Statistical Inference on KGs

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Knowledge bases on the Web

Motivation

- There are some serious challenges related to Knowledge Graphs
  - **Growth:** knowledge graphs are highly incomplete!
    - *Knowledge extraction:* extract new entities and relations
    - *Link prediction:* add (or guess) new relations between entities
  - **Validation:** knowledge graphs are not always correct!
    - *Entity resolution:* merge duplicate entities, split wrongly merged ones
    - *Error detection:* remove false assertions
  - **Interface:** how to make it easier to access knowledge?
    - *Semantic parsing:* interpret the meaning of queries
    - *Question answering:* computing answers using knowledge graphs
  - **Intelligence:** can AI emerge from knowledge graphs?
    - *Automatic reasoning* and planning
    - Generalization and abstraction

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We talked about it in the previous lectures

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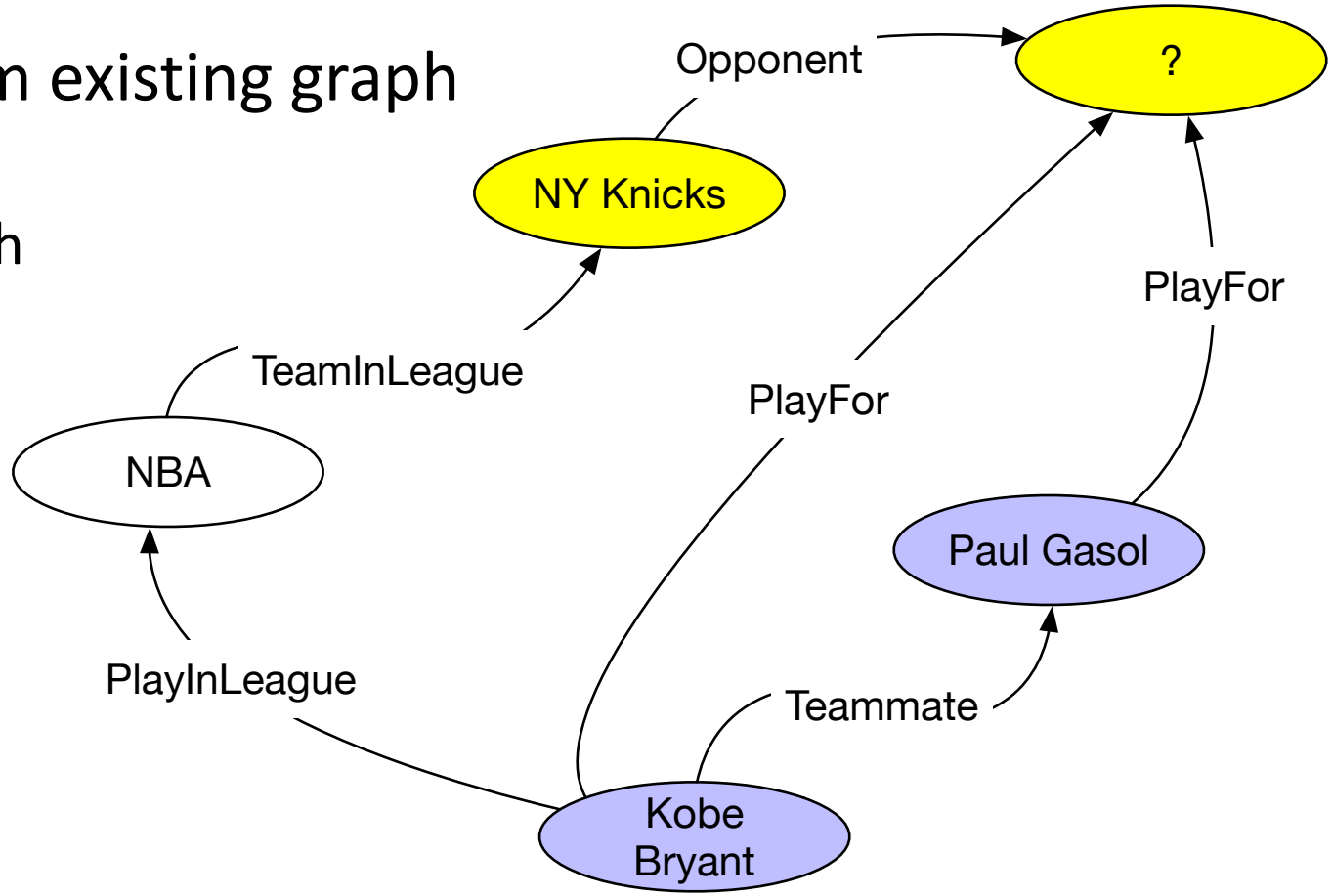
Link Prediction

- **Goal:** Add knowledge from existing graph
  - No external source
  - Reasoning within the graph
- **Some solutions**
  - Rule-based methods
  - Probabilistic models
  - Factorization models
  - Embedding models



