Universal Representation Learning of Knowledge Bases by Jointly Embedding Instances and Ontological Concepts

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Outline

- **Background: Knowledge Graphs and Embeddings**
- Formulation: Two-view Knowledge Graphs
- JOIE Modeling: Cross-view & Intra-view
- Experimental Results
- Conclusion & Future Work

Knowledge graphs (KGs) Are Everywhere

UCLA ScAi

General-purpose KGs

Baidu 知识图谱

Google KNOWLEDGE GRAPH

DBpedia

WIKIDATA

yago select knowledge

NELL

Freebase

Bio & Medical KGs

MeSH

neXtprot

STRING

GENEONTOLOGY Unifying Biology

PubMed

Product Graphs & E-commerce

product graph

ebay

Alibaba.com

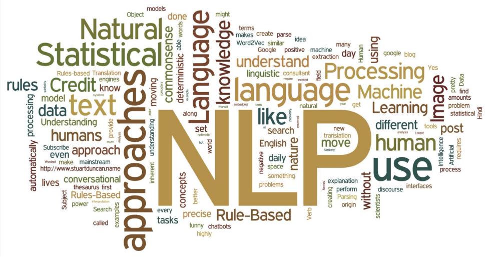
Common-sense KGs & NLP

WORDNET

ConceptNet An open, multilingual knowledge graph

Knowledge Graphs Are Foundational

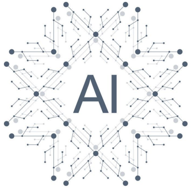
- Foundational to knowledge-driven AI systems
- Enable many downstream applications (NLP tasks, QA systems, etc)



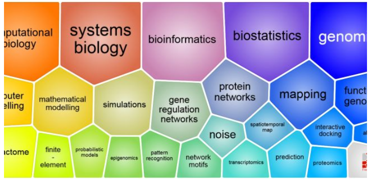
Natural Language Processing

QA & Dialogue systems

Knowledge Graphs

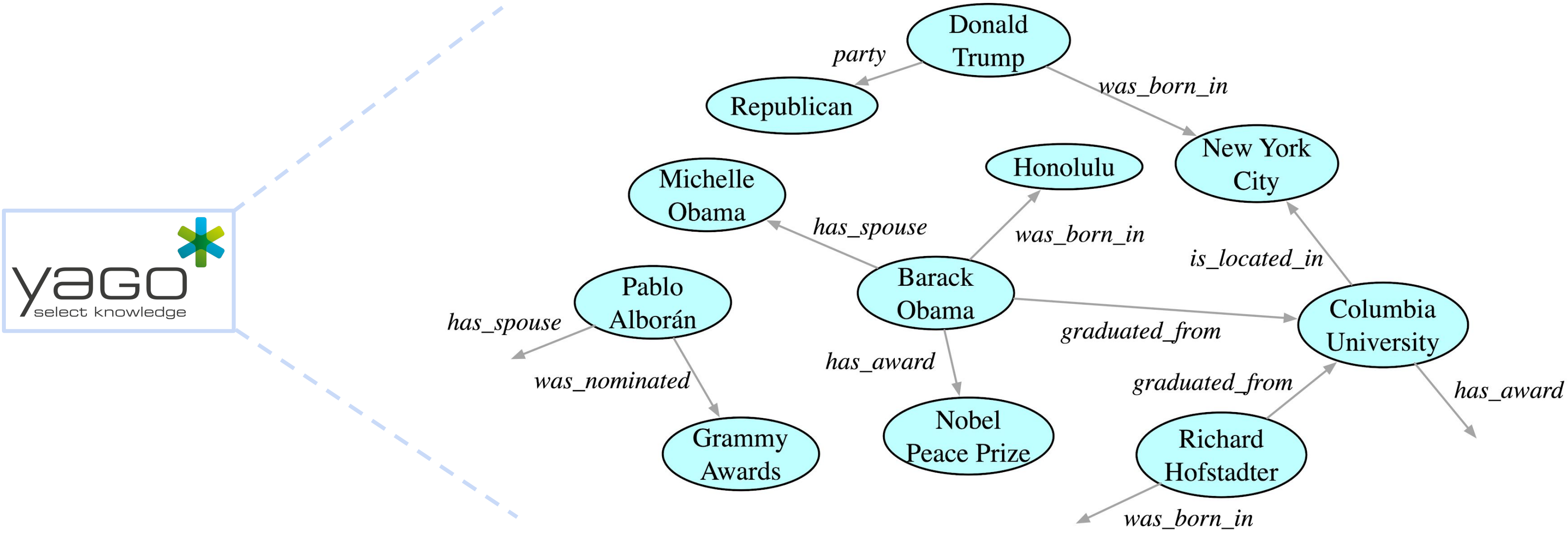


Recommendation Systems



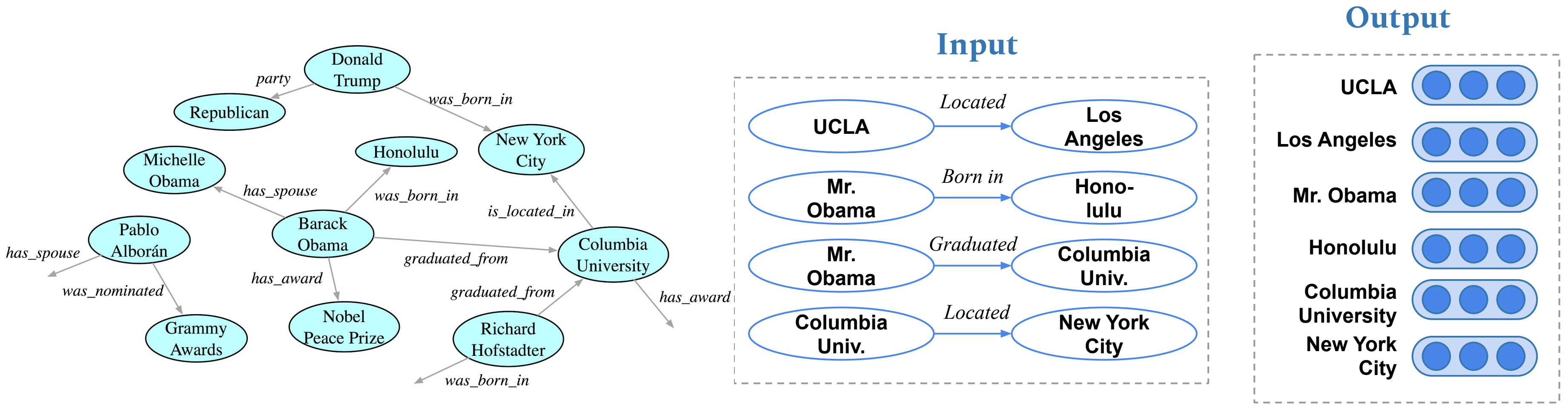
Computational Biology

KG Example From YAGO



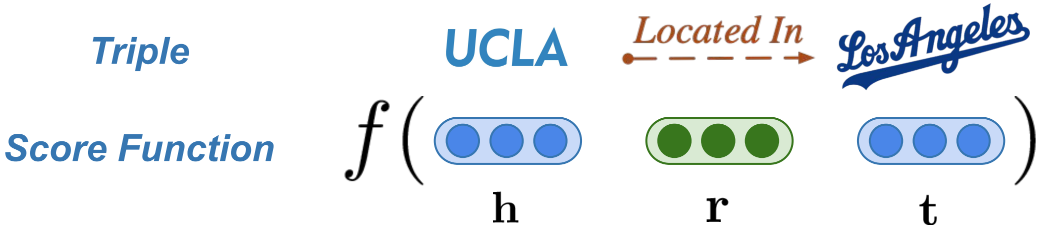
KG Embedding From Triples

- Knowledge graph embeddings represent entities and relations as latent vectors or matrices and support effective relation learning and inference.
- **Input:** Relation facts (triples)
- **Output:** Embedding representations of objects and relations



