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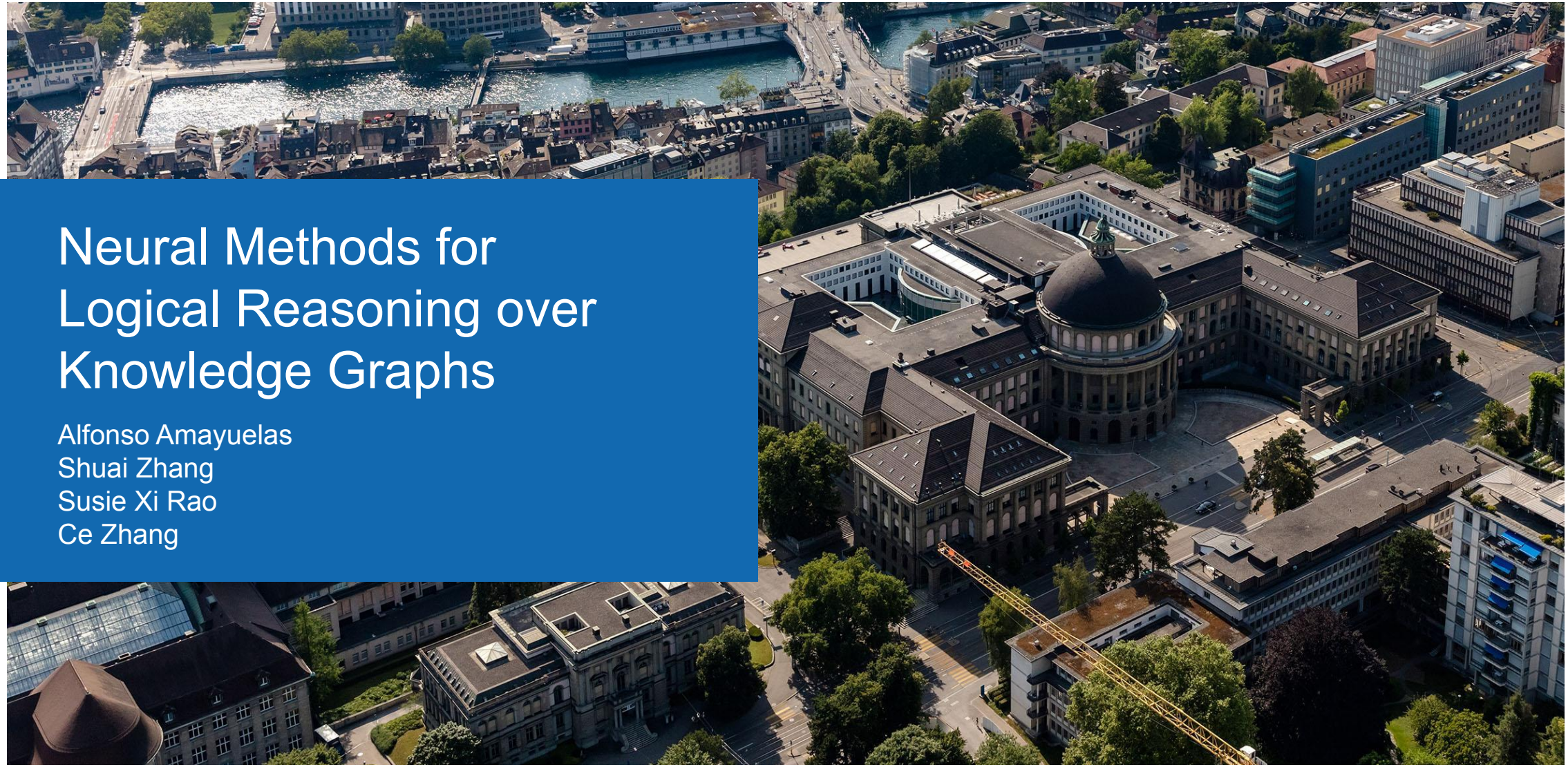
DS3Lab: Data Science, Data Systems, Data Services