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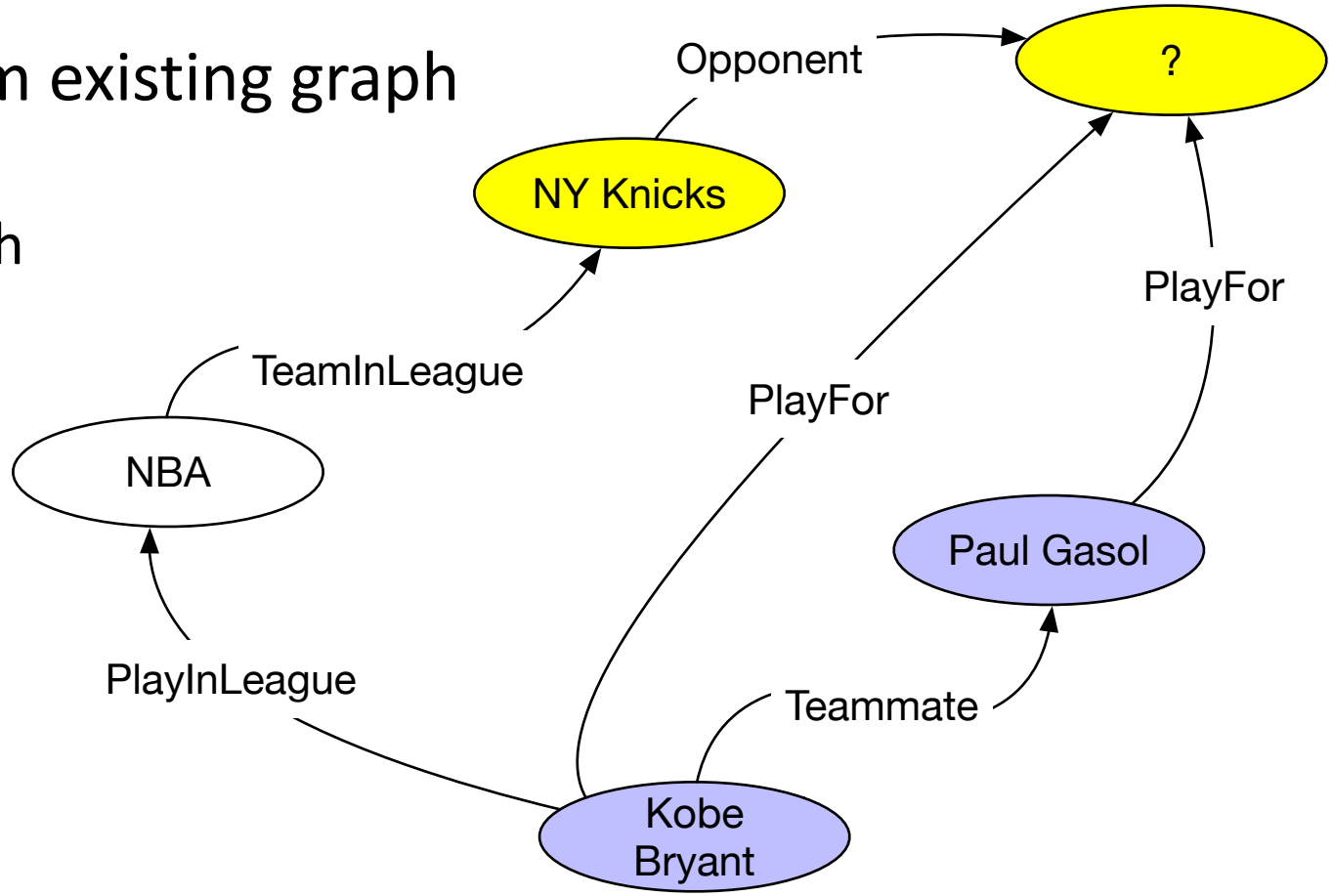

Link Prediction with Rules

- Goal: We want to make the predictions by applying rules that we extract from the graph => *rule mining*
- Rule mining is an important research topic in several communities
- **Association rule mining:** process of discovering rules that associate items together

$I = \{i_1, i_2, \ldots, i_m\}$ is a set of items
Transaction $t \subseteq I$ is a subset of items
Transaction database $T = \{ t_1, t_2, t_3, \ldots, t_n \}$. We assume *T* is large
An *association rule* is defined as $X \rightarrow Y \; where \; X, Y \subseteq I \; and \; X \cap Y = \emptyset$

- A famous algorithm for association mining is the *Apriori* algorithm [1]

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[1] J. Leskovec, A. Rajaraman, and J. D. Ullman, *Mining of massive datasets*. Cambridge University Press, 2014. Chapter 6.

Link Prediction with Rules

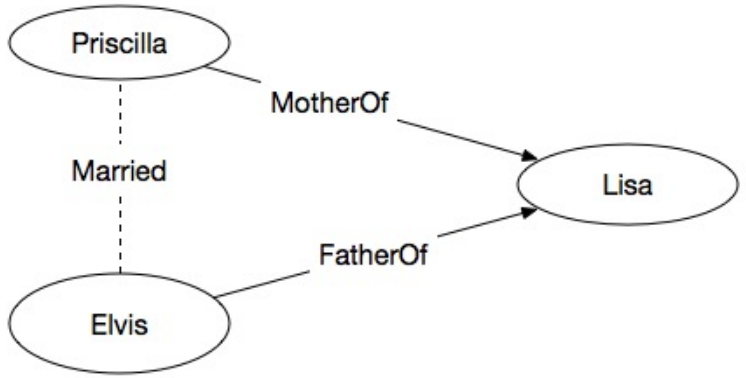
- **Association rule mining:** process of discovering rules that associate items together

In our case, we can assume that a transaction is a connected subgraph

$$t_i = \{mother(Priscilla, Lisa), father(Elvis, Lisa), married(Priscilla, Elvis)\}$$

If we observe that this transaction occurs *often,* then we can infer the rule

$$mother(x, y), father(z, y) \rightarrow married(x, z)$$



Link Prediction with Rules

- **Inductive Logic Programming (ILP):** field of machine learning that deduces logical rules from ground facts

Input:
- A background knowledge B (mostly a set of atoms, e.g. *married(obama,michelle)*)
- A set of positive examples E^+ (some facts that hold)
- A set of negative examples E^- (some facts that do not hold)

Goal:
Calculate an hypothesis *h* s.t. $B \wedge h$ entails E^+ and does not entail E^-

- Several ILP systems have been designed to extract rules from the Web, e.g. SHERLOCK [1] and DL-Learner [2]

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[1] S. Schoenmackers, O. Etzioni, D. S. Weld, and J. Davis, "Learning First-order Horn Clauses from Web Text," in EMNLP 2010, pp. 1088–1098.
[2] J. Lehmann, "DL-Learner: learning concepts in description logics," *Journal of Machine Learning Research*, vol. 10, no. Nov, pp. 2639–2642, 2009.

