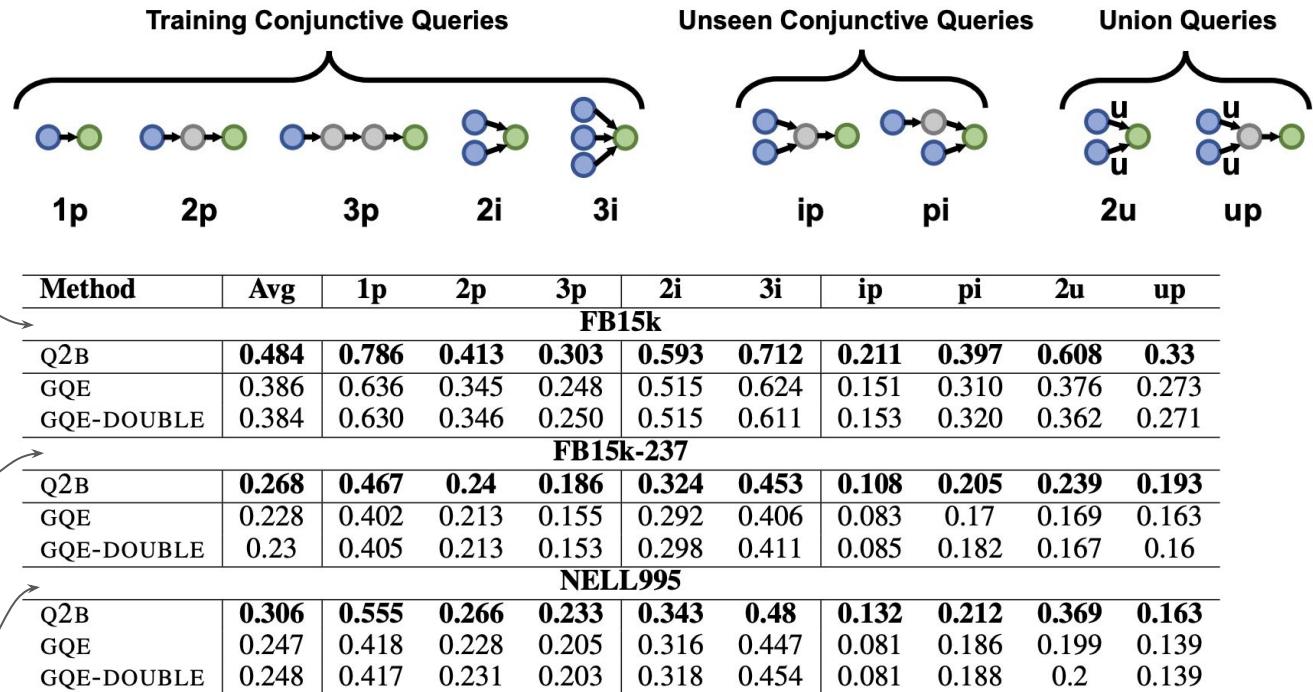
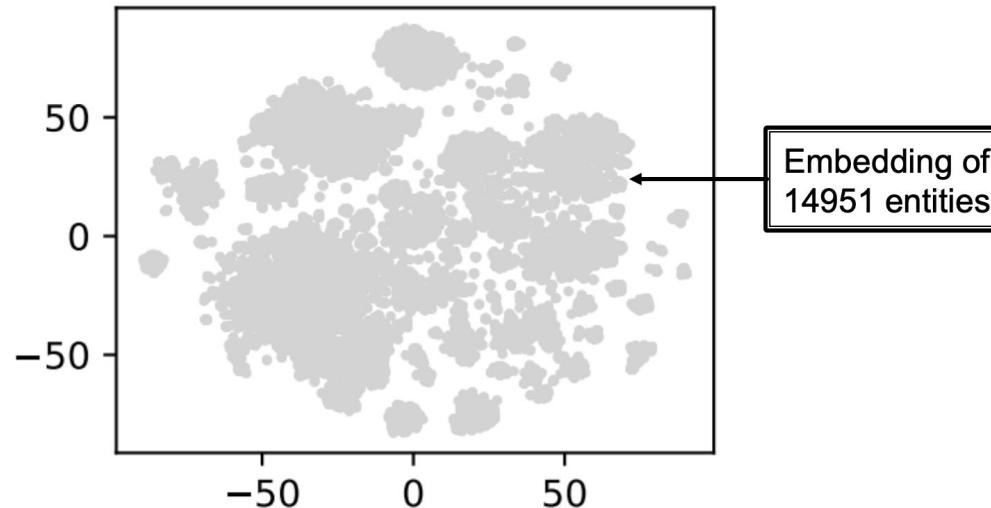