Neural Methods for Logical Reasoning over Knowledge Graphs

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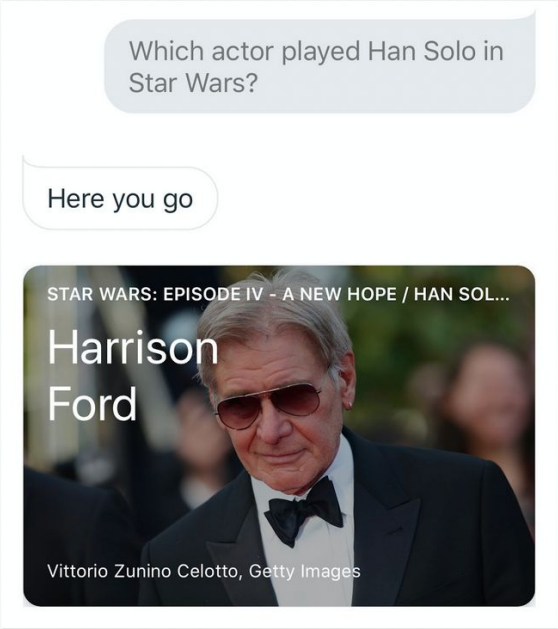
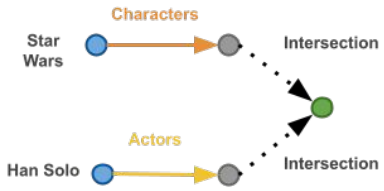
But users want to ask more complex queries