Learning KG Embeddings

- Key of existing KG embedding methods: Triple score function

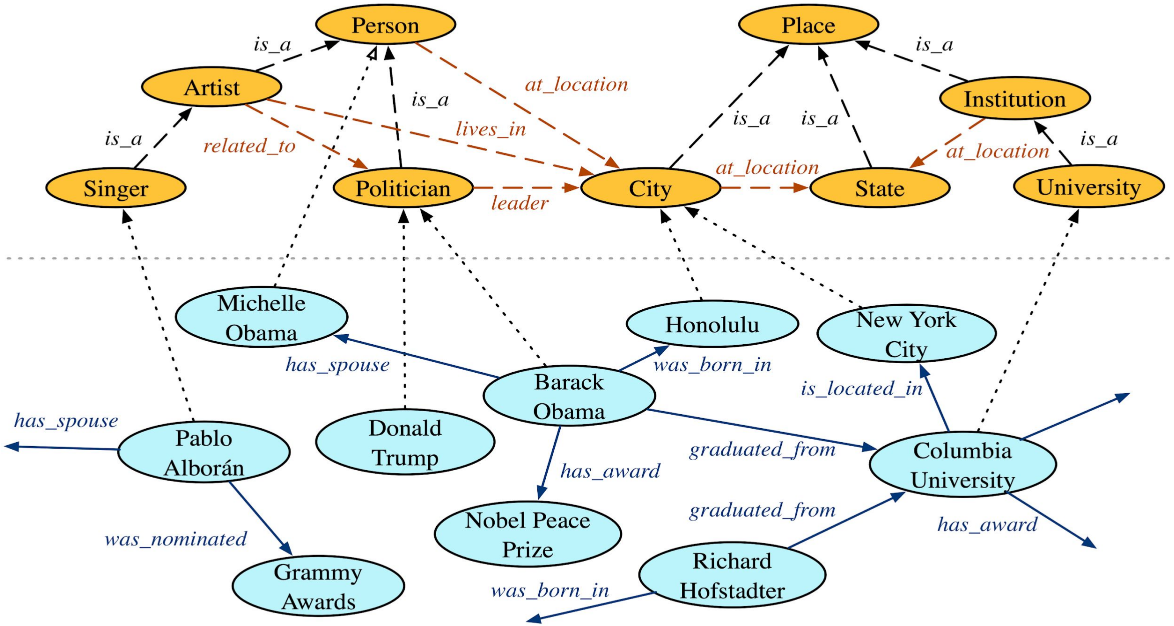


- Previous research employ various arithmetic methods to capture observed relations of entities in a single KG (for example, translational distance or similarity)

Model	Score Function	Embeddings
TransE (Bordes et al., 2013)	$-\|\|\mathbf{h}+\mathbf{r}-\mathbf{t}\|\|$	$\mathbf{h},\mathbf{r},\mathbf{t}\in\mathbb{R}^k$
TransX	$-\|\|g_{r,1}(\mathbf{h})+\mathbf{r}-g_{r,2}(\mathbf{t})\|\|$	$\mathbf{h},\mathbf{r},\mathbf{t}\in\mathbb{R}^k$
DistMult (Yang et al., 2014)	$(\mathbf{h}\circ\mathbf{t})\cdot\mathbf{r}$	$\mathbf{h},\mathbf{r},\mathbf{t}\in\mathbb{R}^k$
HolE (Nickel et al., 2016)	$(\mathbf{h}\star\mathbf{t})\cdot\mathbf{r}$	$\mathbf{h},\mathbf{r},\mathbf{t}\in\mathbb{R}^k$
ComplEx (Trouillon et al., 2016)	$\mathrm{Re}\langle\mathbf{r},\mathbf{h},\bar{\mathbf{t}}\rangle$	$\mathbf{h},\mathbf{r},\mathbf{t}\in\mathbb{C}^k$
ConvE (Dettmers et al., 2017)	$\langle\sigma(\mathrm{vec}(\sigma([\mathbf{r},\mathbf{h}]*\Omega))\mathbf{W}),\mathbf{t}\rangle$	$\mathbf{h},\mathbf{r},\mathbf{t}\in\mathbb{R}^k$
RotatE (Sun et al., 2017)	$-\|\|\mathbf{h}\circ\mathbf{r}-\mathbf{t}\|\|^2$	$\mathbf{h},\mathbf{r},\mathbf{t}\in\mathbb{C}^k$, $\|r_i\|=1$

Drawbacks & Limitation

- Most existing approaches embed instance-level knowledge.
- KGs have both specific instances and general ontological concepts.