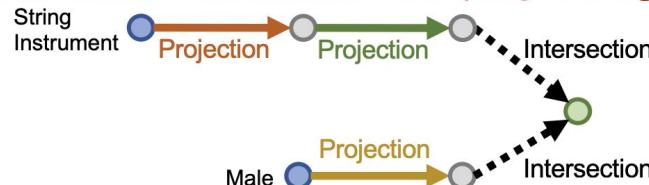
Table 2: H@3 results of QUERY2BOX vs. GQE on FB15k, FB15k-237 and NELL995.

# Query2Box

## Query Embedding

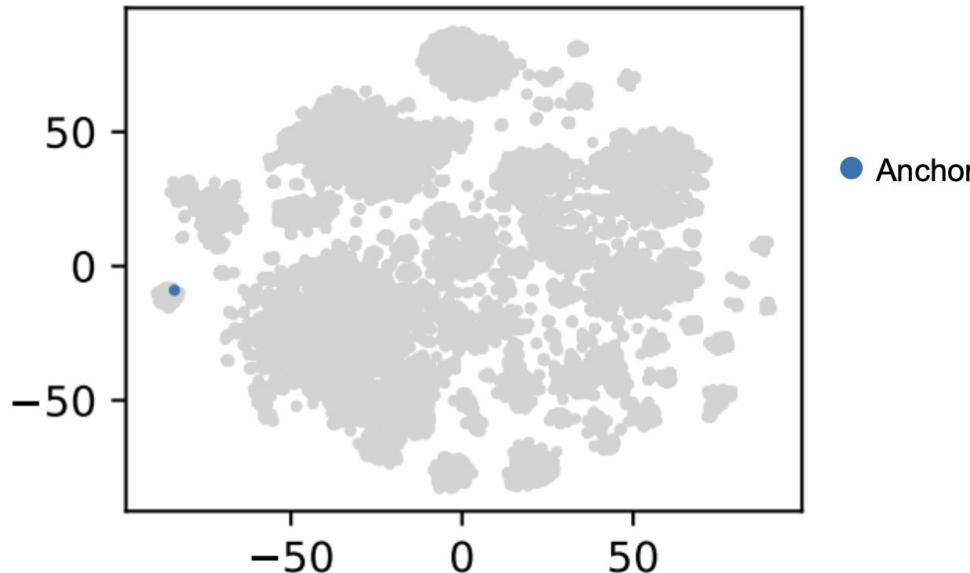


“List male instrumentalists who play string instruments”



