UCLA Samueli Computer Science

Graph Learning Session

Incorporating Ontological Information in Knowledge Graph Learning and Applications

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Bio

- Currently final-year Ph.D. candidate at UCLA co-advised by Yizhou Sun and Wei Wang in UCLA Data Mining Group.
- My research interests include knowledge graph, graph representation learning, KG-empowered applications (NLP, Bioinformatics, recommender systems, etc.).
- Before joining UCLA, I graduated in 2017 from Department of Automation, Tsinghua University.

Past Experiences

- PhD Research Intern, IBM, 2020
- Applied Science Intern, Amazon Product Graph, 2019
- Research Intern, NEC Labs America, 2018

Today's Agenda

- Background: Knowledge graphs and representation learning
- **JOIE:** Joint learning on instance and ontology view on knowledge graphs
- Two JOIE-inspired applications: Bioinformatics (**Bio-JOIE**) and Recommender Systems (**P-Companion**)
- Summer intern project at MSAI: **DocGraph**

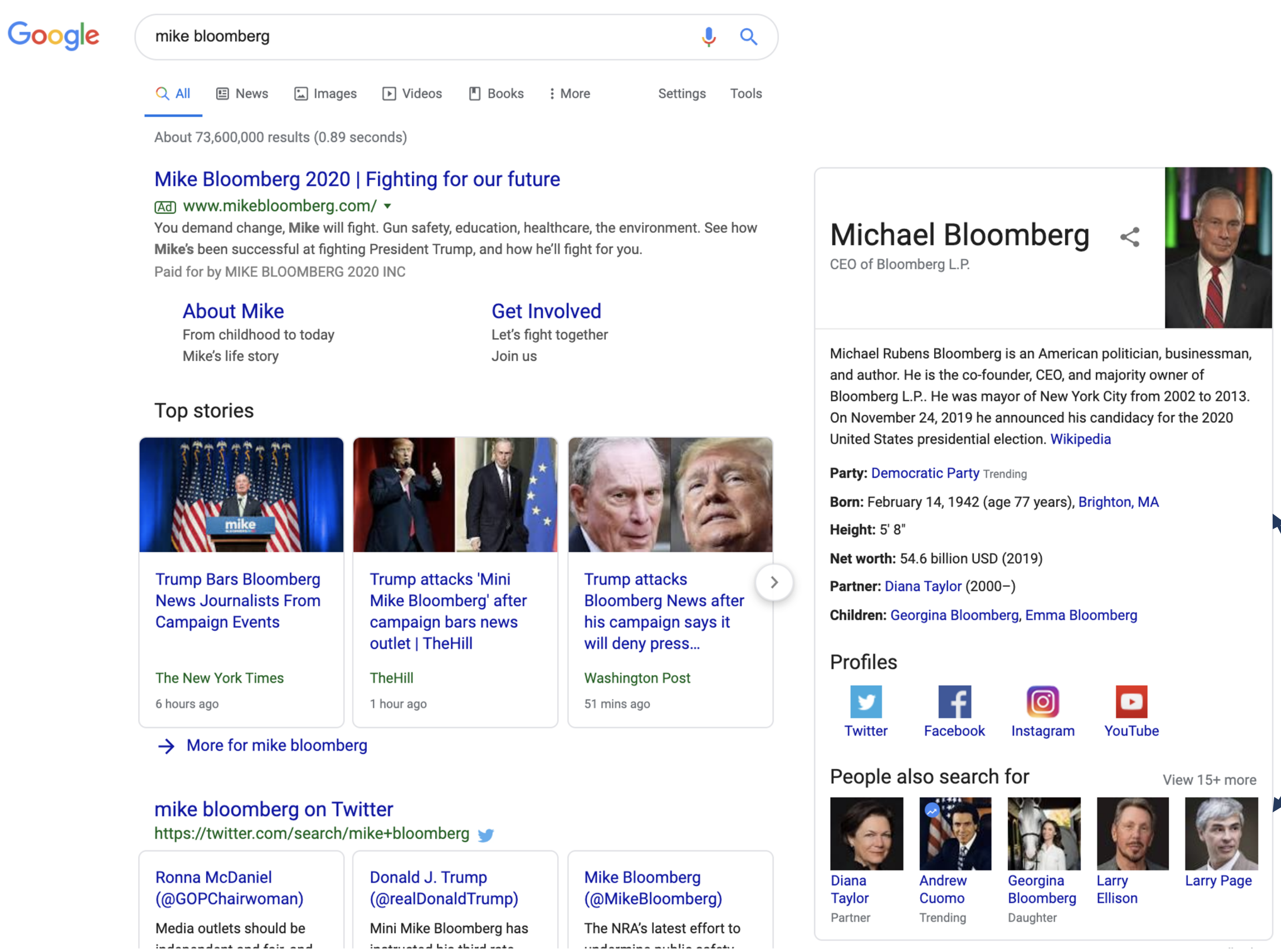
Papers

- Universal representation learning of knowledge bases by jointly embedding instances and ontological concepts (KDD'19)
- Bio-JOIE: Joint representation learning of biological knowledge bases (ACM BCB'20, Best Student Paper)
- P-Companion: A principled framework for diversified complementary product recommendation (CIKM'20)

Background: Knowledge Graphs and Representation Learning on KG

What is a KG? What is the structure of a KG?

KG: Whenever you google…



Facts from KG

Knowledge graphs (KGs) Are Everywhere

General-purpose KGs

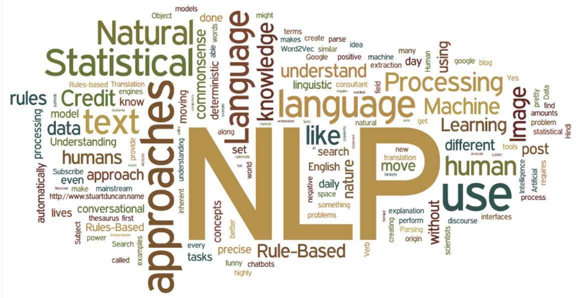
Bio & Medical KGs

Product Graphs & E-commerce

Common-sense KGs & NLP

Knowledge Graphs Are Important

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



Natural Language Processing

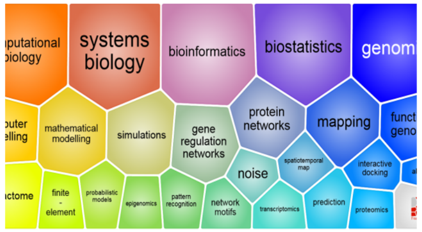
Sorry, I don't know that one.

QA & Dialogue systems

Knowledge Graphs

ebay amazon NETFLIX

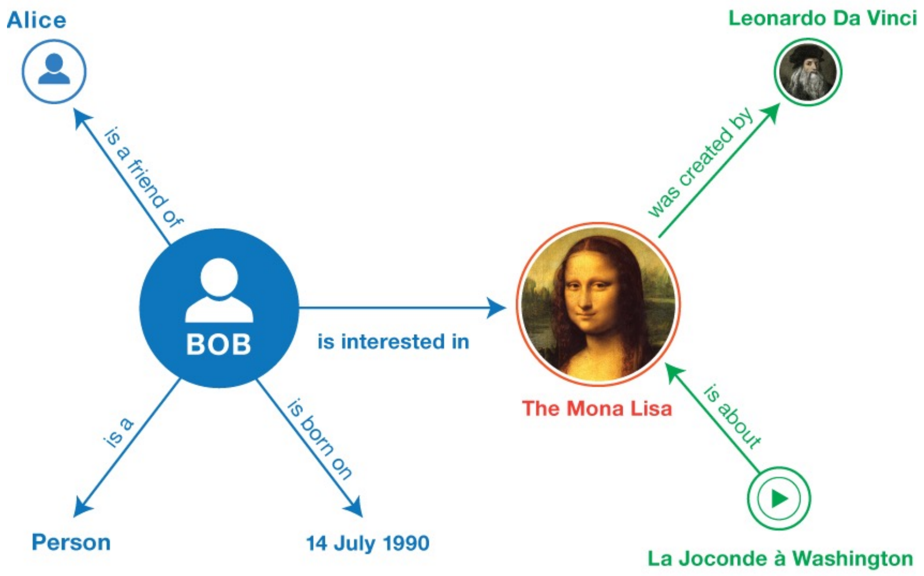
Recommender Systems



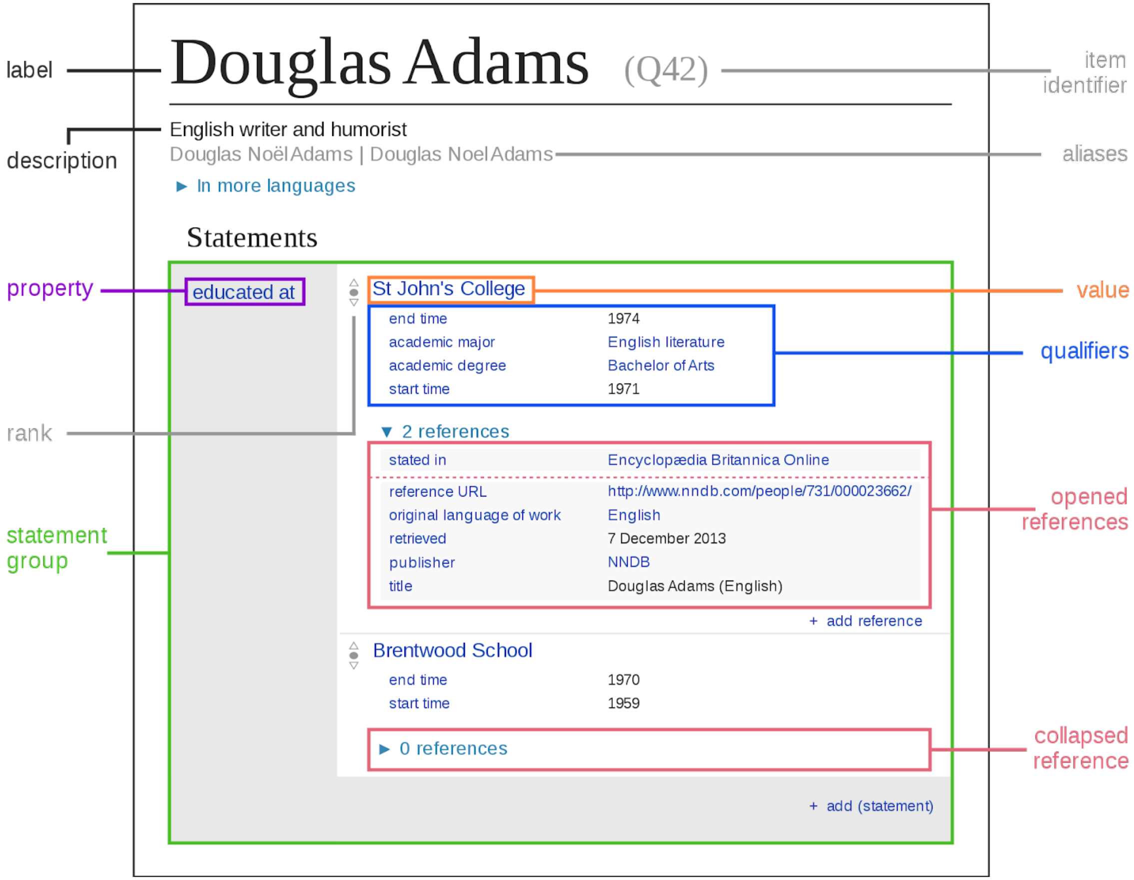
Computational Biology

How are KGs structured or formatted?

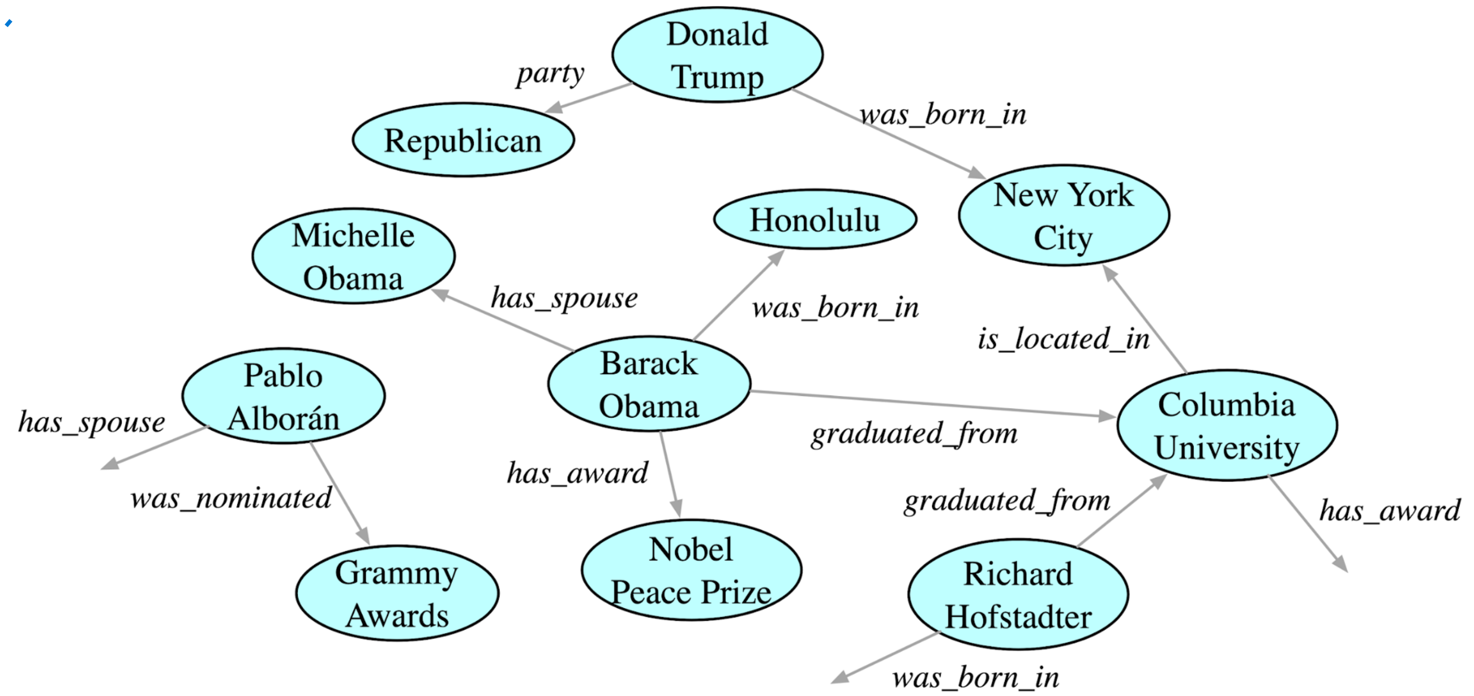
- **Triples (RDF)**
  - Represented by: a node for the subject, a node for the object, and an arc/node for the predicate.
  - Example: Semantic Web, medical ontologies, etc.



- **Label-property**
  - Entity, labels, properties, qualifiers, etc.
  - Example: Wikidata

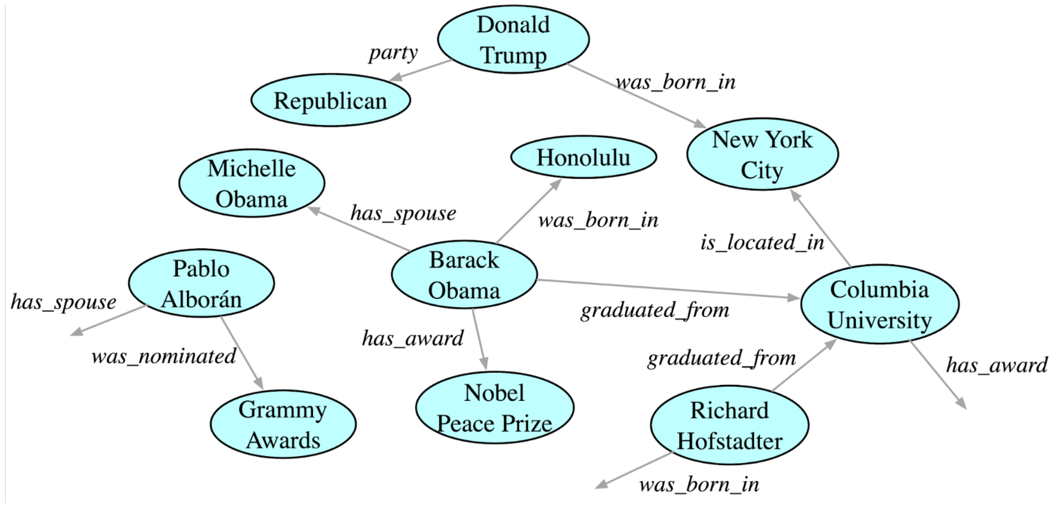


A KG Snapshot from YAGO, made with triples

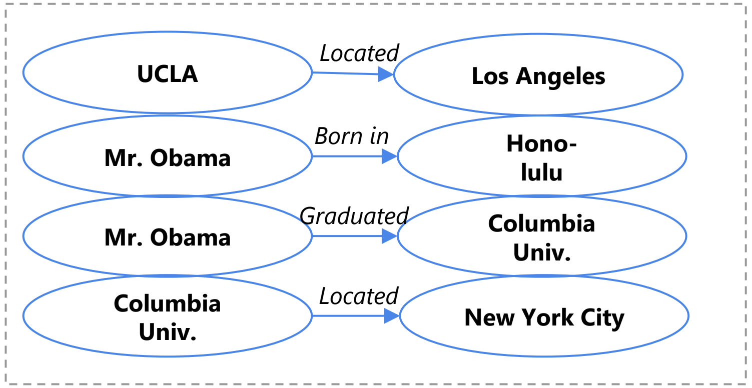


KG Embeddings From Triples

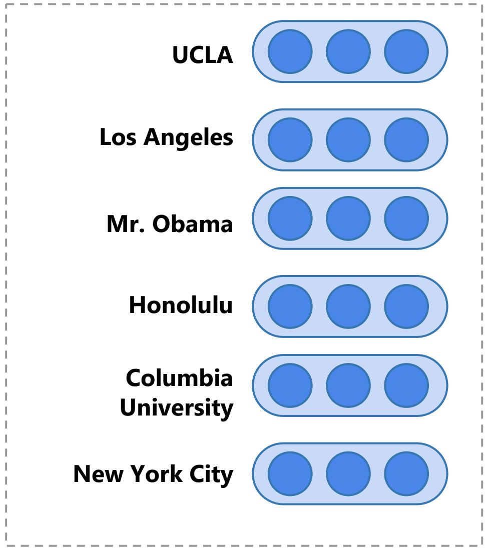
- Knowledge graph embeddings represent entities and relations as latent vectors or matrices and support effective relation learning and inference.
- **Input**: Relation facts (triples)
- **Output**: Embedding representations of objects and relations