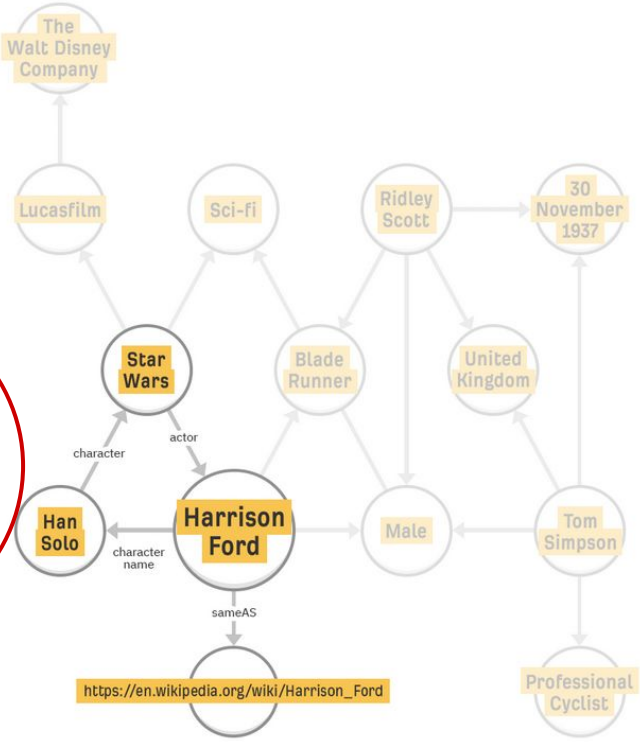


Natural Language Processing



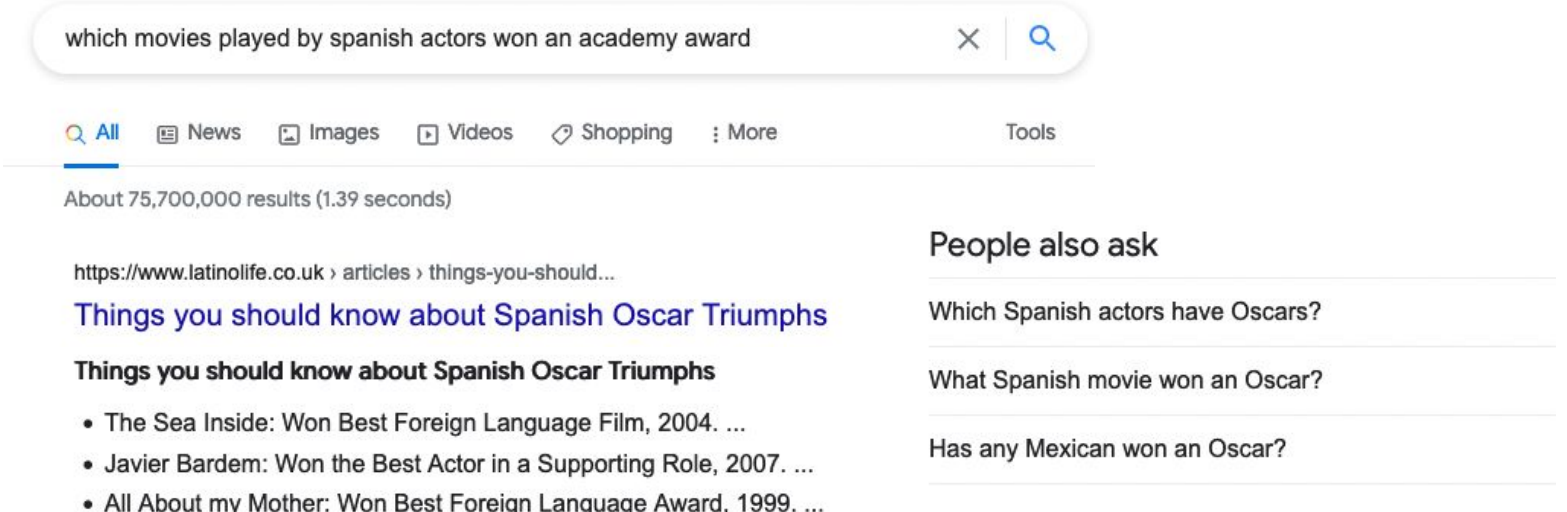
((Star Wars, characters) ∧ (Han Solo, playedBy))

Ask the Knowledge Graph



We will focus on this

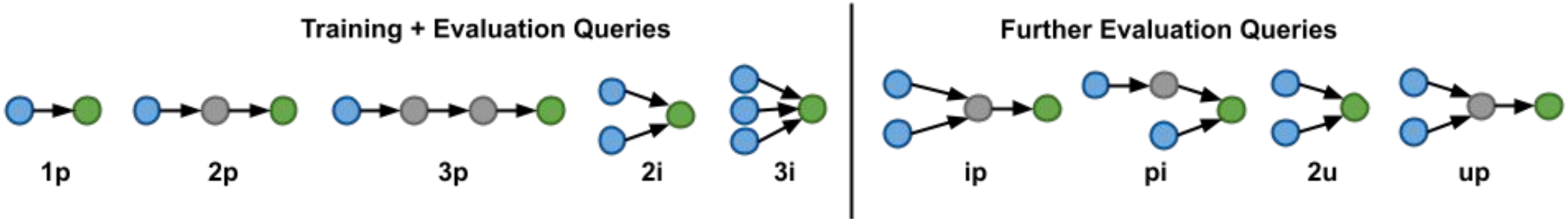
Here is where the problem starts...



Motivation: Logical Reasoning over Knowledge Graphs

Can we do multi-hop reasoning i.e. answer complex queries on an incomplete massive KG?

Our goal: Apply full First-order logic: *Existential, Negation, Conjunction, Disjunction*



Why is it complicated?