# Query2Box

Query Embedding

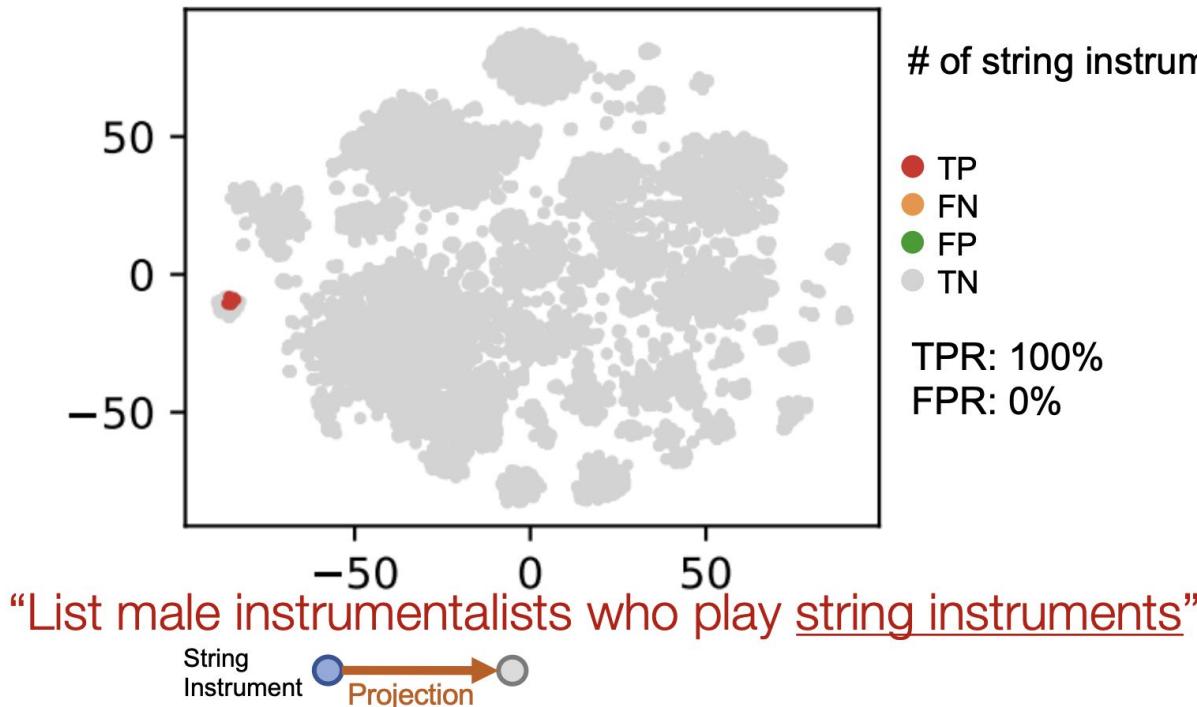


“List male instrumentalists who play string instruments”