Link Prediction with Rules: AMIE

One big problem of rule association mining and ILP methods is that they either assume CWA or require negative samples

Knowledge Graphs operate under OWA: what is not known might still be true!

Link Prediction with Rules: AMIE

- **AMIE [1]** is a system where rules are extracted with a "rule-association" mining mindset
- Horn rules are constructed incrementally and in parallel
  - They start considering a rule with a single atom, e.g. *fatherOf(X,Y)*
  - Then add another atom which shares at least one variable, e.g. *motherOf(Z,Y)*
  - When the rule is closed (e.g. each variable appears in at least two atoms), it is evaluated using confidence: Only rules with high confidence are kept

$$conf(rule) = \frac{count(body \ \wedge \ head)}{count(body)}$$

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[1] L. A. Galárraga, C. Teflioudi, K. Hose, and F. Suchanek, "AMIE: Association Rule Mining Under Incomplete Evidence in Ontological Knowledge Bases," in *WWW*, 2013, pp. 413–422.

Link Prediction with Rules: AMIE

- An important novelty of the AMIE system is the introduction of the notion of *Partial Completeness Assumption*

Definition: Let KG' be the graph which contain all true facts which are not known in KG. The assumption consists of assuming that if $r(x,y) \in KG$ then $\nexists\, y'.r(x,y') \in KG'$

Standard confidence

$$conf(\overrightarrow{B} \Rightarrow r(x,y)) := \frac{supp(\overrightarrow{B} \Rightarrow r(x,y))}{\#(x,y) : \exists z_1, ..., z_m : \overrightarrow{B}}$$

PCA-based confidence

$$conf_{pca}(\overrightarrow{B} \Rightarrow r(x,y)) := \frac{supp(\overrightarrow{B} \Rightarrow r(x,y))}{\#(x,y) : \exists z_1, ..., z_m, y' : \overrightarrow{B} \wedge r(x,y')}$$

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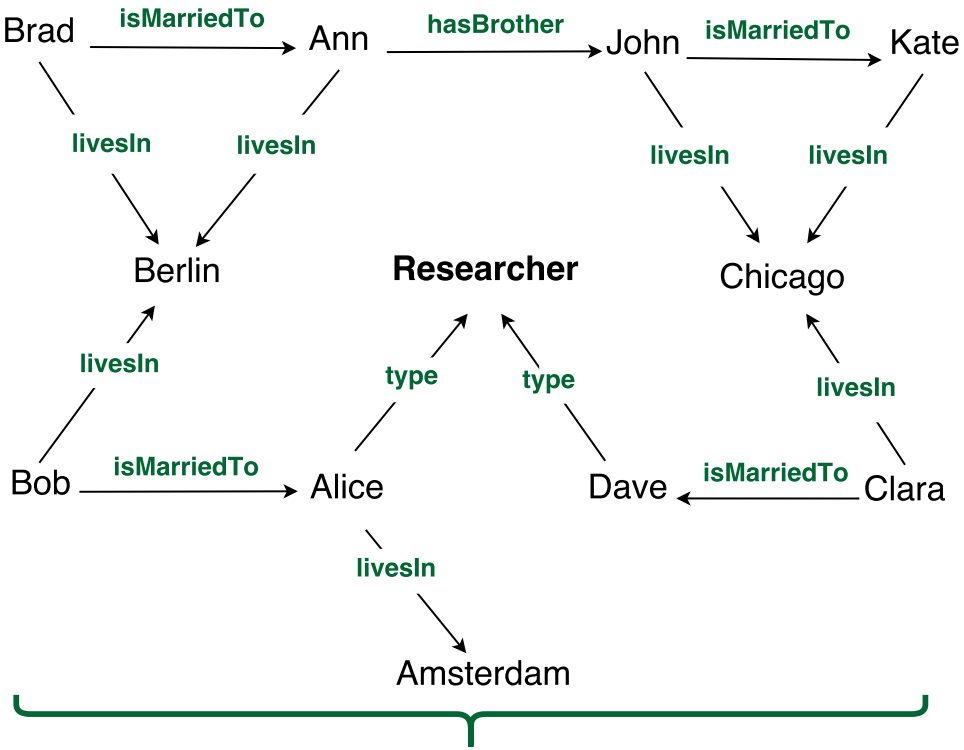
Evaluation

System	Top n	Predictions	Precision
ALEPH	7	2997	27%
AMIE	13	3180	66%
ALEPH	9	5031	26%
AMIE	29	5003	47%
ALEPH	17	8457	30%
AMIE	52	8686	45%

	Top 20 rules	Top 30 rules	All rules
Confidence	0.76	0.63	0.33
PCA Confidence	0.32	0.29	0.29