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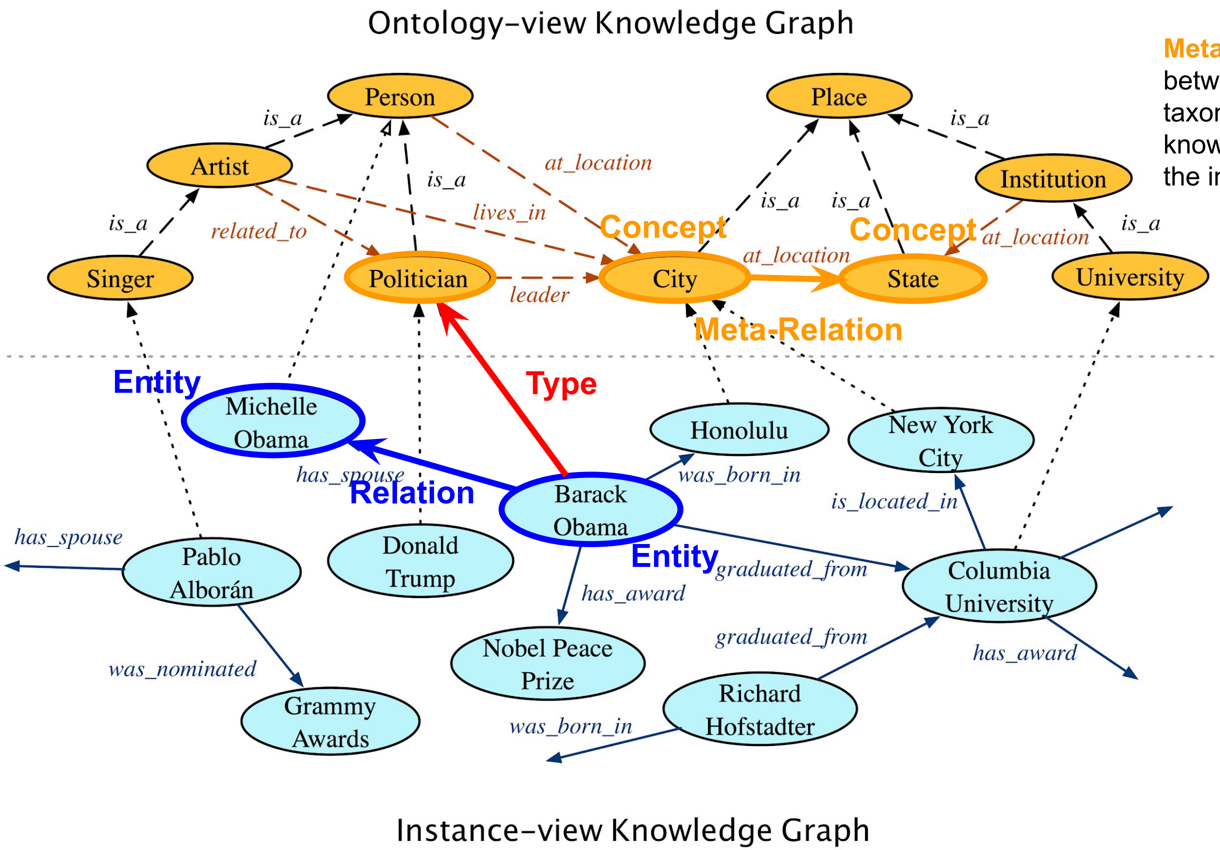
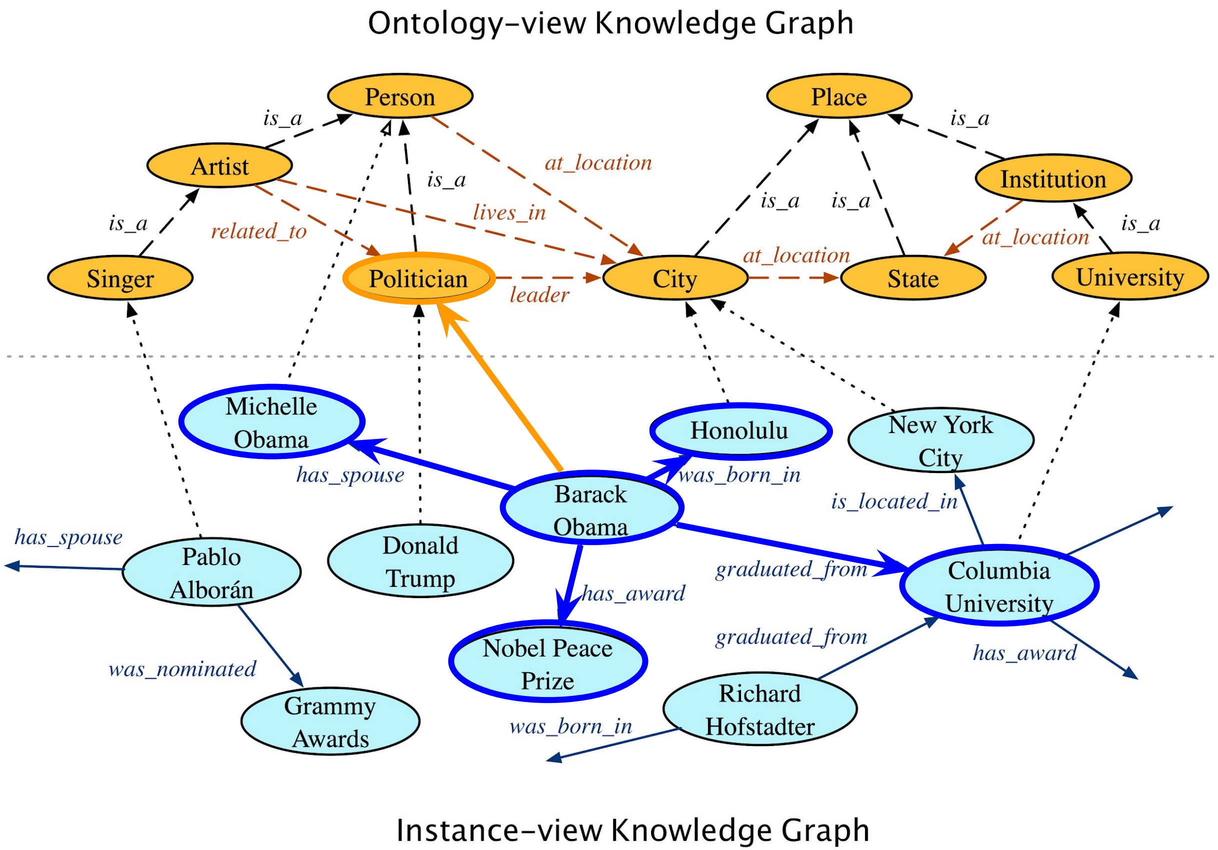
Two-view KG: More than a instance view



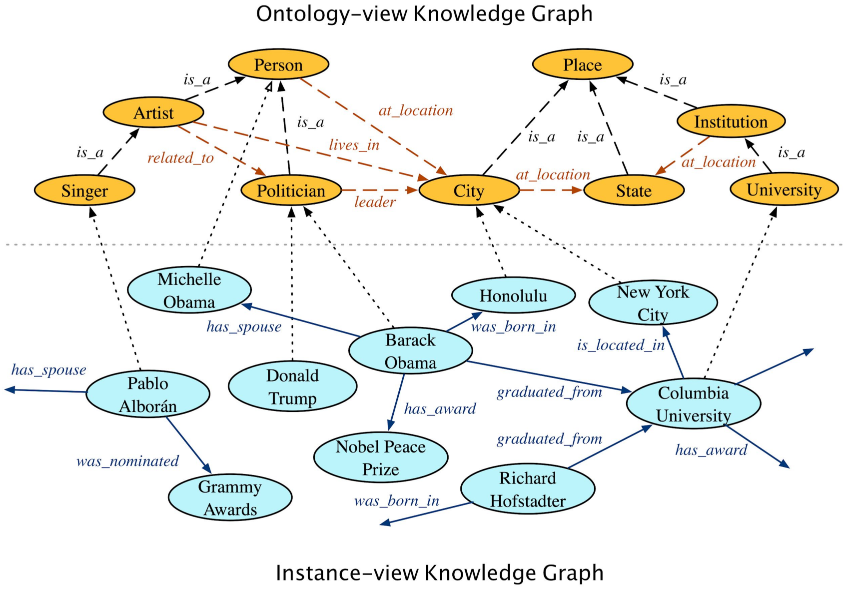
Meta-relation: Relations between concepts, including taxonomy, common-sense knowledge, which differ from the instance view.