Input

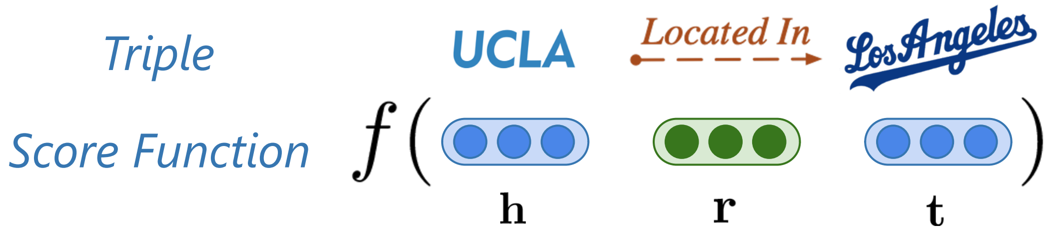


Output



Learning KG Embeddings

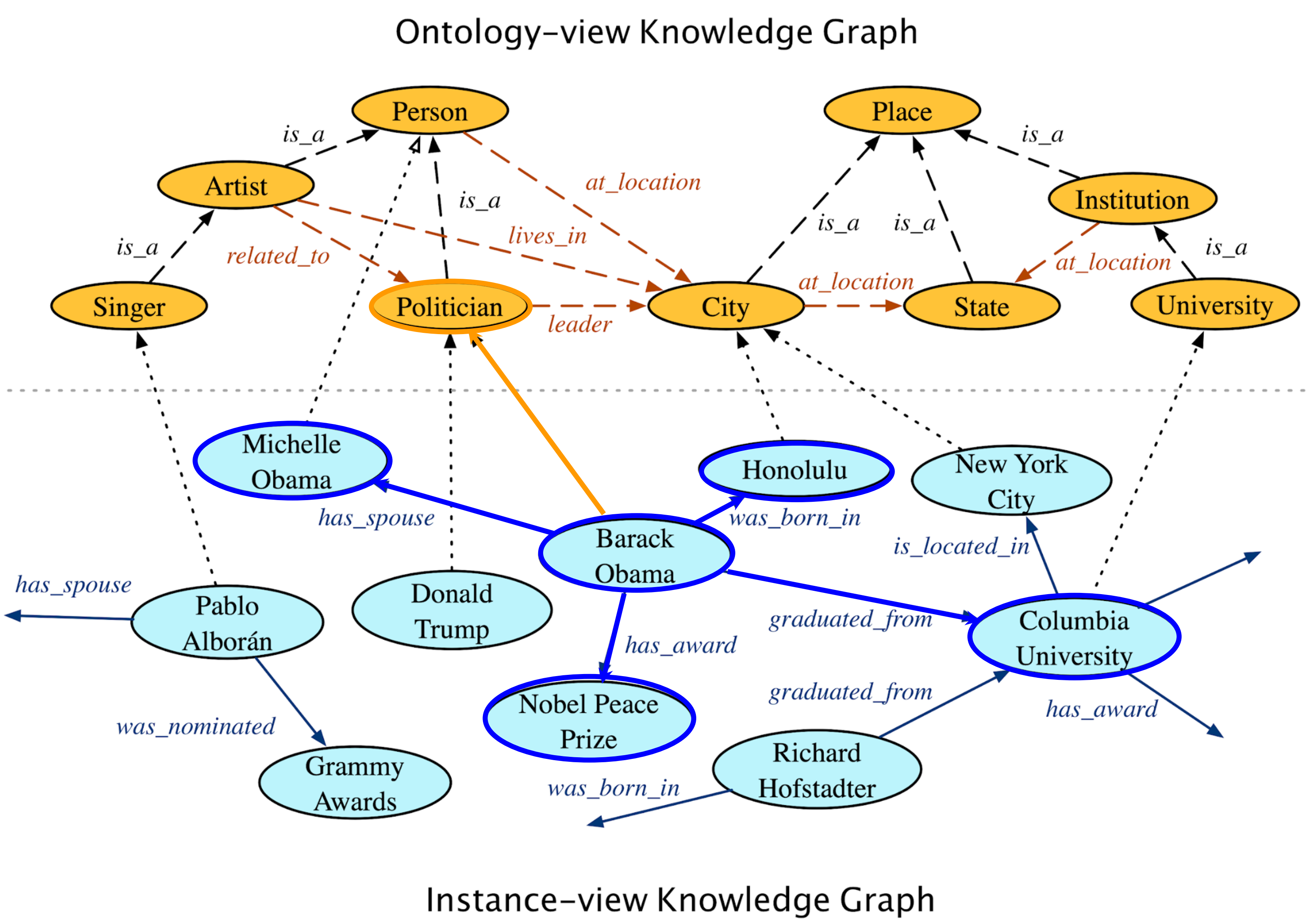
- Key of existing KG embedding methods: Triple score function



- 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., 2019)	$-\|\|\mathbf{h}\circ\mathbf{r}-\mathbf{t}\|\|^2$	$\mathbf{h},\mathbf{r},\mathbf{t}\in\mathbb{C}^k, \|r_i\|=1$

A different view: How can we learn “Obama”?

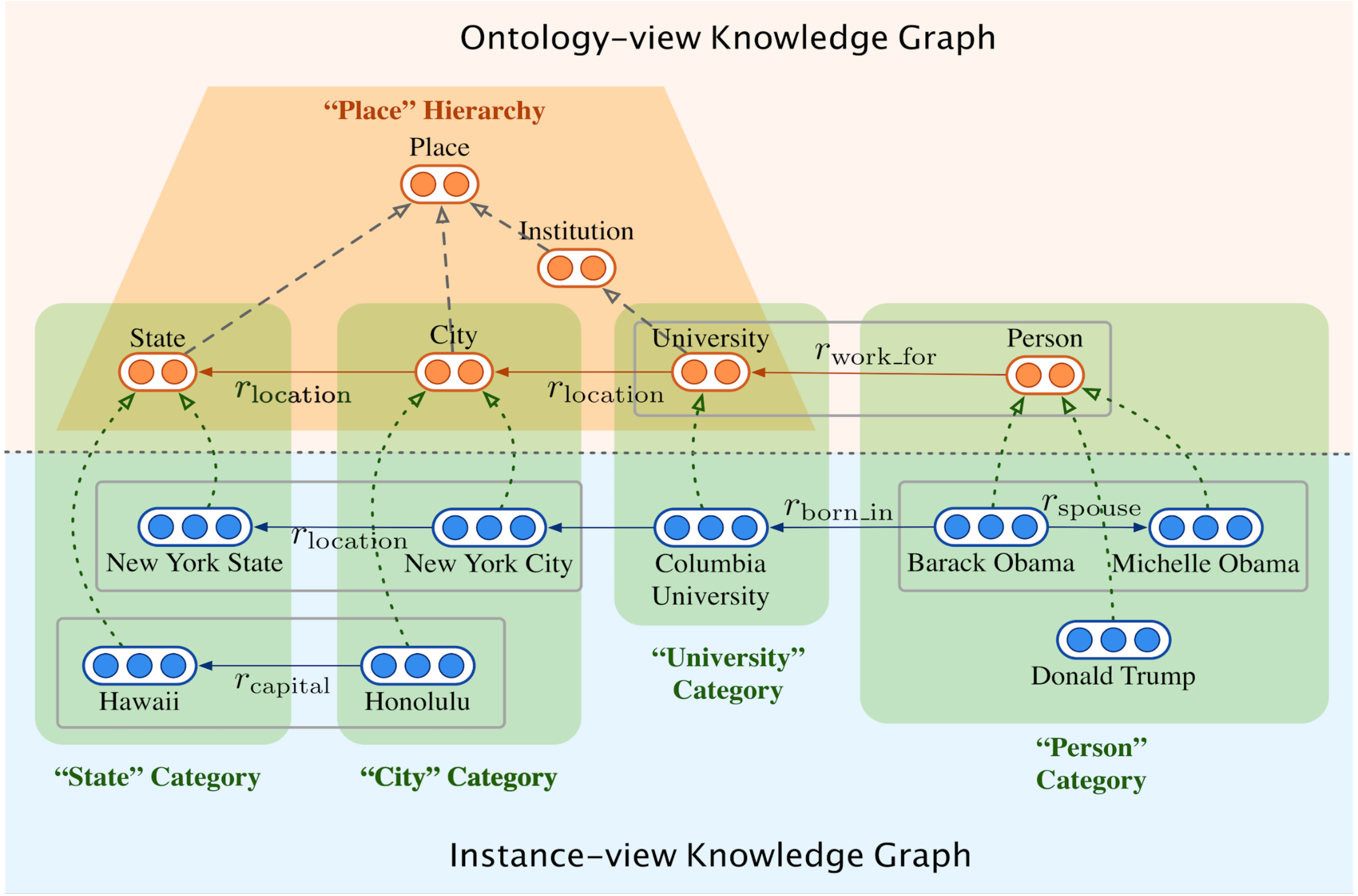


JOIE: Universal representation learning of knowledge bases by jointly embedding instances and ontological concepts

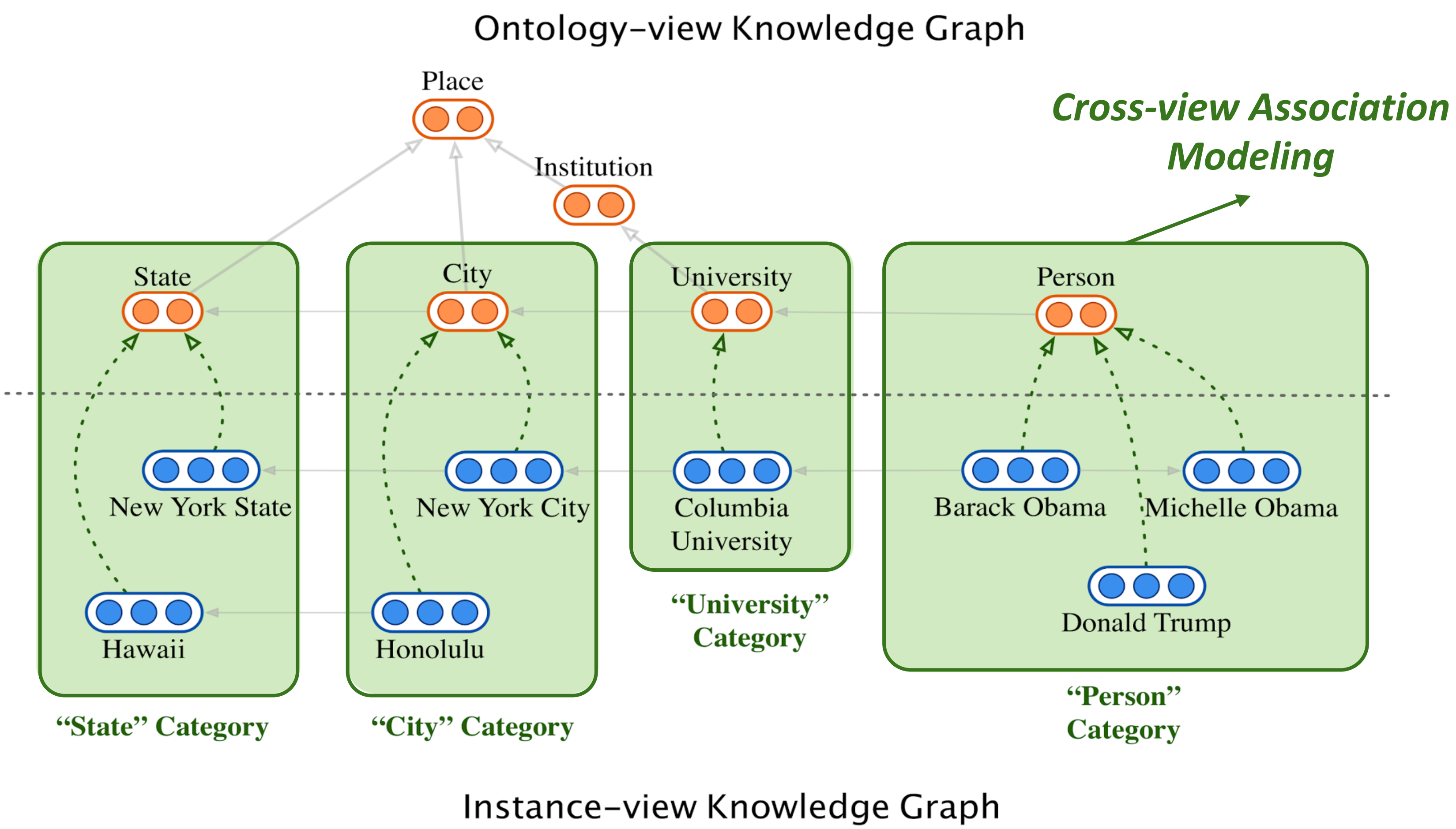
How can we manage to jointly learn the instance and ontology?

JOIE: Learning on Instance & Ontology View

- Cross-view Association model
- Intra-view model



JOIE: Cross-view Association



JOIE: Cross-view Association Modeling

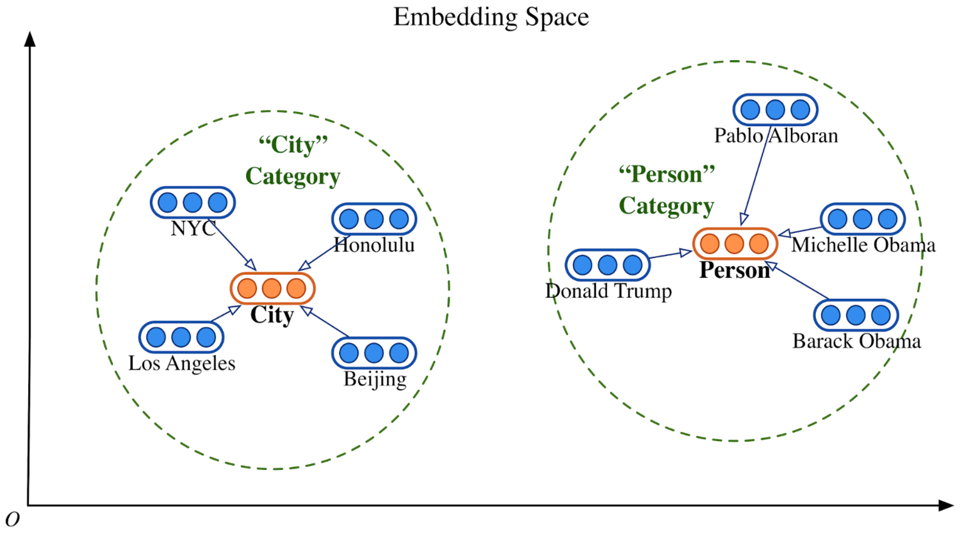
- **Goal:** capture associations between the entities **e** and corresponding concepts **c**
- **Cross-view Grouping (CG)**

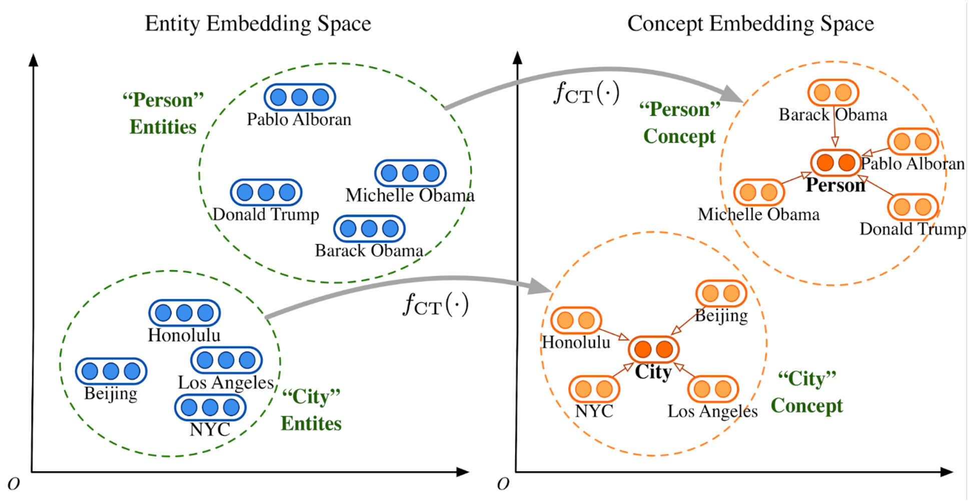
$$J_{\text{Cross}}^{\text{CG}} = \frac{1}{|\mathcal{S}|} \sum_{(e,c)\in\mathcal{S}} \left[||\mathbf{c} - \mathbf{e}||_2 - \gamma^{\text{CG}} \right]_+$$

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

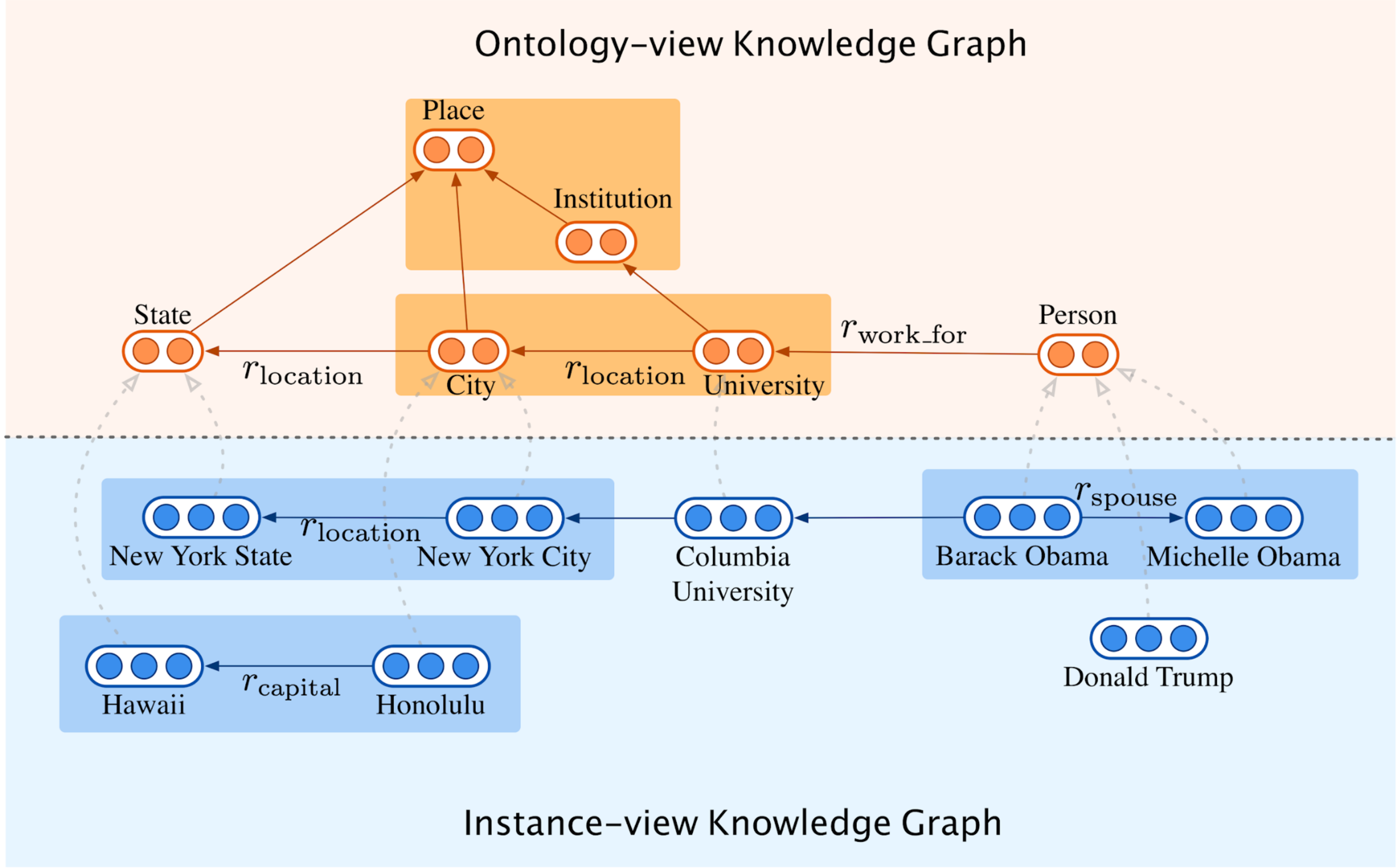
$$f_{\text{CT}}(\mathbf{e}) = \sigma(\mathbf{W}_{\text{ct}} \cdot \mathbf{e} + \mathbf{b}_{\text{ct}})$$