String  
Instrument

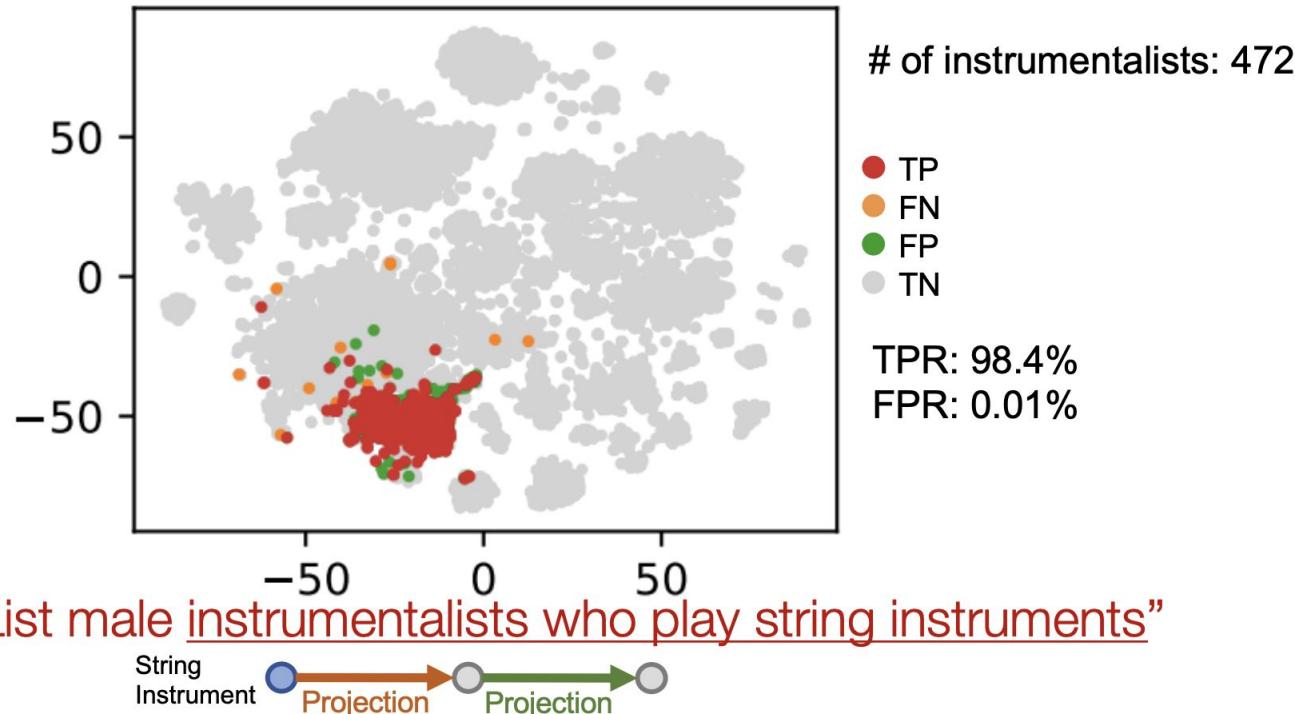
# Query2Box

## Query Embedding



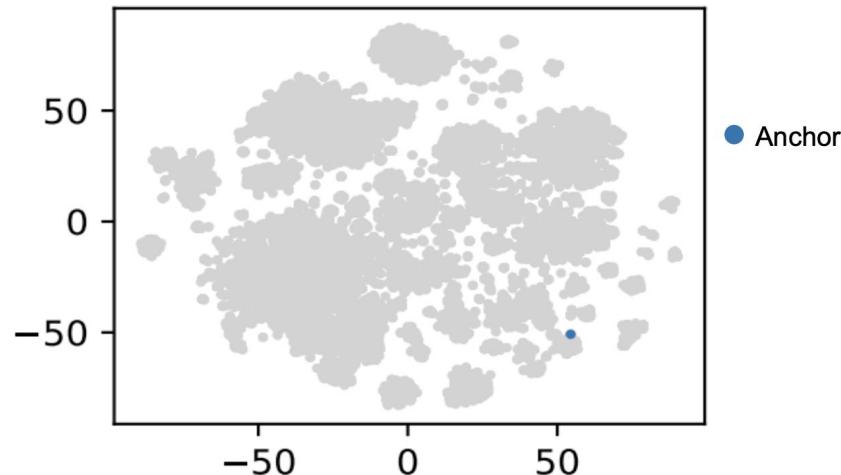
# Query2Box

## Query Embedding



# Query2Box

## Query Embedding

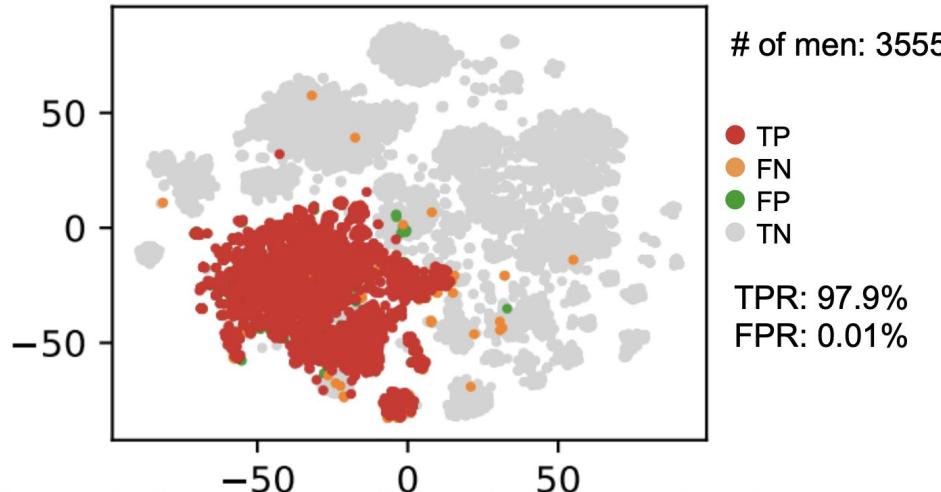


“List male instrumentalists who play string instruments”

Male

# Query2Box

## Query Embedding

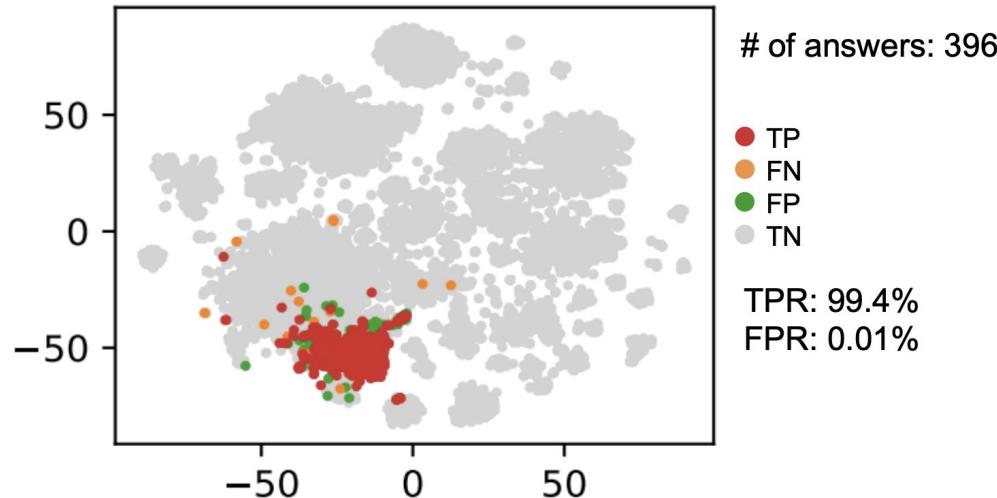


“List male instrumentalists who play string instruments”