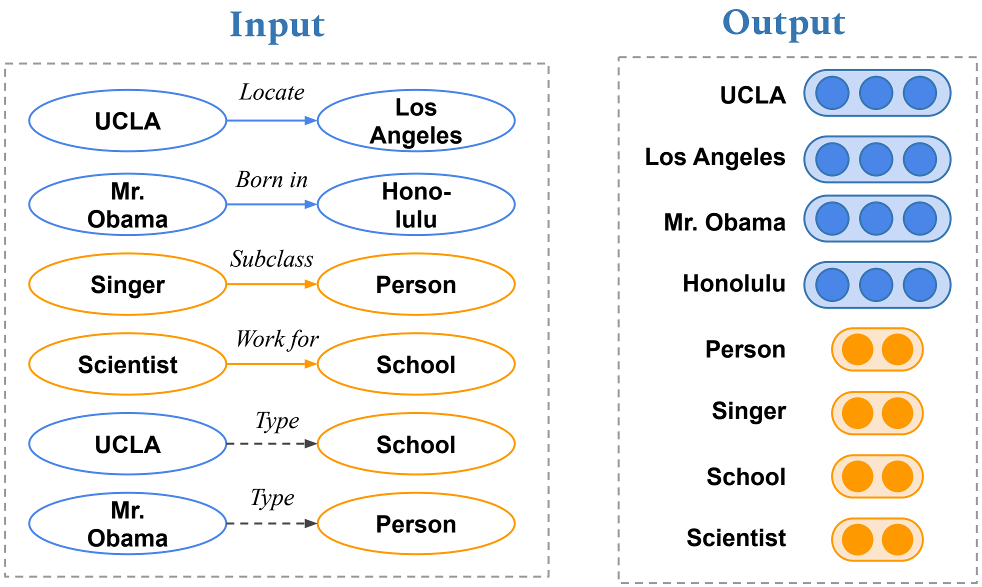
Two-view KG: More than just a set of triples



Problem Formulation

- **Input:** Instance-view KG triples, ontology-view KG triples, cross-view type links
- **Output:** Embeddings of entities, concepts, relations and meta-relations





Why Two-view KG Embeddings?

- Many existing KGs, such as YAGO and DBpedia, have constructed two views.
- Two views represent different levels of abstraction for relational knowledge, and can be used to enhance each other.
- Embeddings of a two-view KG provide more natural and clearer knowledge organization and curation, and are in line with human cognition.

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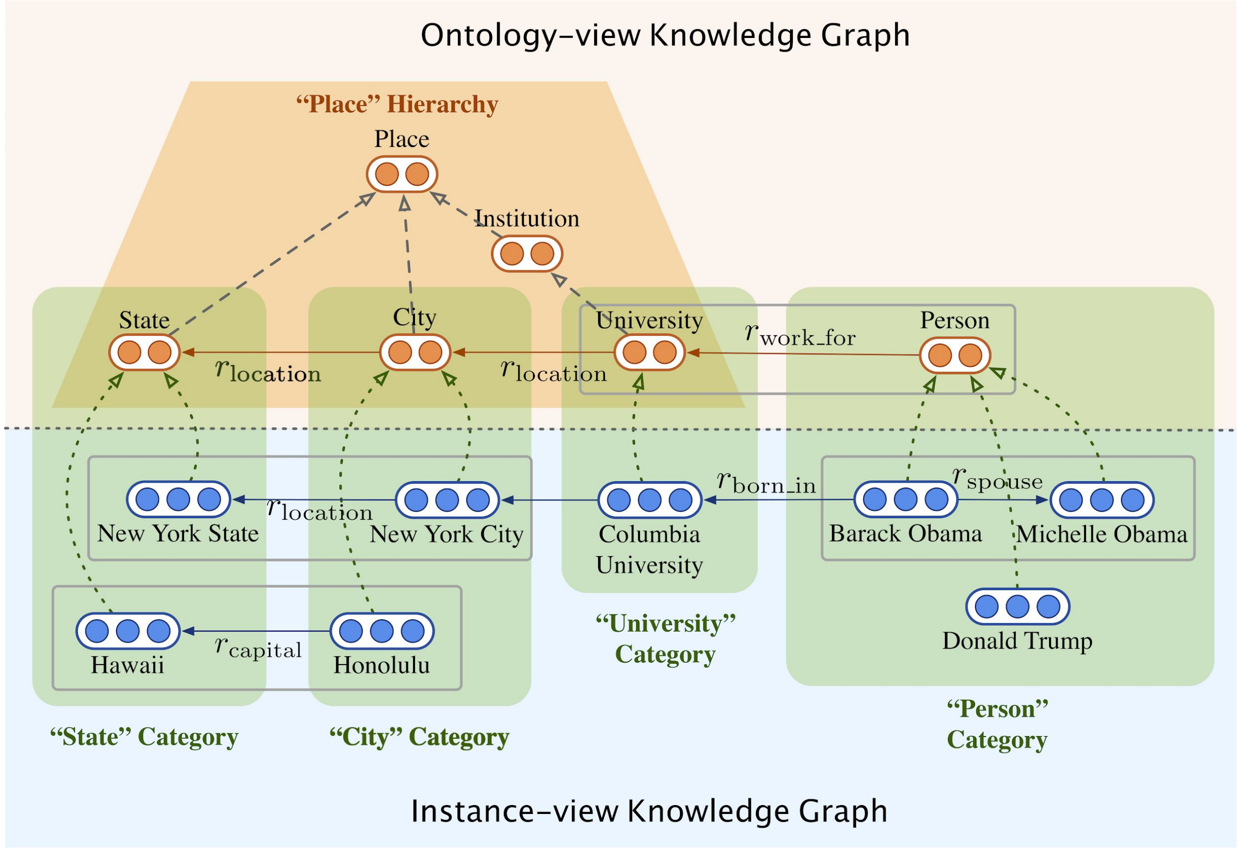
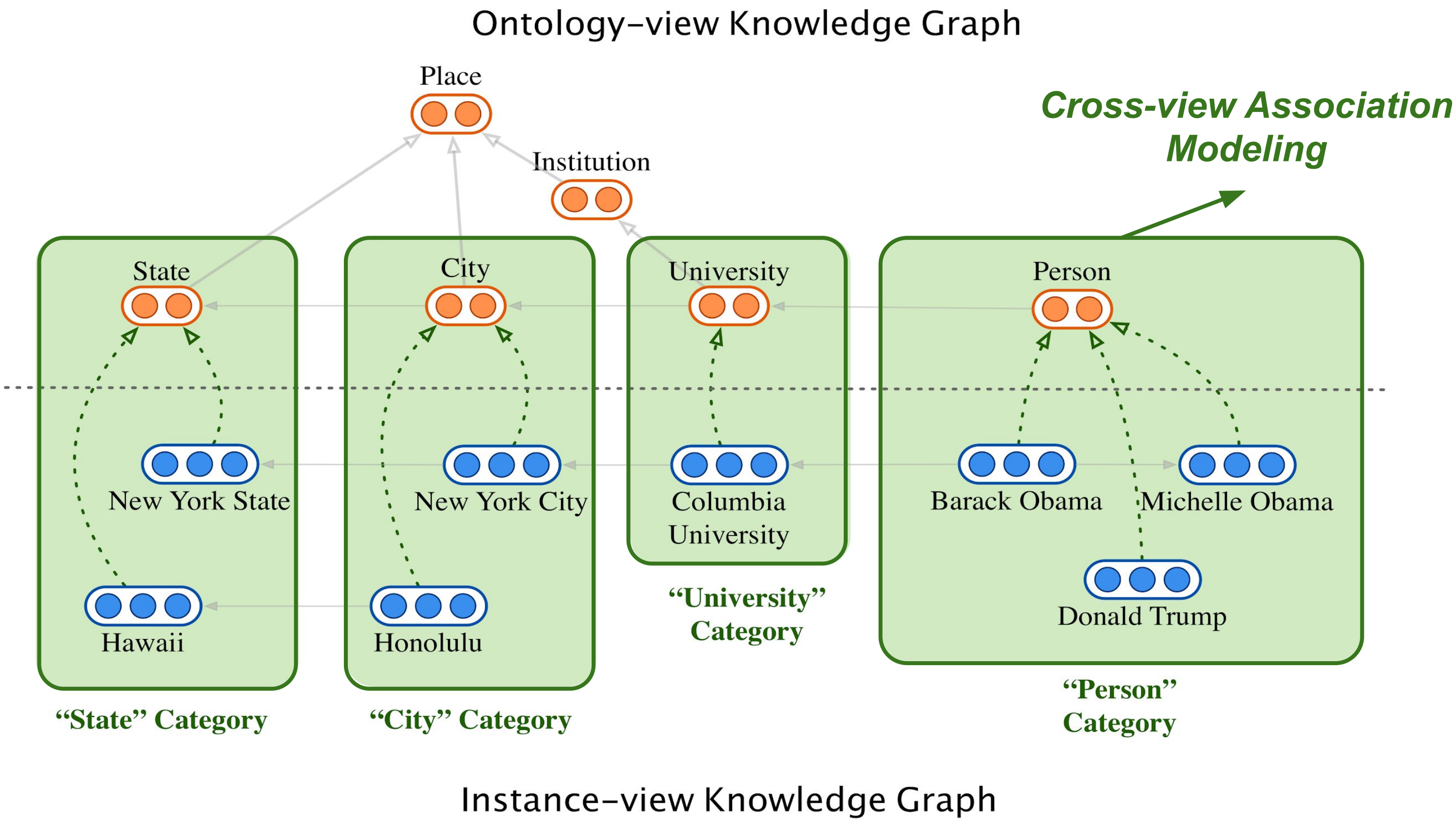
JOIE: Modeling