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





JOIE: Intra-view



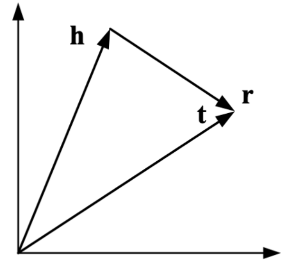
JOIE: Intra-view Model

- 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

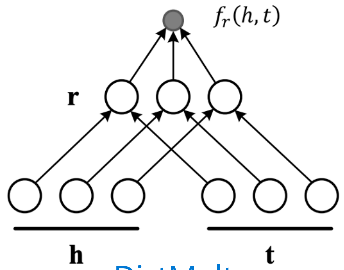
$$f_{\mathrm{TransE}}(\mathbf{h},\mathbf{r},\mathbf{t}) = -||\mathbf{h}+\mathbf{r}-\mathbf{t}||_2$$
$$f_{\mathrm{Mult}}(\mathbf{h},\mathbf{r},\mathbf{t}) = (\mathbf{h}\circ\mathbf{t})\cdot\mathbf{r}$$
$$f_{\mathrm{HolE}}(\mathbf{h},\mathbf{r},\mathbf{t}) = (\mathbf{h}\star\mathbf{t})\cdot\mathbf{r}$$

- Training on contrastive margin loss

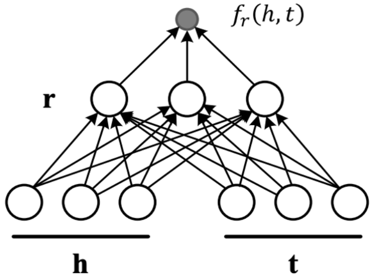
$$J_{\mathrm{Intra}}^{\mathcal{G}} = \frac{1}{|\mathcal{G}|}\sum_{\substack{(h,r,t)\in\mathcal{G}\\ \wedge(h',r,t')\notin\mathcal{G}}}\left[\gamma^{\mathcal{G}} + f(\mathbf{h}',\mathbf{r},\mathbf{t}') - f(\mathbf{h},\mathbf{r},\mathbf{t})\right]_+$$



TransE



DistMult



HolE

JOIE: Joint Training & Model Summarization

- 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
  - Optional: Hierarchical-aware modeling on ontological view specifically for taxonomy meta relations
- Joint training on cross-view loss and intra-view loss

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

JOIE: Experiment Setup

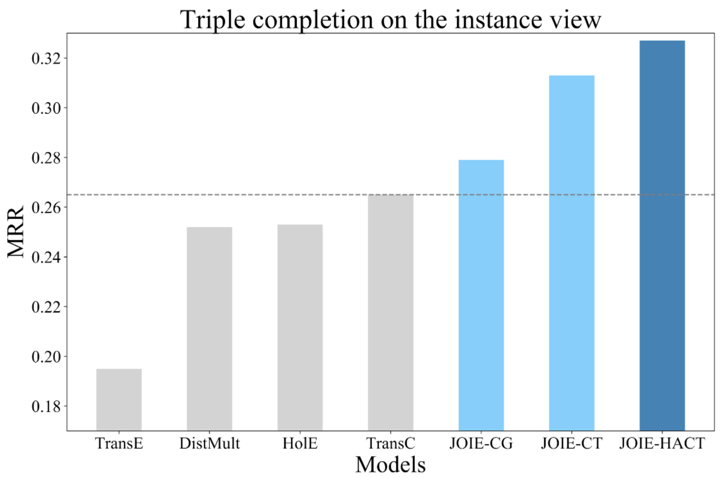
- Datasets: YAGO26K-906 (from YAGO) and DB111K-184 (from DBpedia), ontology-view leveraged from ConceptNet
- Tasks: *Triple completion* and *entity typing*
- Evaluation metrics
  - Triple completion: *MRR, Hit@K score (K=1,3,10)*
  - Entity typing: *Accuracy (Hit@1), Hit@3 Score*
- Baselines: TransE,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

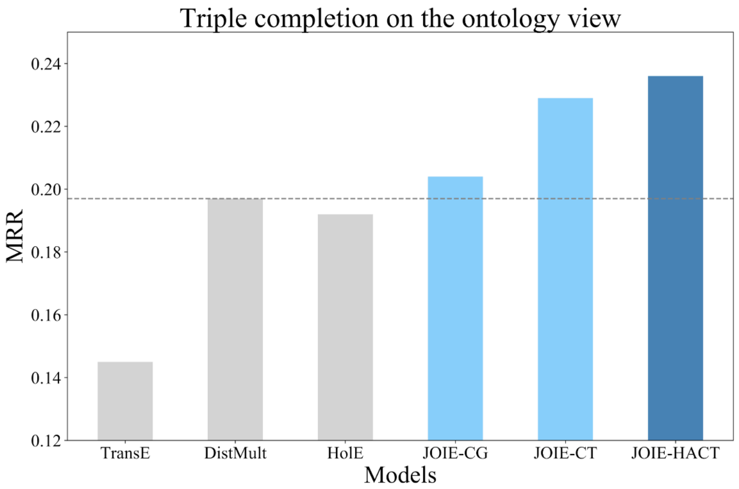
Dataset	Instance Graph $\mathcal{G}_I$			Ontology Graph $\mathcal{G}_O$			Type Links $\mathcal{S}$
	#Entities	#Relations	#Triples	#Concepts	#Meta-relations	#Triples	
YAGO26K-906	26,078	34	390,738	906	30	8,962	9,962
DB111K-174	111,762	305	863,643	174	20	763	99,748

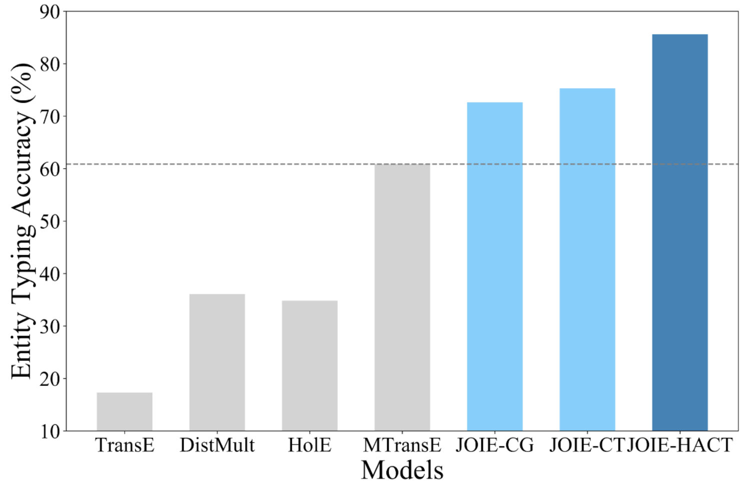
JOIE: Results

Triple Completion

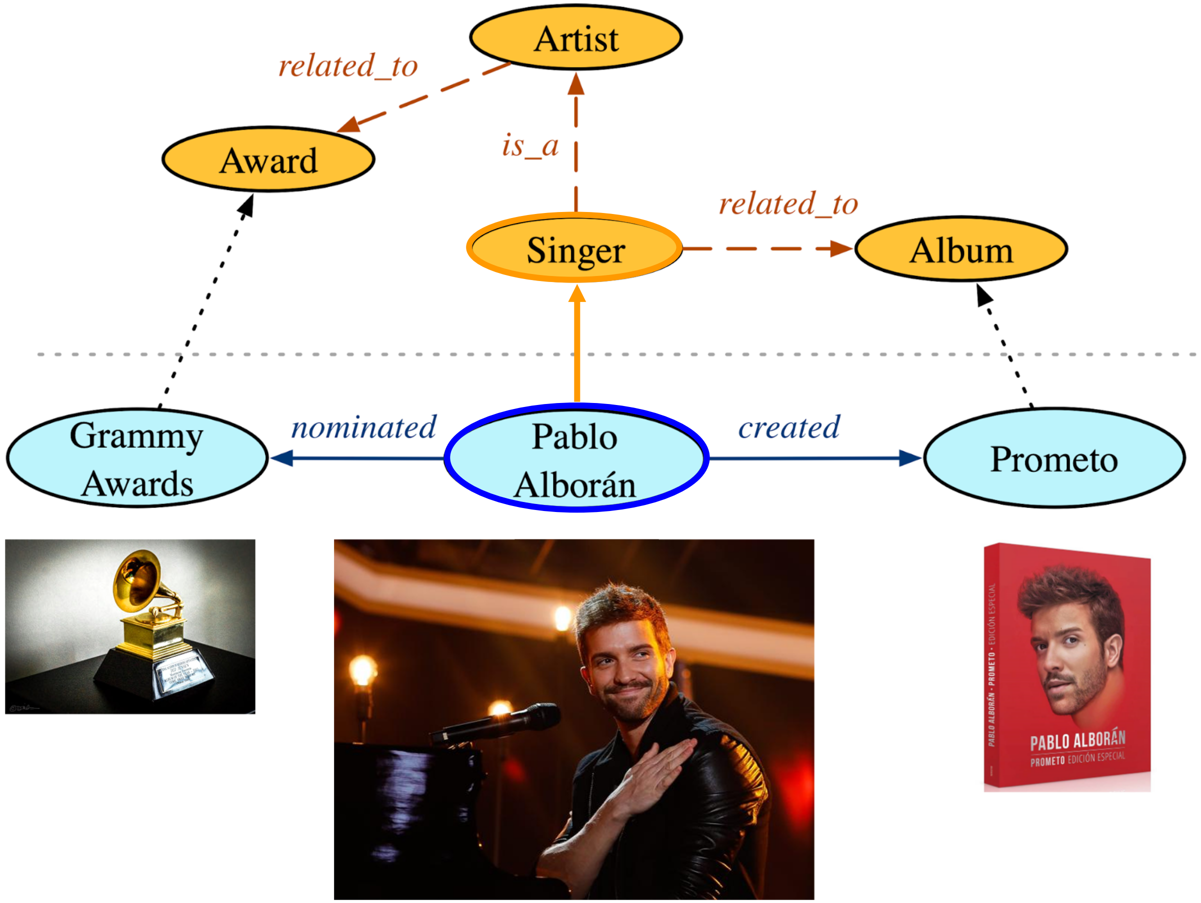
Entity Typing







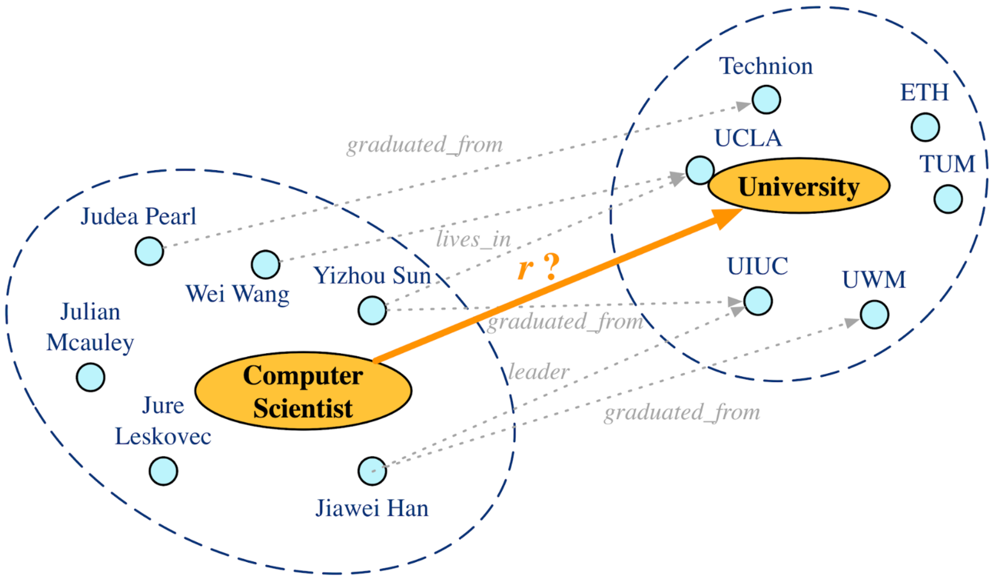
Case Study: Long-tail Entity Typing



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

Case Study: Ontology Population

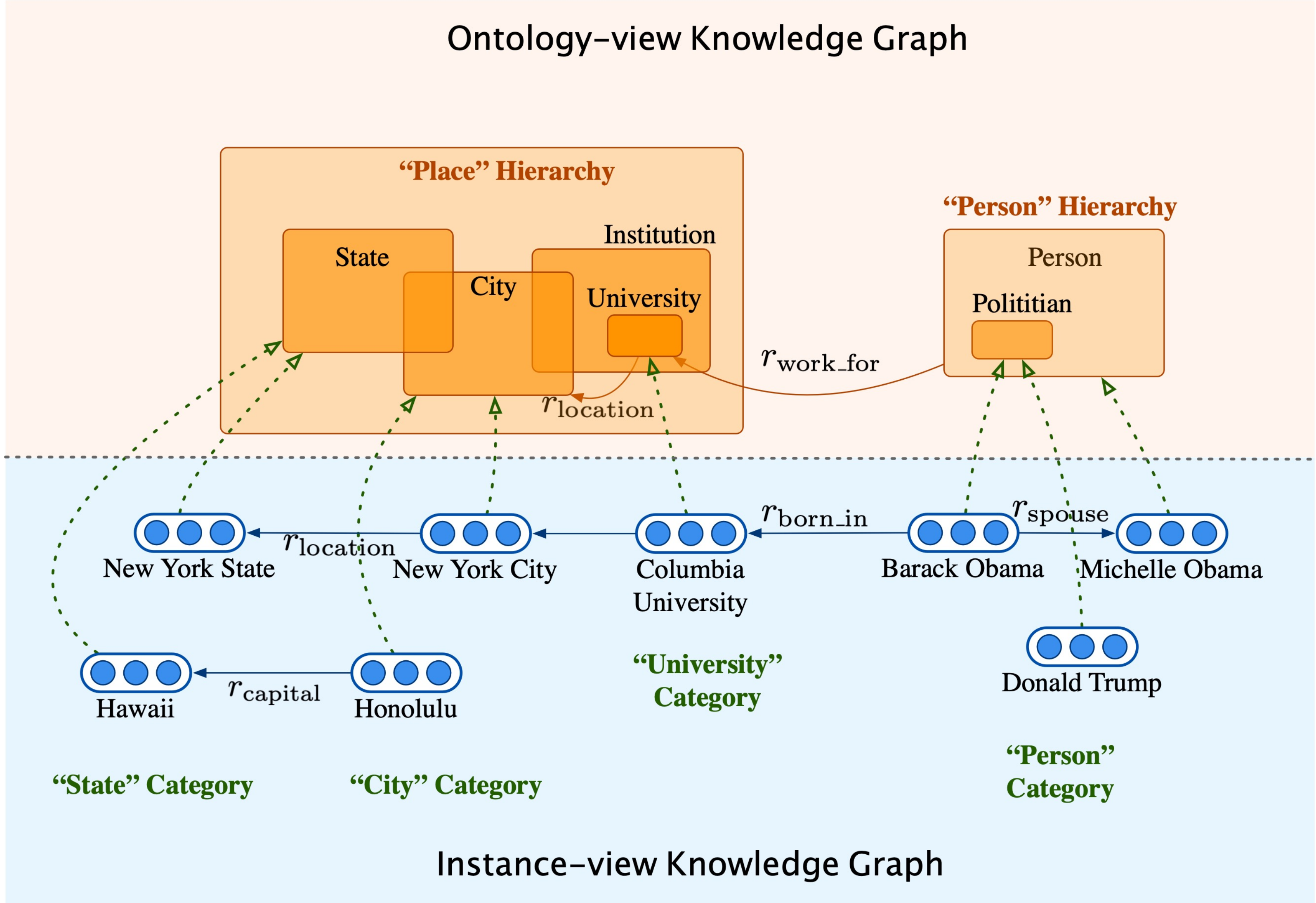


Examples of ontology population

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)

Extension: JOIE + Ontological Box Embedding

Use box embedding to better capture the hierarchy in ConceptNet (common sense) ontology.



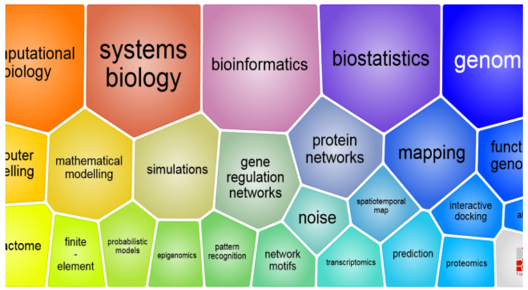
Application 1: KG in Bioinformatics

Bio-JOIE: Joint representation learning of biological knowledge bases

A story of protein interaction networks and gene ontology.
Multiple species, more views, more informational.

