

Knowledge Graph Embeddings: From Theory to Practice

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Outline

Theoretical Overview

- Introduction
- Anatomy of a Knowledge Graph Embedding Model
- Evaluation Protocol and Metrics
- Advanced KGE Topics
- Open Research Questions

1h 30m



Applications

15 m



Software Ecosystem

15 m



Hands-on Session

1h 15m



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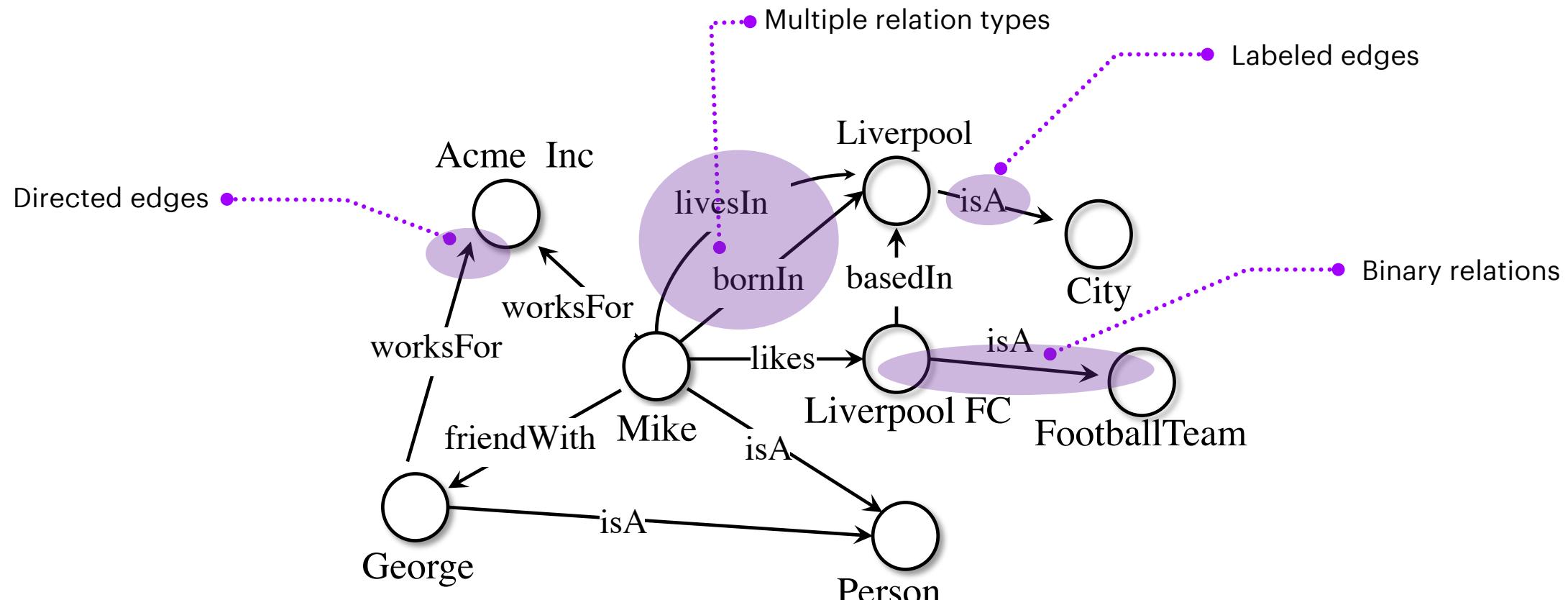
Software Ecosystem

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1h 15m

Knowledge Graph



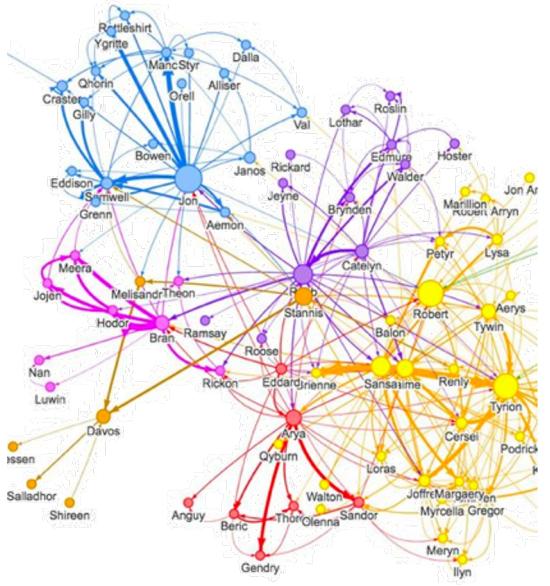
$$\mathcal{G} = \{(s, p, o)\} \subseteq \mathcal{E} \times \mathcal{R} \times \mathcal{E}$$

\mathcal{E} : set of entities of \mathcal{G}

\mathcal{R} : set of relations of \mathcal{G}

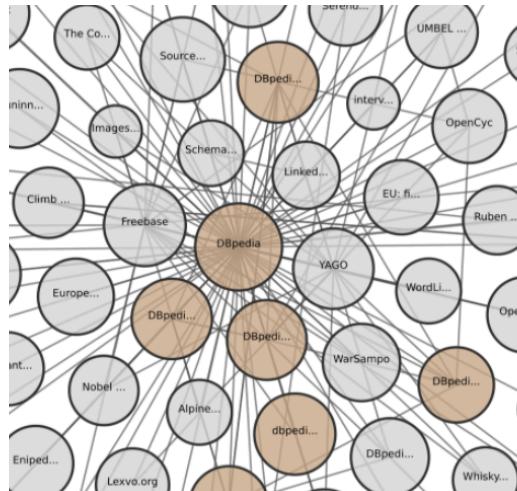
In-depth overview of Knowledge Graphs in
[Hogan et al. 2020]

SOCIAL NETWORKS



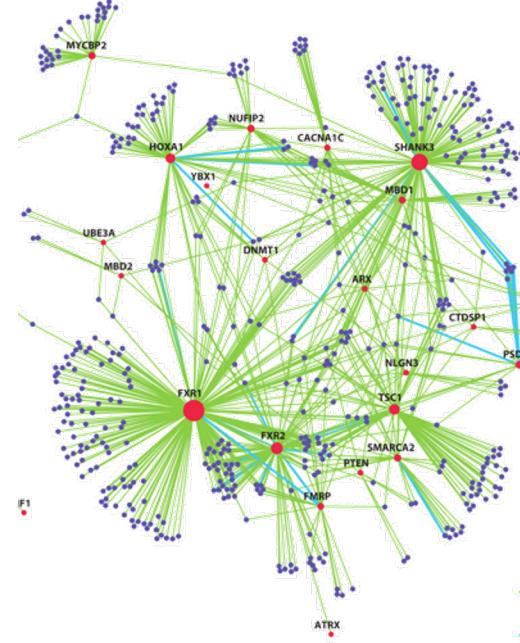
[\[neo4j.com\]](https://neo4j.com)

COLLABORATIVE WEB-BASED KNOWLEDGE BASES



[\[lod-cloud.net\]](https://lod-cloud.net)

PROTEIN-PROTEIN INTERACTION NETWORKS

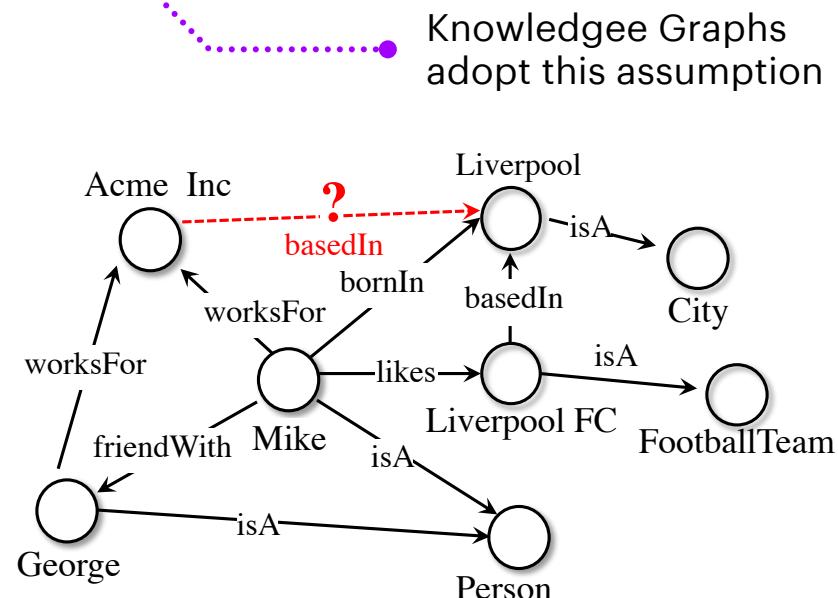


[\[ebi.ac.uk\]](https://ebi.ac.uk)

Knowledge Graph	Statements	Entities
 yago select knowledge	120 M	10 M
 WIKIDATA	610 M	51 M
 DBpedia	1.3 B	6 M
 GDELT	3.5 B	364 M

Knowledge Graphs & The Open World Assumption

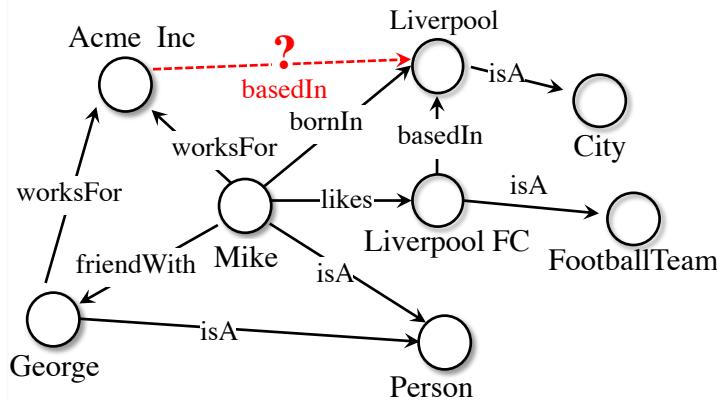
- **Closed World Assumption (CWA)**: absence of a fact means it is necessarily false.
- **Open World Assumption (OWA)**: absence of a fact does not imply fact is false. We simply do not know.



Machine Learning on Knowledge Graphs/ Statistical Relational Learning

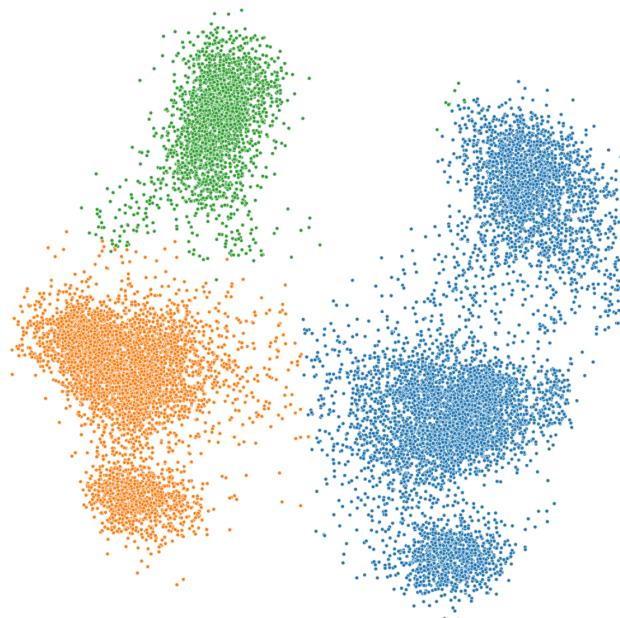
LINK PREDICTION / TRIPLE CLASSIFICATION

- Knowledge graph completion
- Content recommendation
- Question answering



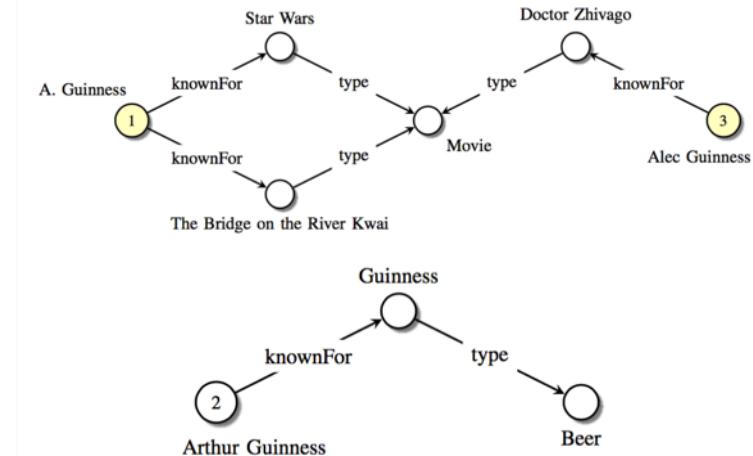
COLLECTIVE NODE CLASSIFICATION / LINK-BASED CLUSTERING

- Customer segmentation



ENTITY MATCHING

- Duplicate detection
- Inventory items deduplication

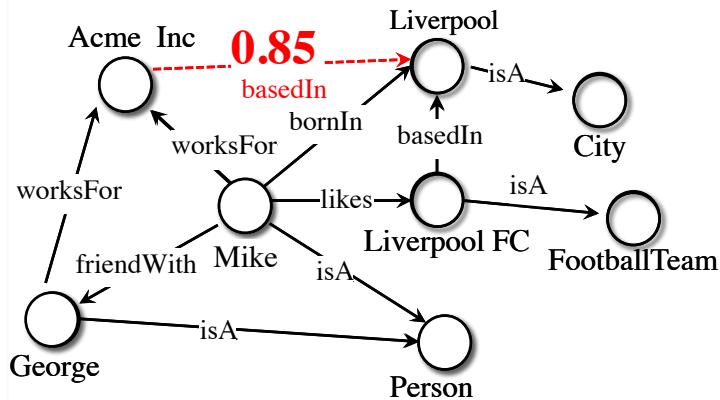


Pic from [Nickel et al. 2016a]

Machine Learning on Knowledge Graphs/ Statistical Relational Learning

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Assigning a score proportional to the likelihood that an unseen triple is true.

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Triple Classification

- Binary classification task
- Binary classification metrics
- Test set requires positives and ground truth negatives

Traditional Statistical Relational Learning

- **Logic Programming:** predict new links from facts and extracted rules.
- **Inductive Logic Programming (ILP):** predict new links from rules extracted from correlated facts.
- **Rule Mining:** e.g. AMIE+: extracts Horn clauses based on their support in the KG.
- **Graphical Models:**

[Gallaraga et al. 2015]

- Conditional Random Fields (CRFs)
- Probabilistic Relational Models
- Relational Markov Networks
- Relational Dependency Networks

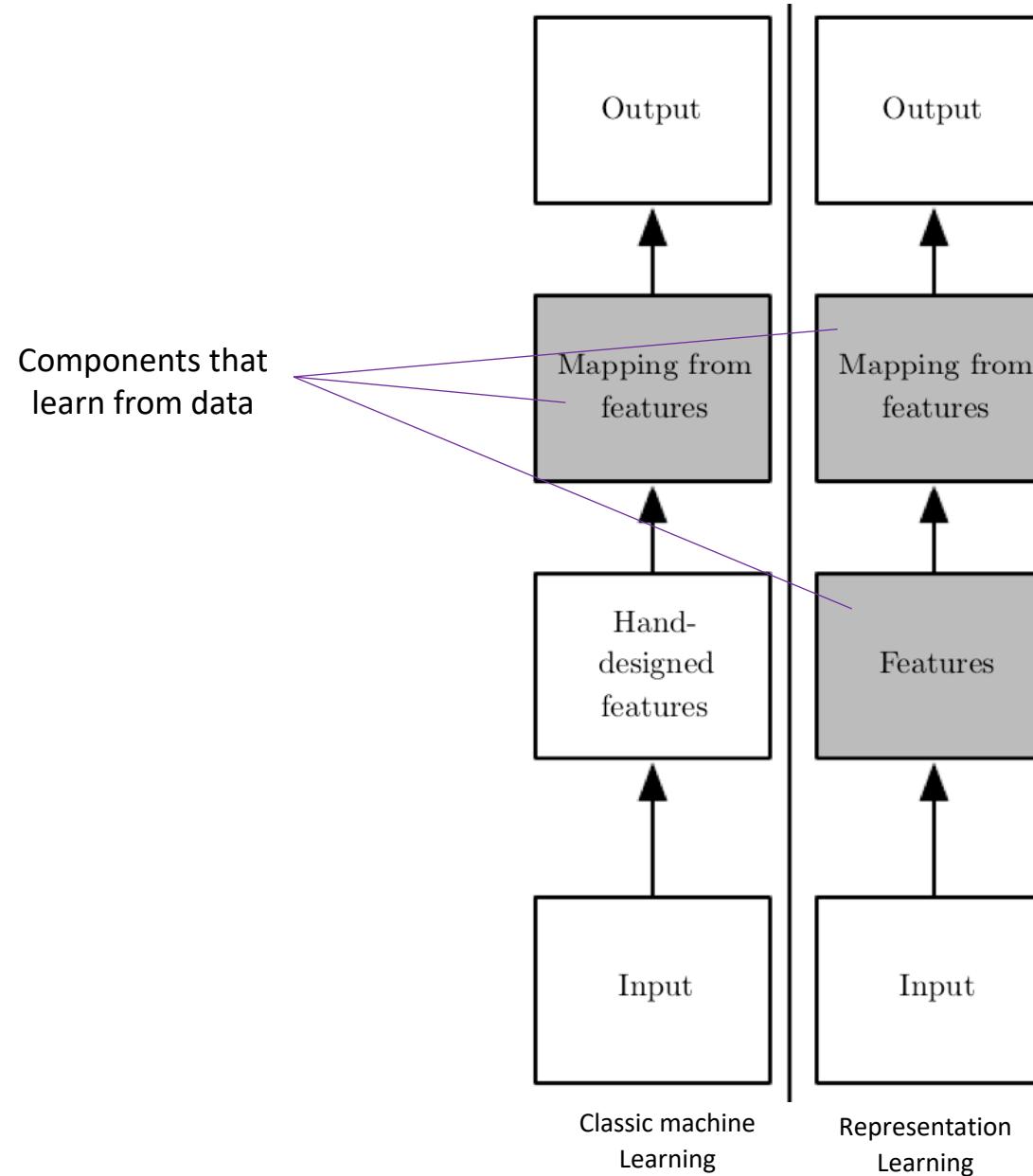
[Getoor & Taskar 2007]

Limitations

- Limited Scalability to KG size
- Limited modeling power
- Non-differentiable approaches

Introducing (Graph) Representation Learning

- Manual feature engineering on graphs is hard and time-consuming...
- ... what if instead we *learn* representations of nodes and edges?