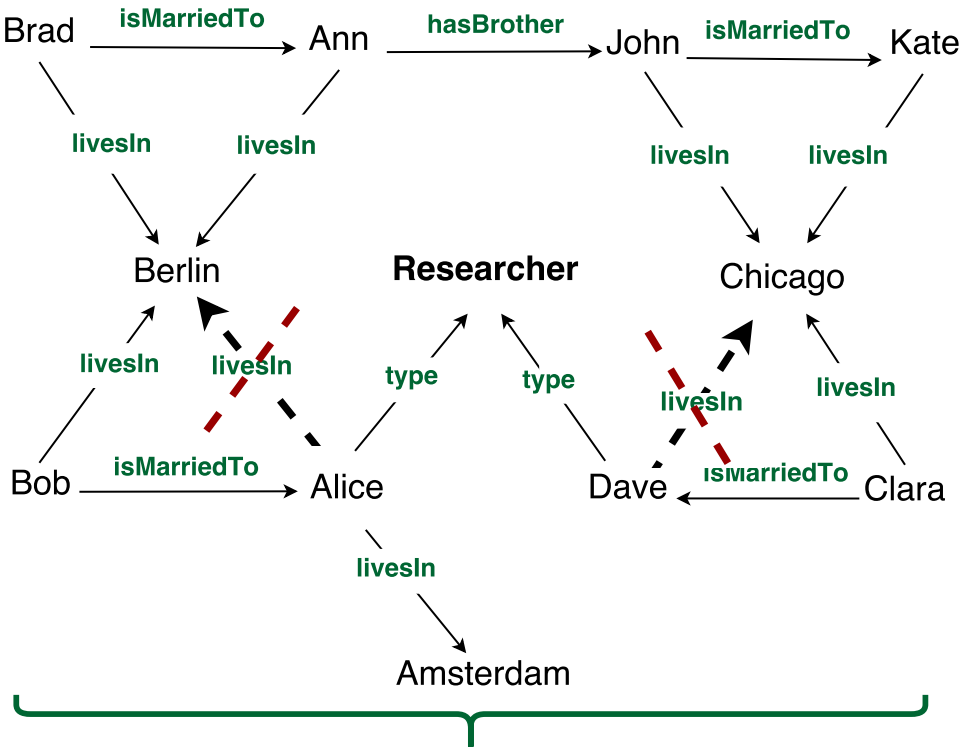
$$isCitizenOf(x, y) \Rightarrow livesIn(x, y)$$
$$hasAdvisor(x, y) \wedge graduatedFrom(x, z) \Rightarrow worksAt(y, z)$$
$$wasBornIn(x, y) \wedge isLocatedIn(y, z) \Rightarrow isCitizenOf(x, z)$$
$$hasWonPrize(x, G.\ W.\ Leibniz) \Rightarrow livesIn(x, Germany)$$

Link Prediction with Rules: Non-monotonic Learning



$$r: \; livesIn(X, Z) \leftarrow isMarriedTo(Y, X), livesIn(Y, Z)$$

Link Prediction with Rules: Non-monotonic Learning



$$r: \; livesIn(X, Z) \leftarrow isMarriedTo(Y, X), livesIn(Y, Z), not \; researcher(X)$$

Link Prediction with Rules: Non-monotonic Learning

- We developed a technique to mine non-monotonic rules [1].
- Focus on **unary** rules (binary rules are converted with *propositionalization*)
- **Step 1.** Mine association Horn clauses from the KG. We can use FPGrowth, an off-the-shelf popular algorithm
- **Step 2.** Determine normal and abnormal substitutions for every rule (see next slide)
- **Step 3.** Find all exception candidates (=predicates for unary rules) for every rule
- **Step 4.** Rank exception candidates and select the best ones

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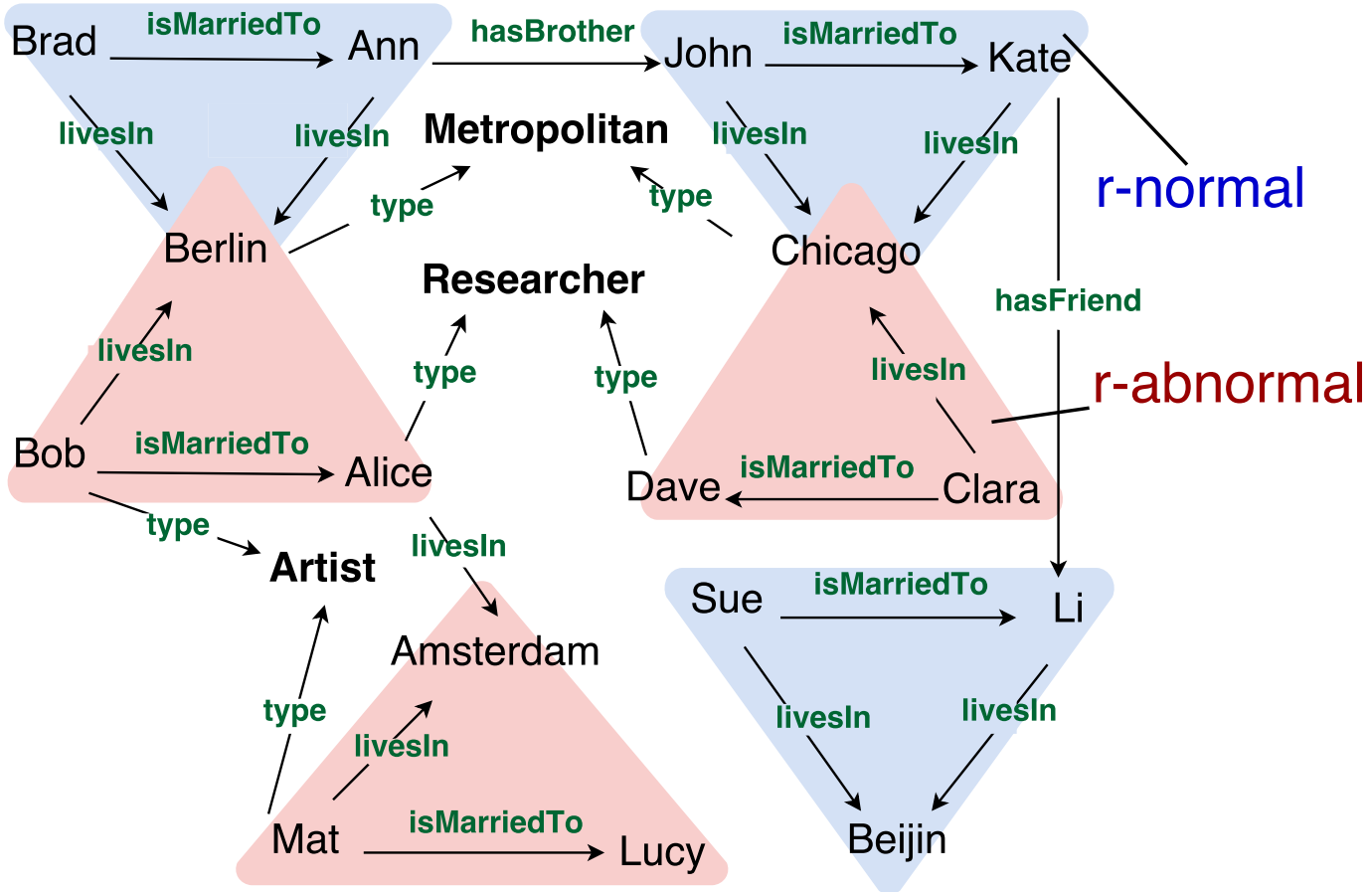
[1] M. H. Gad-Elrab, D. Stepanova, J. Urbani, and G. Weikum, "Exception-Enriched Rule Learning from Knowledge Graphs," in *ISWC*, 2016, pp. 234–251.