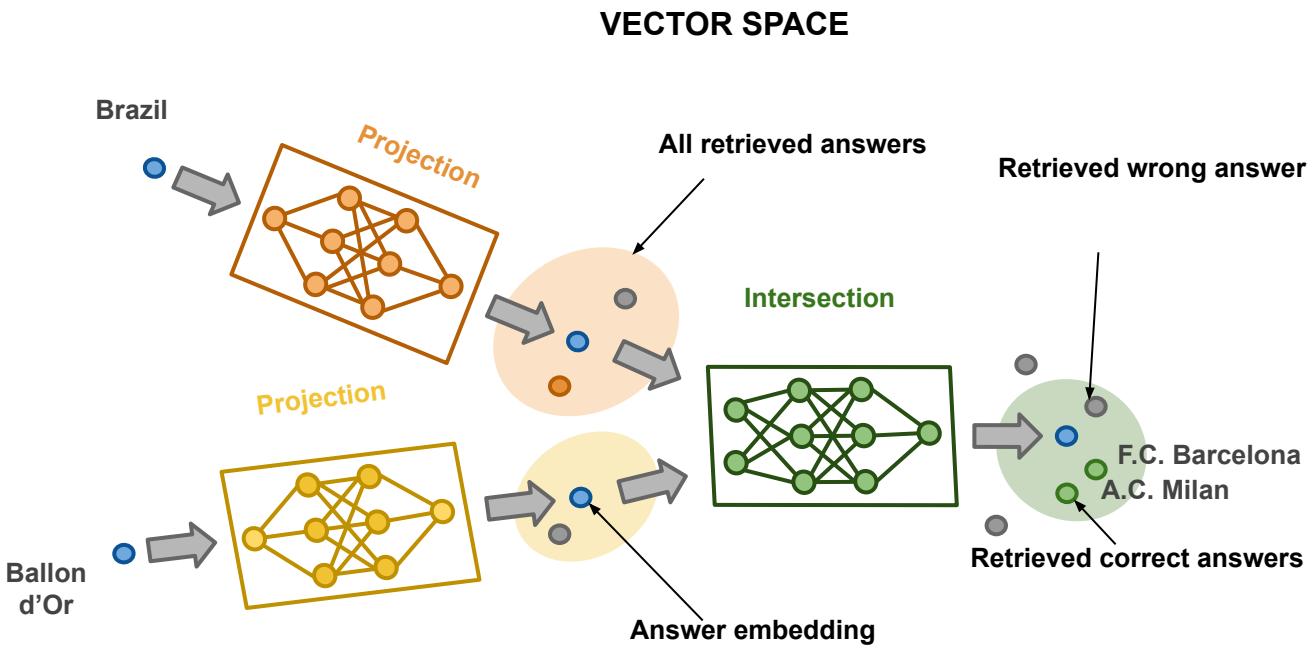
1. Increase in query-hops => Increase in complexity of traditional methods
2. Knowledge graphs are incomplete and very large in real cases

How the system works

Query: *"List the teams where Brazilian football players who were awarded a Ballon d'Or played"*

Input: Query in logical statements: *(((Brazil, CitizenOf), (Ballon d'Or, Winner)), Team)*

Output: Rank of all entities, according to the value of the negative random sampling. Done by near-neighbor search via *Locality Sensitivity Hashing*



The model uses low-dimensional one-point vector embeddings to represent the entities.

The logical operations are defined by Neural Networks

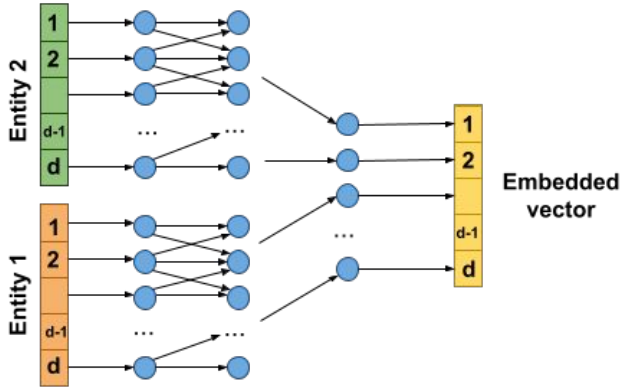
Multi-Layer Perceptron (**MLP**)

MLP: Operators are defined by a simple Multi-Layer Perceptron Neural Network

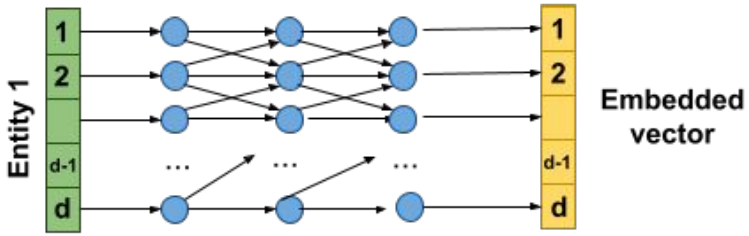
Why Neural Networks? Good results in basic KG tasks [5]

(+) Flexibility to “learn” any operator

(-) Hard to understand what they really learn



2-input operator



1-input operator

Operators:

- Projection $P(s_i, r_j) = NN_k(s_i, r_j), \forall i \in S, \forall j \in |R|$
- Intersection $I(s_i, s_j) = NN_k(s_i, s_j), \forall i, j \in S$
- Negation $N(s_i) = NN_k(s_i), \forall s_i \in S$