Pic from [Goodfellow et al. 2016]

Can we re-use traditional deep learning tools?

- CNNs are designed for grids (e.g. images)
- RNNs/word2vec for sequences (e.g. text)

But graphs are more complex:

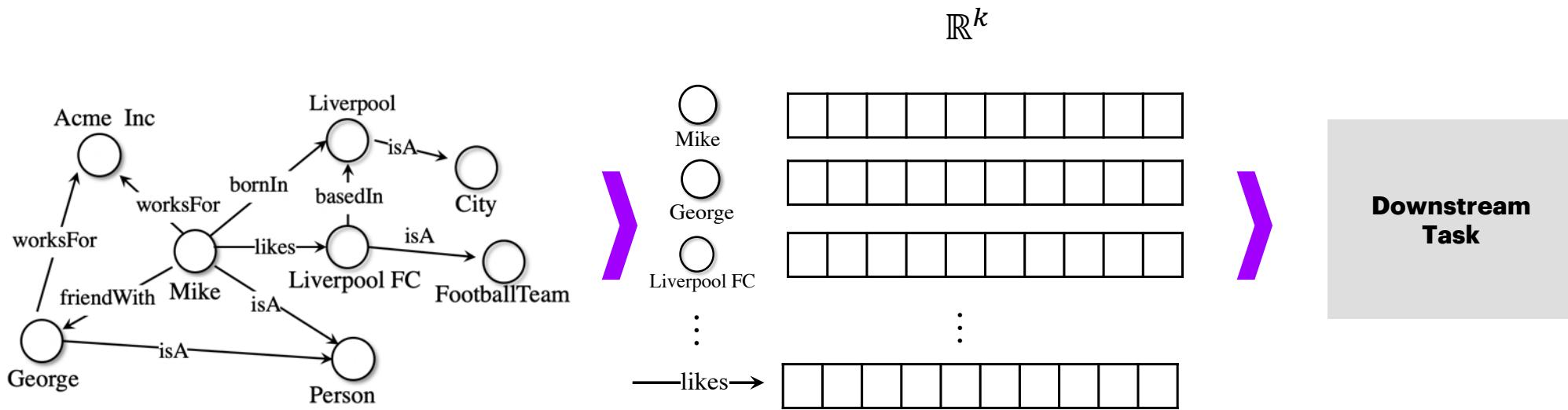
- No spatial locality
- No fixed-node ordering (graph isomorphism problem)
- Multimodal (concepts, text, numbers, timestamps, etc.)

We need ad-hoc models!

From AAAI-19 tutorial on Graph Representation Learning [Hamilton & Tang 2019]

Graph Representation Learning

Learning representations of nodes and edges



Node Representation/Graph Feature based Methods

PRA, LINE, DeepWalk, node2vec

Graph Neural Networks (GNNs)

GCNs, Graph Attention Networks

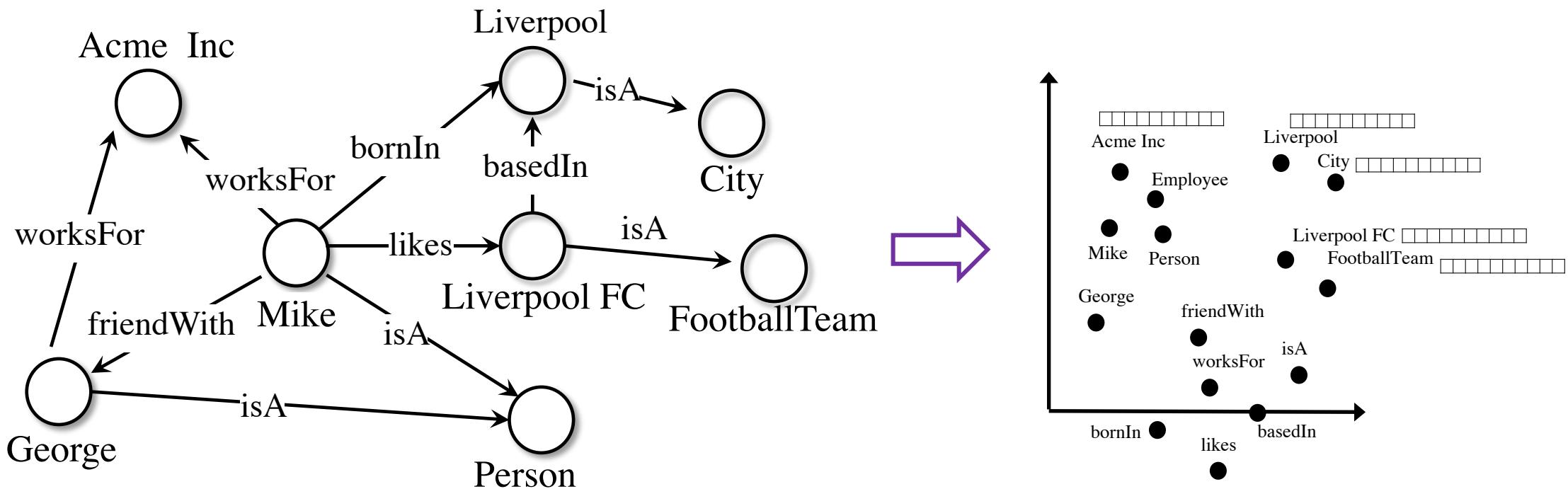
For a complete overview of graph feature-based models and GNNs:
[Hamilton & Sun 2019]
[Hamilton 2020]

Knowledge Graph Embeddings (KGE) TransE, DistMult, ComplEx, ConvE

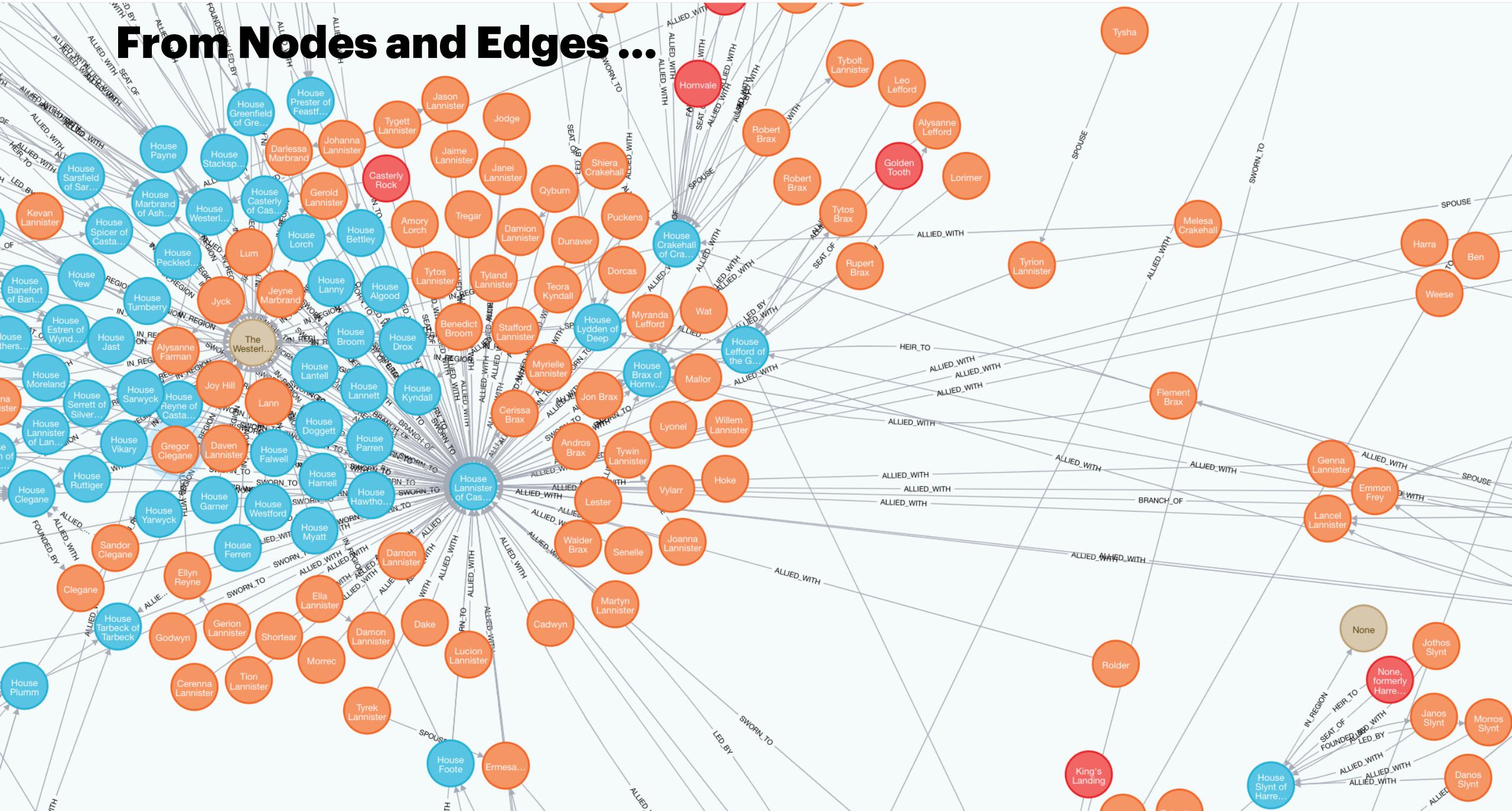
Scope of this tutorial

Knowledge Graph Embeddings (KGE)

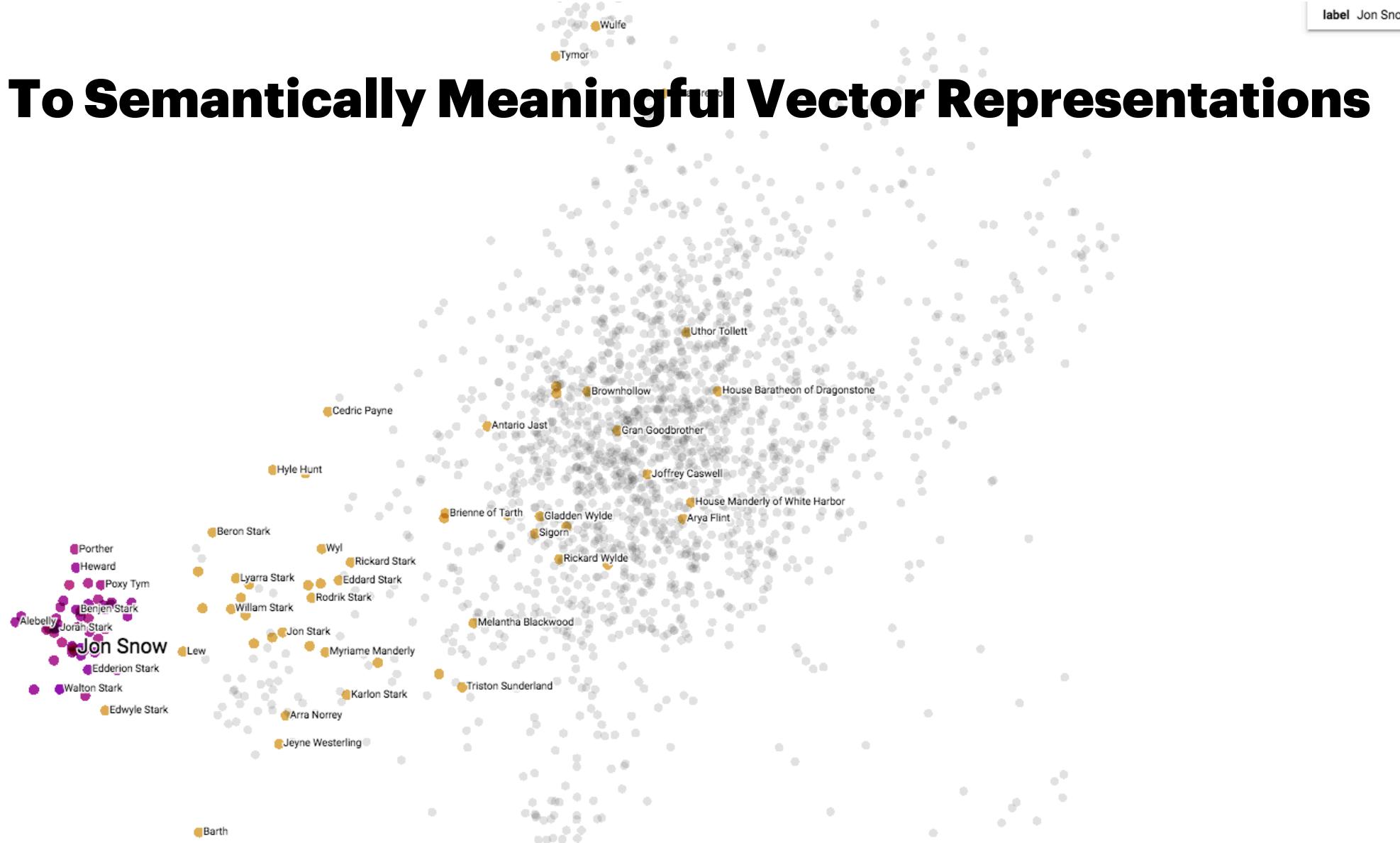
Automatic, supervised learning of **embeddings**, i.e. projections of entities and relations into a continuous low-dimensional space.



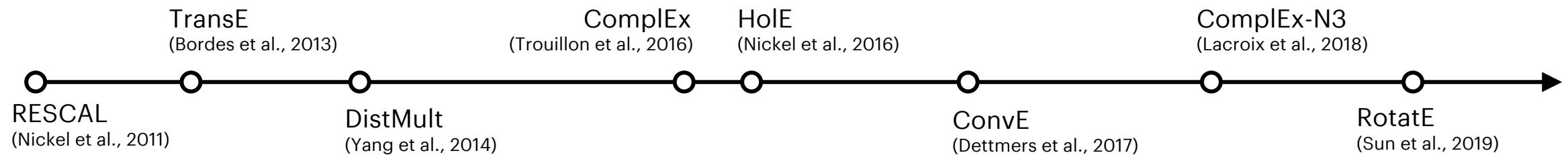
From Nodes and Edges .



... To Semantically Meaningful Vector Representations



(Some) KGE models in recent published literature:



KGE Design Rationale: Capture KG Patterns

Symmetry

<Alice marriedTo Bob>

Asymmetry

<Alice childOf Jack>

Inversion

<Alice childOf Jack>
<Jack fatherOf Alice>

Composition

<Alice childOf Jack>
<Jack siblingOf Mary>
<Alice nieceOf Mary>

But also:

- Hierarchies
- Type constraints
- Transitivity
- Homophily
- Long-range dependencies

Model	Symmetry	Antisymmetry	Inversion	Composition
SE	✗	✗	✗	✗
TransE	✗	✓	✓	✓
TransX	✓	✓	✗	✗
DistMult	✓	✗	✗	✗
ComplEx	✓	✓	✓	✗
RotatE	✓	✓	✓	✓

[Sun et al. 2019]

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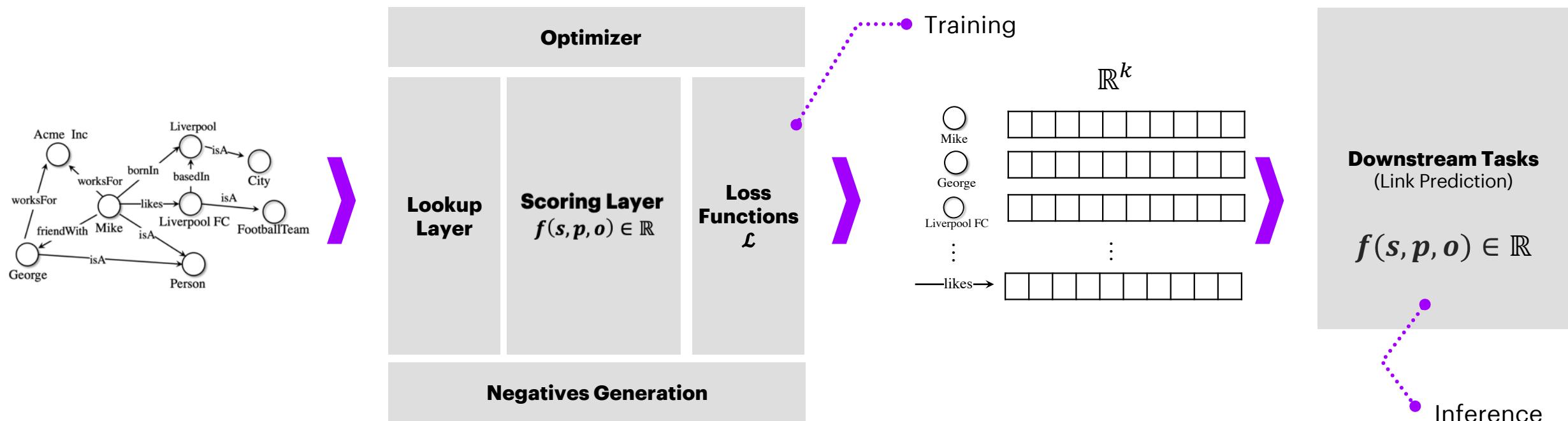
Software Ecosystem

15 m

Hands-on Sessions

1h 15m

At a Glance



Anatomy of a Knowledge Graph Embedding Model

- Knowledge Graph (KG) \mathcal{G}
- Scoring function for a triple $f(t)$
- Loss function \mathcal{L}
- Optimization algorithm
- Negatives generation strategy

Scoring function f

f assigns a score to a triple (s, p, o)

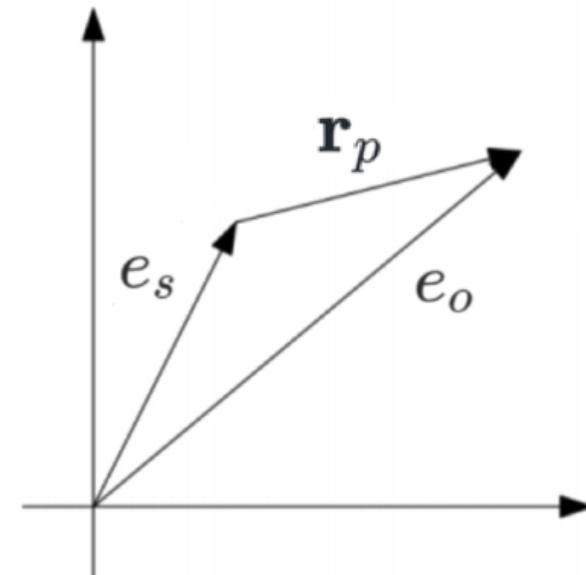
High score = high changes for the triple to be a true fact.