Abnormal substitutions



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Link Prediction

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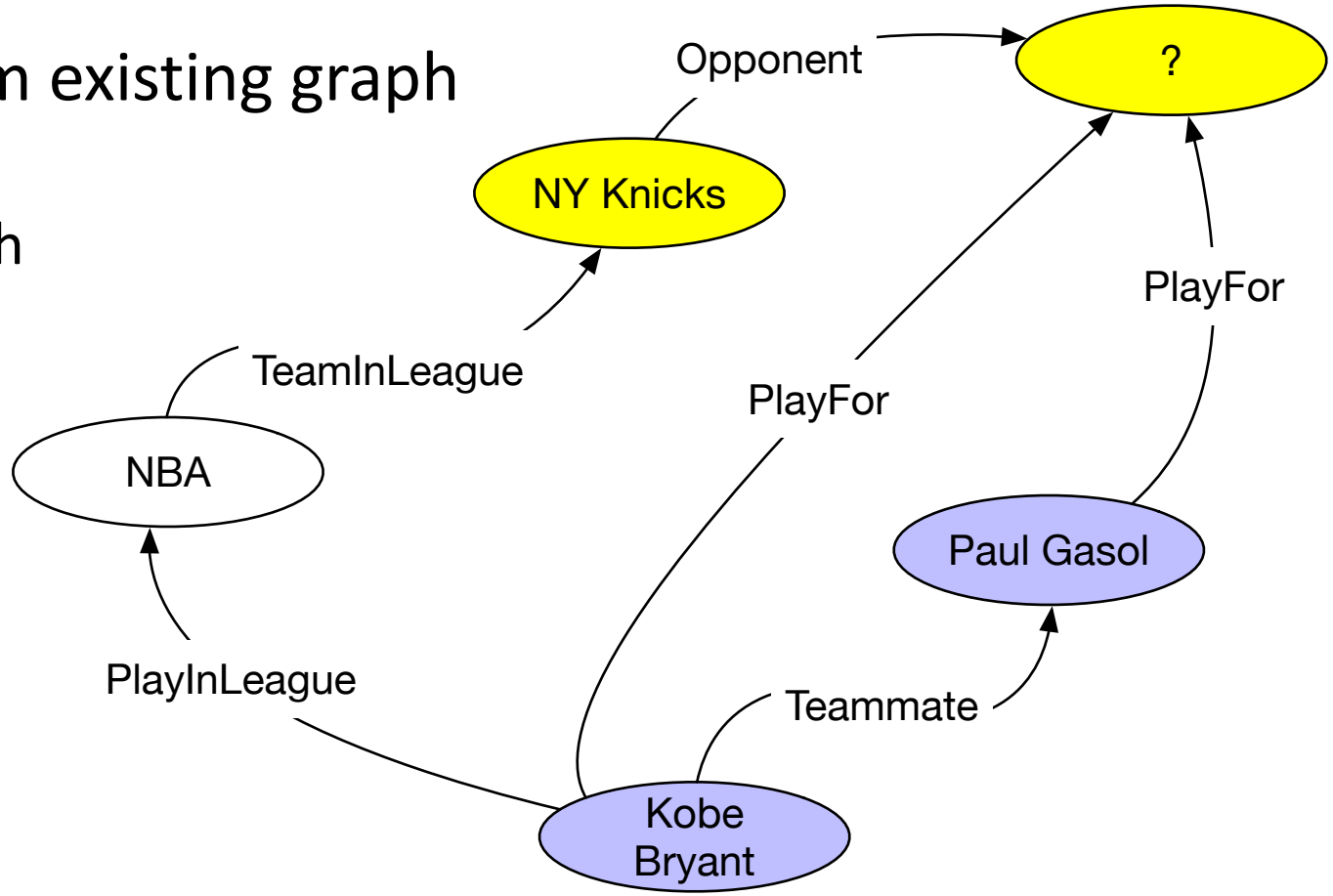
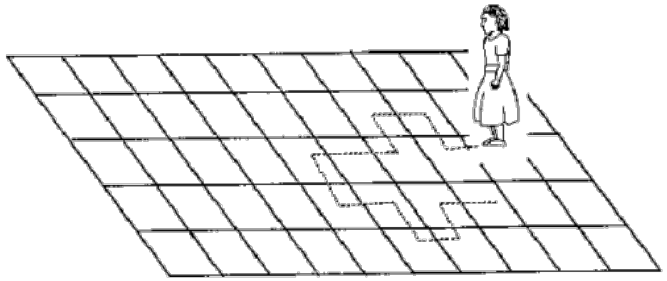