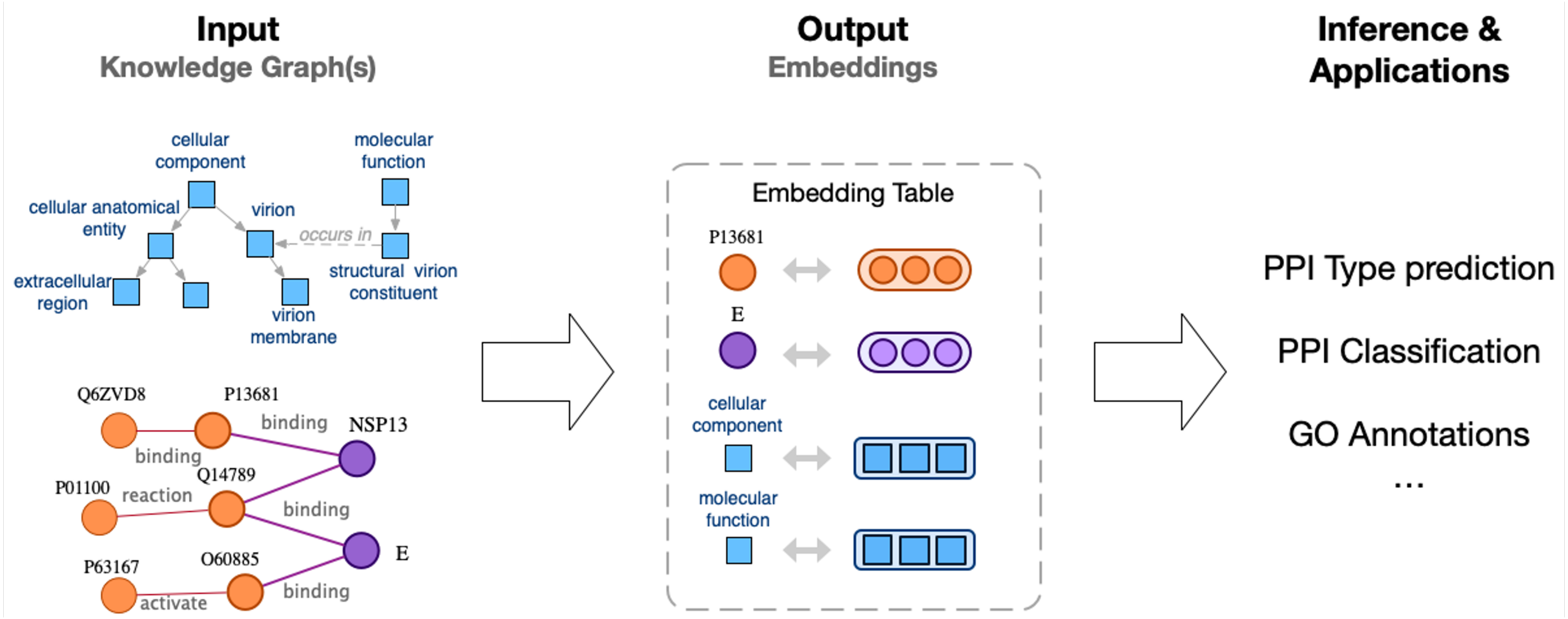
Application 1: Bio-JOIE

Knowledge Graphs



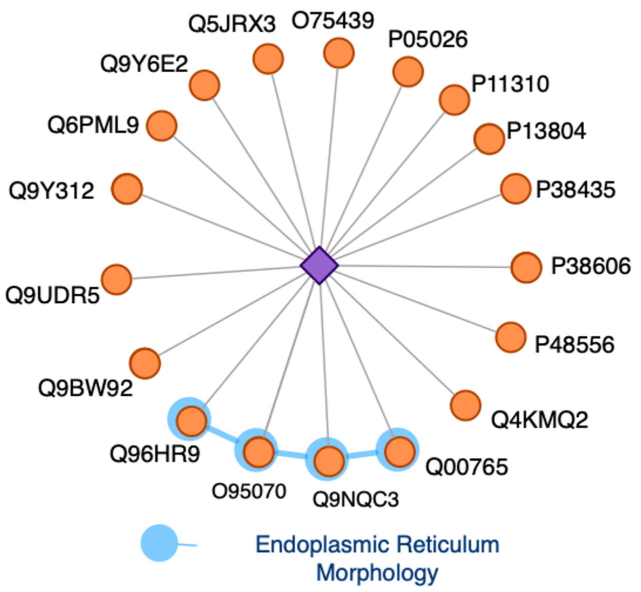
Computational Biology & Bioinformatics

KG Embedding for Medical Knowledge

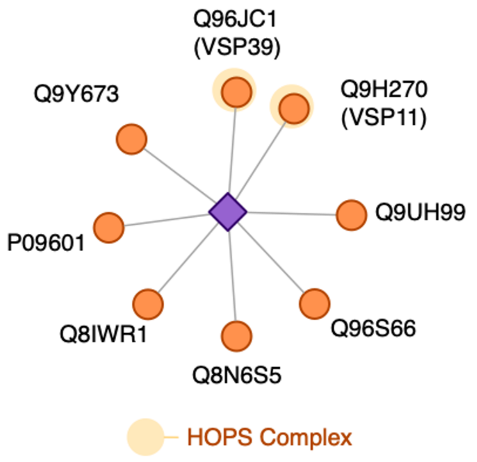


Similar Ontology-Instance Views in Bioinformatics

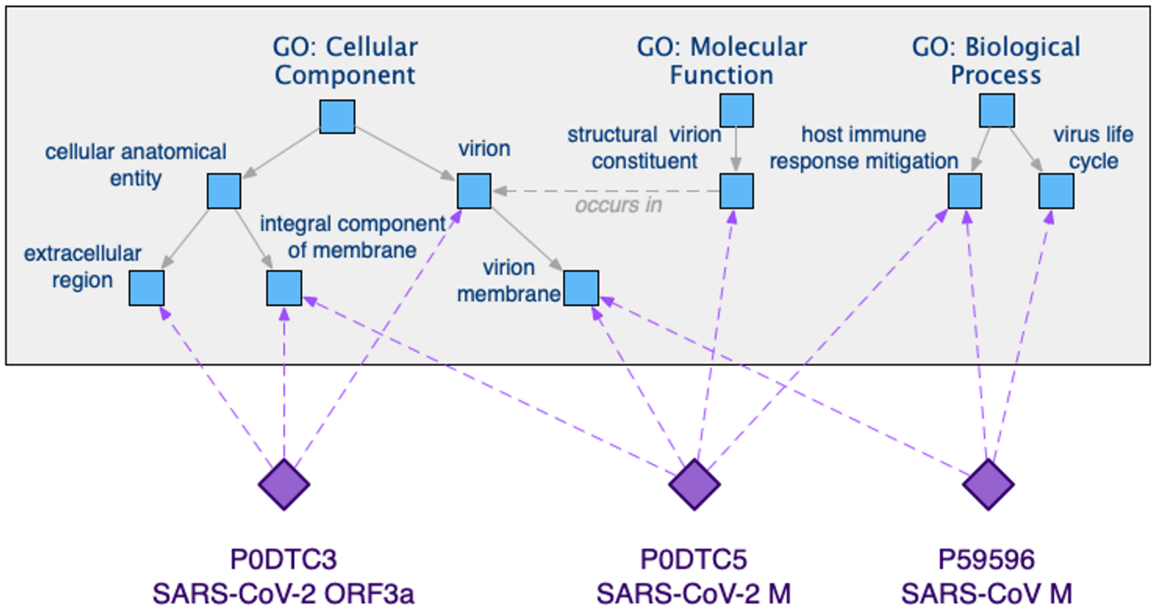
SARS-CoV-2 Human host interactions (Left) and SARS-CoV-2 Gene Ontology (GO) annotations (Right)



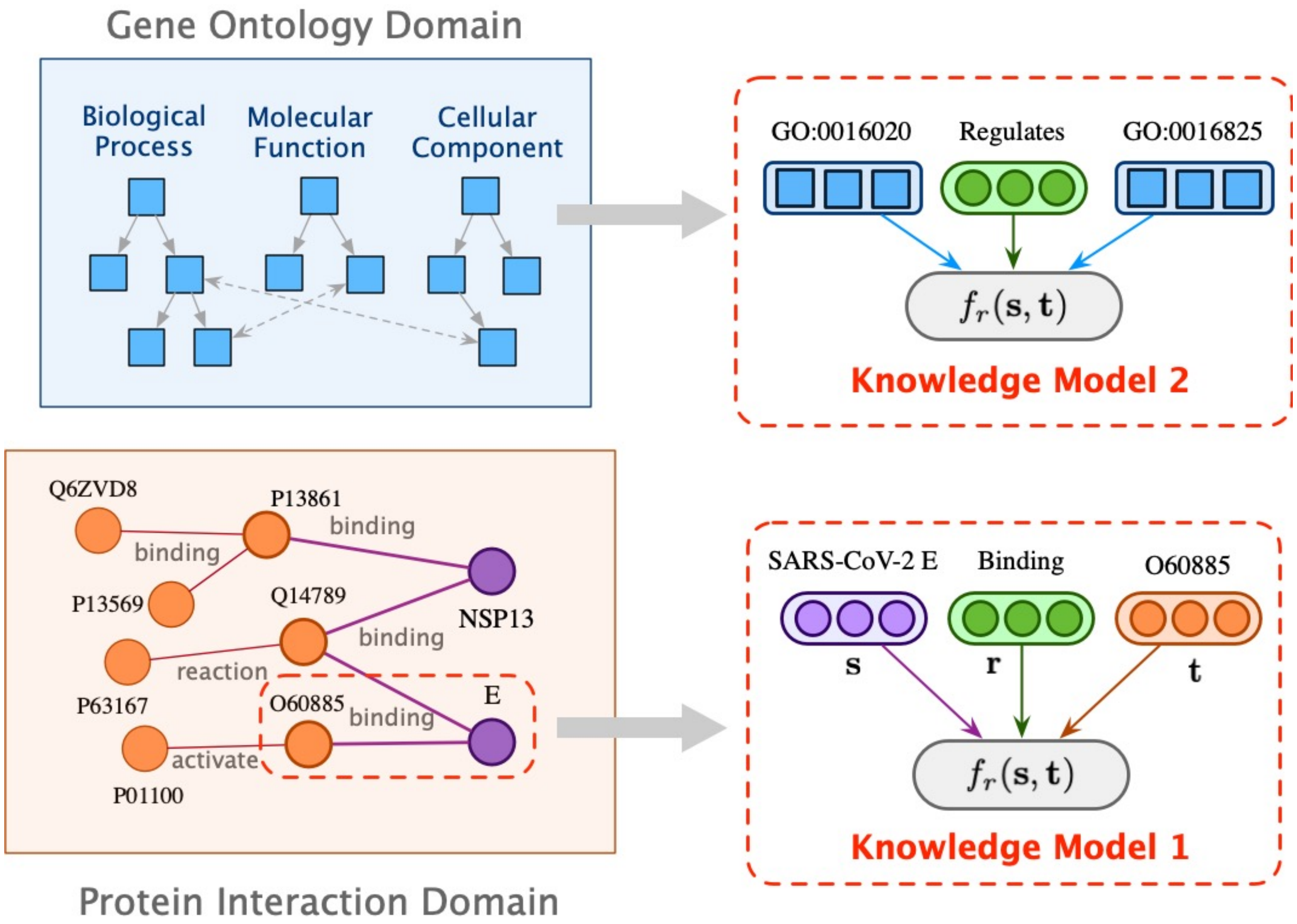
SARS-CoV-2 M Protein (P0DTC5)



SARS-CoV-2 ORF 3a Protein (P0DTC3)

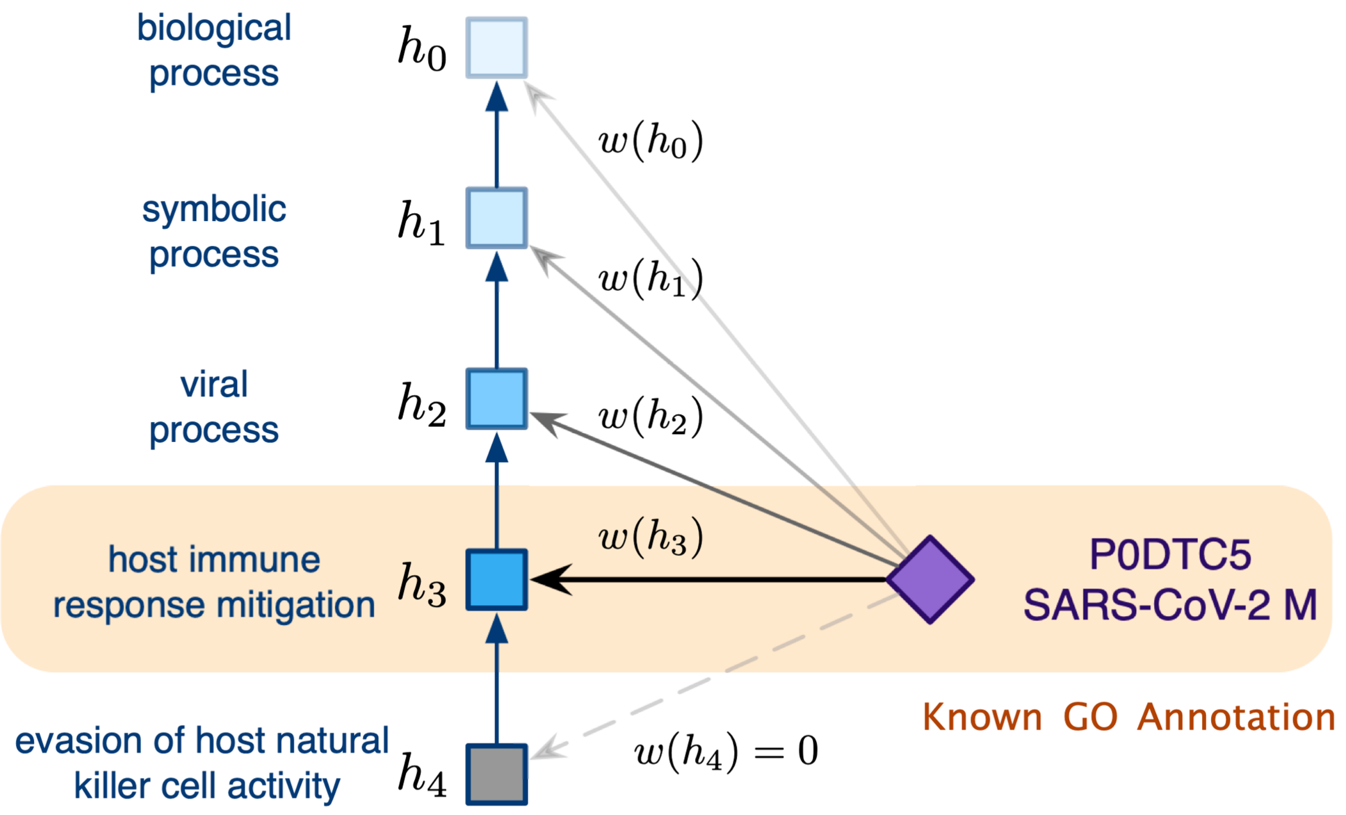


Bio-JOIE: Extension from JOIE



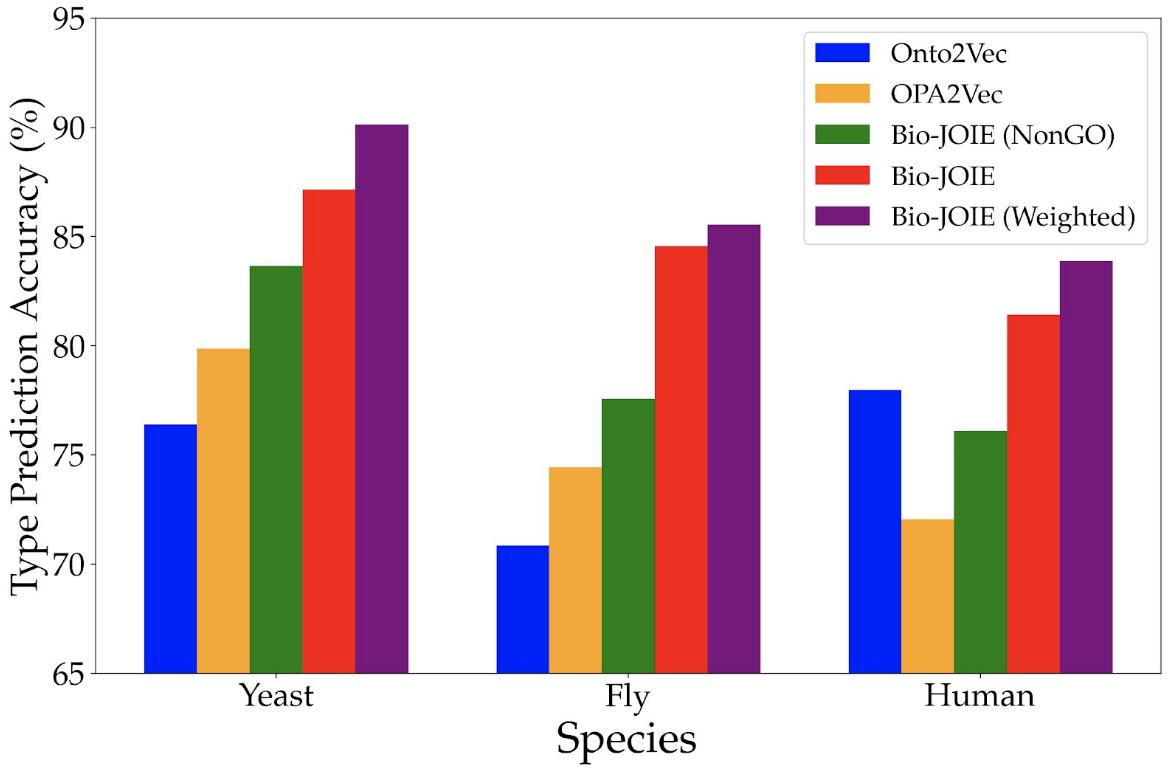
New in Bio-JOIE: Weighted Alignment

Intuition: Assign higher weights to association of protein and a specific GO term compared to a general GO term, in terms of known GO annotations



Bio-JOIE: PPI Prediction

Task: Interaction type prediction given pairs of proteins
Evaluation metric: Prediction accuracy
Baselines: Onto2Vec (variants: Parent, Ancestor, Sum, Mean) , OPA2Vec, Bio-JOIE (NonGO)



Bio-JOIE: PPI Prediction, different GO aspects

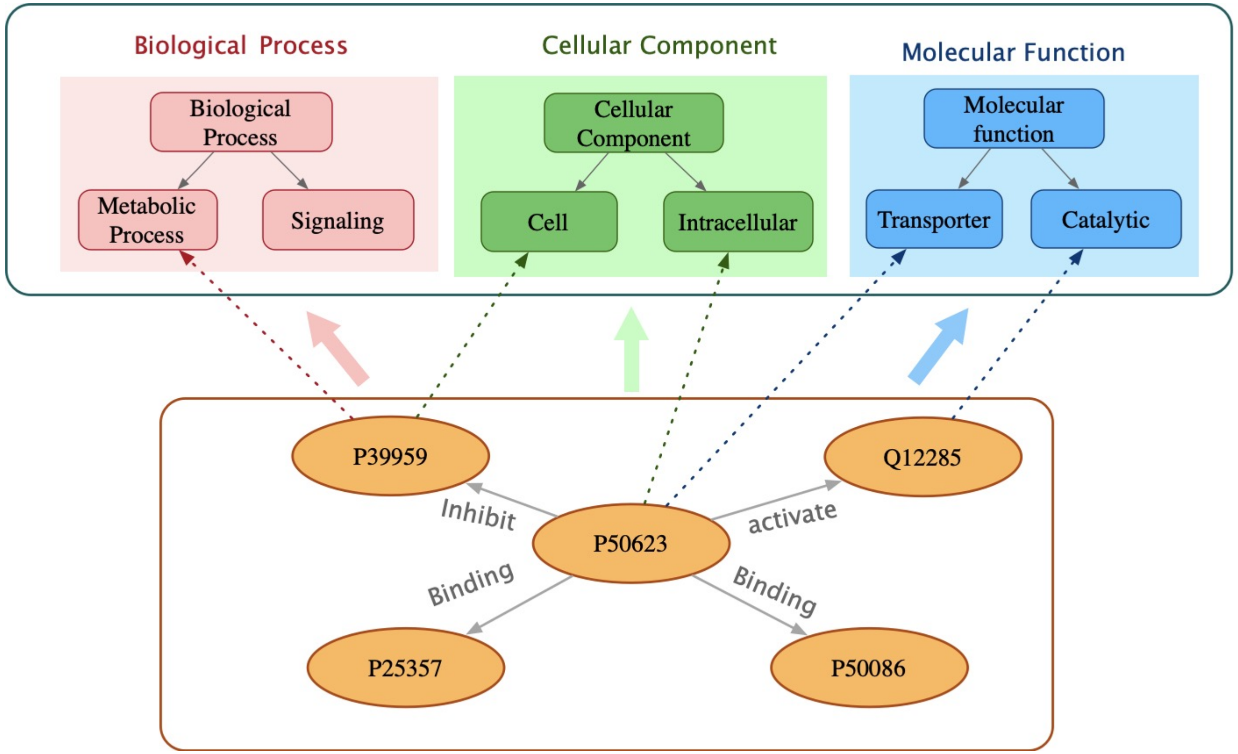
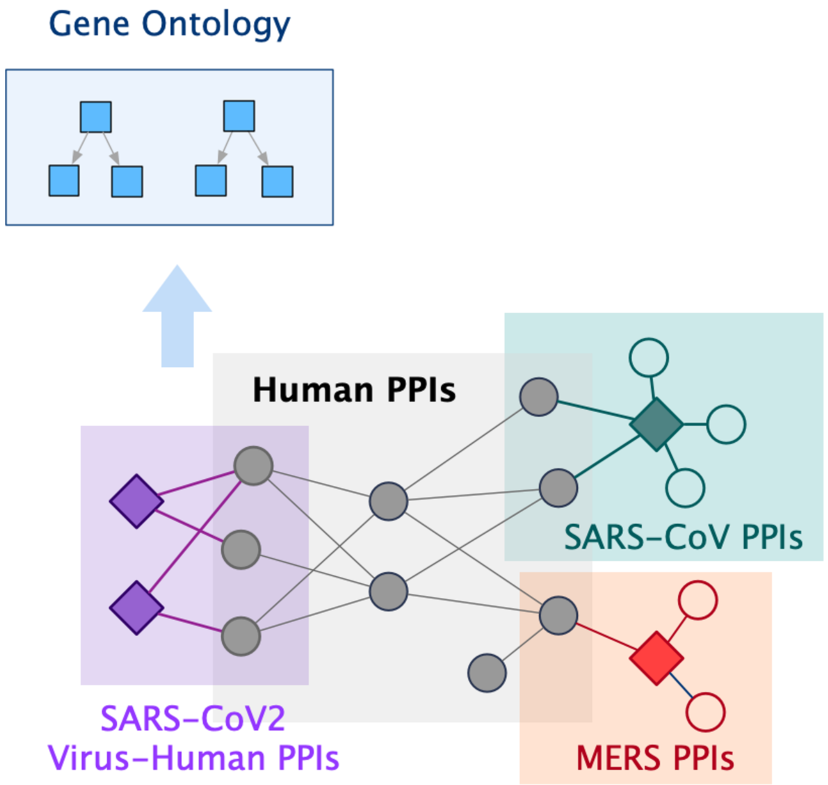