Translation-based Scoring Functions

- **TransE:** Translating Embeddings [Bordes et al. 2013]

$$f_{TransE} = -\|(\mathbf{e}_s + \mathbf{r}_p) - \mathbf{e}_o\|_n$$

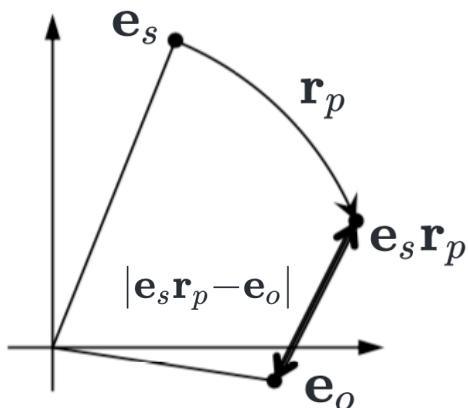


Translation-based Scoring Functions

- **RotatE**: relations modelled as *rotations* in complex space \mathbb{C} : element-wise product between complex embeddings.

[Sun et al. 2019]

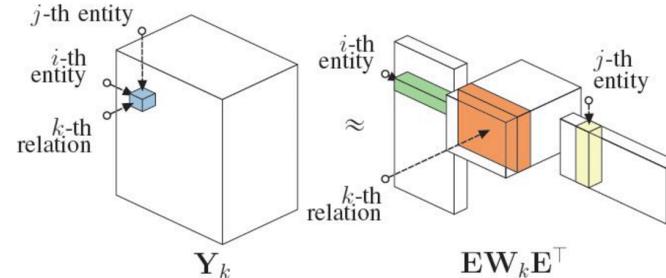
$$f_{RotatE} = -\|\mathbf{e}_s \circ \mathbf{r}_p - \mathbf{e}_o\|_n$$



Factorization-based Scoring Functions

- **RESCAL**: low-rank factorization with tensor product

$$f_{RESCAL} = \mathbf{e}_s^T \mathbf{W}_r \mathbf{e}_o$$



[Nickel et al. 2011]

- **DistMult**: bilinear diagonal model. Dot product.

$$f_{DistMult} = \langle \mathbf{r}_p, \mathbf{e}_s, \mathbf{e}_o \rangle$$

[Yang et al. 2015]

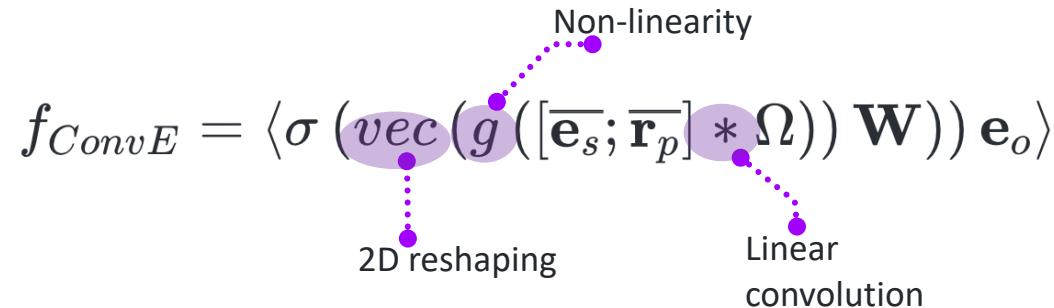
- **ComplEx**: Complex Embeddings (Hermitian dot product):
(i.e. extends DistMult with dot product in \mathbb{C})

$$f_{ComplEx} = \text{Re}(\langle \mathbf{r}_p, \mathbf{e}_s, \overline{\mathbf{e}}_o \rangle)$$

[Trouillon et al. 2016]

“Deeper” Scoring Functions

- **ConvE**: reshaping + convolution



[Dettmers et al. 2017]

- **ConvKB**: convolutions and dot product

[Nguyen et al. 2018]

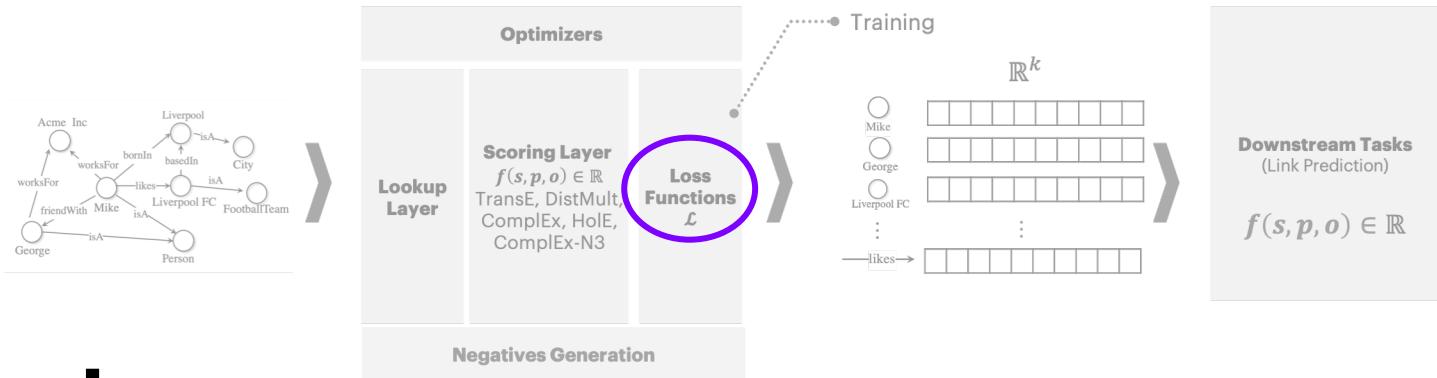
$$f_{ConvKB} = \text{concat} (g ([\mathbf{e}_s, \mathbf{r}_p, \mathbf{e}_o]) * \Omega) \cdot W$$

Computationally expensive!

Other Recent Models

- HolE [Nickel et al. 2016]
- SimplE [Kazemi et al. 2018]
- QuatE [Zhang et al. 2019]
- MurP [Balažević et al. 2019]
- ...

Loss function \mathcal{L}



Pairwise Margin-Based Hinge Loss

Pays a penalty if score of positive triple < score of synthetic negative by a margin γ

$$\mathcal{L}(\Theta) = \sum_{t^+ \in \mathcal{G}} \sum_{t^- \in \mathcal{C}} \max(0, [\gamma + f(t^-; \Theta) - f(t^+; \Theta)])$$

Score assigned to a **synthetic negative** Score assigned to **true** triple

[Bordes et al. 2013]

Negative Log-Likelihood / Cross Entropy

$$\mathcal{L}(\Theta) = \sum_{t \in \mathcal{G} \cup \mathcal{C}} \log(1 + \exp(-y f(t; \Theta)))$$

Label of the triple t $y \in \{-1, 1\}$

[Trouillon et al. 2016]

Loss function \mathcal{L}

Binary Cross-Entropy

$$\mathcal{L} = -\frac{1}{N} \sum_{t \in \mathcal{G} \cup \mathcal{C}} y \cdot \log(\sigma(f(t; \Theta))) + (1 - y) \cdot \log(1 - f(t; \Theta))$$

[Dettmers et al. 2017]

Self-Adversarial

$$\mathcal{L} = -\log \sigma(\gamma + f(t^+; \Theta)) - \sum_{t \in \mathcal{G}} p(t^-; \Theta) \underbrace{\log \sigma(-f(t^-; \Theta) - \gamma)}_{\text{Weight for the negative sample } t^-}$$

[Sun et al. 2019]

Many more: Multiclass Negative Log-likelihood, Absolute Margin, etc.

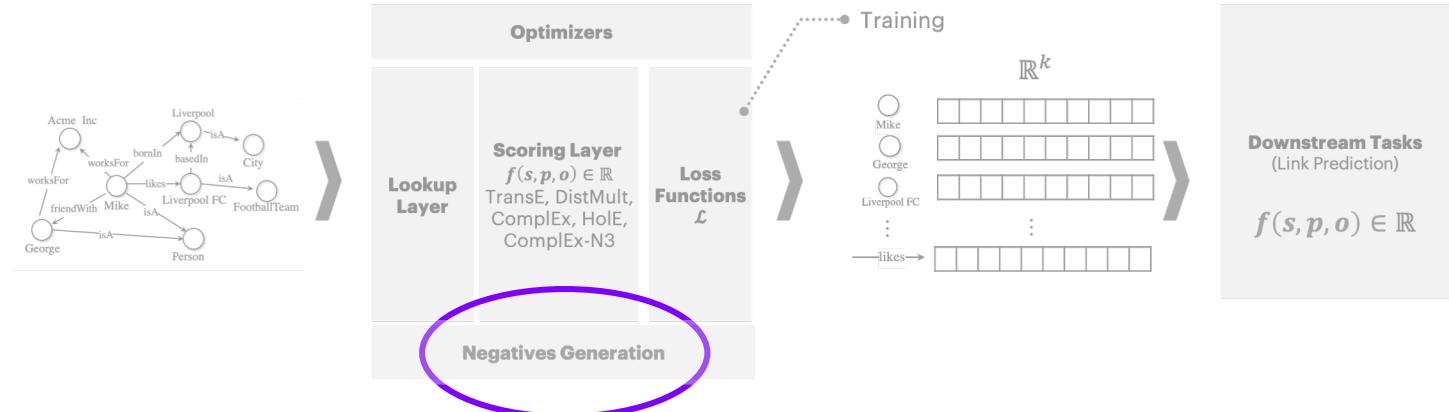
Regularizers

- L1, L2
- L3 [Lacroix et al. 2018]
- Dropout (ConvE) [Dettmers et al. 2017]

Initialization

- Random (Uniform)
- Random (Normal)
- Glorot

Negatives Generation



Where do negative examples come from? (i.e. false facts)

Local Closed World Assumption: the KG is only *locally* complete

“Corrupted” versions of a triple as synthetic negatives:

$$\mathcal{C} = \{(\hat{s}, p, o) | \hat{s} \in \mathcal{E}\} \cup \{(s, p, \hat{o}) | \hat{o} \in \mathcal{E}\}$$

“corrupted subject”

“corrupted” object

The predicate is
unaltered

Synthetic Negatives: Example

$\mathcal{E} = \{Mike, Liverpool, AcmeInc, George, LiverpoolFC\}$

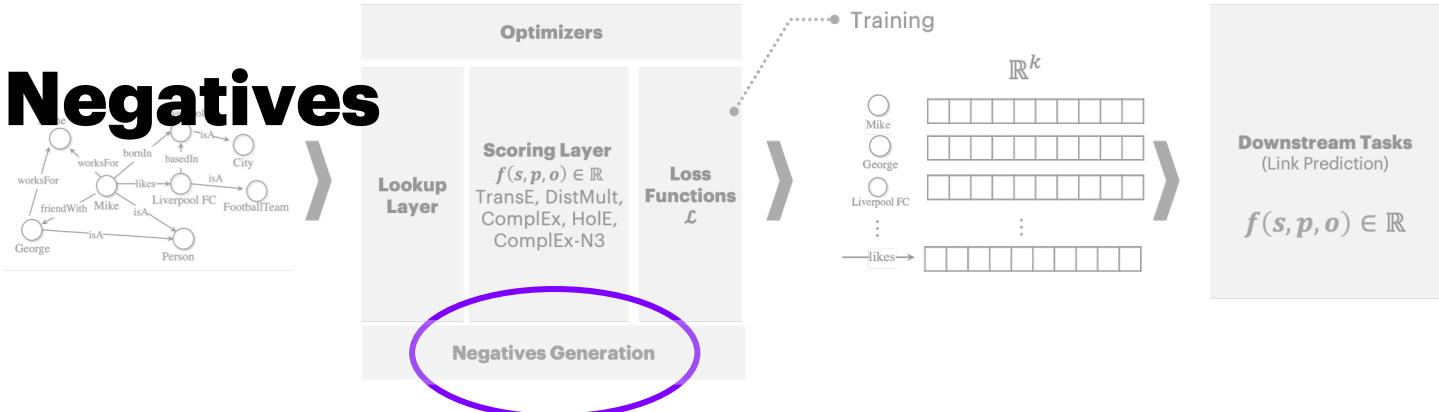
$\mathcal{R} = \{bornIn, friendWith\}$

$t \in \mathcal{G} = (Mike \text{ bornIn } Liverpool)$

$\mathcal{C}_t =$

Mike	bornIn	AcmeInc
Mike	bornIn	LiverpoolFC
George	bornIn	Liverpool
AcmeInc	bornIn	Liverpool

Training with Synthetic Negatives

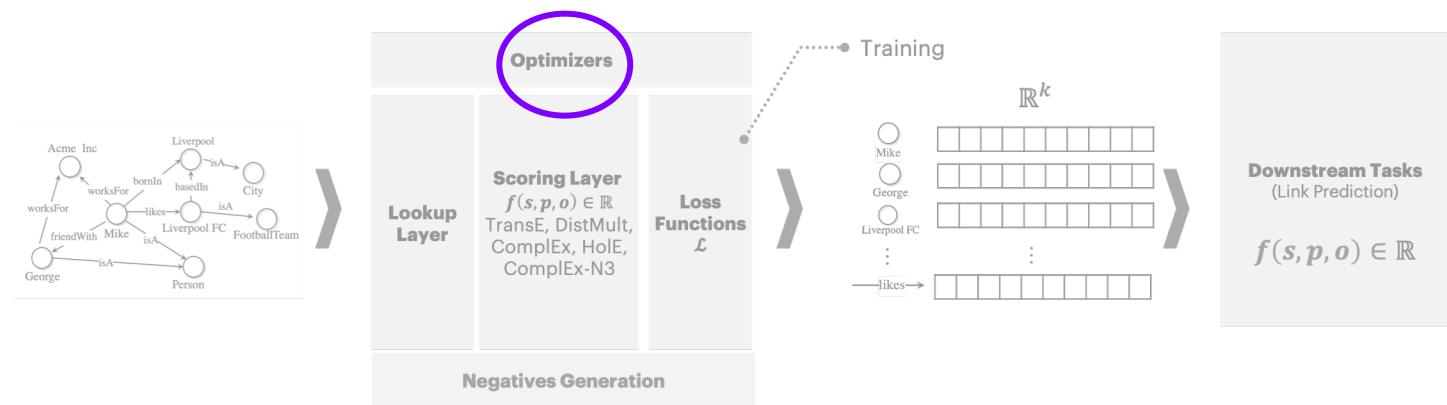


Uniform sampling: generate all possible synthetic negatives and sample n negatives for each positive t.

Complete set: no sampling. Use all possible synthetic negatives for each positive t. (mind scalability)

1-n scoring: batches of $(s, p, *)$ or $(*, p, o)$ labeled as positives (if included in training KG) or negatives (if not in training KG).
[Dettmers et al. 2017]

Training Procedure and Optimizer



Optimizer: learn optimal parameters (e.g. embeddings). Off-the-shelf SGD variants:
(AdaGrad, Adam)

$$\min_{\Theta} \mathcal{L}(\Theta)$$

Reciprocal Triples

Injection of reciprocal triples in training set.