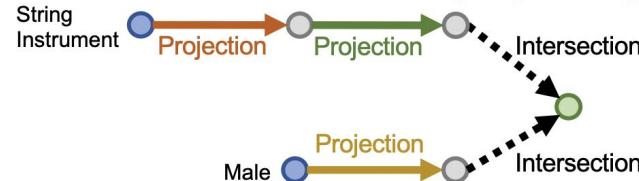


# Query2Box

## Query Embedding



"List male instrumentalists who play string instruments"



# Neural Reasoning

## Pros

- No database & query engine needed
- No SPARQL / other queries
- We can work with incomplete KGs:  
infer new facts and predict links

## Cons

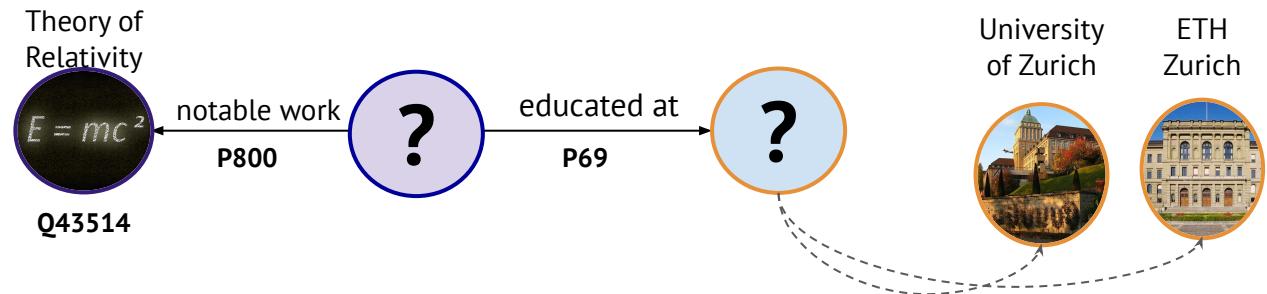
- **Hardly scalable** to large graphs
- Often **not explainable** results
- Computationally **expensive**
- Problems handling **literals**

# Challenges: Answer Verbalization

Input Question

Where was the author of the theory of relativity educated?

Answer

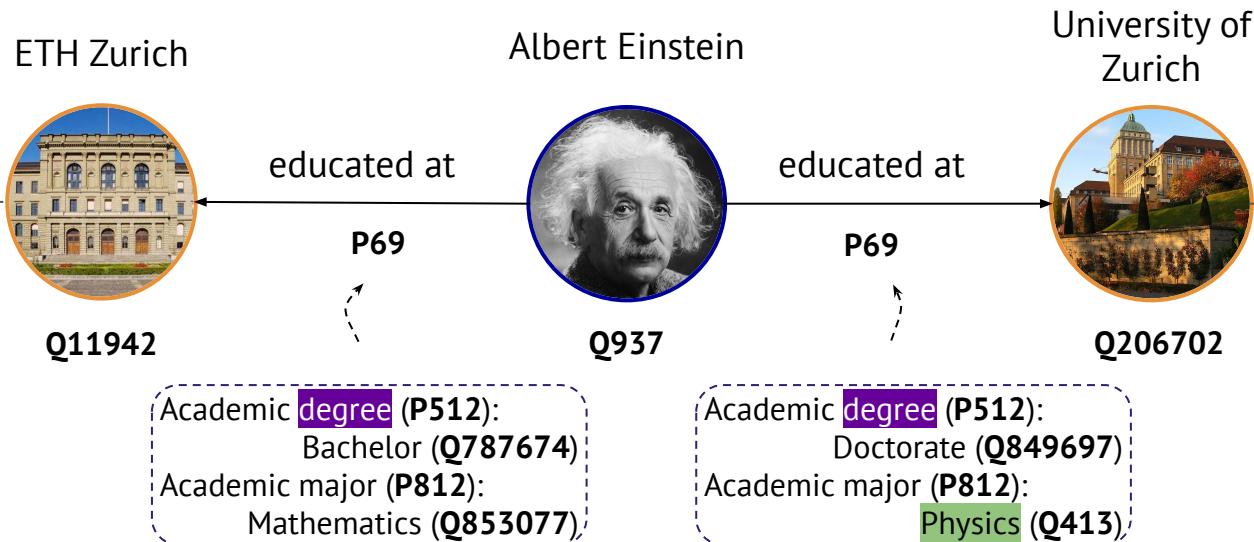


Human-friendly Answer

The author of the theory of relativity educated at the University of Zurich and ETH Zurich.