- Cross-view Association model
- Intra-view model

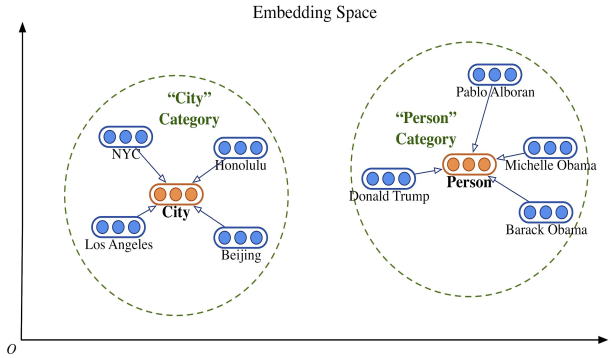


JOIE: Cross-view Association Model



JOIE: Cross-view Model

- **Goal:** capture associations between the entities **e** and corresponding concepts **c**



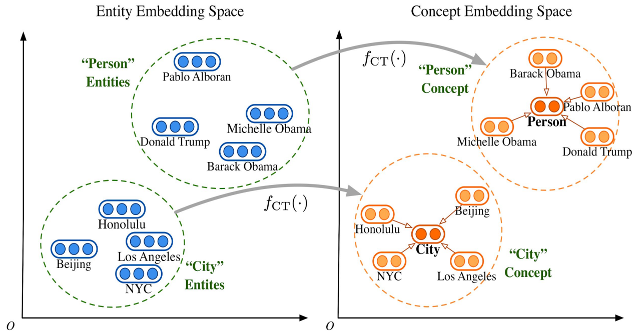
- **Cross-view Grouping (CG)**

$$J_{\text{Cross}}^{\text{CG}} = \frac{1}{|\mathcal{S}|} \sum_{(e,c)\in\mathcal{S}} \left[||\mathbf{c} - \mathbf{e}||_2 - \gamma^{\text{CG}} \right]_+$$