<Alice childOf Jack>
<Jack childOf⁻¹ Alice>

[Dettmers et al. 2017]
[Lacroix et al. 2018]

Model Selection

- Grid search
 - Mind the size of the grid!
 - Early stopping
- Random search
- Quasi-random + Bayesian [Ruffinelli et al. 2020]

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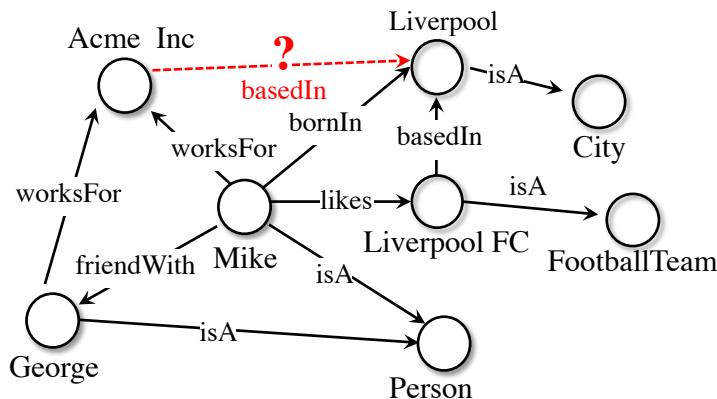
15 m

Hands-on Sessions

1h 15m

The Task

LINK PREDICTION / TRIPLE CLASSIFICATION



Assigning a score proportional to the likelihood that an unseen triple is true.

Link Prediction

- Learning to rank problem
- Information retrieval metrics
- No ground truth negatives in test set required

Triple Classification

- Binary classification task
- Binary classification metrics
- Test set requires positives and ground truth negatives

Learning-To-Rank problem:

How well are positive triples ranked against **synthetic negatives** built under the **Local Closed World Assumption**.

Same procedure
used in training

Evaluation Metrics

Mean Rank (MR)

$$MR = \frac{1}{|Q|} \sum_{i=1}^{|Q|} rank_{(s,p,o)_i}$$

Mean Reciprocal Rank (MRR)

$$MRR = \frac{1}{|Q|} \sum_{i=1}^{|Q|} \frac{1}{rank_{(s,p,o)_i}}$$

Hits@N

$$Hits@N = \sum_{i=1}^{|Q|} 1 \text{ if } rank_{(s,p,o)_i} \leq N$$

Example How unseen, test positive triples rank against **synthetic negatives?**

s	p	o	score	rank
Mike	born_in	Leeds	0.789	1
Mike	born_in	Liverpool	0.753	2
Mike	born_in	Germany	0.695	3
George	born_in	Liverpool	0.456	4
Mike	born_in	George	0.234	5

s	p	o	score	rank
Mike	friend_with	George	0.901	1
Mike	friend_with	Jim	0.345	2
Acme	friend_with	George	0.293	3
Mike	friend_with	Liverpool	0.201	4
France	friend_with	George	0.156	5

*

Unseen positive
triples (test set)

$$MR = 1.5$$

$$MRR = 0.75$$

$$Hits@1 = 0.5$$

$$Hits@3 = 1.0$$

Benchmark Datasets

The diagram illustrates the relationships between four knowledge graph datasets: Freebase, WordNet, FB15K-237, WN18RR, YAGO3-10, and YAGO. Freebase is connected to FB15K-237. WordNet is connected to both FB15K-237 and YAGO3-10. YAGO is connected to both WN18RR and YAGO3-10.

	FB15K-237	WN18RR	YAGO3-10	YAGO
Training	272,115	86,835	1,079,040	
Validation	17,535	3,034	5,000	
Test	20,466	3,134	5,000	
Entities	14,541	40,943	123,182	
Relations	237	11	37	

Link Prediction: SOTA Results

	FB15K-237	WN18RR	YAGO3-10
Literature Best	0.35*	0.48*	0.49*
TransE (AmpliGraph)	0.31	0.22	0.51
DistMult (AmpliGraph)	0.31	0.47	0.50
ComplEx (AmpliGraph)	0.32	0.51	0.49
HoIE (AmpliGraph)	0.31	0.47	0.50
ConvE (AmpliGraph)	0.26	0.45	0.30
ConvE (1-N, AmpliGraph)	0.32	0.48	0.40
ConvKB (AmpliGraph)	0.23	0.39	0.30

		<i>FB15K-237</i>		<i>WNRR</i>	
		MRR	Hits@10	MRR	Hits@10
<i>First</i>	RESCAL (Wang et al., 2019)	27.0	42.7	42.0	44.7
	TransE (Nguyen et al., 2018)	29.4	46.5	22.6	50.1
	DistMult (Dettmers et al., 2018)	24.1	41.9	43.0	49.0
	ComplEx (Dettmers et al., 2018)	24.7	42.8	44.0	51.0
	ConvE (Dettmers et al., 2018)	32.5	50.1	43.0	52.0
<i>Ours</i>	RESCAL	35.7	54.1	46.7	51.7
	TransE	31.3	49.7	22.8	52.0
	DistMult	34.3	53.1	45.2	53.1
	ComplEx	34.8	53.6	47.5	54.7
	ConvE	33.9	52.1	44.2	50.4
<i>Recent</i>	TuckER (Balazevic et al., 2019)	35.8	54.4	47.0	52.6
	RotatE (Sun et al., 2019a)	33.8	53.3	47.6	57.1
	SACN (Shang et al., 2019)	35.0	54.0	47.0	54.4
<i>Large</i>	DistMult (Salehi et al., 2018)	35.7	54.8	45.5	54.4
	ComplEx-N3 (Lacroix et al., 2018)	37.0	56.0	49.0	58.0

[<https://github.com/Accenture/AmpliGraph>]

[Ruffinelli et a. 2020]

Comparing SOTA Results is Tricky

- Different training strategies (e.g. synthetic negatives)
- Reciprocal relations in training set?
- Unfair or suboptimal hyperparameters selection
- Evaluation protocol: how to behave with tie ranks?
- Ablation studies!

Read discussion in [Ruffinelli et al 2020]

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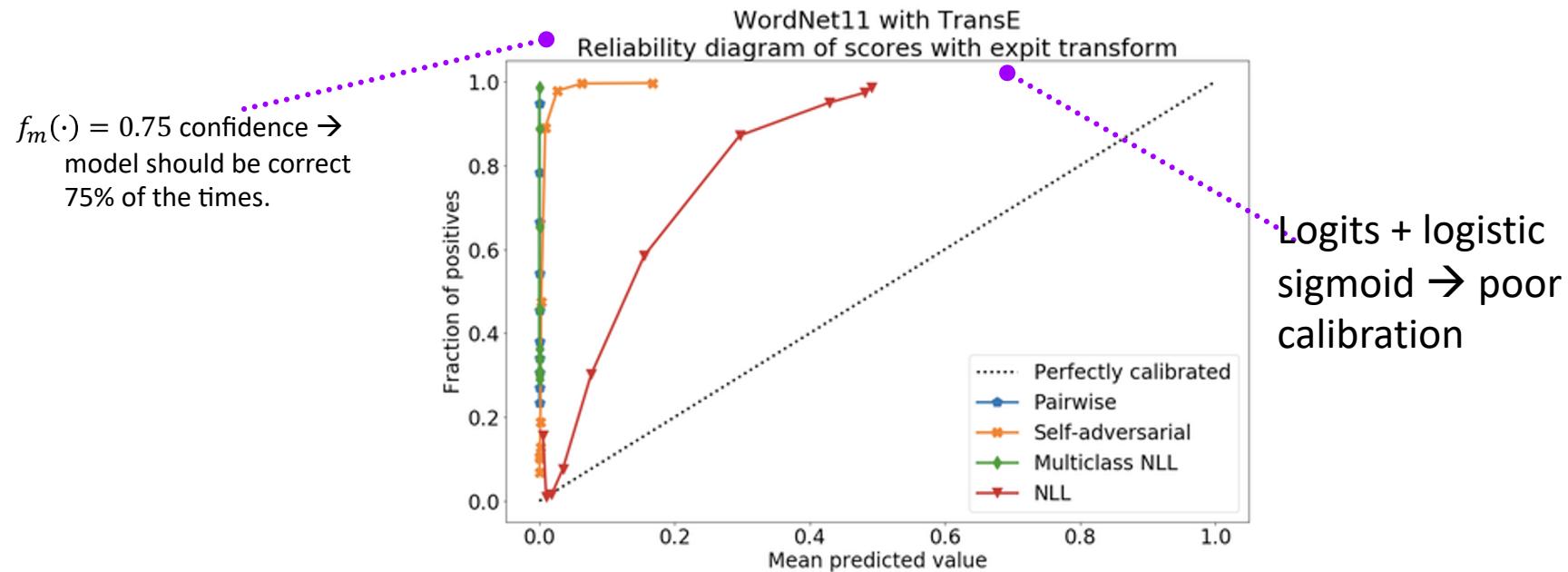
Hands-on Sessions

1h 15m

Calibration

Probabilities Generated by KGE models are Uncalibrated!

[Tabacof & Costabello 2020]

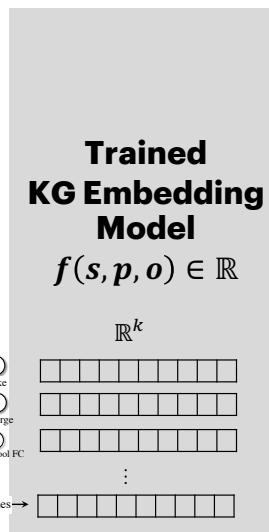
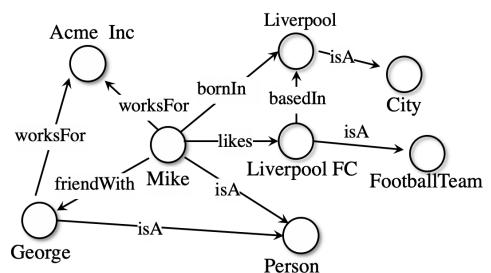


- **Mistrust** in model discoveries
- **Poor Interpretability** in high-stakes scenarios (i.e. drug-target discovery)

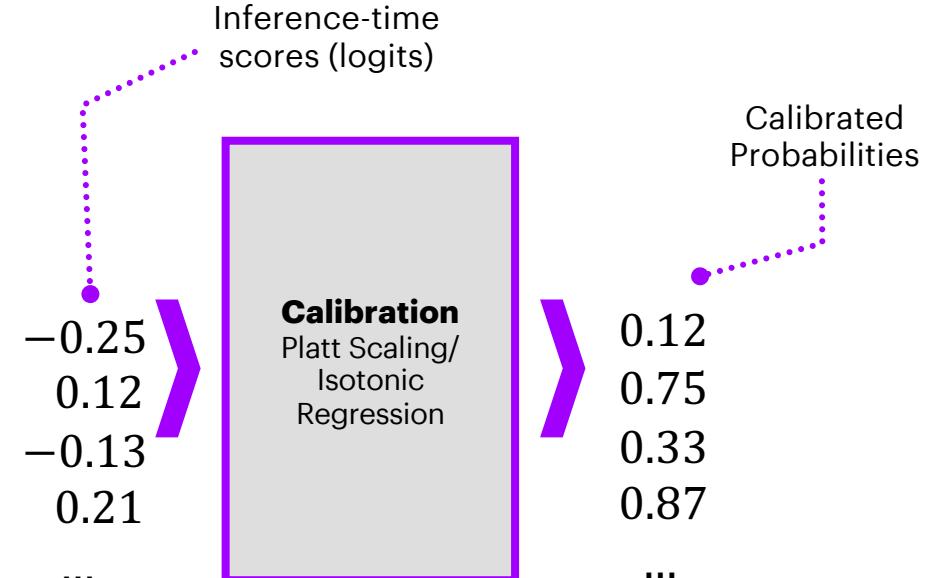
How can we calibrate KGE models? How to do so without ground truth negatives?

Calibrating With Ground Truth Negatives

(Available w/ Triple Classification Datasets)



Calibration dataset
(Ground truth positives + **negatives**)



LiverpoolFC	isa	City	-1
AcmeInc	isa	Company	1
George	worksFor	Mike	-1
AcmeInc	basedIn	Liverpool	1
...

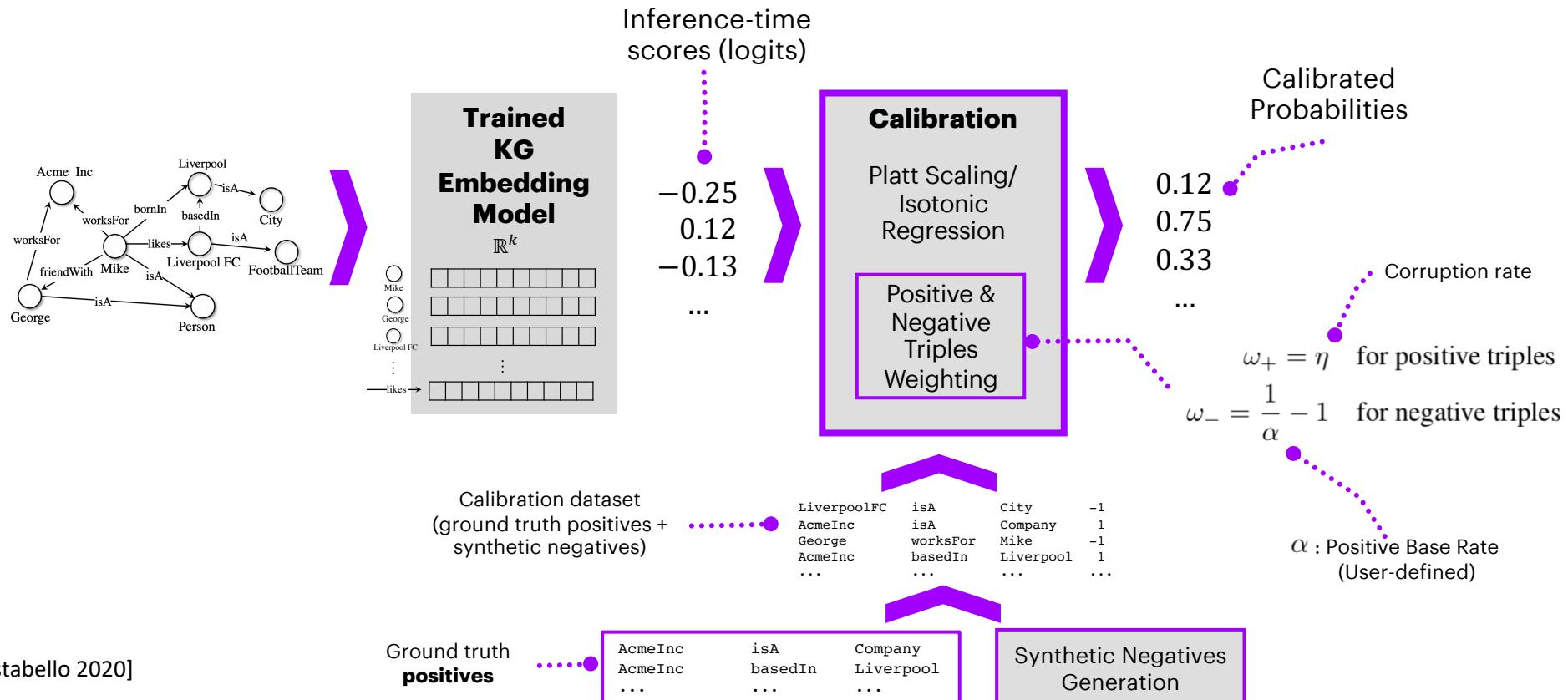
$$\alpha = \frac{P}{P + N}$$

Positive Base Rate
(Automatically Inferred)

[Tabacof & Costabello 2020]

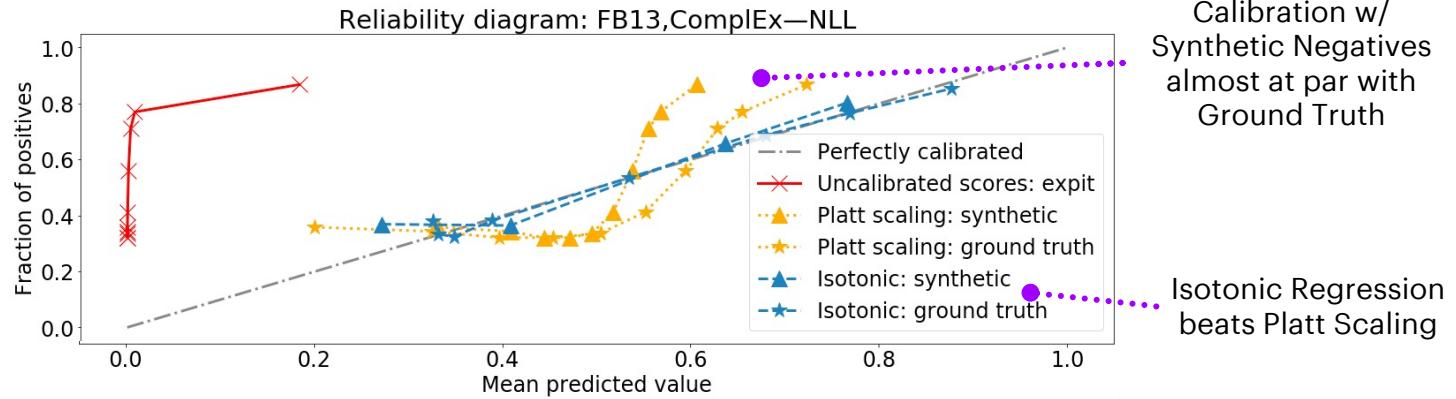
Calibrating With Synthetic Negatives

(No Ground Truth Negatives Available)