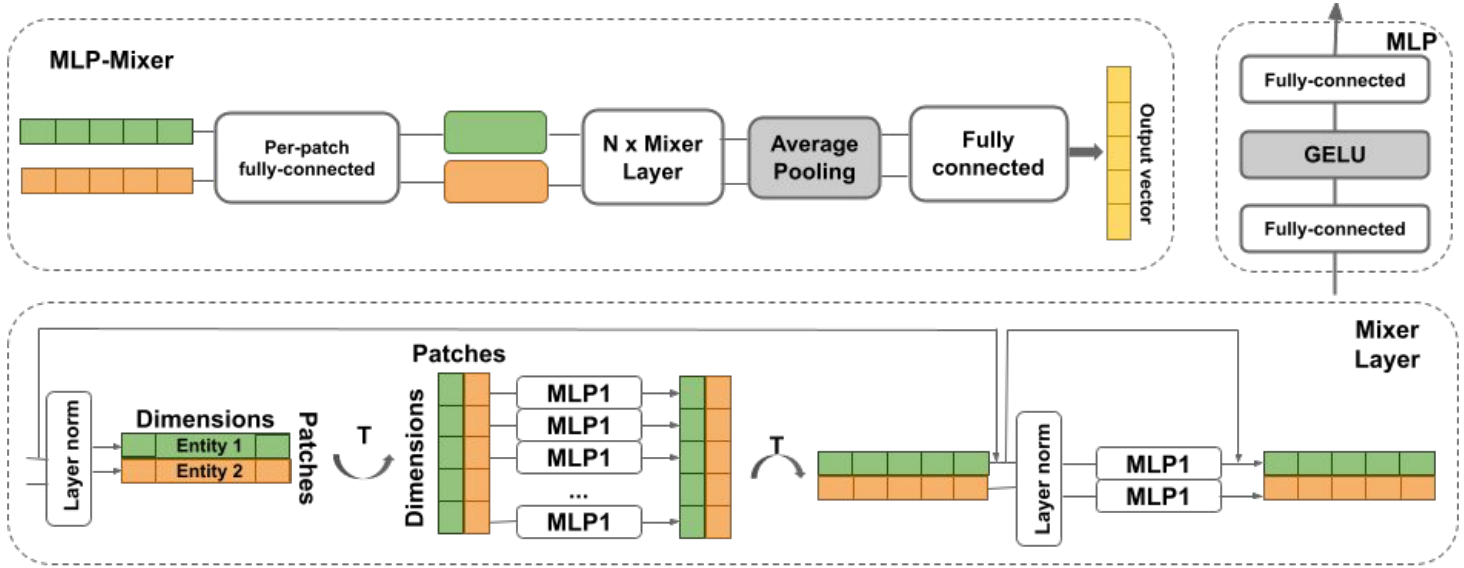
where s_i represents an entity variable and r_j a relation

!*Notice* we do not have a Union operator because we represent queries in DNF

Multi-Layer Perceptron Mixer (**MLP-Mixer**)

MLP-Mixer [6] is a Neural Network Architecture built for Image Processing with the purpose of removing convolutions.

MLP-Mixer Modules



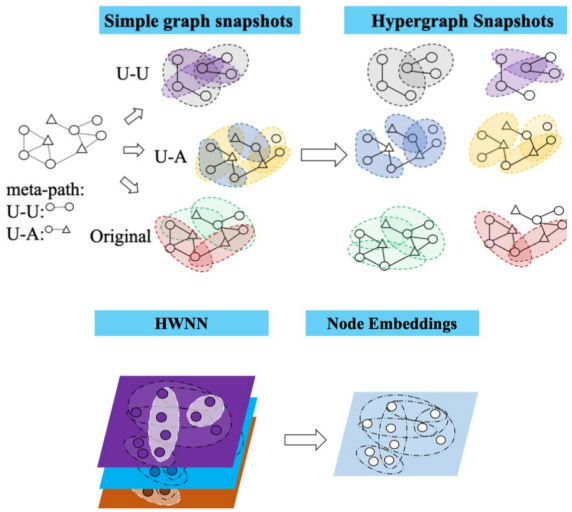
2-input Operators:

- Projection $P(s_i, r_j) = MLP_{mix}(s_i, r_j) \forall i \in S, \forall j \in |R|$
- Intersection $I(s_i, s_j) = MLP_{mix}(s_i, s_j), \forall i, j \in S$