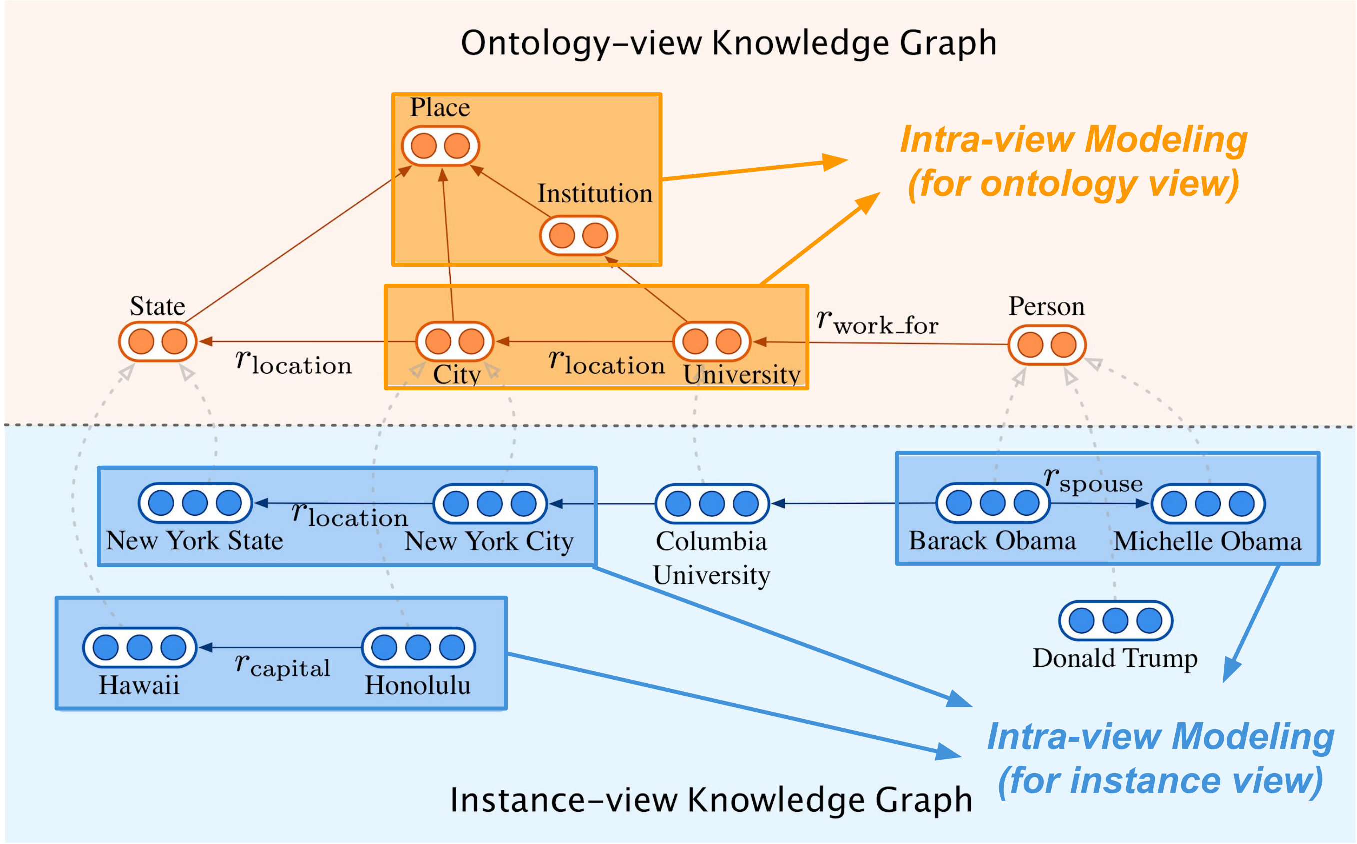
- **Cross-view Transformation (CT)**

$$f_{\text{CT}}(\mathbf{e}) = \sigma(\mathbf{W}_{\text{ct}} \cdot \mathbf{e} + \mathbf{b}_{\text{ct}})$$

$$J_{\text{Cross}}^{\text{CT}} = \frac{1}{|\mathcal{S}|} \sum_{\substack{(e,c)\in\mathcal{S} \\ \wedge (e,c')\notin\mathcal{S}}} \left[\gamma^{\text{CT}} + ||\mathbf{c} - f_{\text{CT}}(\mathbf{e})||_2 - ||\mathbf{c}' - f_{\text{CT}}(\mathbf{e})||_2 \right]_+$$



JOIE: Intra-view Model



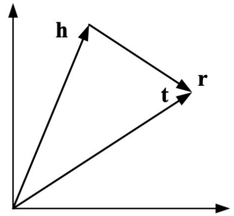
JOIE: Intra-view Model for Instance View

- Goal: To embed the relational structures in the instance view of the KB
- Apply any KG embedding techniques on instance view
  - Three representatives: TransE, DistMult, and HolE

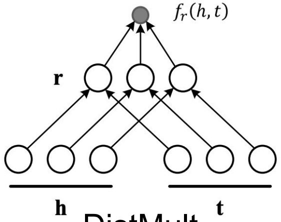
$$f_{\text{TransE}}(\mathbf{h},\mathbf{r},\mathbf{t}) = -||\mathbf{h}+\mathbf{r}-\mathbf{t}||_2$$
$$f_{\text{Mult}}(\mathbf{h},\mathbf{r},\mathbf{t}) = (\mathbf{h}\circ\mathbf{t})\cdot\mathbf{r}$$
$$f_{\text{HolE}}(\mathbf{h},\mathbf{r},\mathbf{t}) = (\mathbf{h}\star\mathbf{t})\cdot\mathbf{r}$$

- Training on marginal ranking loss

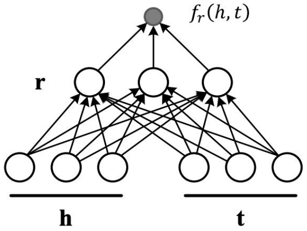
$$J_{\text{Intra}}^{\mathcal{G}} = \frac{1}{|\mathcal{G}|}\sum_{\substack{(h,r,t)\in\mathcal{G}\\ \wedge(h',r,t')\notin\mathcal{G}}}\left[\gamma^{\mathcal{G}} + f(\mathbf{h}',\mathbf{r},\mathbf{t}') - f(\mathbf{h},\mathbf{r},\mathbf{t})\right]_+$$



TransE



DistMult



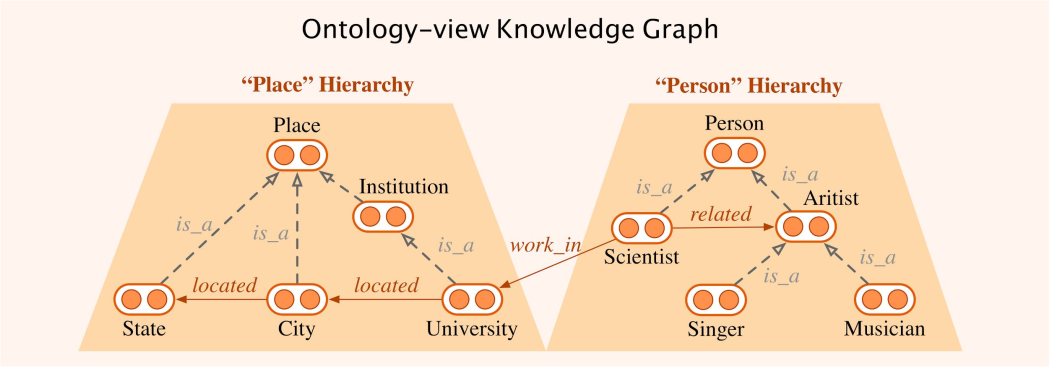
HolE

JOIE: Intra-view Model for Ontology View

- We can still follow the same techniques as the instance view. $J_{\text{Intra}} = J_{\text{Intra}}^{\mathcal{G}_I} + \alpha_1 \cdot J_{\text{Intra}}^{\mathcal{G}_O}$
- However, the hierarchical structure of the ontology-view represents critical semantics, with special meta relations such as "*is_a*" and "*subclass*".

c_l : Scientist c_h :Person

$$g_{\text{HA}}(\mathbf{c}_h) = \sigma(\mathbf{W}_{\text{HA}} \cdot \mathbf{c}_l + \mathbf{b}_{\text{HA}})$$



- Similar to CT model, we model such hierarchical structures in,

$$J_{\text{Intra}}^{\text{HA}} = \frac{1}{|\mathcal{T}|} \sum_{\substack{(c_l, c_h) \in \mathcal{T} \\ \wedge (c_l, c_h') \notin \mathcal{T}}} \left[\gamma^{\text{HA}} + ||\mathbf{c}_h - g(\mathbf{c}_l)||_2 - ||\mathbf{c_h}' - g(\mathbf{c_l})||_2\right]_+$$