Link Prediction with Random Walks

- Rules are expensive to calculate and are “brittle”. [1] proposes a different approach, called Path Ranking Algorithm (PRA), which is a process based on *random walks*

Definition: Given a graph and a starting point, we select a neighbor of it at random, and move to this neighbor; then we select a neighbor of this point at random, and move to it etc. The (random) sequence of points selected this way is a random walk on the graph. [2]



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[1] N. Lao, T. Mitchell, and W. W. Cohen, “Random walk inference and learning in a large scale knowledge base,” in *EMNLP*, 2011, pp. 529–539.
[2] L. Lovász, “Random walks on graphs: A survey,” *Combinatorics, Paul erdos is eighty*, vol. 2, no. 1, pp. 1–46, 1993.

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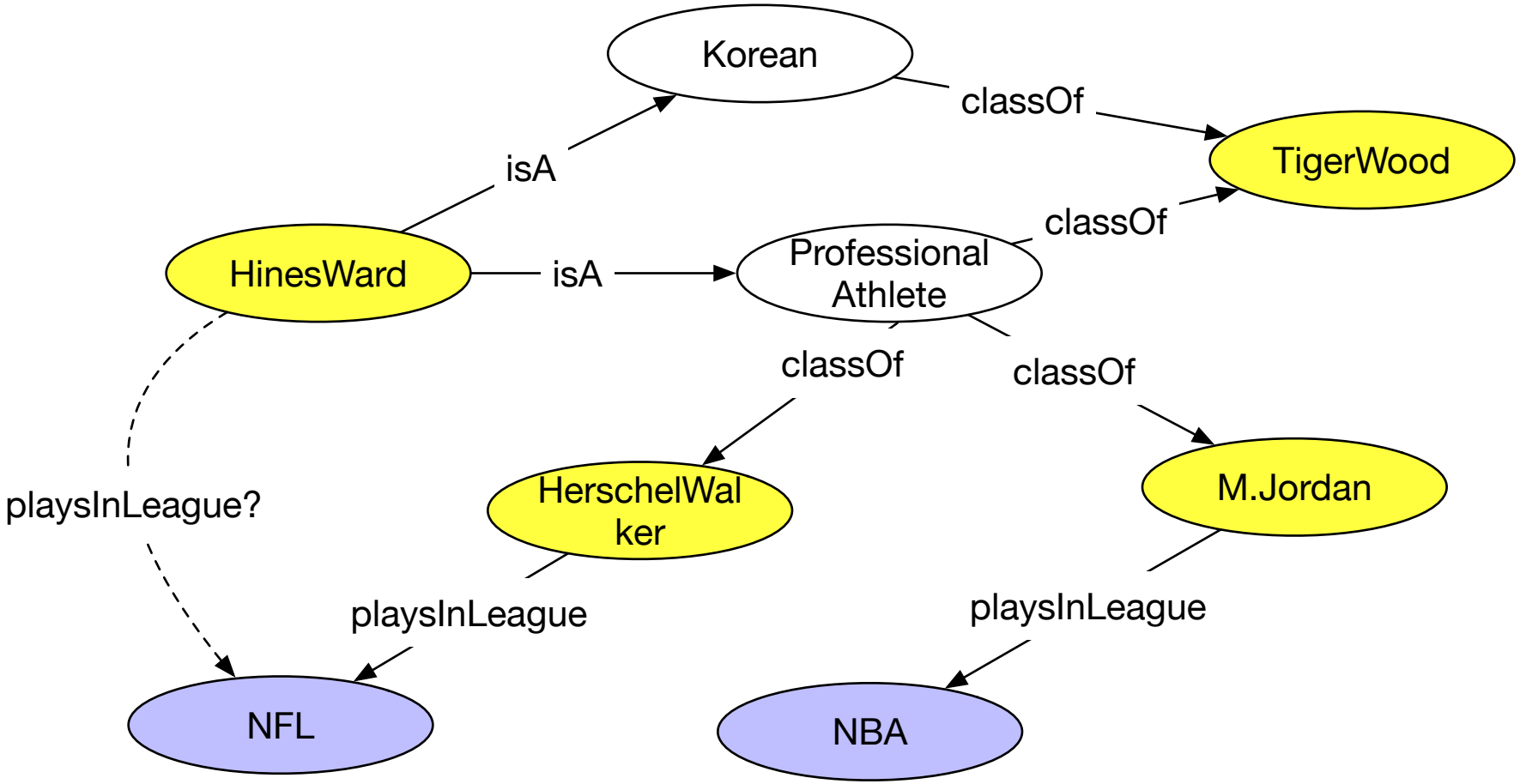