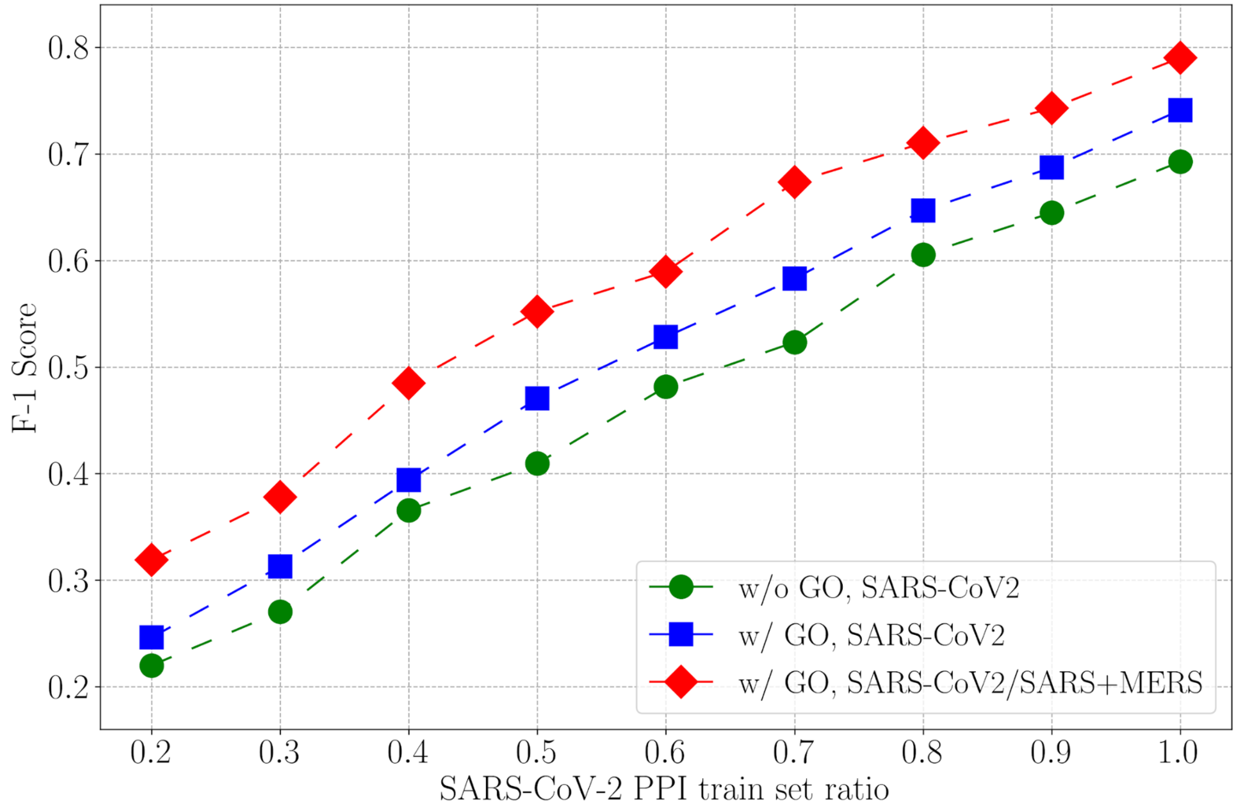
Table: Comparison of Bio-JOIE performance on combinations of three different aspects in GO.

#	Aspects	Yeast	Fly	Human
1	BP	0.8794	0.8402	0.8153
	CC	0.8499	0.8272	0.8054
	MF	0.8539	0.8386	0.8165
2	BP+CC	0.8717	0.8473	0.8271
	BP+MF	0.8673	0.8471	0.8163
	CC+MF	0.8569	0.8466	0.8170
3	AllGO	**0.9012**	**0.8555**	**0.8389**

Experiment: SARS-CoV-2 PPI Classification

Task: Virus-human PPI classification by embeddings learned from multiple gene ontology aspects and similar viruses

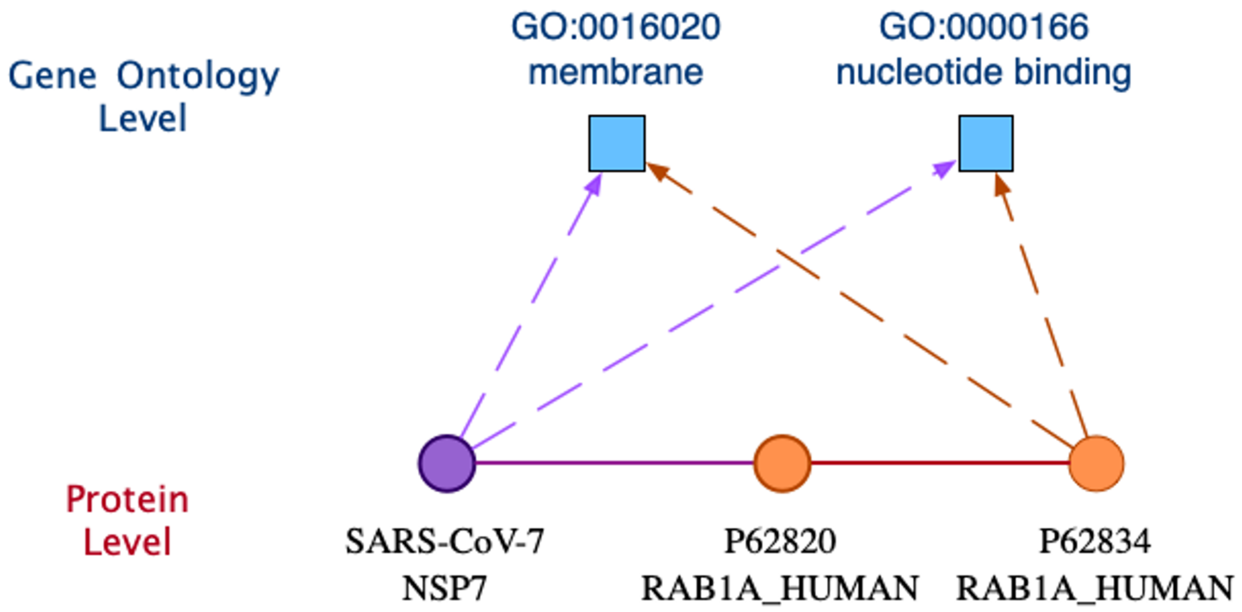




Experiment: SARS-CoV-2 Target Prediction

SARS-CoV-2 Protein	Top Predicted Human Target Proteins
NSP7	P62834(0.685), P51148(0.879), P62070(0.418), P67870, O14578, Q8WTV0(0.854), P53618(0.350), Q9BS26, O94973, Q7Z7A1

Diving deep into the top-1 prediction:



Application 2: KG in Recommendation

P-Companion: A principled framework for diversified complementary product recommendation

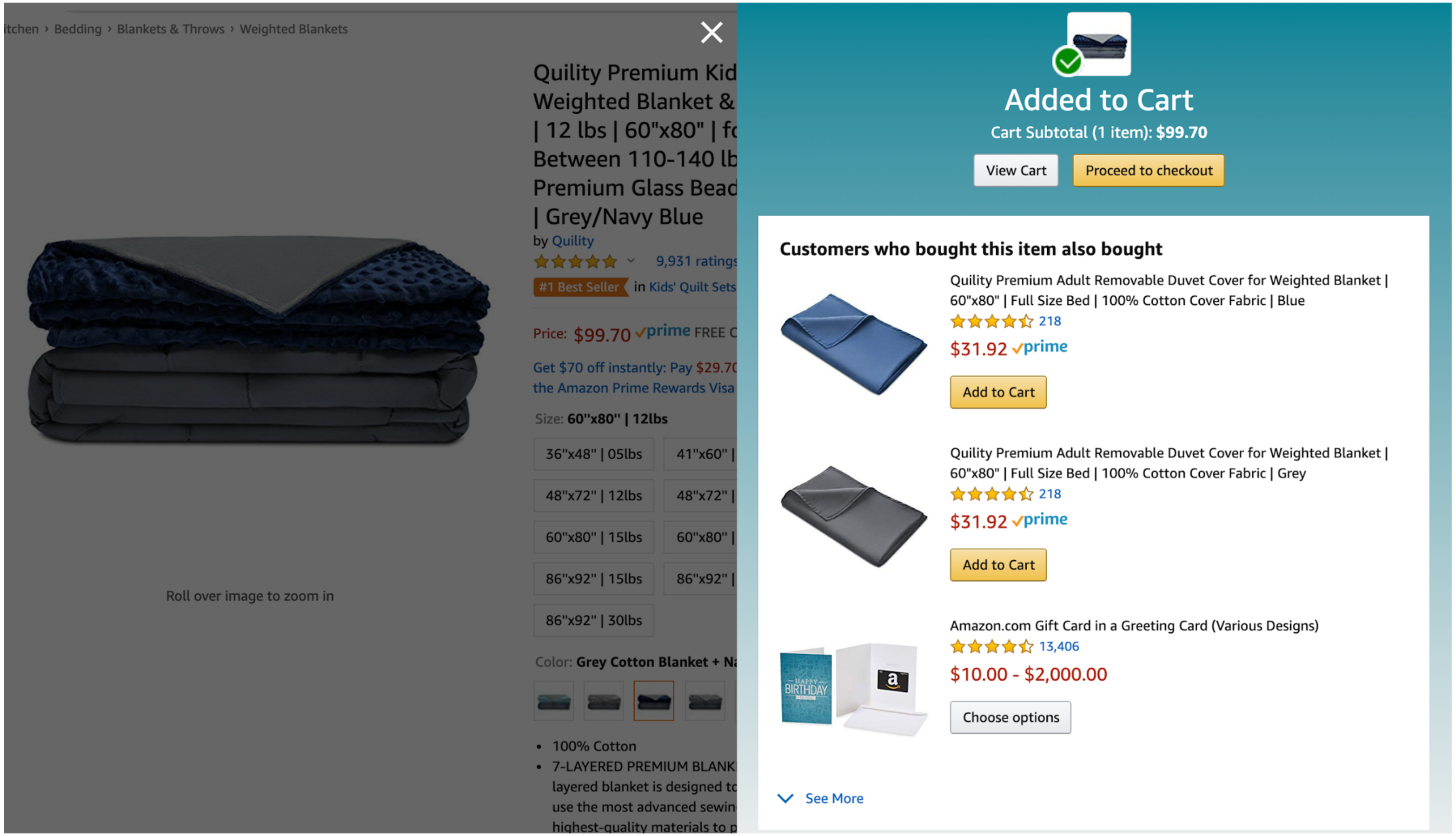
How can we manage to jointly learn the instance and ontology?

Application 2: Recommender System

Knowledge Graphs

Recommender Systems

Task: Complementary Recommendation



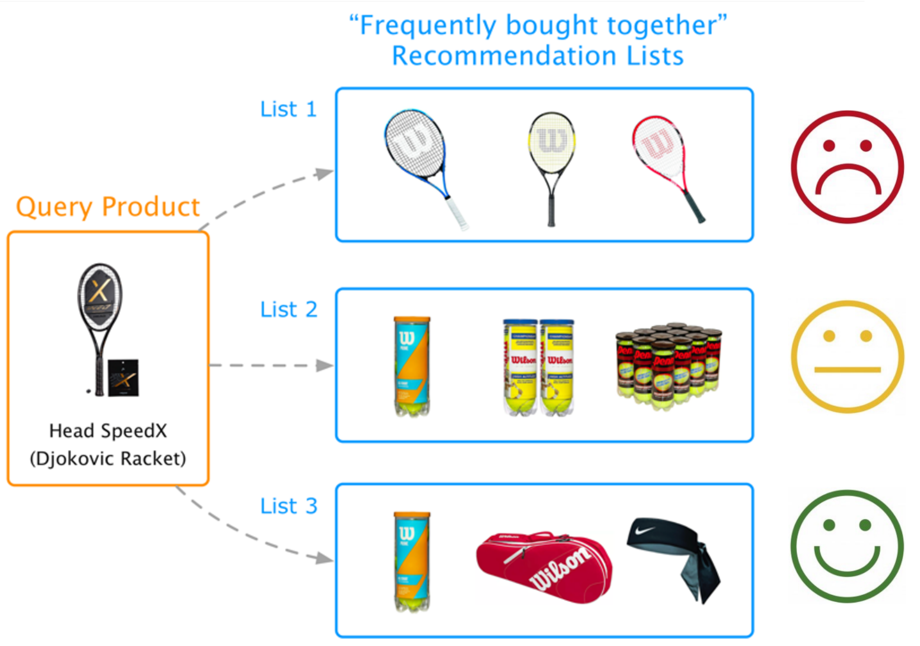
"How about just buying more? I want to go to the space." said J. Bezos

Task: Complementary Recommendation

Think about one customer who plans to buy a tennis racket (e.g., Head SpeedX Djokovic racket).

What would you recommend for him to purchase together?

- List 1: three more tennis rackets? → Sorry, we are not looking for substitutes!
- List 2: three sets of tennis balls? → Hmm, not bad, but only need one is good enough. Can we do better?
- List 3: one tennis ball pack, one bag and one headband? → Sound good this time!



Problem Definition

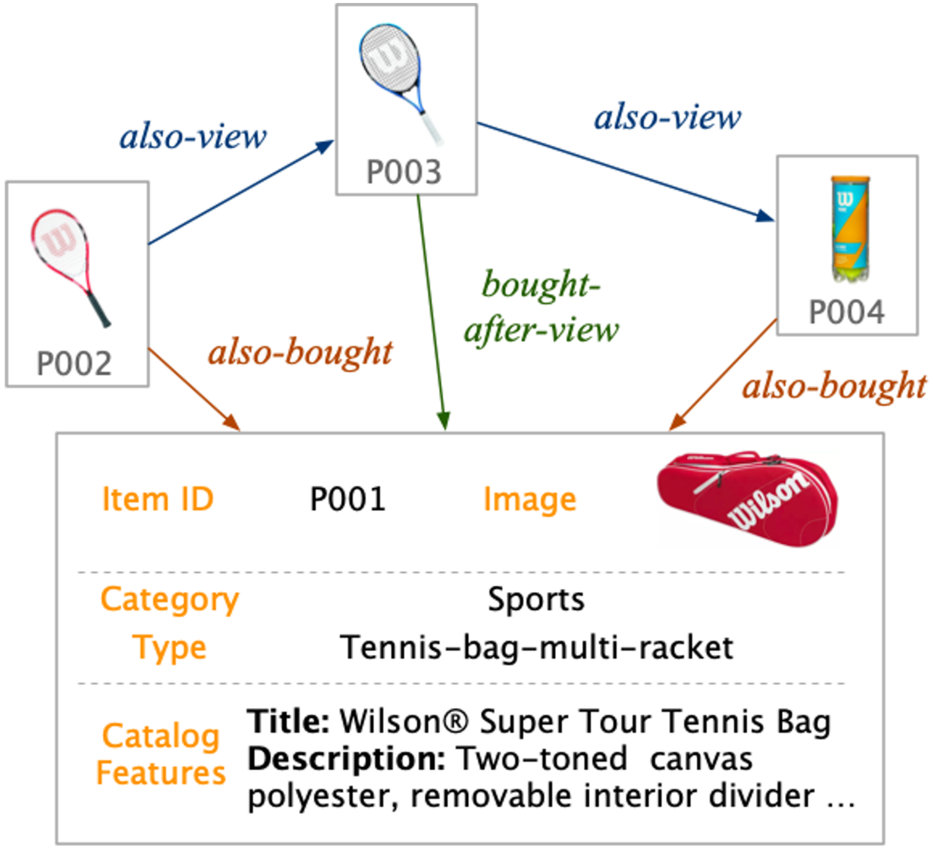
- Given the input as catalog features (including item type) and customers behavior data, for a query item ***i***, we recommend a set of items ***S*(i)**, aiming at optimizing their co-purchase probability and recommendation diversity.

query item ***i***

Recommendation set ***S*(i)**

"Behavior-based" Product Graphs (PG)

- Behavior based product graph → Attributed heterogeneous information networks (KG)
- **Node:** Product items with attributes (title, description, category, keywords)
- **Edges:** Customer browsing/purchase behaviors (such as also-bought, also-view, bought-after-view, as important indicators of substitutes or complements)
- Note that there are many alternative ways to construct product graphs, with different modeling goals.