JOIE: Summary & Model Highlights

- Two model components: Cross-view model and intra-view model
- Cross-view association model $\Rightarrow J_{\text{Cross}}$
  - Categorical grouping (CG)
  - Categorical transformation (CT)
- Intra-view model $\Rightarrow J_{\text{Intra}}$
  - Can apply any KG embedding on each view
  - Hierarchical-aware modeling on ontological view specifically for taxonomy meta relations
- Joint training on cross-view loss and intra-view loss

$$J = J_{\text{Intra}} + \omega \cdot J_{\text{Cross}}$$

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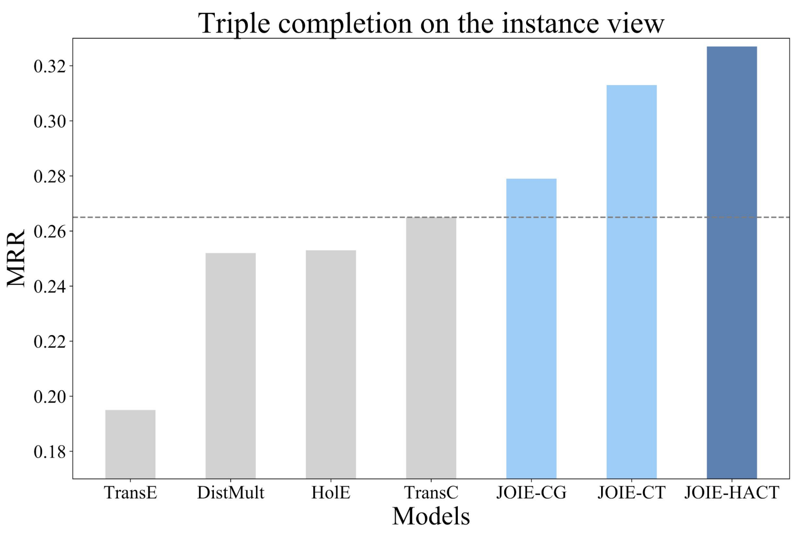
Experiment Setup

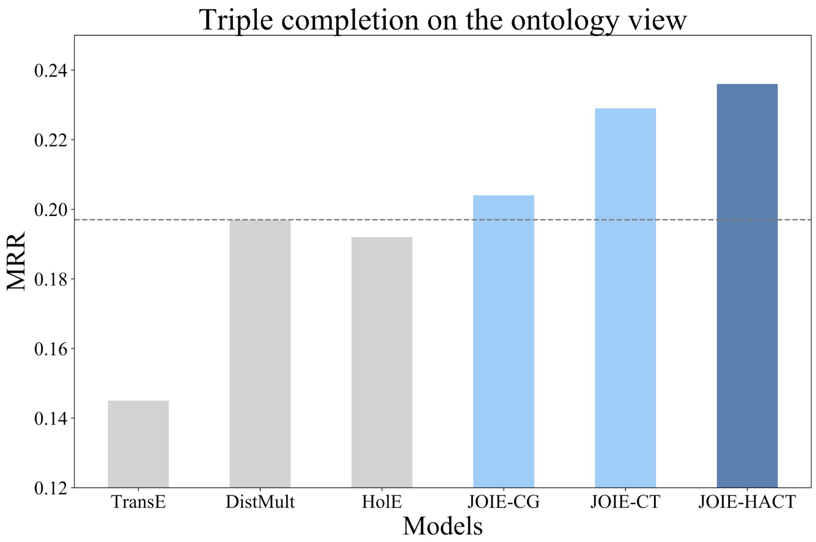
- Datasets: YAGO26K-906 (from YAGO) and DB111K-184 (from DBpedia)
- Tasks: **Triple completion** and **entity typing**
- Evaluation metrics
  - Triple completion: MRR, Hit@*K* score (*K*=1,3,10)
  - Entity typing: Accuracy (Hit@1), Hit@3 Score
- Baselines: TransE, DistMult, HolE, TransC, MTransE

Dataset	Instance Graph $\mathcal{G}_I$			Ontology Graph $\mathcal{G}_O$			Type Links $\mathcal{S}$
	#Entities	#Relations	#Triples	#Concepts	#Meta-relations	#Triples	
YAGO26K-906	26,078	34	390,738	906	30	8,962	9,962
DB111K-174	111,762	305	863,643	174	20	763	99,748

Task 1: Triple Completion

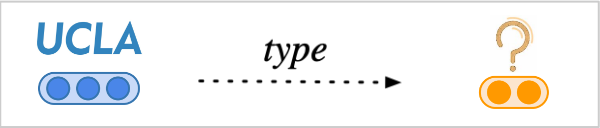
- Given the head and predicate of a triple, what is the most likely tail (answer)?