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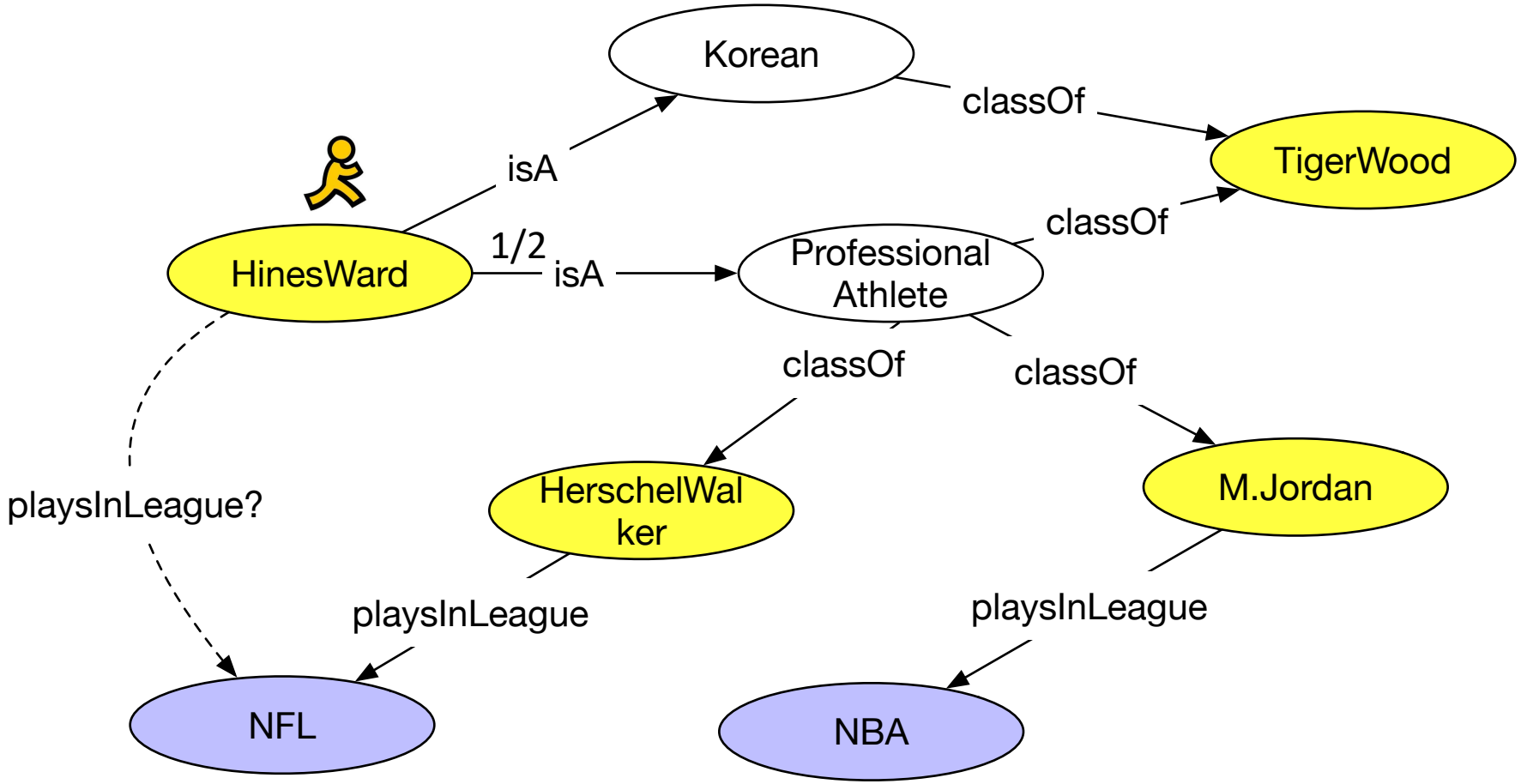

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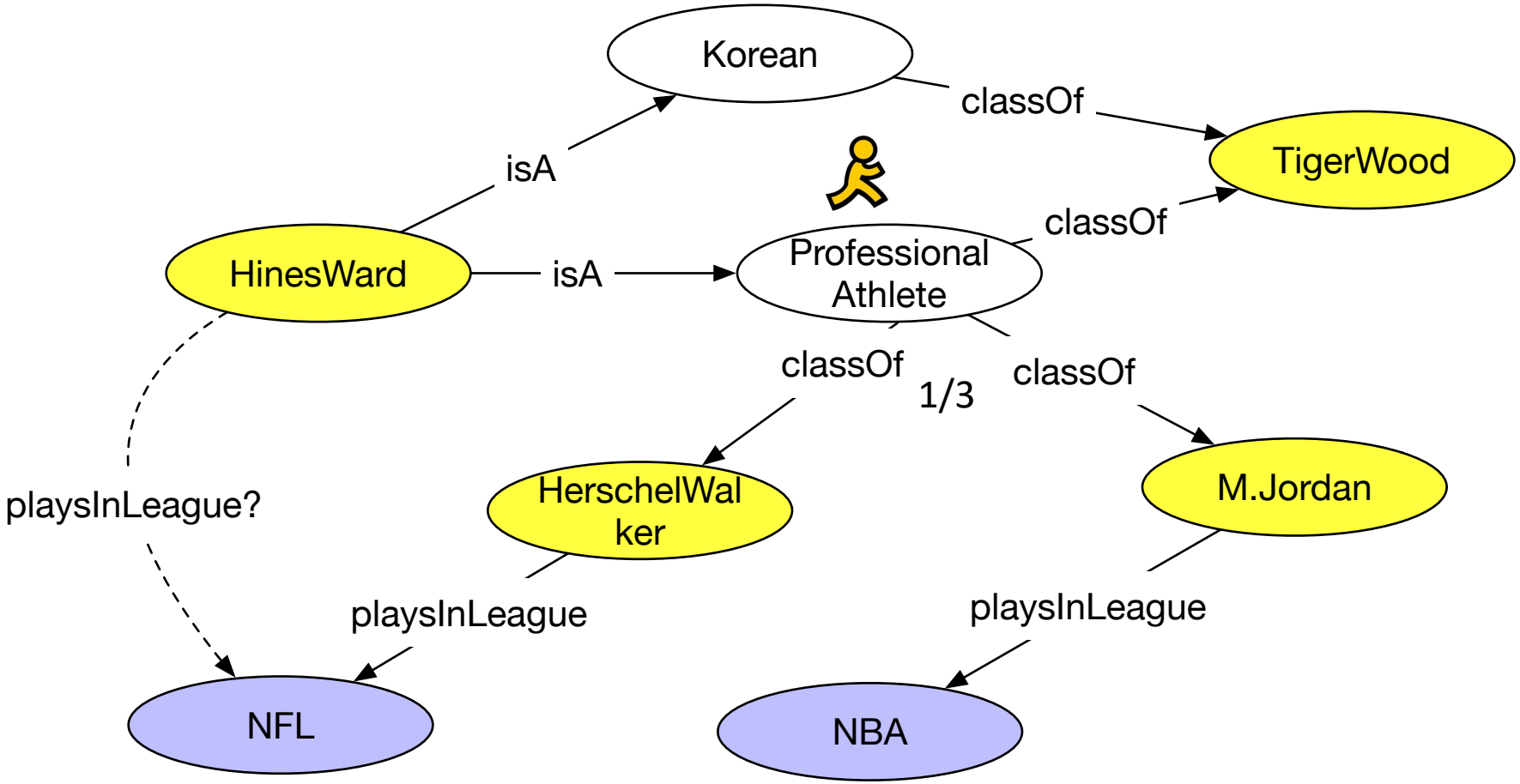