Calibration is Effective

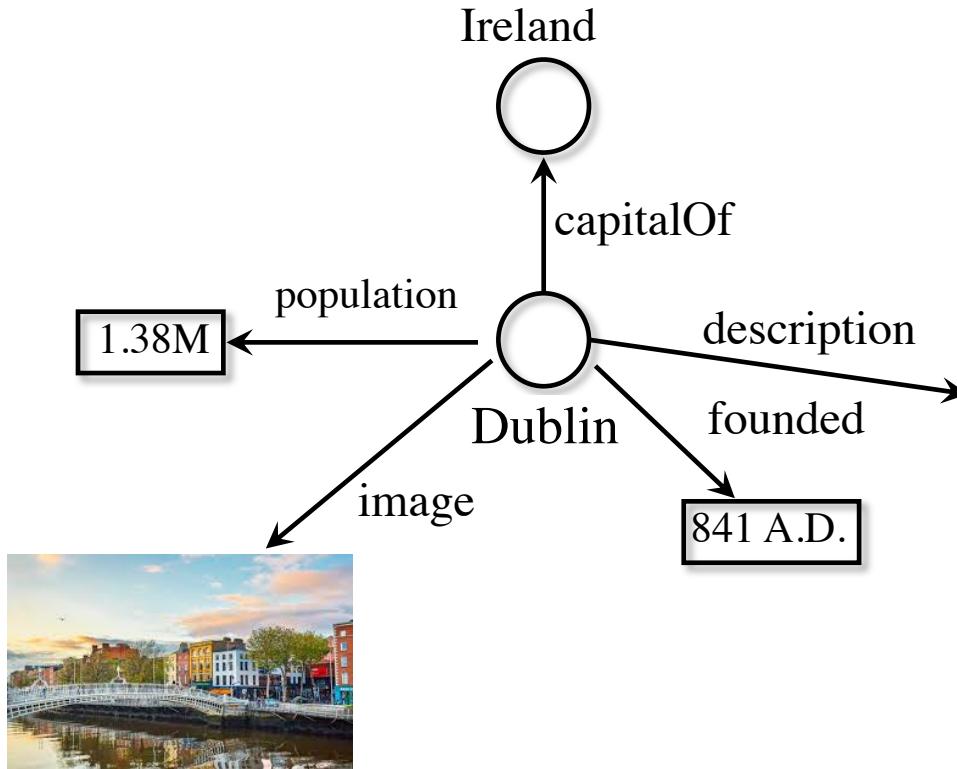
[Tabacof & Costabello 2020]



- All calibration techniques work **considerably better** than uncalibrated settings
- More **trustworthy and interpretable** predictions

Multimodal Knowledge Graphs

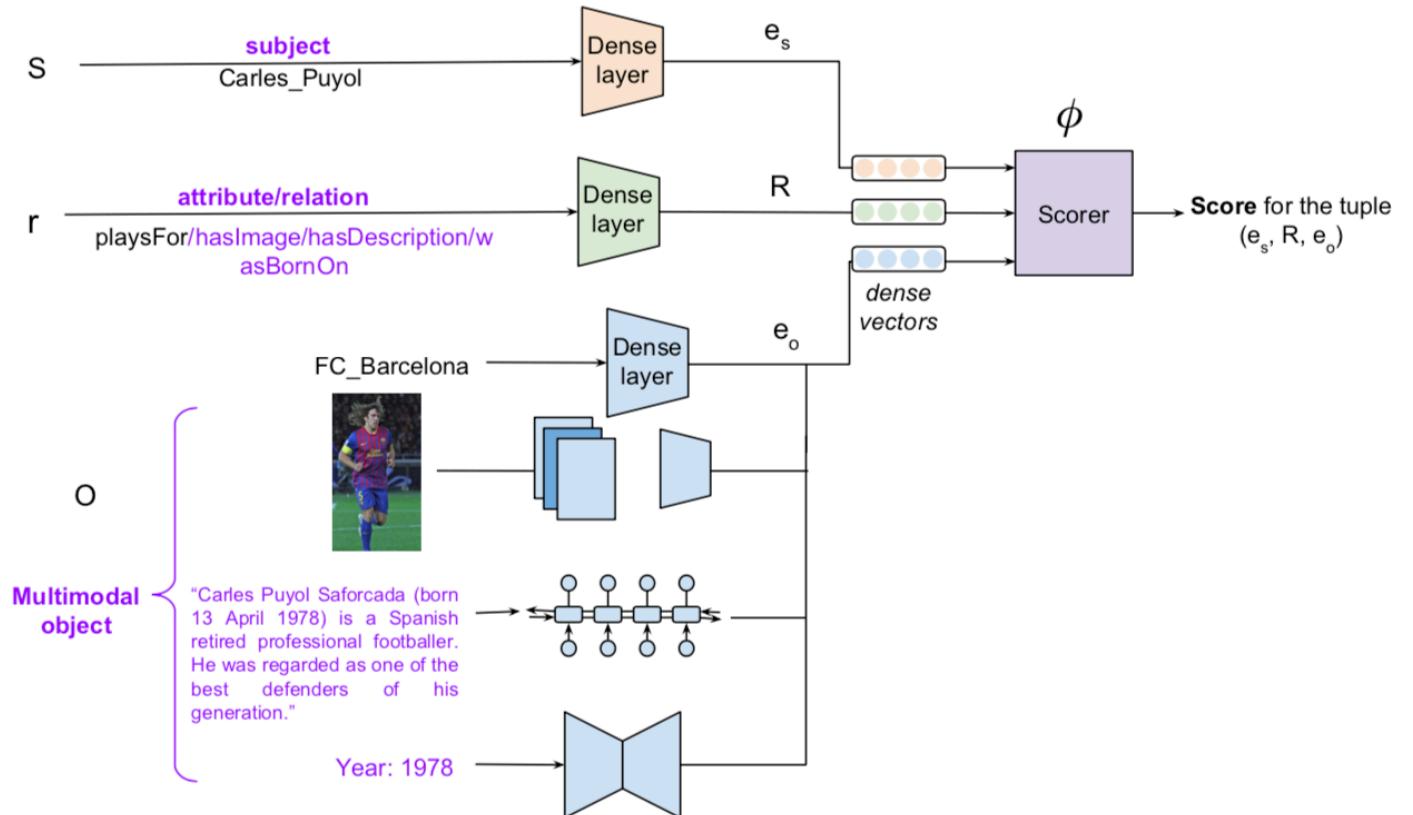
Many real-world graphs includes **multi-modal attributes**.



Dublin (/dʌblɪn/, Irish: Baile Átha Cliath [bəl̥e: 'kl̥iəh]) is the capital and largest city of Ireland. Dublin is in the province of Leinster on Ireland's east coast, at the mouth of the River Liffey. The city has an urban area population of 1,345,402. The population of the Greater Dublin Area, as of 2016, was 1,904,806 people. Founded as a Viking settlement, the Kingdom of Dublin became Ireland's principal city following the Norman invasion. The city expanded rapidly from the 17th century and was briefly the second largest city [...]

Multimodal Knowledge Graph Embeddings

- KBLRN [Garcia-duran et al.2017]
- LiteralE [Kristiadi et al. 2018]
- MKBE [Pezeshkpour et al. 2018]

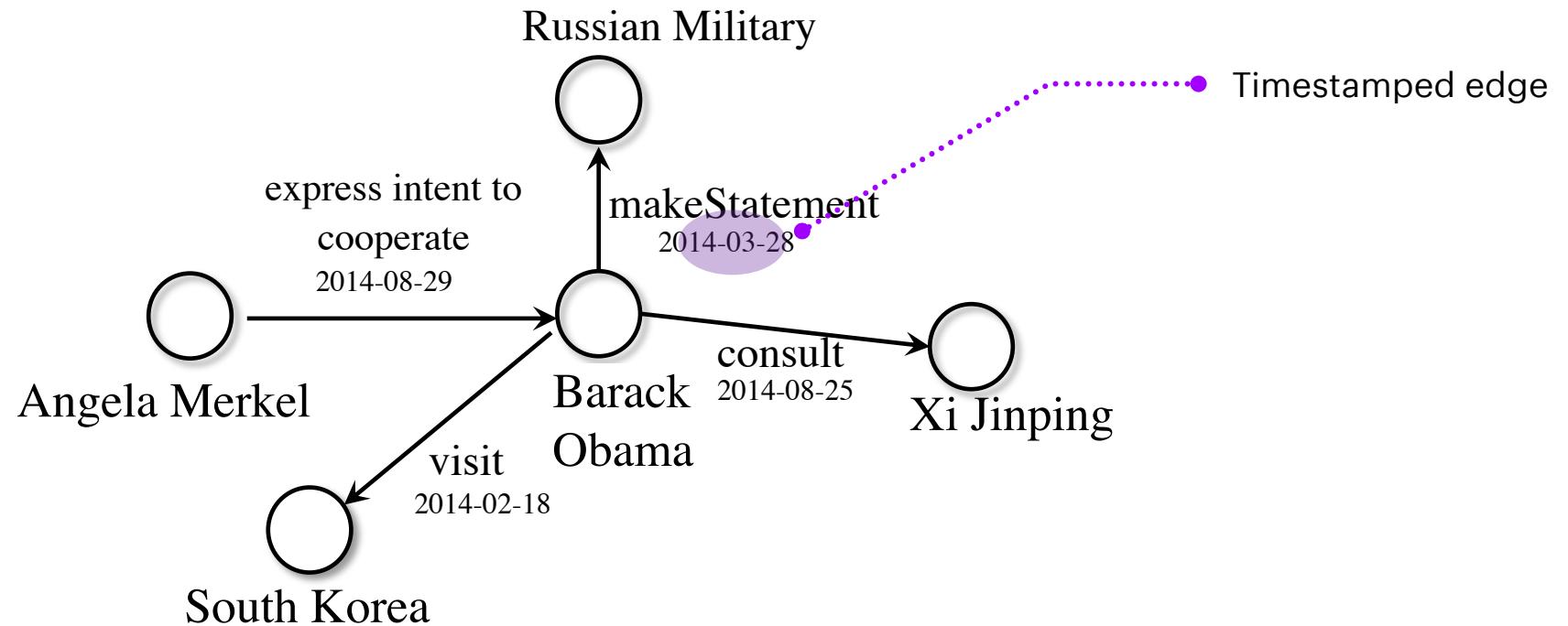


[Gesese et al. 2019] surveys recent literature

[Pezeshkpour et al. 2018]

Temporal Knowledge Graphs

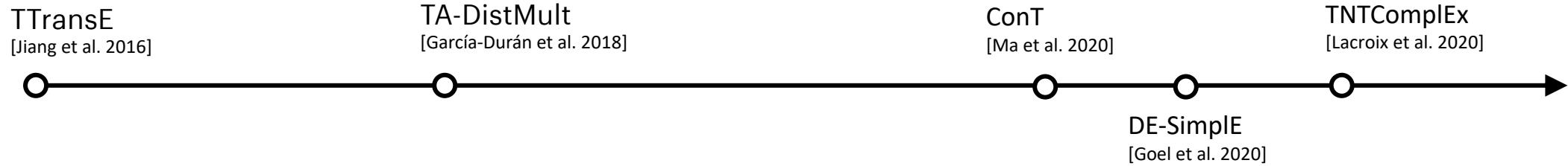
Many real-world graphs represents timestamped concepts.



	ICEWS14	ICEWS05-15	Yago15k	Wikidata
Entities	6869	10094	15403	432715
Predicates	460	502	102	814
Timestamps	365	4017	170	1726
SI	72826	368962	110441	7224361

Table from [Lacroix et al. 2020]

Time Awareness: Temporal KGE models



TNTComplEx

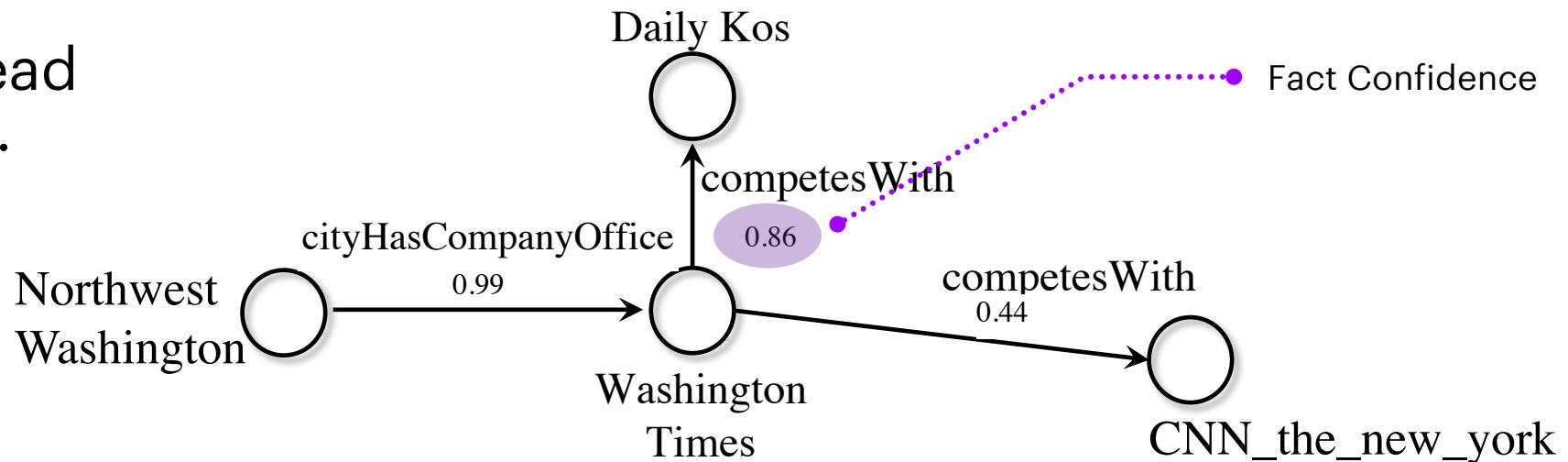
- Embeddings for each timestamp
- Order 4 tensor decomposition problem
- ComplEx as decomposition method

	ICEWS14	ICEWS15-05	Yago15k
TA	0.48	0.47	0.32
DE-SimplE	0.53	0.51	-
ComplEx	0.47 (0.47)	0.49 (0.49)	0.35 (0.36)
TComplEx	0.56 (0.61)	0.58 (0.66)	0.35 (0.36)
TNTComplEx	0.56 (0.62)	0.60 (0.67)	0.35 (0.37)

[Lacroix et al. 2020]

Uncertain Knowledge Graphs

Automatic KG generation may lead to *uncertain* facts.



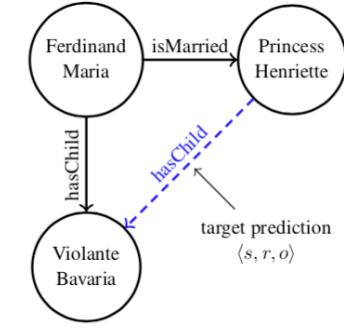
UKGE [Chen et al. 2019]

- Jointly training of KGE model + probabilistic soft logic to predict likelihood of unseen triples
- Logical rules are required as additional input

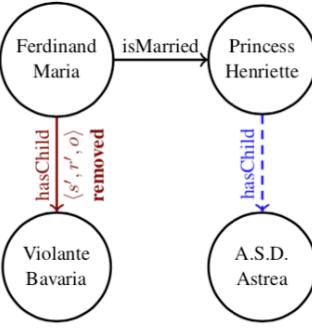
Robustness

KGE suffer from adversarial modifications

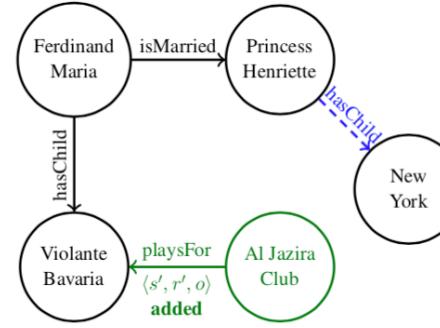
Link Prediction



(a) KG, with the target prediction



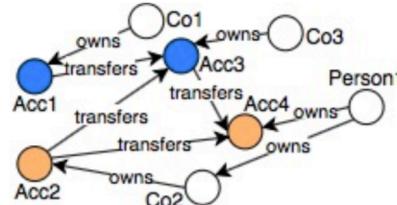
(b) After removing a fact



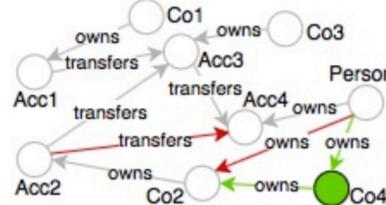
(c) After adding a fact

[Pezeshkpour et al. 2019]

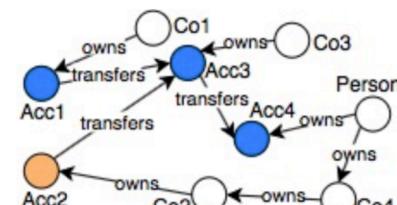
Node Classification



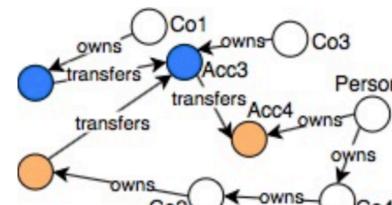
(a) Original



(b) Adversarial perturbations



(c) Adversarial attack



(d) Adversarial robustness

[Bhardwaj 2020]

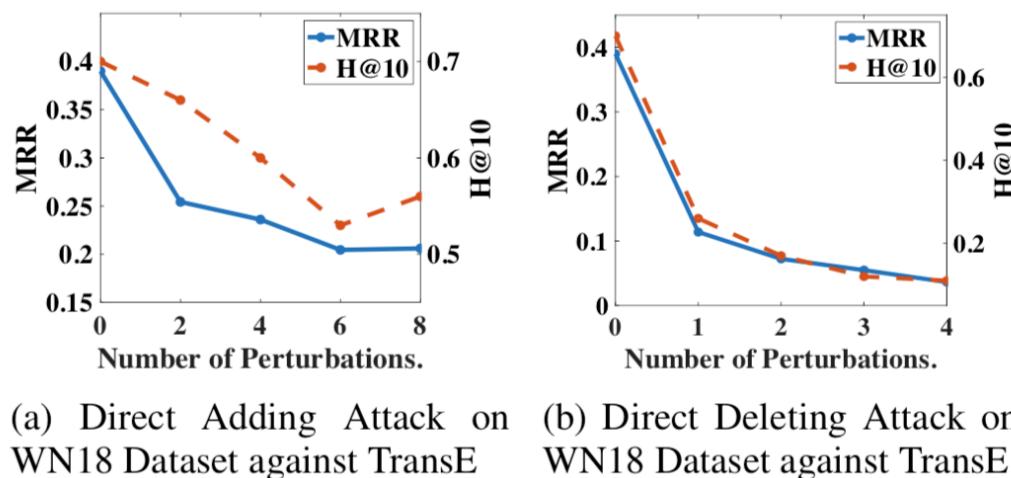
Robustness

Zhang et al. 2019

Generates input perturbations from the latent space by scoring all possible perturbations