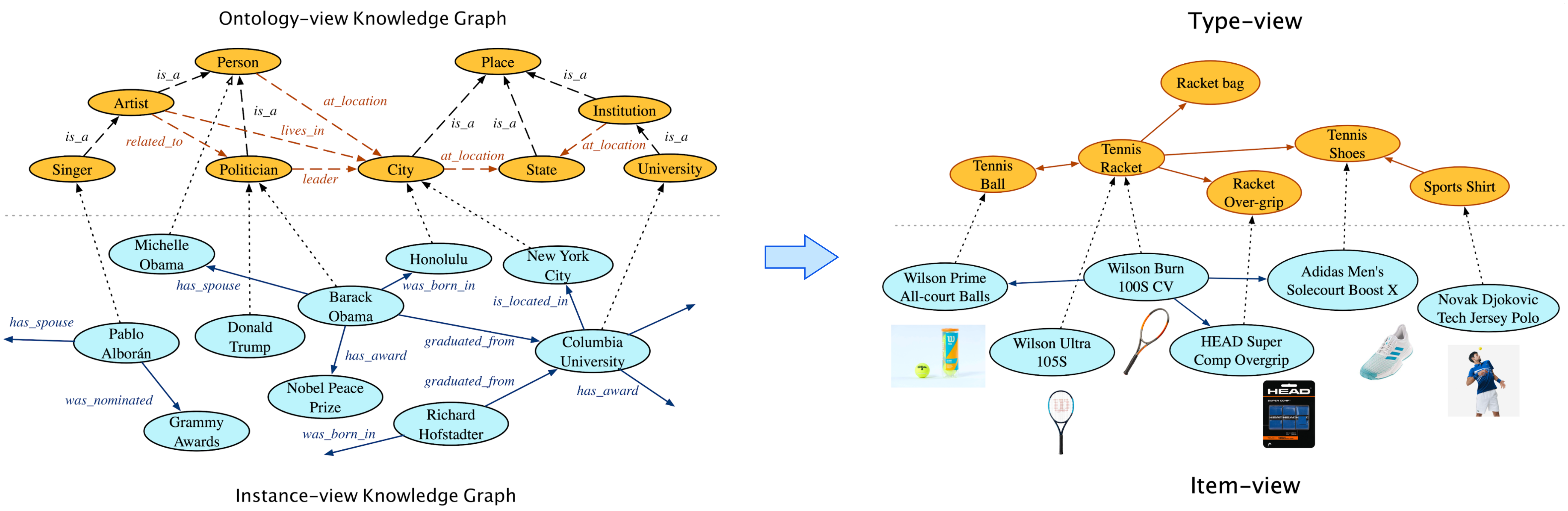
Product Node: P001

*Quick Comparison of KG and PG

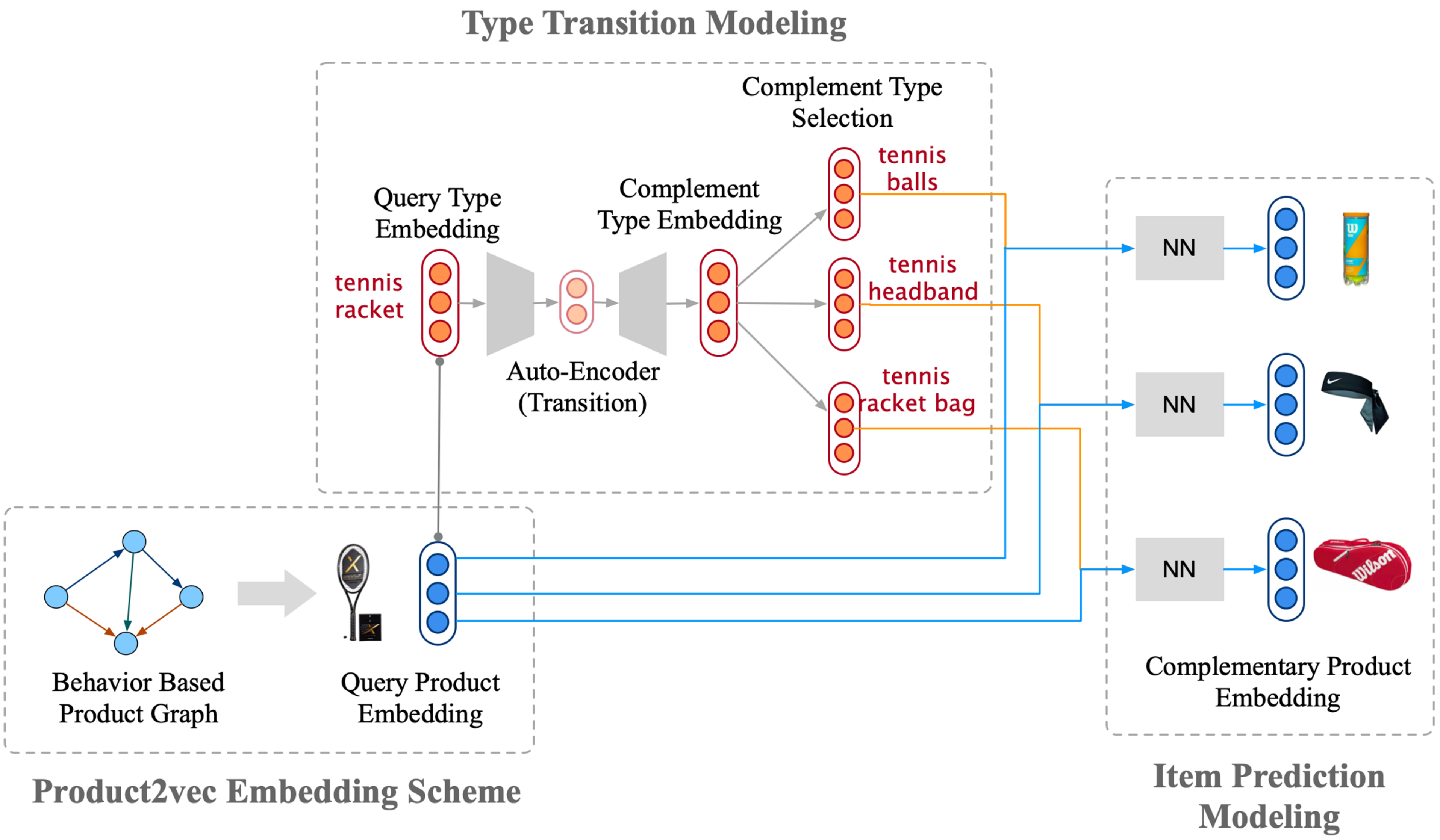
Comparison	Knowledge Graphs	Product Graphs
Source	Established facts	Product catalog, use-product interaction
Quality	Observed facts are well-established and plausible.	Much noisier
Quantity of relations	Typically, thousands of possible relations in real world, such as born_in, director_of, etc	A few relations defined from specified user behavior, such as also_view and also_bought
Attributes	Entity types, numerical features, descriptions, and many other additional features	
Logic rules	Available for logical inference and refinement.	Possibly a few rules. Similar products may have similar complements.
Downstream tasks	Knowledge completion, relation extraction, question answering, etc.	Recommendation, searching, personalization, etc.

Connecting KG to PG

Product item to product type relation in PG is like entity-concept association in KG.

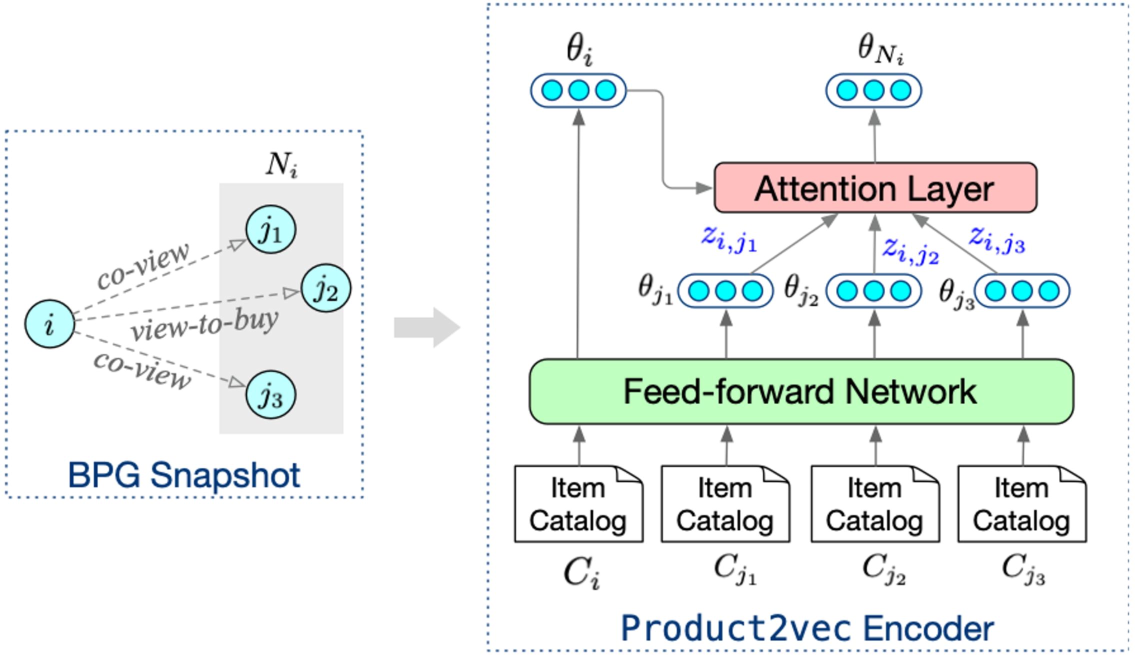


Product Companion: Workflow



Base Module: Product2vec

- GNN-based product representation learning framework
- FNN transforms the original textual features to latent embeddings and later aggregate the information from similar products selectively by the attention layer.



FNN Model:

$$\theta_i = FFN(C_j) = \sigma\left(\sigma\left(C_i W^{(1)} + b^{(1)}\right) W^{(2)} + b^{(2)}\right) W^{(3)} + b^{(3)}$$

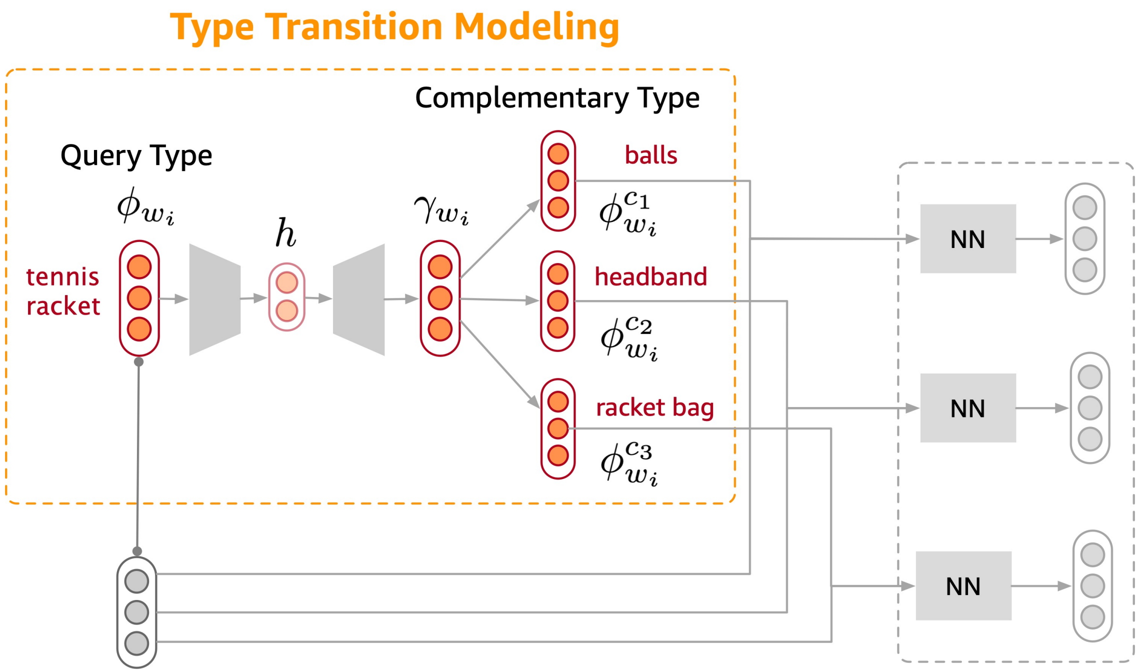
Attention Weight:

$$z_{i,j} = \mathrm{softmax}_j\left(\theta_i^T \theta_j\right) = \frac{\exp(\theta_i^T \theta_j)}{\sum_{j' \in N_i} \exp(\theta_i^T \theta_{j'})}$$

Product2Vec training loss:

$$L = \sum_{i \in \mathcal{I}} \sum_{y \in \{\pm 1\}} \left\{\max\left(\epsilon - y \cdot \left(\lambda - ||\theta_i - \theta_{N_i}||_2^2\right)\right)\right\}$$

Module 2: Complementary Type Transition



Auto-encoder based type transition model:

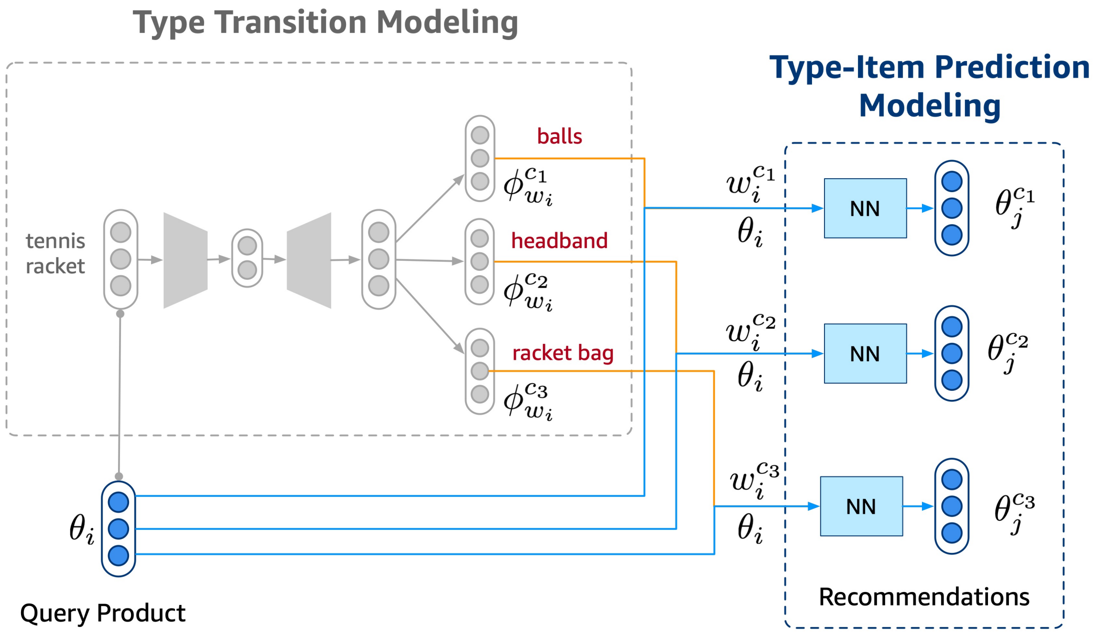
$$h = \mathrm{Dropout}\left(\mathrm{ReLU}\left(\phi_{w_i} W^{(4)} + b^{(4)}\right)\right)$$

$$\gamma_{w_i} = hW^{(5)} + b^{(5)}$$

Training loss:

$$\min \sum_{i,j \in \mathcal{T}} \left(\max \left\{ 0, \epsilon_w - y_{i,j} \left(\lambda_w - \|\gamma_{w_i} - \phi_{w_j}^c\|_2^2 \right) \right\} \right)$$

Module 3: Complementary Item Prediction



Item prediction neural model:

$$\theta_i^{w_c} = \theta_i \odot (\phi_{w_c}^c W^{(6)} + b^{(6)}),$$
$$s.t., \ ||\phi_{w_c}^c - \gamma_{w_i}||_2^2 \leq \beta$$

Training loss:

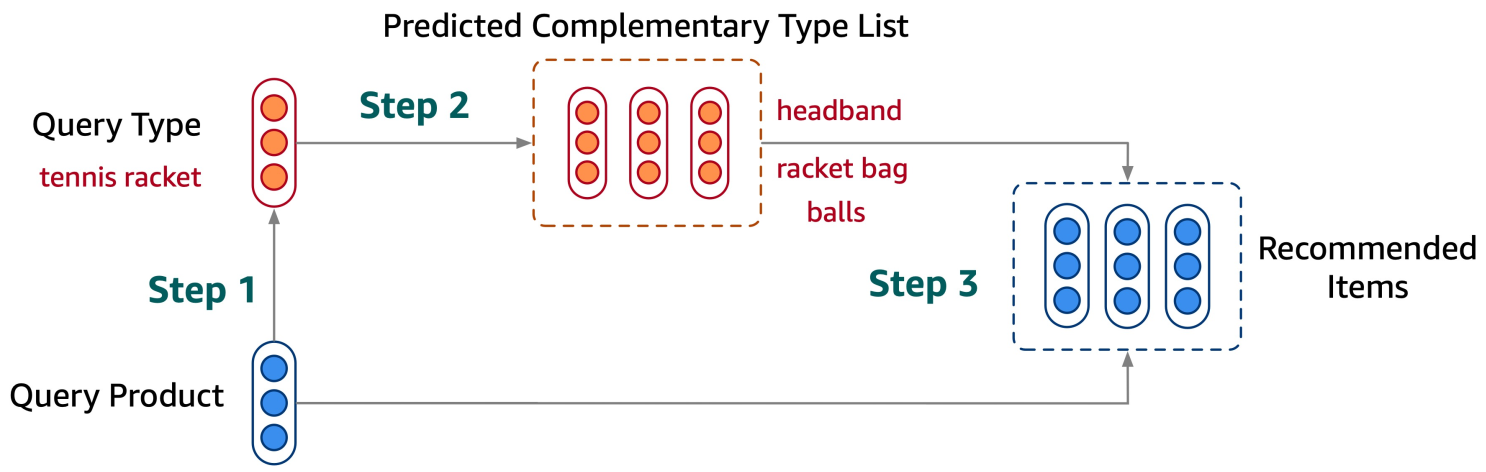
$$\min \sum_{i,j \in \mathcal{T}} \max \{0, \epsilon_i - y_{i,j} (\lambda_i - \|\theta_i^{w_c} - \theta_j\|_2^2)\}$$

Joint Training and Inference

Joint training on type transition and item prediction:

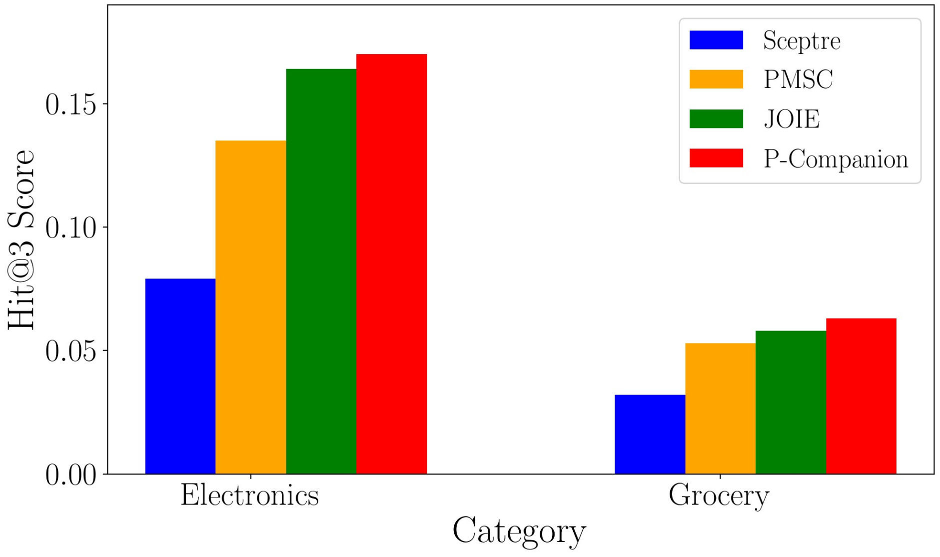
$$\min \sum_{i,j \in \mathcal{T}} \alpha \underbrace{\boxed{\left(\max\left\{0, \epsilon_i - y_{i,j}\left(\lambda_i - \|\theta_i^{w_j} - \theta_j\|_2^2\right)\right)\right\}}}_{\text{Item prediction loss}} + (1-\alpha) \underbrace{\boxed{\left(\max\left\{0, \epsilon_w - y_{i,j}\left(\lambda_w - \|\gamma_{w_i} - \phi_{w_j}^c\|_2^2\right)\right\}\right)}}_{\text{Type transition loss}}$$

Inference stage:



Evaluation: From history purchase data

- Given a pair **(i , j)**, associated with type **wi** and **wj**, from co-purchase record as ground truth, we ask our model as well as all baselines to output recommendation list (with predicted complementary types), and consider the following:
  - whether item **j** is in the list. → ***Item level***
  - Whether type **wj** is in the predicted types → ***Type level***
- Metric: Hit@K score (both item level and type level, if applicable)
- Baselines: Sceptre, PMSC, JOIE



Dataset		Electronics	Grocery
Model & Setting		Hit@60	Hit@60
Sceptre		0.124	0.085
PMSC		0.179	0.139
JOIE		0.200	0.155
P-Companion	1 type × 60 items	0.138	0.088
	3 types × 20 items	0.198	0.153
	5 types × 12 items	0.222	**0.189**
	6 types × 10 items	**0.227**	0.187

Case Study: Type Transition Prediction

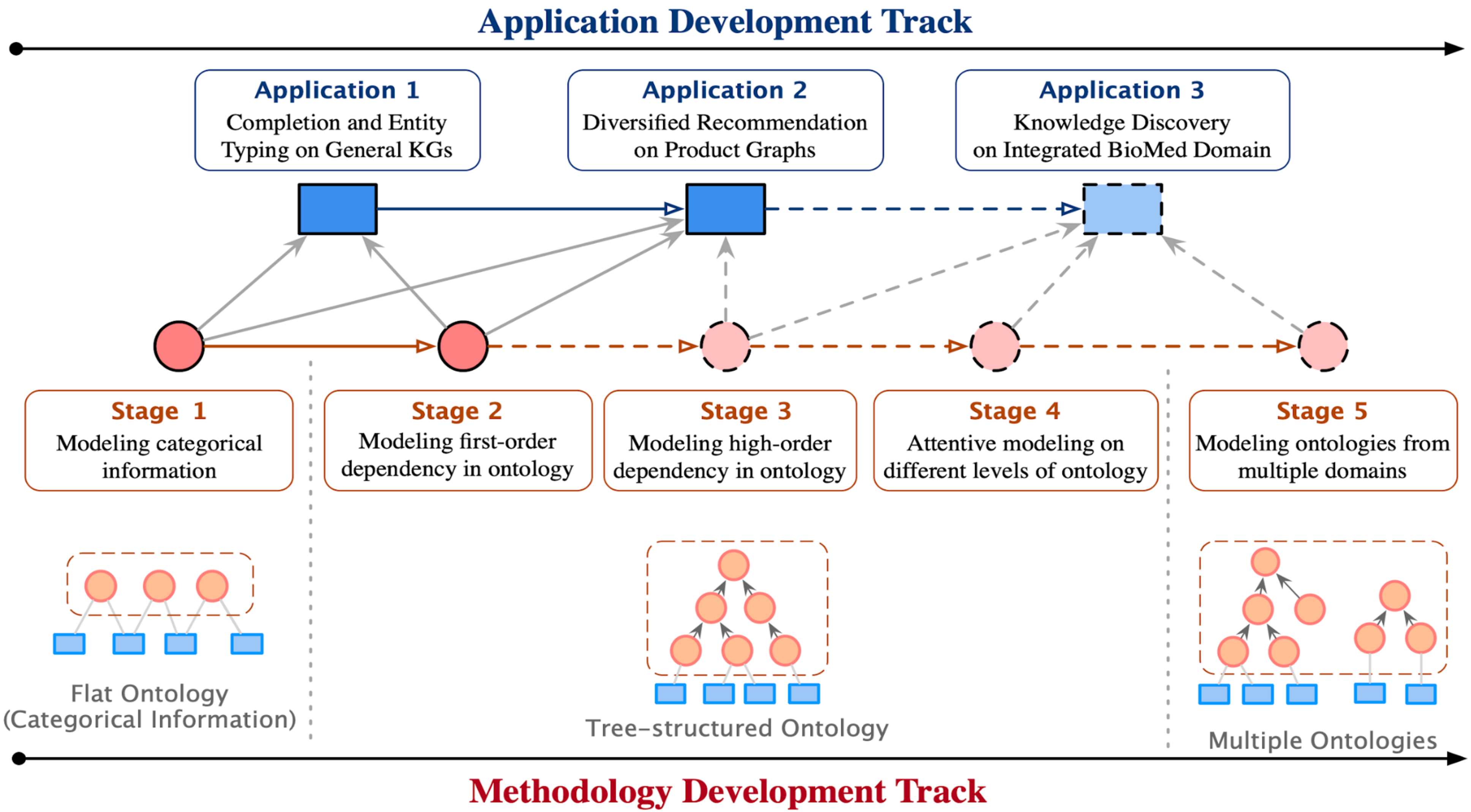
- Examples of Predicted Top-3 Complementary Type Predictions

Query Type	Predicted Complementary Types
camera-power-adapter	(1) sec-digit-card (2) micro-sd-card (3) hdmi-cable
cell-phone-battery	(1) cell-phone-screen-protect (2) battery-charge-case (3) flip-cell-phone-carry-case
roast-coffee-bean	(1) fridge-coffee-cream (2) whole-bean (3) white-tea
fly-fish-line	(1) fluorocarbon-fish-line (2) surf-fish-rod (3) fly-fish-reel

Case Study: Product Recommendation

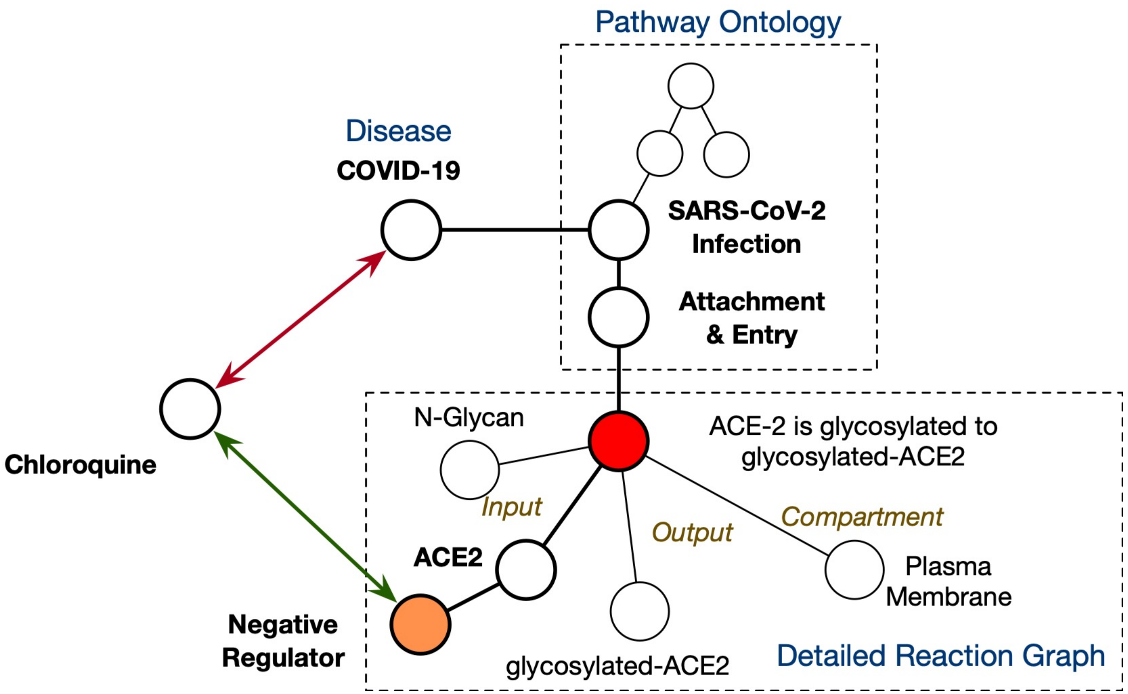
Category	Query Item	Co-Purchase	Top-5 Recommendations from P-Companion
Electronics			
Grocery			
All-Group (Pet home)		None	
All-Group (Fishing tools)		None	

Research Development Map (Ongoing)

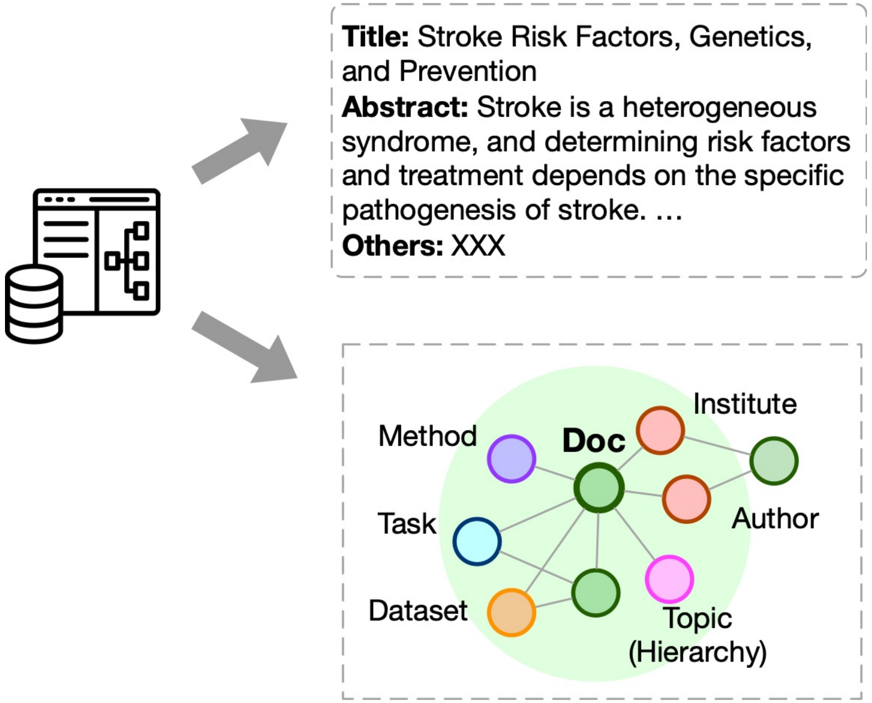


KG Representation with Graph Attributes

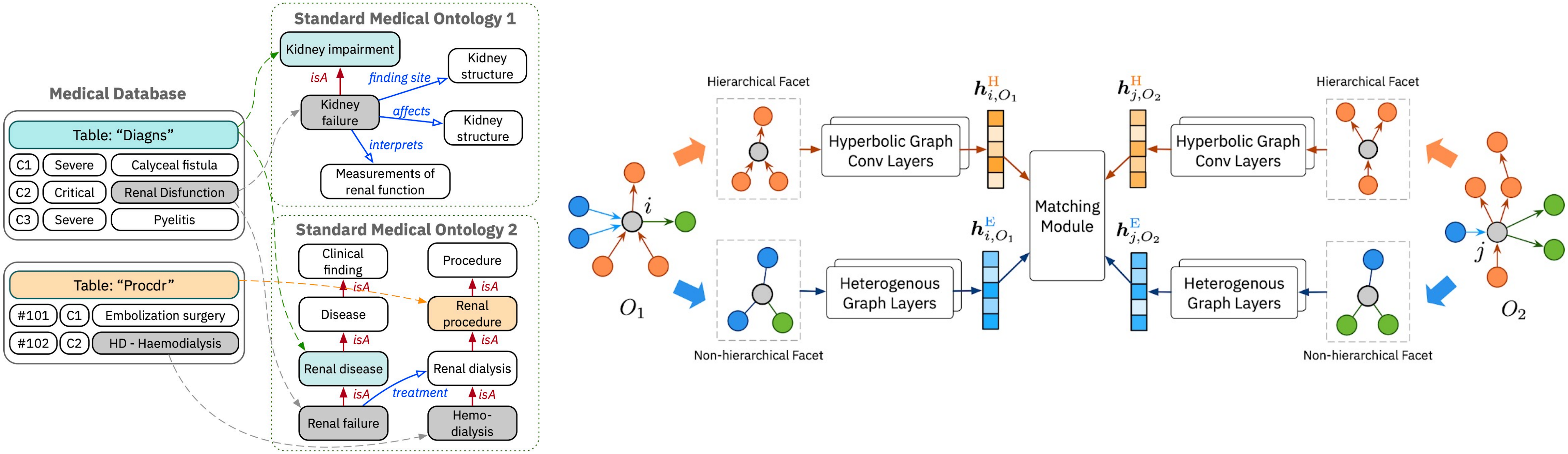
Example 1: Reaction Graph in Bio-KG



Example 2: Document Structured Knowledge



Hybrid-GNN Data-Ontology Matching

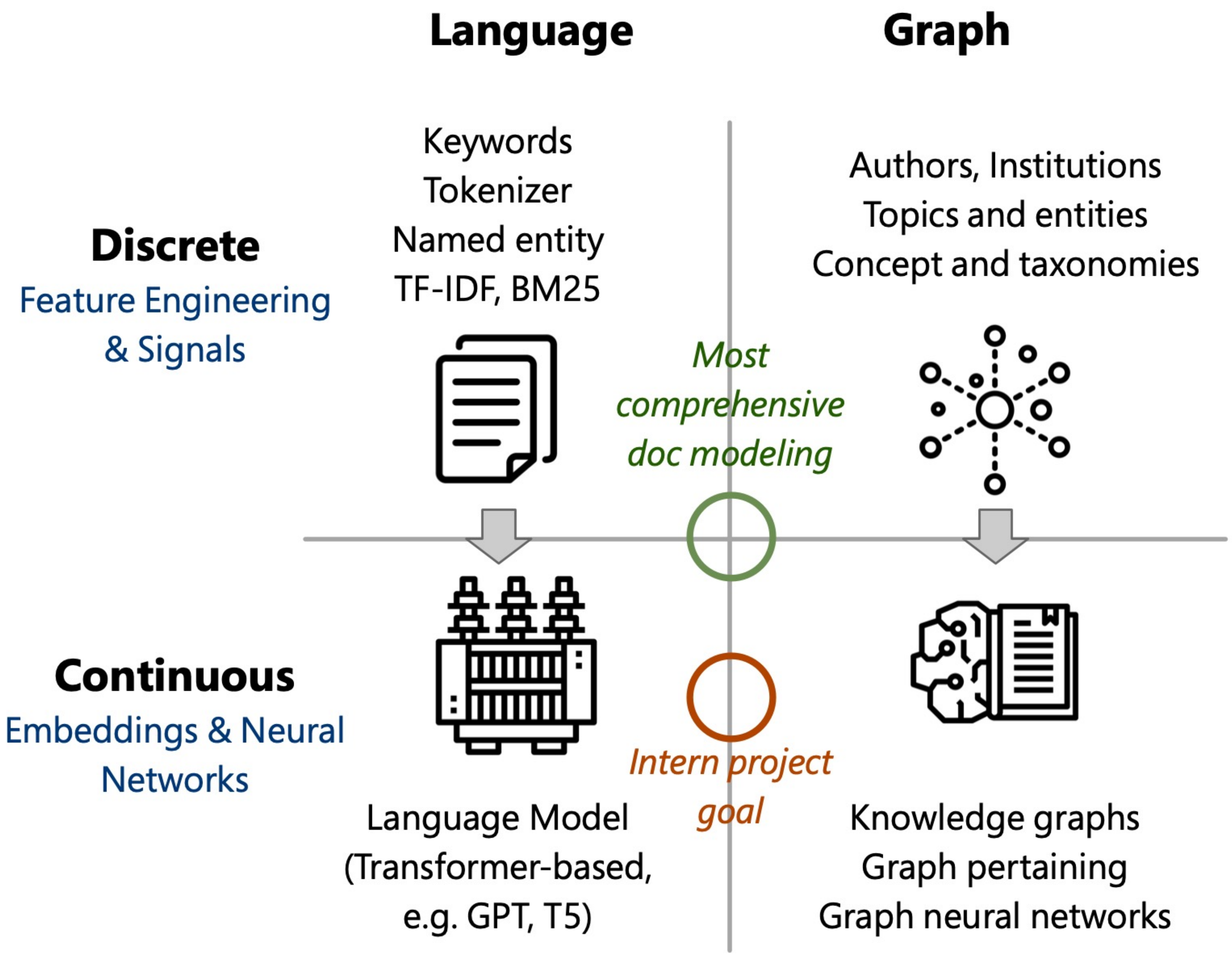


Summary

- Knowledge graphs often have ontological information, which is important for learning and inference but sparsely investigated.
- Joint learning on the instance and ontology views improves the KG embeddings. That is, incorporating ontologies in KGs is beneficial.
- Ontology-enhanced KG modeling can be applied in a wide selection of interdisciplinary applications, such as protein-protein interaction prediction in bioinformatics and diversified product recommendation in recommender systems.
- Graph neural networks have shown as a power tool on KG as relational data and graph-related downstream tasks, such as node classification, link prediction.