Insight: Convolutional layers are not performing great -> Intuitively, nearby entities are not initially related

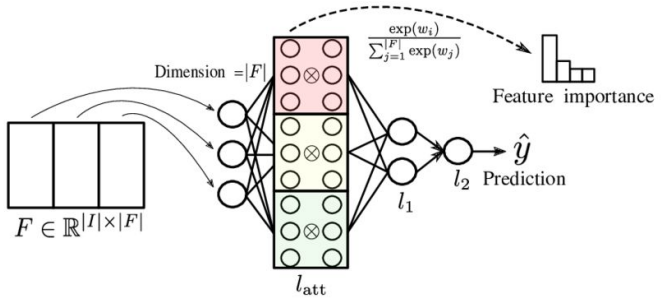
Model variants

Hyper-Graph Embeddings



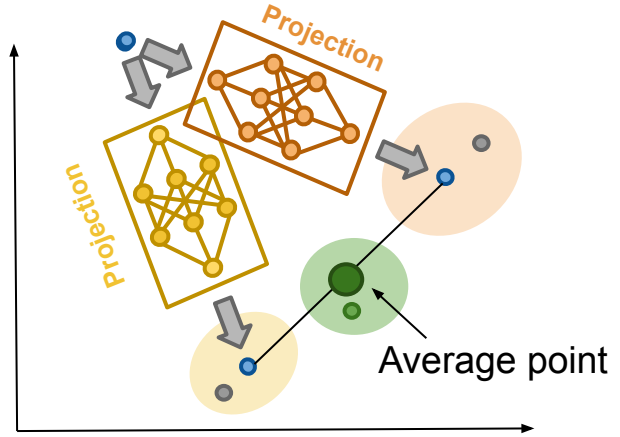
Graph embedding transformation into a series of snapshots to create new node embeddings

Attention mechanism



Include the attention layers in the operators to focus on the "important" parts of the embedding

2-vector Average



NNs may learn different "close" results

We compute the operators twice and average the result

Results: Models vs Baselines

Insights:

1. We see a considerable improvement in all cases
2. Neural Networks seem to be capturing the essence of the logical operations
3. A combination of model variants can potentially lead to a better improvement

	Best model so far (BetaE)			1-point vector encoding (GQE)		
Dataset	**MLP**	**MLP-Mixer**	**2-vector avg**	**MLP**	**MLP-Mixer**	**2-vector avg**
FB15k	5%	4%	9%	36%	35.5%	39%
FB15k-237	7%	9%	11%	28%	29%	31%
NELL995	7%	9%	8%	30%	32%	31%

Table of relative improvements (%)

Results: Negative Queries

Pros: Achieve better results than baseline model

Cons: (1) Hard to understand the representation of a negative entity
(2) Unable to measure query uncertainty

Dataset	Model	2in	3in	inp	pin	pni	avg
FB15K	MLP	**17.2**	**17.8**	**13.5**	**9.1**	**15.2**	**14.5**
	BetaE	14.3	14.7	11.5	6.5	12.4	11.8
FB15-237	MLP	**6.6**	**10.7**	**8.1**	**4.7**	**4.4**	**6.9**
	BetaE	5.1	7.9	7.4	3.6	3.4	5.4
NELL995	MLP	**5.1**	**8.0**	**10.0**	**3.6**	**3.6**	**6.1**
	BetaE	**5.1**	7.8	**10.0**	3.1	3.5	5.9

19% improvement

22% improvement

4% improvement

(Measure) **MRR: Mean Reciprocal Rank**

Future work

Some points to cover in future work:

- **Logical Disjunction (∨)**: Now we use DNF transformation to handle this query. Look into other methods that create an OR operator.
- **Logic Regularizers**: Logic Neural Networks can be a good fit for this problem. Our initial results seemed discouraging. Further research needed.
- **Query/answer generation**: The structures we use for training and testing may have a great influence on the system performance. Better query generation techniques could have a performance boost.
- **Other embeddings**: There are other types of embeddings unexplored for this problem. Look into other promising graph embeddings (i.e. quantum embeddings)

References

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[6] Tolstikhin, Ilya, et al. "Mlp-mixer: An all-mlp architecture for vision." arXiv preprint arXiv:2105.01601 (2021).

Thank you

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