CRIAGE [Pezeshkpour et al. 2019]

Encoder-decoder based inverter neural network



KGE & Neuro-Symbolic Reasoning

Background knowledge injection with Soft Constraints

[Minervini et al. 2017]

Manually provide rules (or mine with AMIE+) and inject into loss function:

(a) Axioms extracted from YAGO3		(b) Axioms extracted from DBPEDIA	
HASNEIGHBOR	\equiv	HASNEIGHBOR ⁻	ASSOC. BAND
ISMARRIEDTO	\equiv	ISMARRIEDTO ⁻	MUSICAL BAND
PLAYSFOR	\equiv	ISAFFILIATEDTO	\equiv ASSOC. MUSICAL ARTIST
ISCONNECTEDTO	\equiv	ISCONNECTEDTO ⁻	MUSICAL ARTIST

We extend \mathcal{L} with the regularization term $\mathcal{R}_{\mathcal{S}}$:

$$\mathcal{L}_{\mathcal{S}}(\Theta) = \mathcal{L}(\Theta) + \lambda \mathcal{R}_{\mathcal{S}}(\Theta)$$

$\lambda = \infty$ hard constraints

$\lambda = 0$ original model

$$\mathcal{R}_{\mathcal{S}}(\Theta) \triangleq \sum_{p \equiv q \in \mathcal{A}_1} D [\mathbf{r}_p \| \mathbf{r}_q] + \sum_{p \equiv q^- \in \mathcal{A}_2} D [\mathbf{r}_p \| \Phi(\mathbf{r}_q)]$$

$D[x||y] = ||x - y||_2^2$: Divergence measure

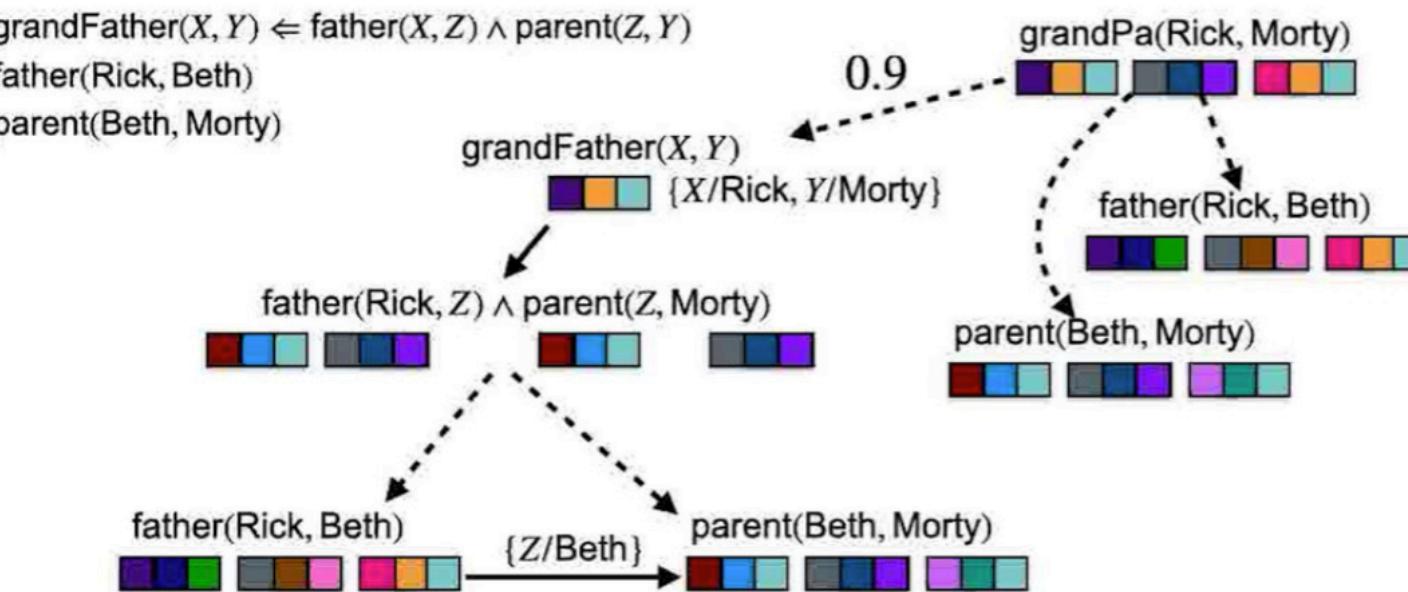
$\Phi(\cdot)$: Model-dependent transformation

\mathcal{A}_1 : equivalent axioms set

\mathcal{A}_2 : inverse axioms set

KGE & Neuro-Symbolic Reasoning: Neural Theorem Provers (NTP)

- Rule-based models + KGE
- Interplay of KGE strengths (good generalization power, scalability) with rule-based interpretability (“small data” capabilities).
- NTP implement reasoning (e.g. backward chaining) in fully differentiable architectures
 - Symbols replaced by embeddings
 - Compare embeddings in Prolog backward chaining instead of matching symbols

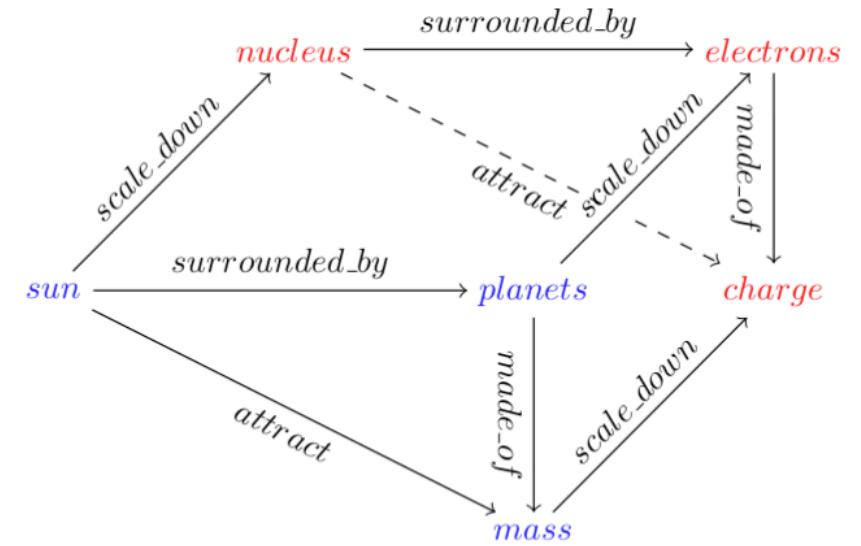


[Rocktäschel et al. 2017]
[Minervini et al. 2020]

Interplay with Other Reasoning Regimes: Analogical Reasoning

ANALOGY [Liu et al 2017]

- Models analogical structures in multi-relational embeddings
- “Differentiable” analogical reasoning combined with KGE models

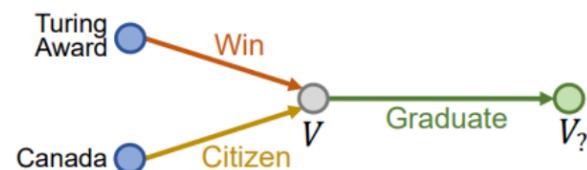


Answering Complex Queries

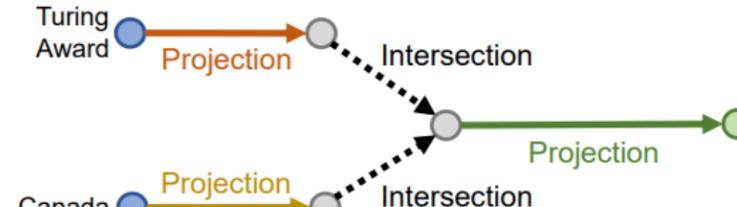
Query2box: reasoning over Knowledge Graphs in a vector space using *box embeddings* to answer complex queries.

[Ren et al. 2020]

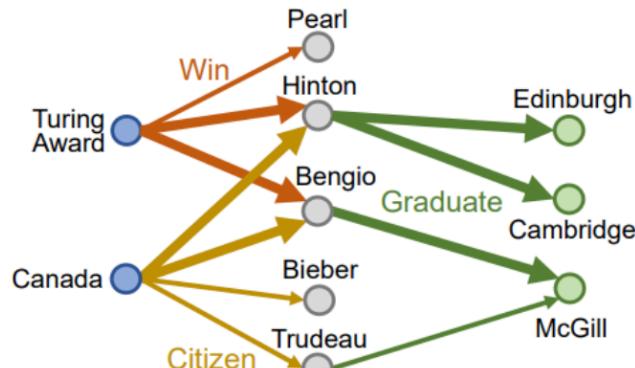
(A) Query q and Its Dependency Graph

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


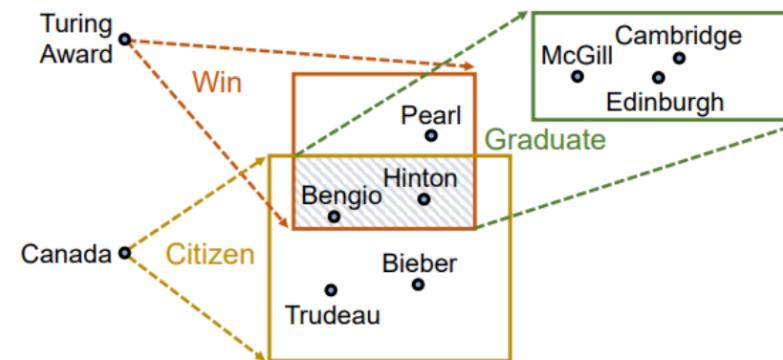
(B) Computation Graph



(C) Knowledge Graph Space



(D) Vector Space



Outline

Theoretical Overview

1h 30m

- Introduction
- Anatomy of a Knowledge Graph Embedding Model
- Evaluation Protocol and Metrics
- Advanced KGE Topics
- **Open Research Questions**

Applications

15 m

Software Ecosystem

15 m

Hands-on Sessions

1h 15m

Open Research Questions

MORE EXPRESSIVE MODELS

Model KG regularities and dependencies while keeping runtime/space complexity low.

SUPPORT FOR MULTIMODALITY

Node and edge attributes, time-awareness still in their infancy.

ROBUSTNESS & INTERPRETABILITY

Techniques to dissect, investigate, explain, and protect from adversarial attacks.

BETTER BENCHMARKS

Agreed-upon fair evaluation protocols, novel datasets.

BEYOND LINK PREDICTION

Multi-path predictions, adoption in larger differentiable architectures to inject background knowledge from graphs.

NEURO-SYMBOLIC INTEGRATION

Integrate KGE non-differentiable reasoning regimes to get the best of different worlds.

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1h 30m

Applications

Q&A

15 m

Software Ecosystem

15 m

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1h 15m

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1h 30m

Applications

15 m



Software Ecosystem

15 m

Hands-on Sessions

1h 15m

Industrial applications:

Pharmaceutical Industry:

Drug Side-effects
Prediction



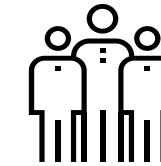
Products:

Product Recommendation



Human Resources:

Career Paths Prediction



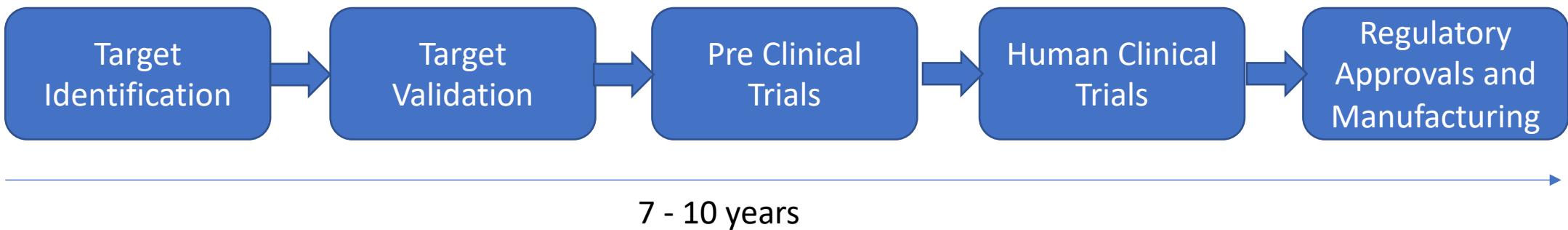
Food & Beverage:

Flavor Combinations

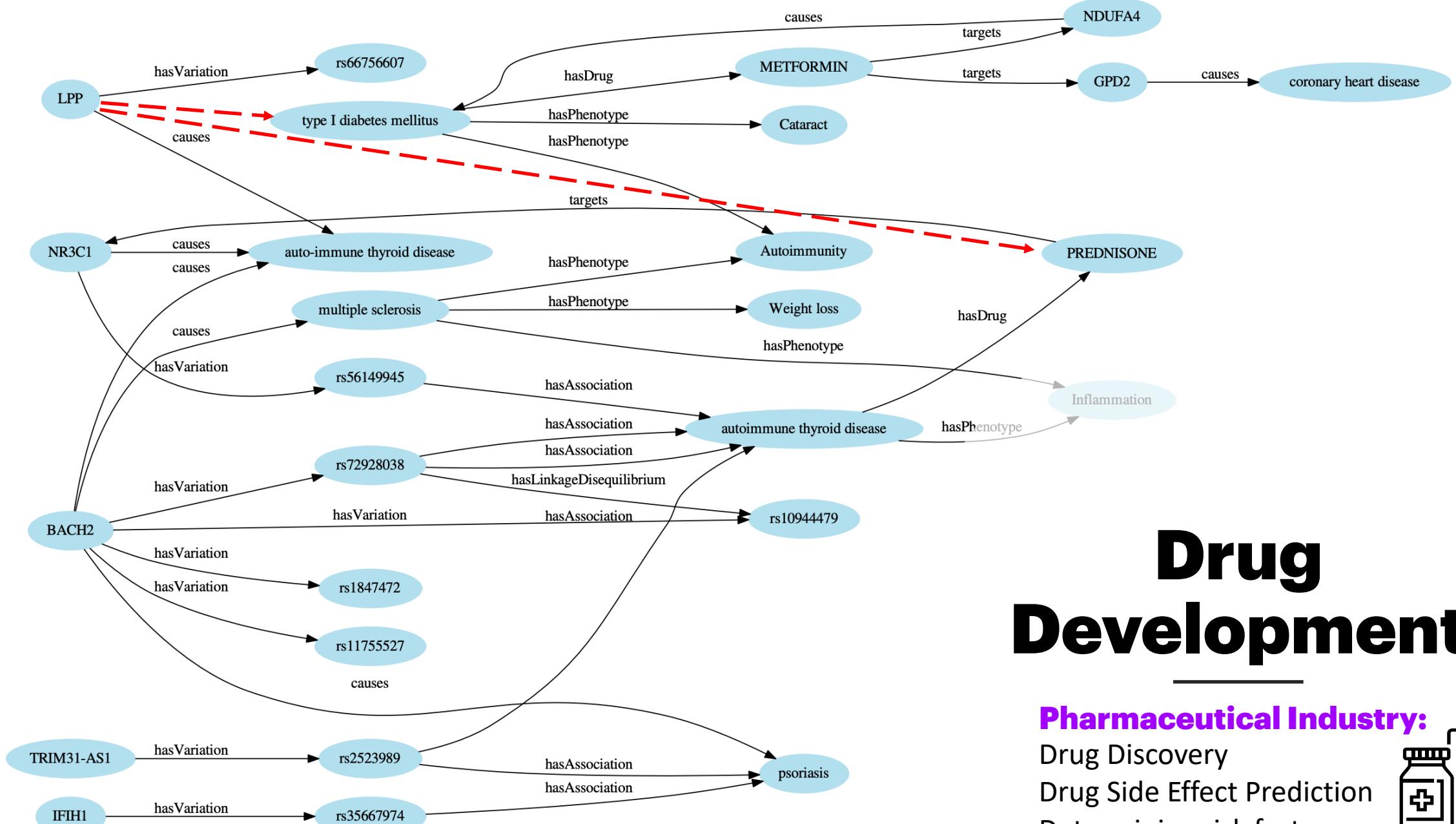


Drug Development

- Drug Development is a time consuming and expensive process which ranges from gene identification, identifying a compound to target the gene, and finally experimentation on animals and humans.



- The initial step of identification of gene/drug takes several years and if not identified correctly may result in loss of time and money.
- “Drug Developers” identify the genes/drugs by reading the latest research before proceeding with experimentation. But it is highly dependent on the experience of the person.