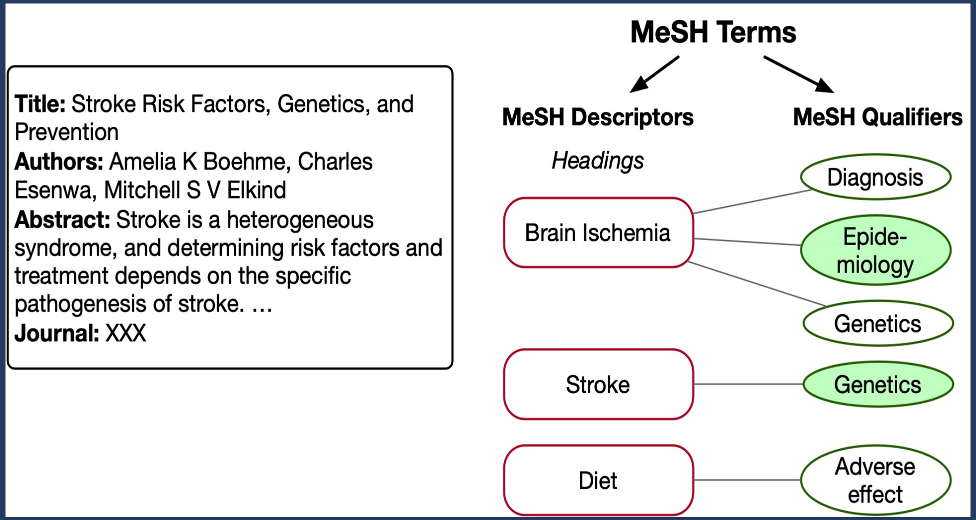
Feature spectrum of document modeling

Knowledge mining and document intelligence

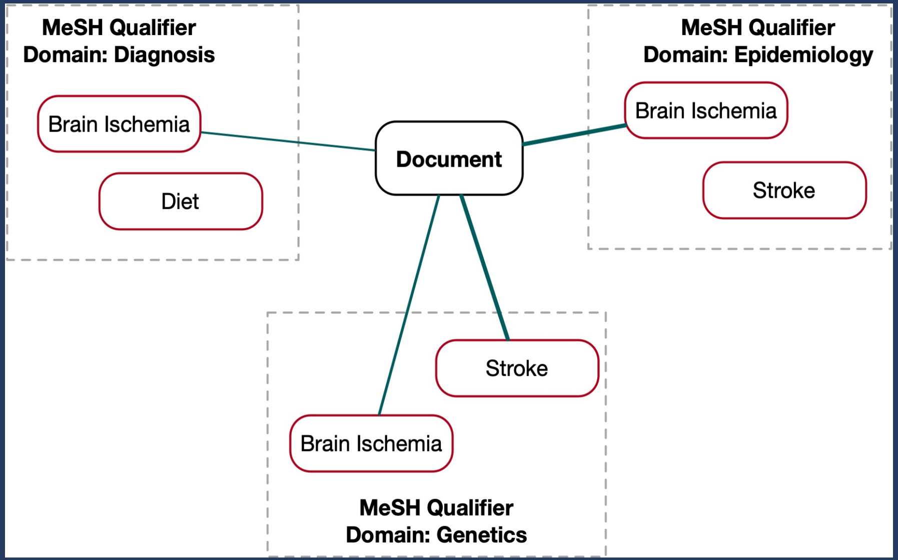


KG-Empowered Document Representation Learning

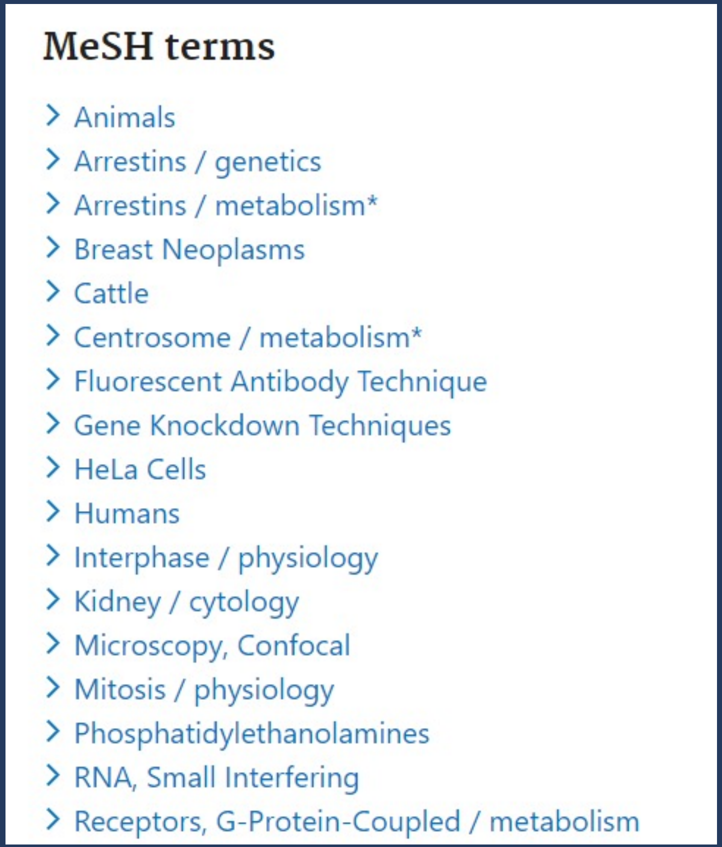
Encoding structured knowledge in documents



Original document



Document connected to KG



MeSH terms

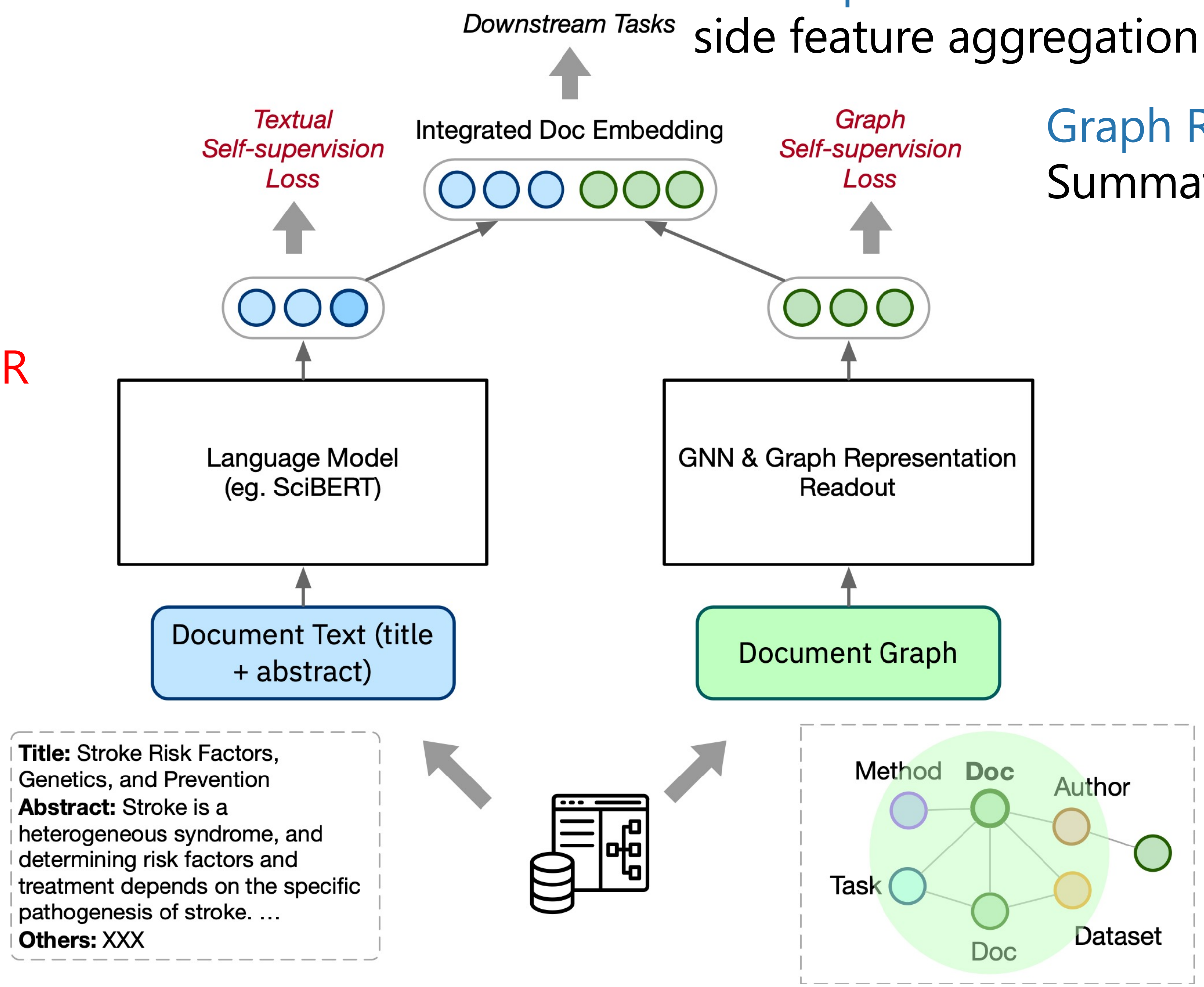
- Animals
- Arrestins / genetics
- Arrestins / metabolism*
- Breast Neoplasms
- Cattle
- Centrosome / metabolism*
- Fluorescent Antibody Technique
- Gene Knockdown Techniques
- HeLa Cells
- Humans
- Interphase / physiology
- Kidney / cytology
- Microscopy, Confocal
- Mitosis / physiology
- Phosphatidylethanolamines
- RNA, Small Interfering
- Receptors, G-Protein-Coupled / metabolism

Proposed Tech Spec (Details, initial version)

Final representation: Text/Graph-side feature aggregation

Graph Readout: MLP+ Summation

Text-side implementation: SPECTER (detached, not trained)
→ Update: Finetune SPECTER

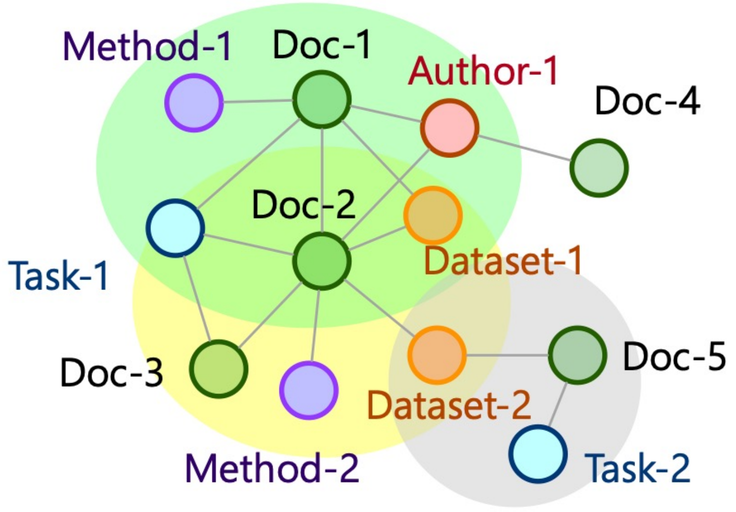


Graph implementation: Original GCN (GAT)
Supervision: Node type classification, edge/link prediction (no graph-level supervision)
→ Update: **GAT**

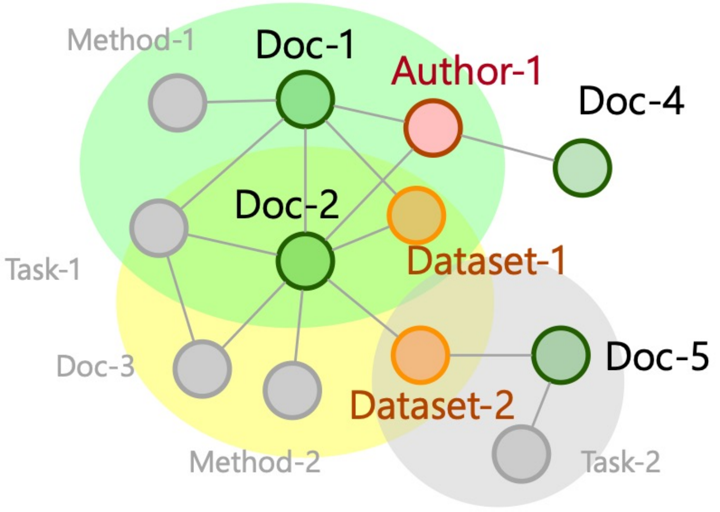
Add Graph-Level Contrastive Loss

- Full-view Graph-level loss + View-selection Subgraph loss

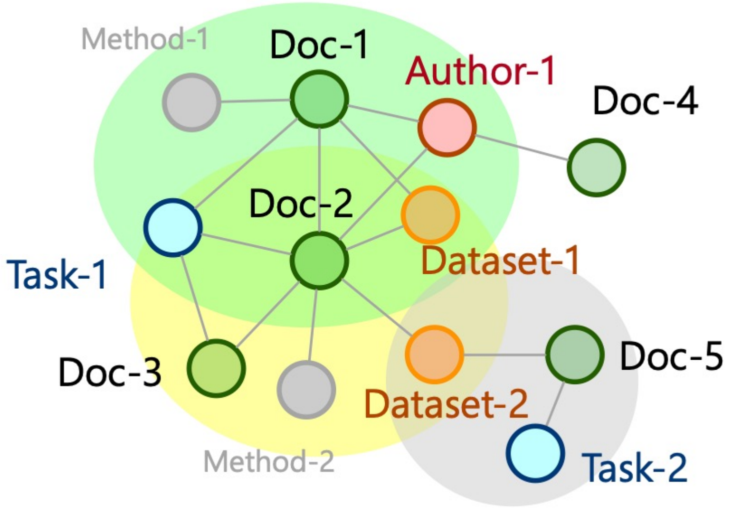
Full-view



Single-view (Dataset)



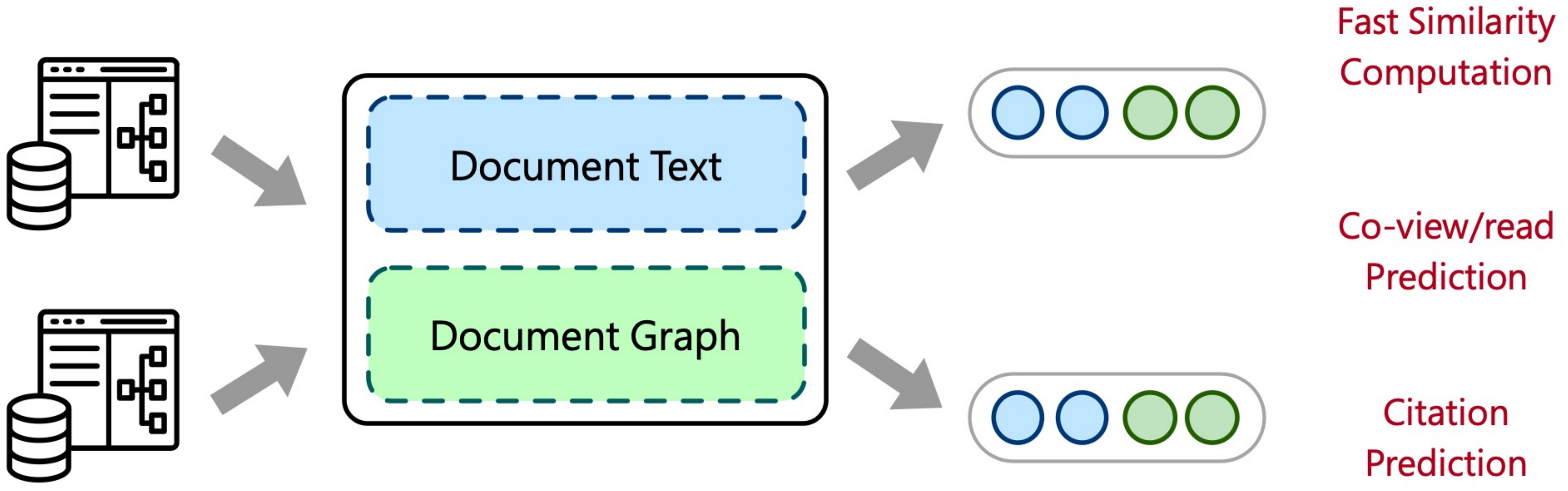
Dual-view



Supporting Doc-related Applications

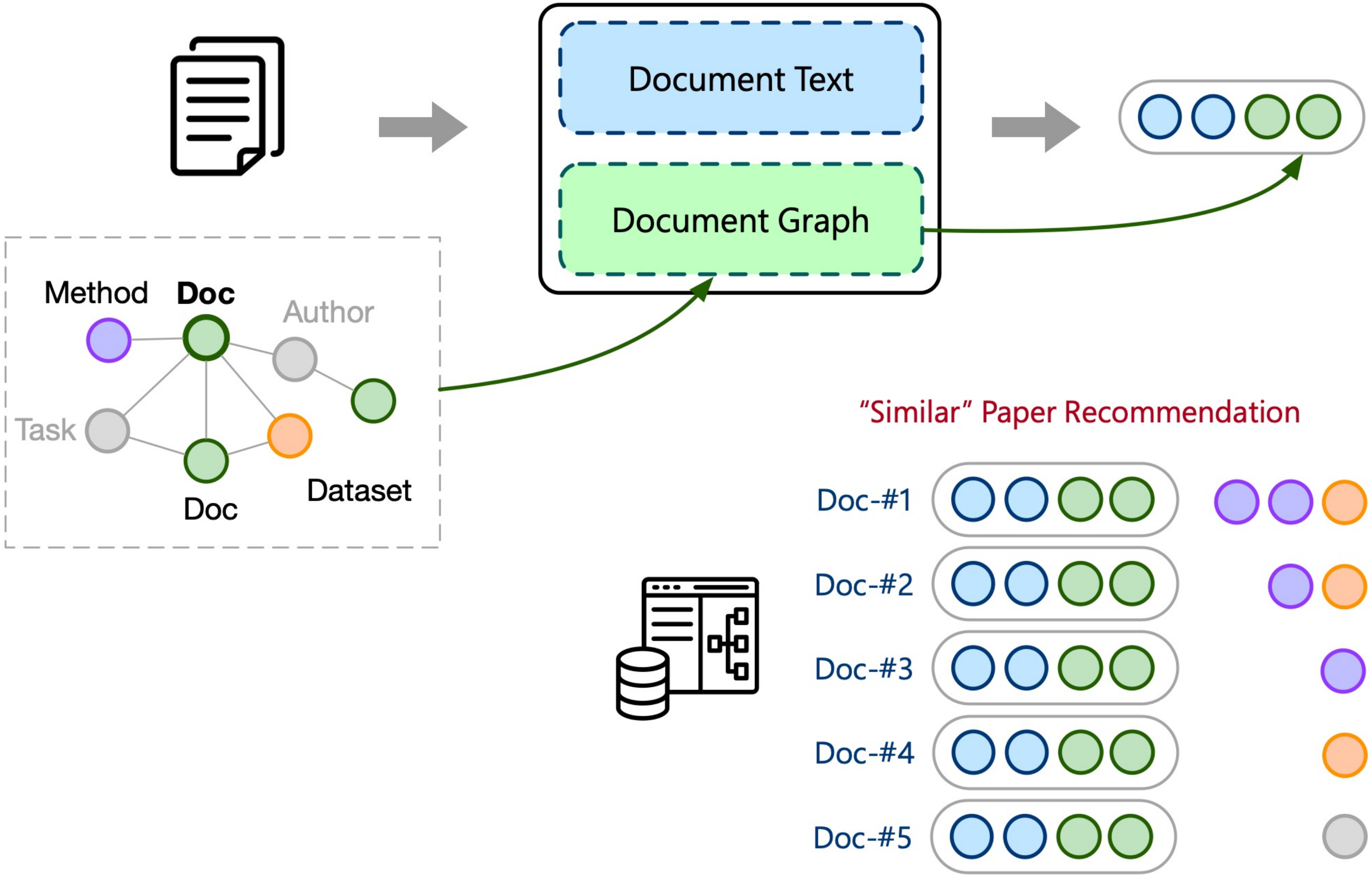
Intermediate output: Document representations → Doc-doc recommendation

Pretrained document embedding for (re)ranking, etc.



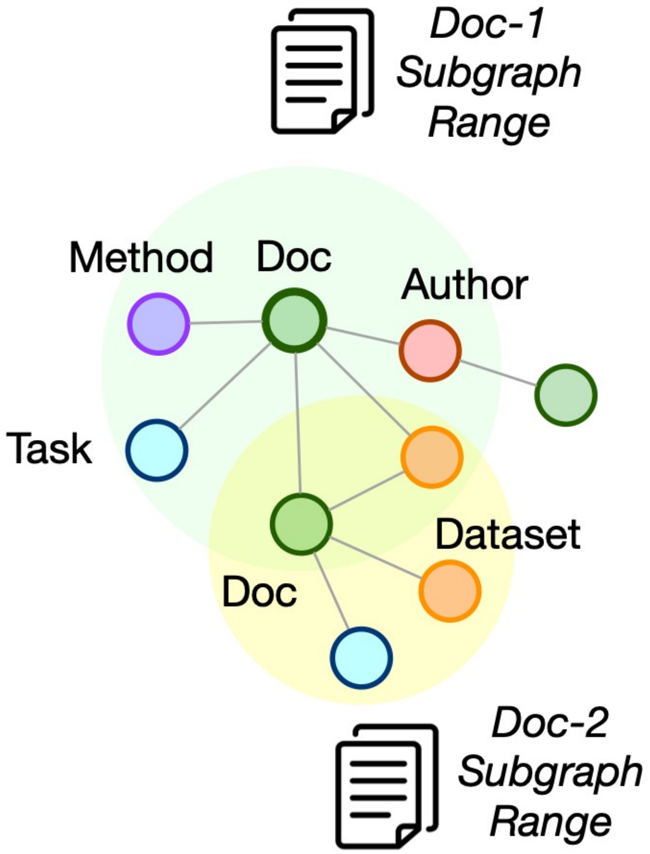
Supporting Doc-related Applications

Controllable, flexible and explainable document recommendation



Supporting Doc-related Applications

Potentially help complete document-level knowledge graphs



Thank you!

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