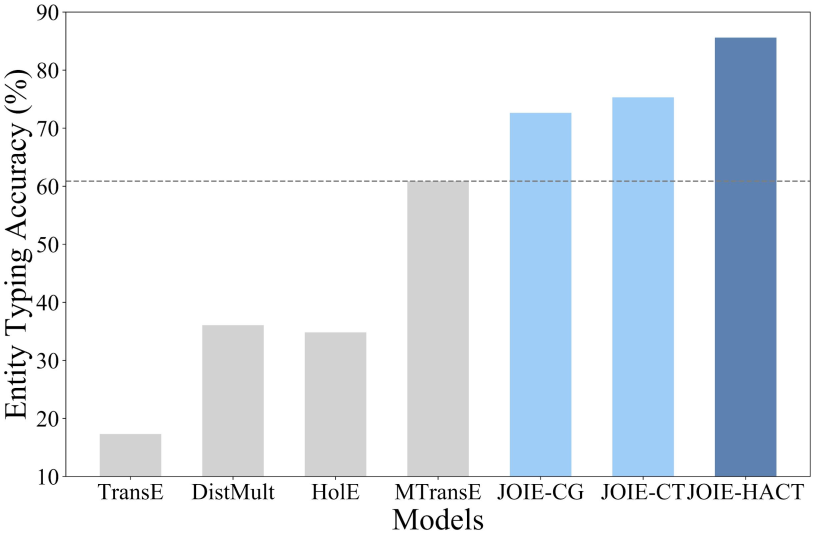




Task 2: Entity Typing

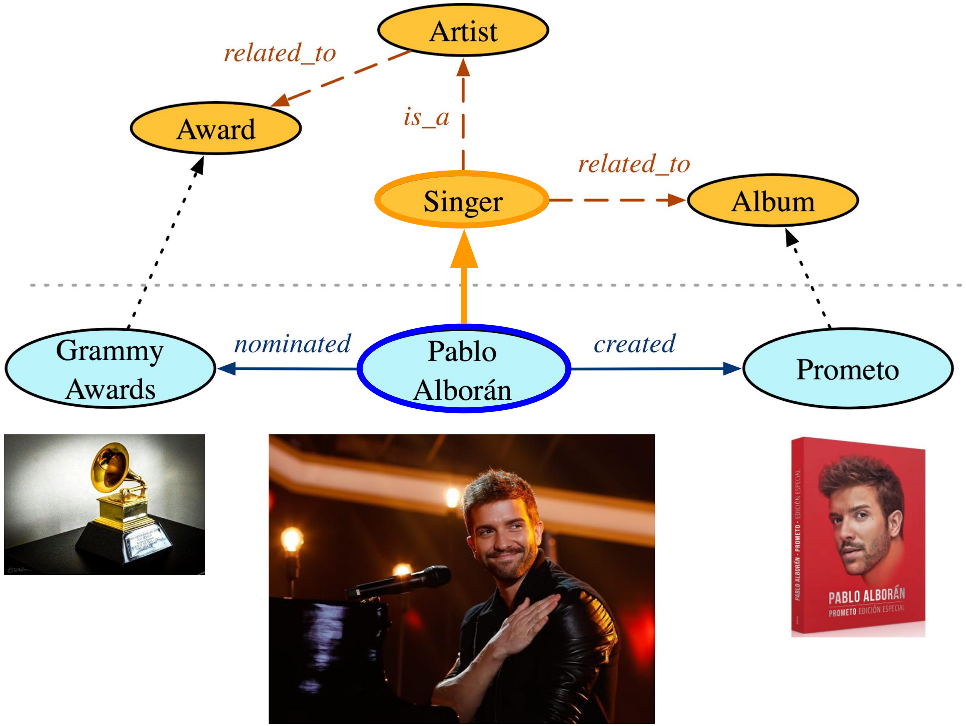
- Given an entity without a known type, what is the most likely type (concept) that it associates with?





Type inference on 30% of all entities on YAGO.

Task 2+: Long-tail Entity Typing



Example of long-tail entity typing

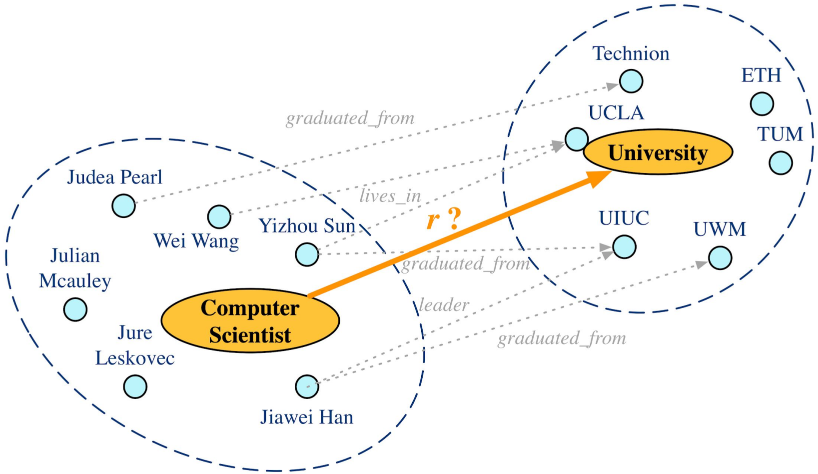
Entity	Model	Top 3 Concept Prediction
Laurence Fishburne	DistMult	football team, club, team
	MTransE	writer, **person**, artist
	JOIE	**person**, artist, philosopher
Warangal City	DistMult	country, village,**city**
	MTransE	administrative region, **city**, settlement
	JOIE	**city**, town, country
Royal Victor -ian Order	DistMult	person, writer, administrative region
	MTransE	election, award, **order**
	JOIE	award, **order**, election

Entity typing accuracy on long-tail entities

Datasets	YAGO26K-906		
Metrics	MRR	Acc.	Hit@3
DistMult	0.156	10.89	25.33
MTransE	0.526	46.45	67.25
JOIE-TransE-CG	0.708	59.97	79.80
JOIE-TransE-CT	0.737	62.05	82.60
JOIE-HATransE-CT	**0.802**	**69.66**	**87.75**

Task 3: Ontology Population

→ JOIE can help enhance the quality of ontology view and make it more complete and informative by populating the instance-level knowledge.



Examples of ontology population

Query	Top 3 Populated Triples with distances
(scientist, ?r, university)	scientist, ***graduated from***, university (0.499) scientist, ***isLeaderOf***, university (1.082) scientist, *isKnownFor*, university (1.098)
(boxer, ?r, club)	boxer, ***playsFor***, club (1.467) boxer, *isAffiliatedTo*, club (1.474) boxer, ***worksAt***, club (1.479)
(scientist, ?r, scientist)	scientist, ***doctoralAdvisor***, scientist (0.204) scientist, ***doctoralStudent***, scientist (0.221) scientist, ***relative***, scientist (0.228)

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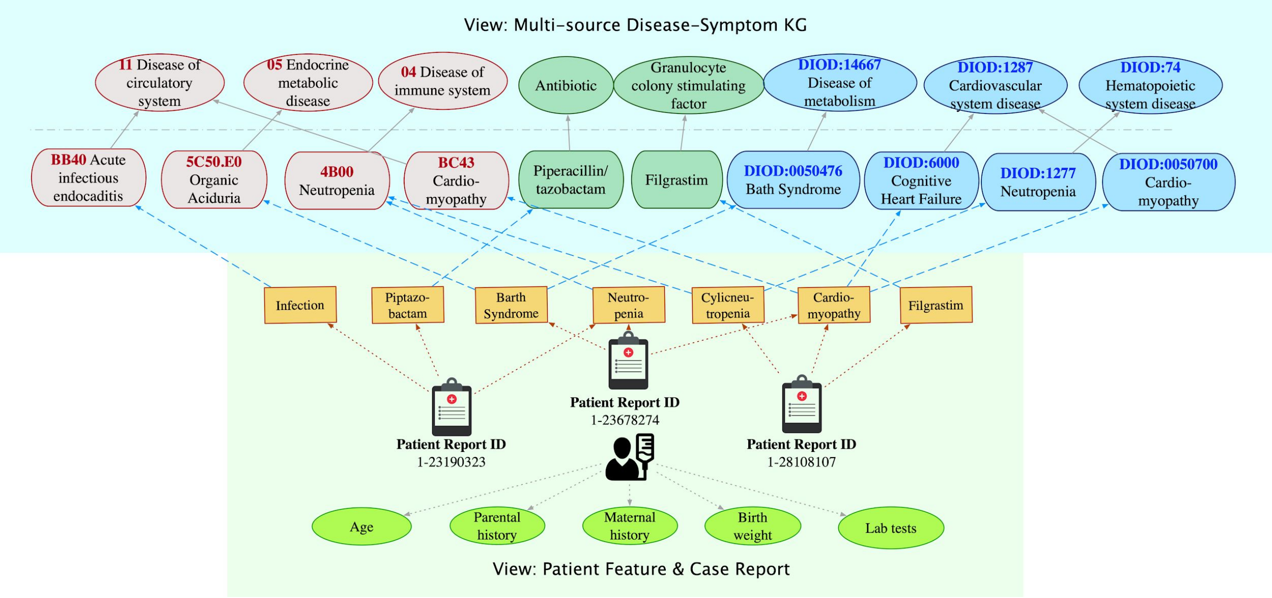
Conclusion & Future Work

- Joint learning on the instance and ontology views improves the KG embeddings.
- Incorporating ontologies in KGs is beneficial.
- Two-view KG modeling can be applied in a wide selection of interdisciplinary applications.
  - Disease-symptom with multiple medical KGs for automated patient case report analysis.



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