Drug Development

Pharmaceutical Industry:
 Drug Discovery
 Drug Side Effect Prediction
 Determining risk factors

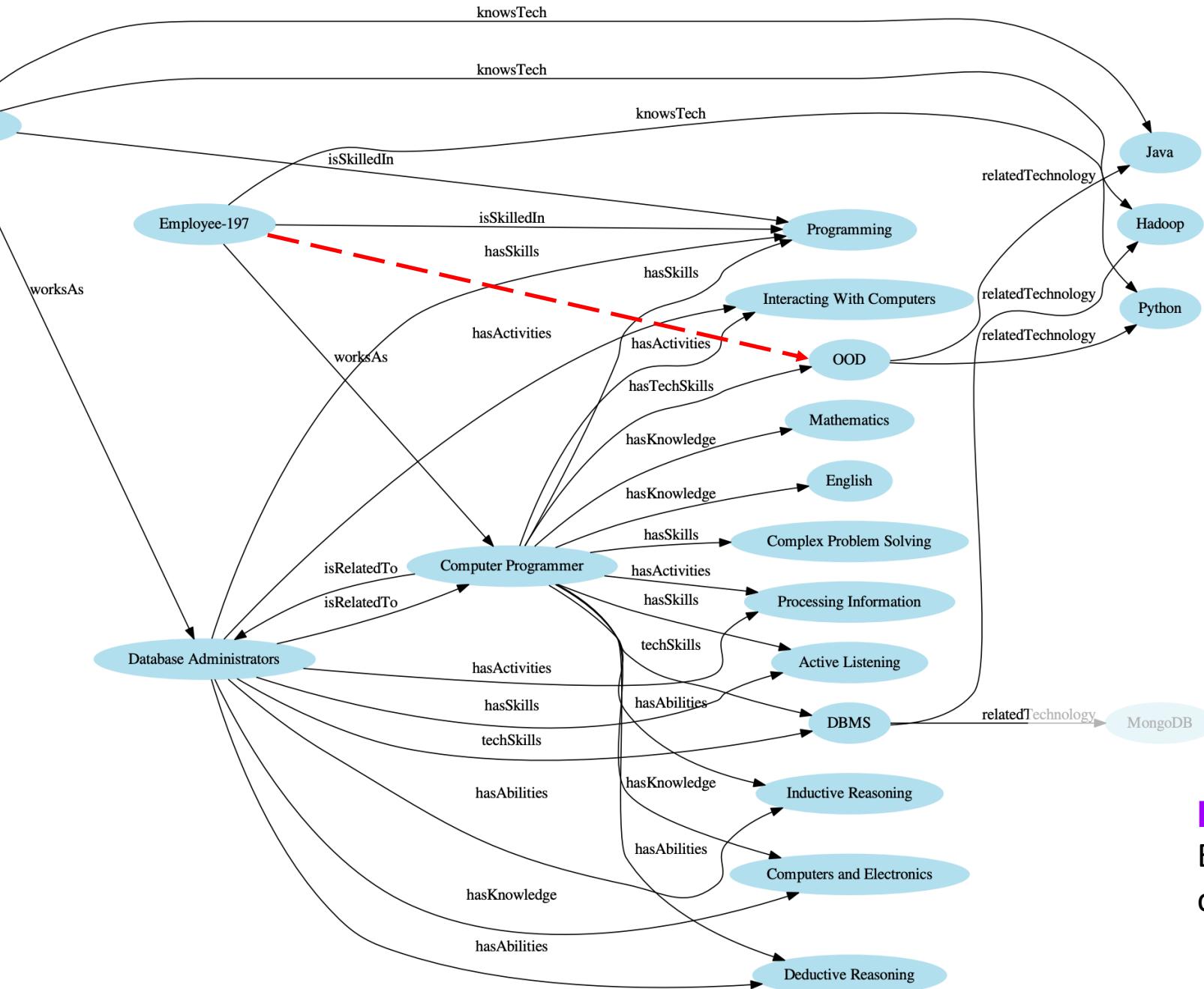


Human Resource

- Technology is evolving at an extremely fast pace. People need to learn new skills to be relevant in the market.
- Due to automation, a lot of roles are becoming obsolete and companies are forced to lay off people.

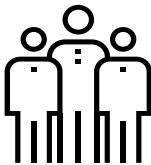
KGEs can be used for following tasks:

- Suggest new technology/tasks for career progression.
- Recommend similar roles within the organization when existing role becomes obsolete.



Human Resource

Human Resources:
Employee Career Progression
or Transition

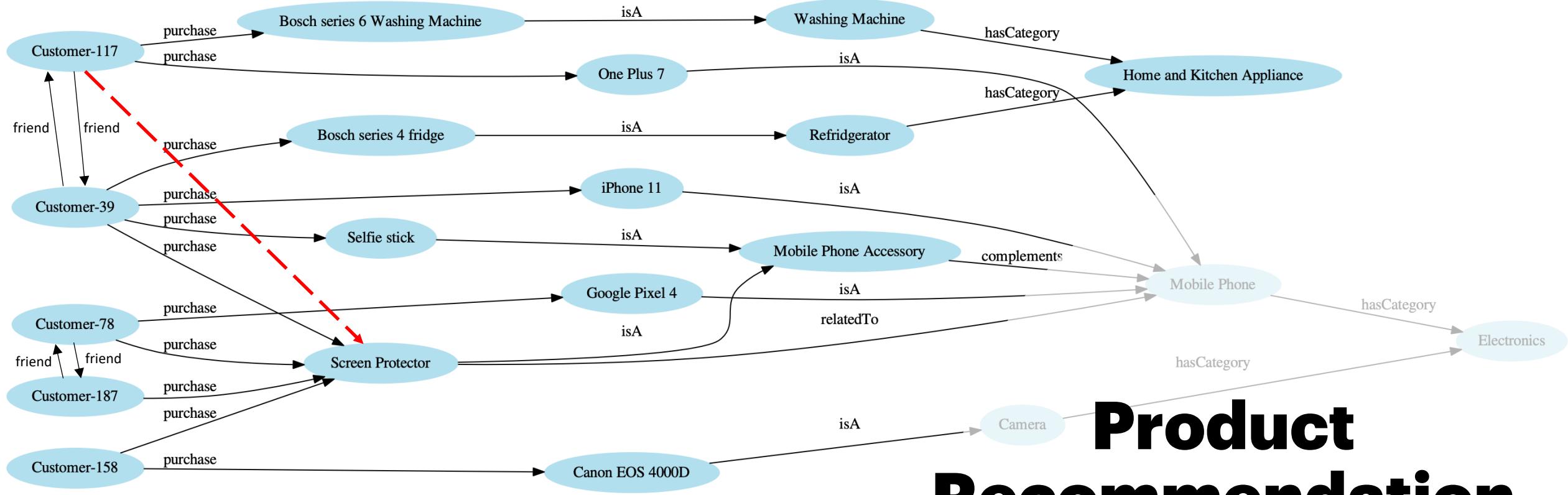


Product Recommendation

KGEs can leverage relation between customers and products.

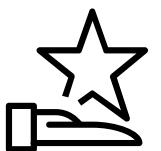
KGEs can be used for following tasks:

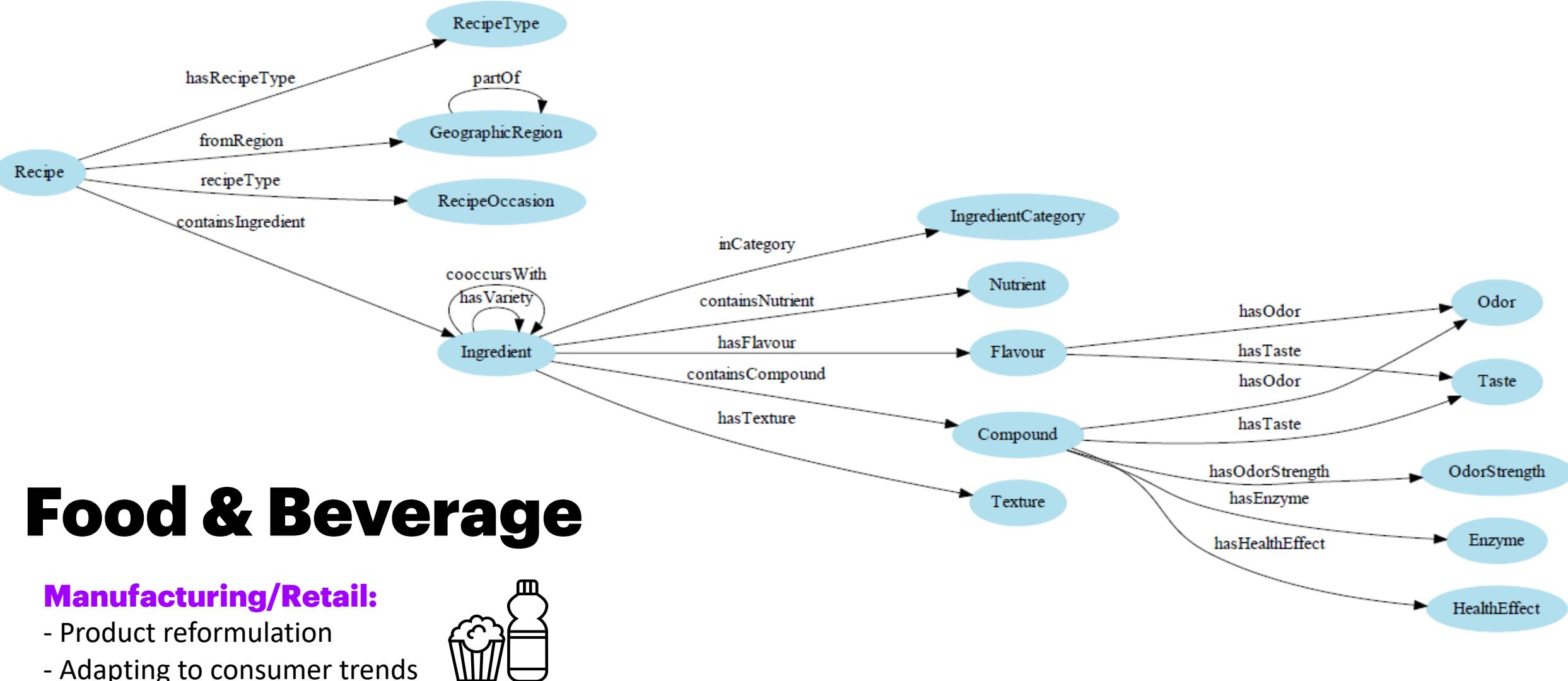
- Recommend new products to customers
- Group customers based on their purchase history

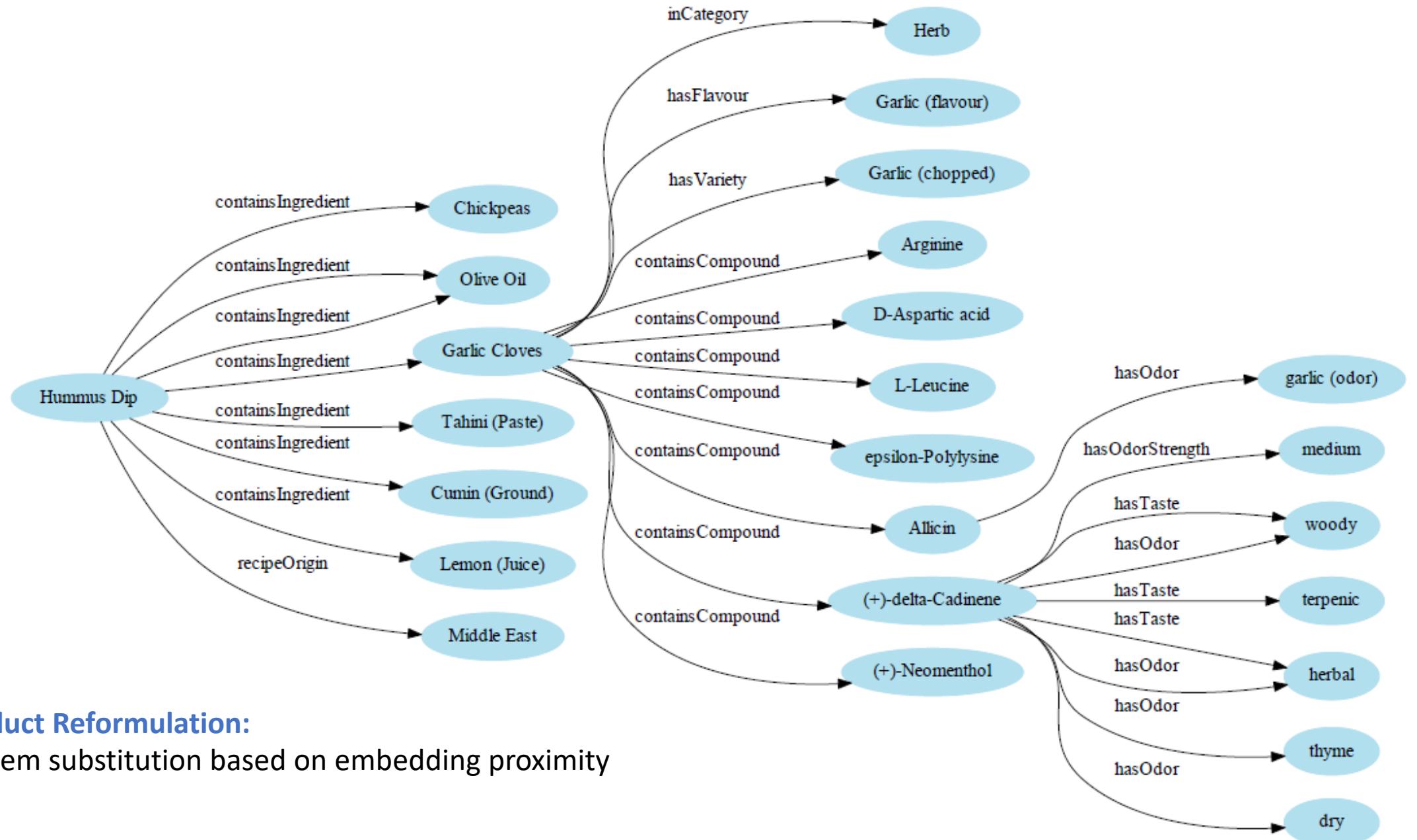


Product Recommendation

Retail:
Product Recommendation
Customer Grouping





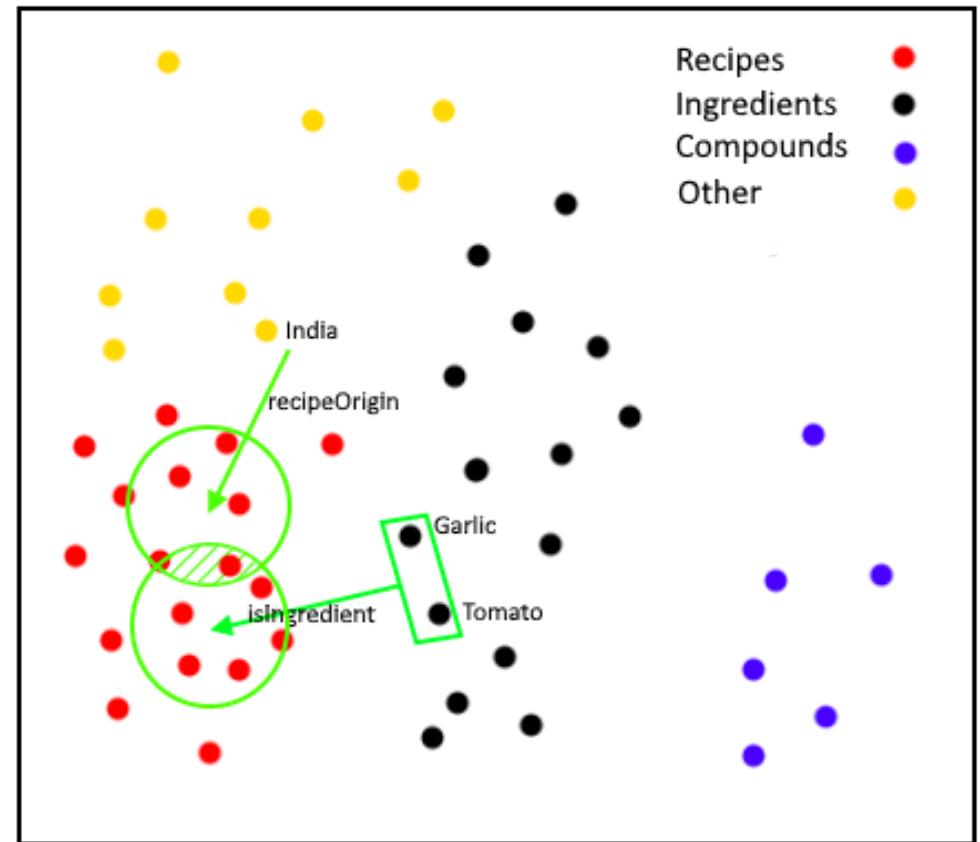


Product Reformulation:

- Item substitution based on embedding proximity

Item Recommendation

- Use vector algebra to find latent region that satisfy input criteria
- Example:
 - “I want *Indian recipes* that *contain garlic and tomato*”
 - $\text{nearest}(\text{avg}(\text{avg}(\text{GARLIC}, \text{TOMATO}) - \text{containsIngredient}, \text{India} - \text{recipeOrigin}))$
- Note: the above is pseudo-code, actual solutions will depend on model, data, fine-tuning, etc
- Alternatively use Bayesian optimization ..



Graph Construction

Datasets

kaggle
yummly™

Pancakes, baking powder,
eggs, all-purpose flour,
raisins, milk, white sugar

Hummus, olive oil,
chickpeas, lemon juice,
tahini, garlic, cumin

...

FOODB

Garlic, (E)-2-Phenyl-2-butenal,
Arginine, D-Aspartic acid
L-Leucine, epsilon-Polylysine,
(±)-erythro-Isoleucine,
Potassium

...

FlavorDB

Flavornet

(+)-delta-Cadinene, 441005,
herbal, woody, thyme, wood,
medicine, dry
1,3-Dithiane, 10451, roasted,
alliaceous

..