# Challenges: Hyper-Relational KGs

Where did **Albert Einstein** receive his **degree** in **physics**?



# Multirelational GNN Encoders for KGs

$$\mathbf{h}_v^{(k)} = f \left( \sum_{u \in \mathcal{N}(v)} \mathbf{W}^{(k)} \mathbf{h}_u^{(k-1)} \right)$$

Vanilla GCN [1]: no relations

$$\mathbf{h}_v^{(k)} = f \left( \sum_{(u,r) \in \mathcal{N}(v)} \mathbf{W}_r^{(k)} \mathbf{h}_u^{(k-1)} \right)$$

R-GCN [2]: a whole matrix  $\mathbf{W}$  per relation

$$\mathbf{h}_v = f \left( \sum_{(u,r) \in \mathcal{N}(v)} \mathbf{W}_{\lambda(r)} \phi(\mathbf{x}_u, \mathbf{z}_r) \right)$$

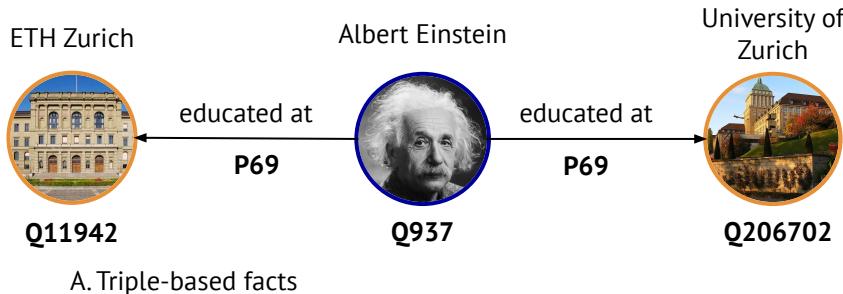
CompGCN [3]: a vector  $\mathbf{z}_r$  per relation +  
composition of  $(h,r)$  +  
only 3 different  $\mathbf{W}$ : input/output/self-loop

[1] Kipf et al. Semi-supervised Classification with Graph Convolutional Networks. ICLR 2017

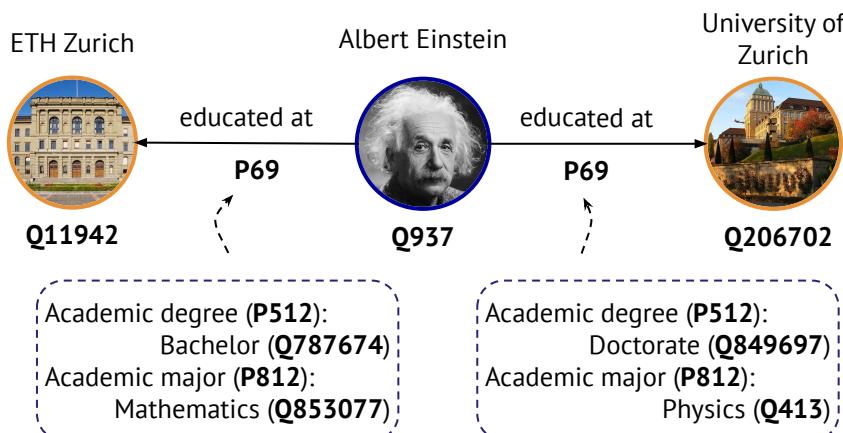
[2] Schlichtkrull et al. Modeling Relational Data with Graph Convolutional Networks. ESWC 2018

[3] Vashisht et al. Composition-Based Multi-Relational Graph Convolutional Networks. ICLR 2020

# Embedding Hyper-Relational KGs



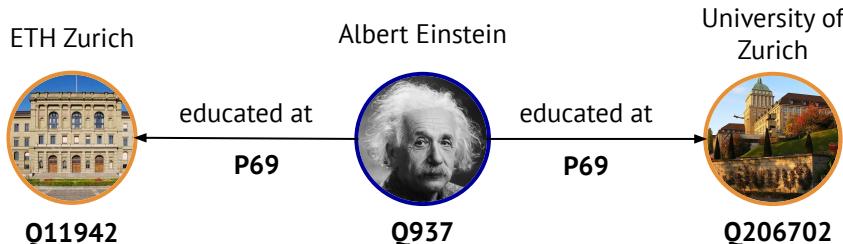
$$\mathbf{h}_v = f \left( \sum_{(u,r) \in \mathcal{N}(v)} \mathbf{W}_{\lambda(r)} \phi(\mathbf{x}_u, \mathbf{z}_r) \right)$$



?