PubChem

(+)-delta-Cadinene Molecular
Weight, 204.35 XLogP3-AA, 3.8
Pathway, gossypol biosynthesis
Pathway, lacinilene C
biosynthesis

..

Data
processing

Triples

Recipe 1, contains, Garlic
Recipe 1, contains, Lemon juice
..

Garlic, hasCompound, Arginine
Garlic, hasCompound, L-Leucine
...

(+)-delta-Cadinene, hasOdor, herbal
(+)-delta-Cadinene, hasOdor, thyme
...

(+)-delta-Cadinene, hasPathway, gossypol
(+)-delta-Cadinene, hasPathway, lacinilene
...



Further reading ..

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1h 15m

Outline

Theoretical Overview

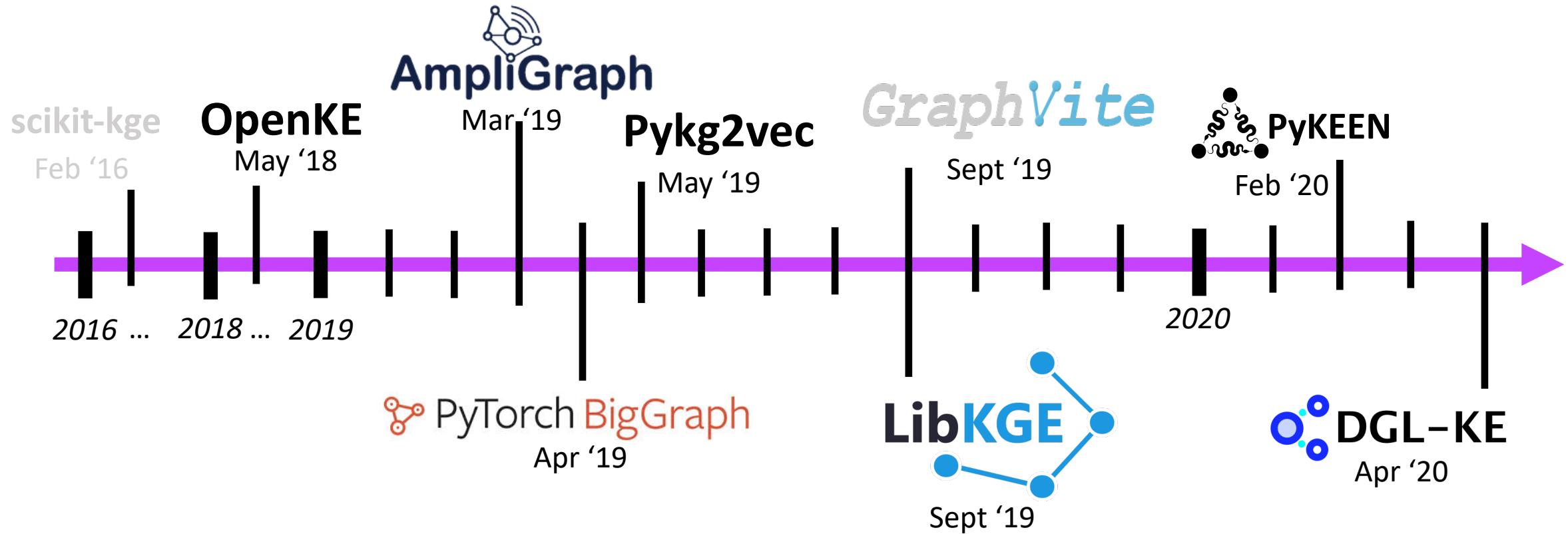
Applications

Software Ecosystem

- Introduction
- What is Out There?
- Libraries Comparison
 - Features
 - Scalability
 - SOTA Reproduced
 - Software Development
- Which Library Should I Use?
- Questions

Hands-on Sessions

KGE's Software Universe



Date reported is first of the following: pre-release/release/tag, in case where there are none of these the date reported is either submission date of a published paper accompanying or induced from repository activity. This is the case for scikit-kge, OpenKE, LibKGE.

Libraries comparison

**... and what we
measured**

Features

Scalability

SOTA Reproduced

Software Development

Features

Models

Pre-trained models

Other Features

...

Models

	<u>TransE</u>	<u>DistMult</u>	<u>ComplEx</u>	<u>TransH</u>	<u>TransD</u>	<u>TransR</u>	<u>RESCAL</u>	<u>Hole</u>	<u>SimplE</u>	<u>Analogy</u>	<u>ConvKB</u>	<u>ConvE</u>
OpenKE	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✗	✗
AmpliGraph	✓	✓	✓	✗	✗	✗	✗	✓	✗	✗	✓	✓
PyTorch BigGraph	✓	✓	✓	✗	✗	✗	✓	✗	✗	✗	✗	✗
GraphVite	✓	✓	✓	✗	✗	✗	✗	✗	✓	✗	✗	✗
DGL-KE	✓	✓	✓	✗	✗	✓	✓	✗	✗	✗	✗	✗
PyKEEN	✓	✓	✓	✓	✓	✓	✓	✓	✓	✗	✓	✓
Pykg2vec	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Lib-KGE	✓	✓	✓	✗	✗	✗	✓	✗	✓	✗	✗	✓
scikit-kge	✓	✗	✗	✗	✗	✓	✓	✓	✗	✗	✗	✗

	<u>RotatE</u>	<u>QuatE</u>	<u>KG2E</u>	<u>NTN</u>	<u>ProjE</u>	<u>RGCN</u>	<u>TuckER</u>	<u>TransM</u>	<u>CP</u>	Other models
OpenKE	✗	✗	✗	✗	✗	✗	✗	✗	✗	
AmpliGraph	✗	✗	✗	✗	✗	✗	✗	✗	✗	
PyTorch BigGraph	✗	✗	✗	✗	✗	✗	✗	✗	✗	
GraphVite	✓	✓	✗	✗	✗	✗	✗	✗	✗	
DGL-KE	✓	✗	✗	✗	✗	✗	✗	✗	✗	
PyKEEN	✓	✗	✓	✓	✓	✓	✓	✗	✗	Complex /DistMultLiteral , ERMLP , StructuredEmbedding , SME
Pykg2vec	✓	✗	✓	✓	✓	✗	✓	✓	✓	SLM , SME , ComplexN3
Lib-KGE	✓	✗	✗	✗	✗	✓	✓	✗	✓	
scikit-kge	✗	✗	✗	✗	✗	✗	✗	✗	✗	ERMLP

Pre-trained Models

	WikiData dump	Freebase	Benchmark datasets
OpenKE	✓ link	✓ fragment ?	✗
AmpliGraph	✗	✗	✓ (upon request)
PyTorch BigGraph	✓ (full)	✗	✗
GraphVite	✓ (Wikidata5m)	✗	✗
DGL-KE	✗	✗	✗
PyKEEN	✗	✗	✗
Pykg2vec	✗	✗	✗
Lib-KGE	✓ (Wikidata5M)	✗	✓ link
scikit-kge	✗	✗	✗

OpenKE requires submitting your name, email and organization before download.
? The size of this embedding suggest it is a fragment.

Other Features

- OpenKE
 - C++ implementation.
- AmpliGraph
 - Benchmarking Aid and pre-processing.
 - Formats: rdf, csv, ntriples.
 - Knowledge discovery API.
 - Visualization.
 - Model selection API.
 - Slack.
 - Colab Tutorials.
- PBG
 - High-level operators.
 - Scalability (partitioning, experimental GPU).
- DGL-KE
 - Scalability (partitioning with METIS, faster than GraphVite and PBG).
- PyKEEN
 - Incorporating multi-modal information.
 - Extensibility (wide range of interchangeable components).
 - Hyperparameters support (Optuna).
- Pykg2vec
 - Metrics summary plots.
 - Automatic discovery for hyperparameters.
 - Interactive results inspector.
- Lib-KGE
 - Hyper param support (includes Bayesian Optimization).
 - Resuming training.
 - Configuration via yaml.
- GraphVite
 - Command line interface.
 - Visualization.
 - Configuration via yaml.
 - Auto-deduction of hyperparameters.
 - Scalability (GPU-CPU hybrid).
 - Node Embedding API.
 - Input data parser.

**scikit-kge is not listed here as it was discontinued*

Scalability

Scalability

	Core Framework	GPU	Distributed Execution CPU	Biggest Graph
OpenKE	PyTorch/Tensorflow	✓	✗	10^8 edges, 4×10^7 nodes [3]
AmpliGraph	Tensorflow	✓	✗ (Coming)	10^8 edges, 10^6 nodes [1]
PyTorch BigGraph	PyTorch	✓	✓	2.4×10^{12} edges, 1.21×10^8 nodes [4]
GraphVite	PyTorch	✓	✓ (GPU-CPU)	1.8×10^{12} edges, 6.6×10^6 nodes [9]
DGL-KE	PyTorch	✓	✓	3.38×10^8 edges, 8.6×10^6 nodes [8]
PyKEEN	PyTorch	✓	✗	-
Pykg2vec	PyTorch/Tensorflow	✓	✗	-
Lib-KGE	PyTorch	✓	✗	-
scikit-kge	-	✗	✗	-

SOTA Reproduced

SOTA Reproduced

	OpenKE	PBG	AmpliGraph	GraphVite	DGL-KE	PyKEEN	Pykg2vec	Lib-KGE	scikit-kge
SOTA reproduced	✓	✓	✓	✓	✓	✗	✓	✓	✓
Models reported	8/10	2/4 ¹	6/6	6/6	6/6	0/22?	10/22	9/9	5/5 ²

¹ page 8, Lerer et. al. 2019.

² page 6, Nickel et. al. 2015.

? Not found.

Software Development

Software Development Metrics

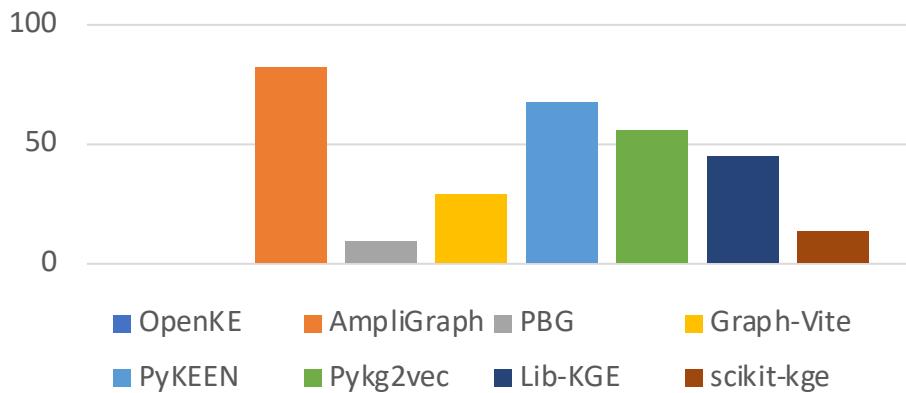
- Documentation ([docstr-coverage](#)) - [PEP 257](#)
 - Counts number of functions, classes, methods, and modules that doesn't have docstrings.
- Tests ([coverage](#))
 - [measures](#) how many lines out of the executable lines were executed.
- Good practices ([pylint](#)) [PEP 8](#)
- Code Complexity ([radon](#)) – McCabe Complexity

Class	A	B	C	D
Number	1-10	10-20	20-40	40+
Code	Well written and structured	Complex Code	Very Complex Code	Extremely Complex Code
Testability	High	Medium	Low	Not Testable
Maintenance Cost and Effort	Less	Medium	High	Very High

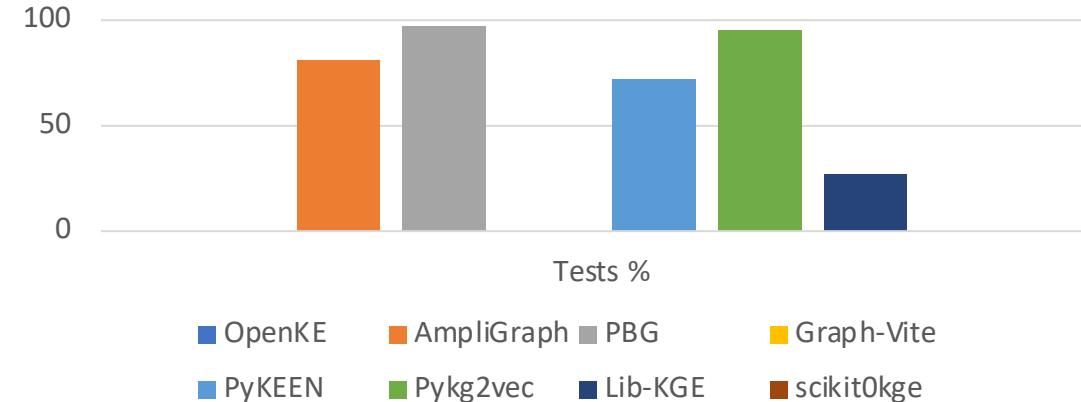
[source](#)

Software Development Metrics

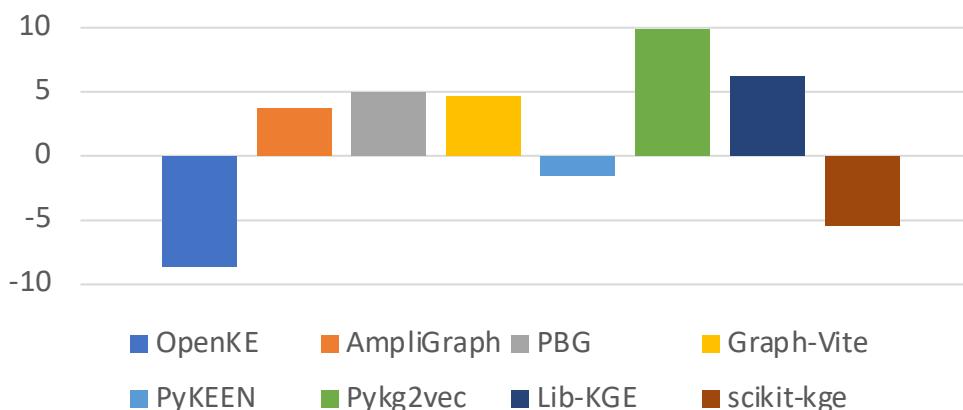
Documentation Coverage [%]



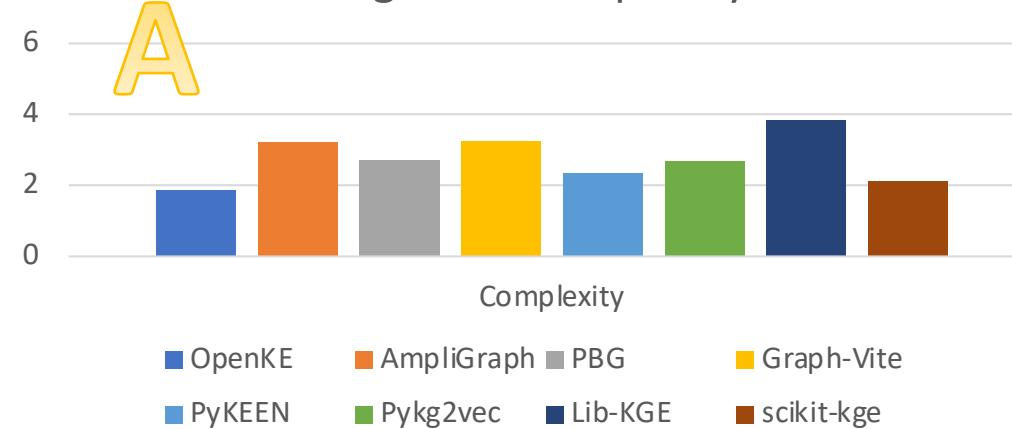
Tests Coverage [%]



Good Practices PEP8 (max 10)



Avg Code Complexity



Which Library Should I Use?

Align your choice with:

- Your task and time that you have for learning the library.
- Your experience.
- Framework the library supports Pytorch/Tensorflow/other?.
- Consider features like scalability, community support, user-friendliness, maturity of the project, accuracy, and supported addons.
- Finally: The choice is yours.

Use tools like [github-statistics](#) to support yourself.

Thank you!

Knowledge Graph Embeddings: From Theory to Practice

Software Ecosystem

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Resources:

- [AmpliGraph](#)
- [Libkge](#)
- [Graphvite](#)
- [DGL-KE](#)
- [Pykeen](#)
- [Pykg2vec](#)
- [OpenKE](#)
- [scikit-kge](#)
- [PyTorch-BigGraph](#)
- [github-statistics](#)
- [Article on how to compare repos](#)

References

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8. Zheng, Da, Xiang Song, Chao Ma, Zeyuan Tan, Zihao Ye, Jin Dong, Hao Xiong, Zheng Zhang, and George Karypis. "DGL-KE: Training Knowledge Graph Embeddings at Scale." ArXiv:2004.08532 [Cs] Proceedings of the 43rd International ACM SIGIR Conference on Research and Development in Information Retrieval (April 18, 2020). <http://arxiv.org/abs/2004.08532>.
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10. Bianchi, Federico, Gaetano Rossiello, Luca Costabello, Matteo Palmonari, and Pasquale Minervini. "Knowledge Graph Embeddings and Explainable AI." ArXiv:2004.14843 [Cs], April 30, 2020. <https://doi.org/10.3233/SSW200011>.

Outline

Theoretical Overview

- Introduction
- Anatomy of a Knowledge Graph Embedding Model
- Evaluation Protocol and Metrics
- Advanced KGE Topics
- Open Research Questions

1h 30m

Applications

15 m

Software Ecosystem

15 m

Hands-on Session

bit.ly/kge-tutorial

1h 15m



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