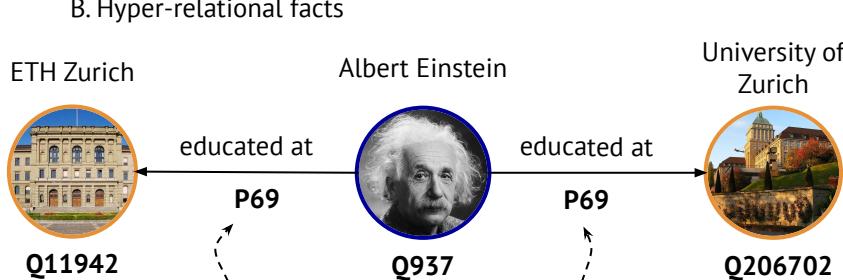
- Qualifying relations and entities can be used as main terms in other facts
- Not all facts might have qualifiers

# Embedding Hyper-Relational KGs



A. Triple-based facts

$$\mathbf{h}_v = f \left( \sum_{(u,r) \in \mathcal{N}(v)} \mathbf{W}_{\lambda(r)} \phi(\mathbf{x}_u, \mathbf{z}_r) \right)$$

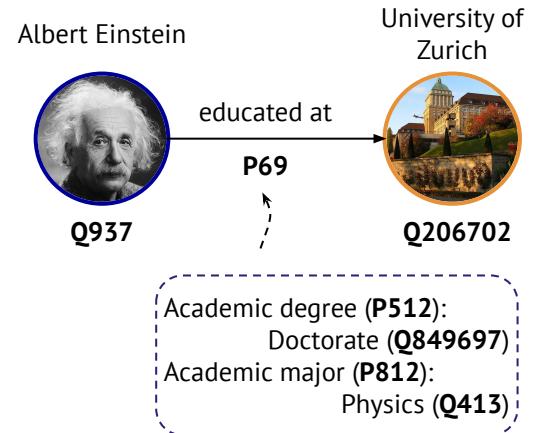
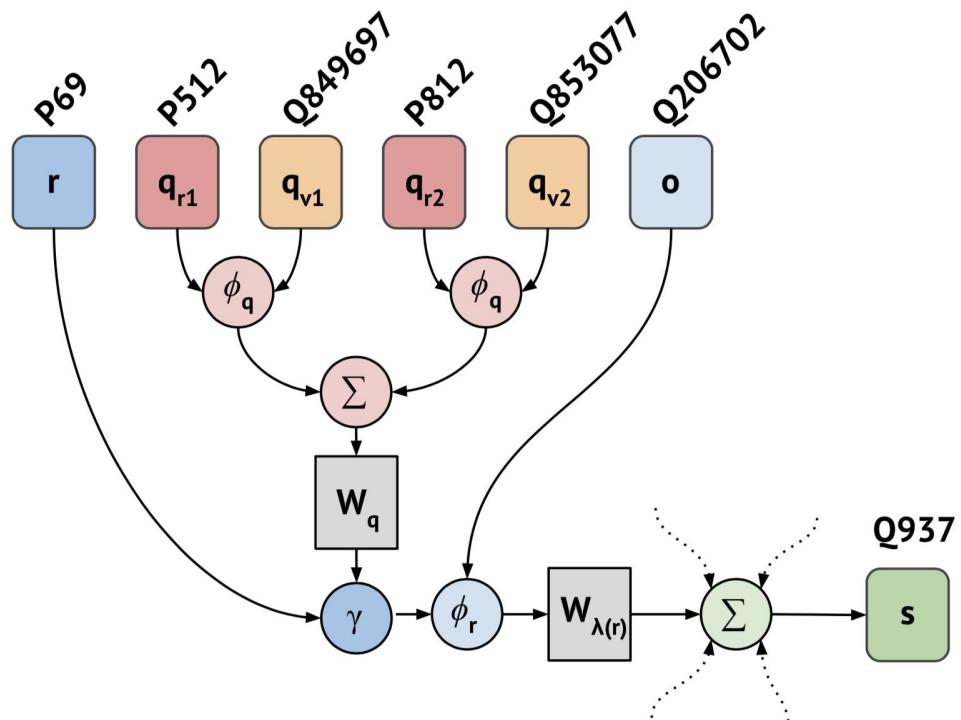


Academic degree (P512):  
Bachelor (Q787674)  
Academic major (P812):  
Mathematics (Q853077)

Academic degree (P512):  
Doctorate (Q849697)  
Academic major (P812):  
Physics (Q413)

$$\mathbf{h}_v = f \left( \sum_{(u,r) \in \mathcal{N}(v)} \mathbf{W}_{\lambda(r)} \phi_r(\mathbf{h}_u, \gamma(\mathbf{h}_r, \mathbf{h}_q)_{vu}) \right)$$

# ★ StarE: Embedding Hyper-Relational KGs



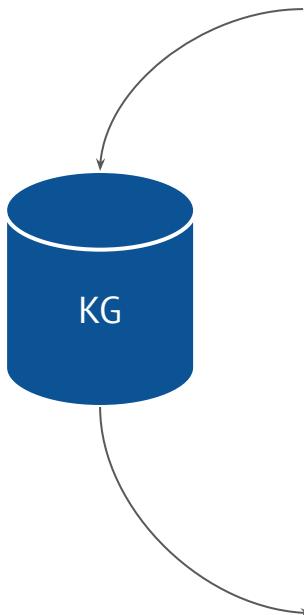
$$\mathbf{h}_v = f \left( \sum_{(u,r) \in \mathcal{N}(v)} \mathbf{W}_{\lambda(r)} \phi_r(\mathbf{h}_u, \gamma(\mathbf{h}_r, \mathbf{h}_q)_{vu}) \right)$$

# Hyper-Relational KGs: Link Prediction

Dataset →	WD50K			WD50K (33)			WD50K (66)			WD50K (100)		
	MRR	H@1	H@10									
Baseline (Transformer (T))	0.275	0.207	0.404	0.218	0.158	0.334	0.270	0.197	0.417	0.351	0.261	0.530
STARE (T) + Transformer(T)	0.308	0.228	0.465	0.246	0.173	0.388	0.297	0.212	0.470	0.380	0.276	0.584
NaLP-Fix	0.177	0.131	0.264	0.204	0.164	0.277	0.334	0.284	0.423	0.458	0.398	0.563
HINGE	0.243	0.176	0.377	0.253	0.190	0.372	0.378	0.307	0.512	0.492	0.417	0.636
Baseline (Transformer (H))	0.286	0.222	0.406	0.276	0.227	0.371	0.404	0.352	0.502	0.562	0.499	0.677
STARE (H) + Transformer(H)	<b>0.349</b>	<b>0.271</b>	<b>0.496</b>	<b>0.331</b>	<b>0.268</b>	<b>0.451</b>	<b>0.481</b>	<b>0.420</b>	<b>0.594</b>	<b>0.654</b>	<b>0.588</b>	<b>0.777</b>

- ★ Hyper-relational models **effectively** leverage qualifiers to improve predictions
- ★ The **more** hyper-relational facts - the **better** are predictions
- ★ The improvement upon triple-only models **grows with the ratio** of hyper-relational edges in the KG

# Challenges: Dialogue & Sequential QA



Turn	Books	Movies	Soccer	Music
$q^0$	<i>When was the first book of the book series The Dwarves published?</i> 2003	<i>Who played the joker in The Dark Knight?</i> Heath Ledger	<i>Which European team did Diego Costa represent in the year 2018?</i> Atlético Madrid	<i>Led Zeppelin had how many band members?</i> 4
$q^1$	<i>What is the name of the second book?</i> The War of the Dwarves	<i>When did he die?</i> 22 January 2008	<i>Did they win the Super Cup the previous year?</i> No	<i>Which was released first: Houses of the Holy or Physical Graffiti?</i> Houses of the Holy
$q^2$	<i>Who is the author?</i> Markus Heitz	<i>Batman actor?</i> Christian Bale	<i>Which club was the winner?</i> Real Madrid C.F.	<i>Is the rain song and immigrant song there?</i> No
$q^3$	<i>In which city was he born?</i> Homburg	<i>Director?</i> Christopher Nolan	<i>Which English club did Costa play for before returning to Atlético Madrid?</i> Chelsea F.C.	<i>Who wrote those songs?</i> Jimmy Page
$q^4$	<i>When was he born?</i> 10 October 1971	<i>Sequel name?</i> The Dark Knight Rises	<i>Which stadium is this club's home ground?</i> Stamford Bridge	<i>Name of his previous band?</i> The Yardbirds



# Thanks!



@migalkin



@michael\_galkin



@mgalkin



mikhail.galkin@iais.fraunhofer.de



migalkin.github.io