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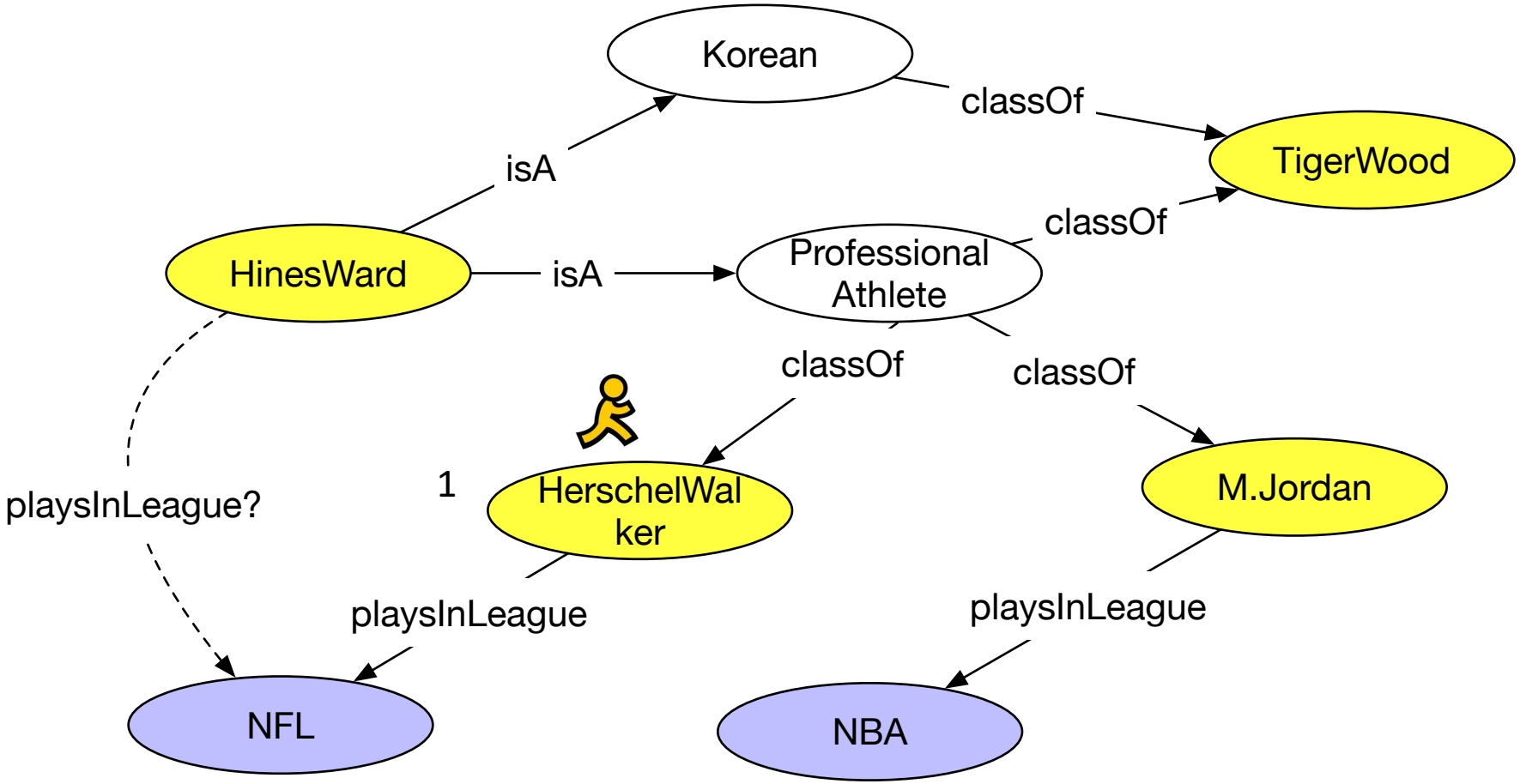

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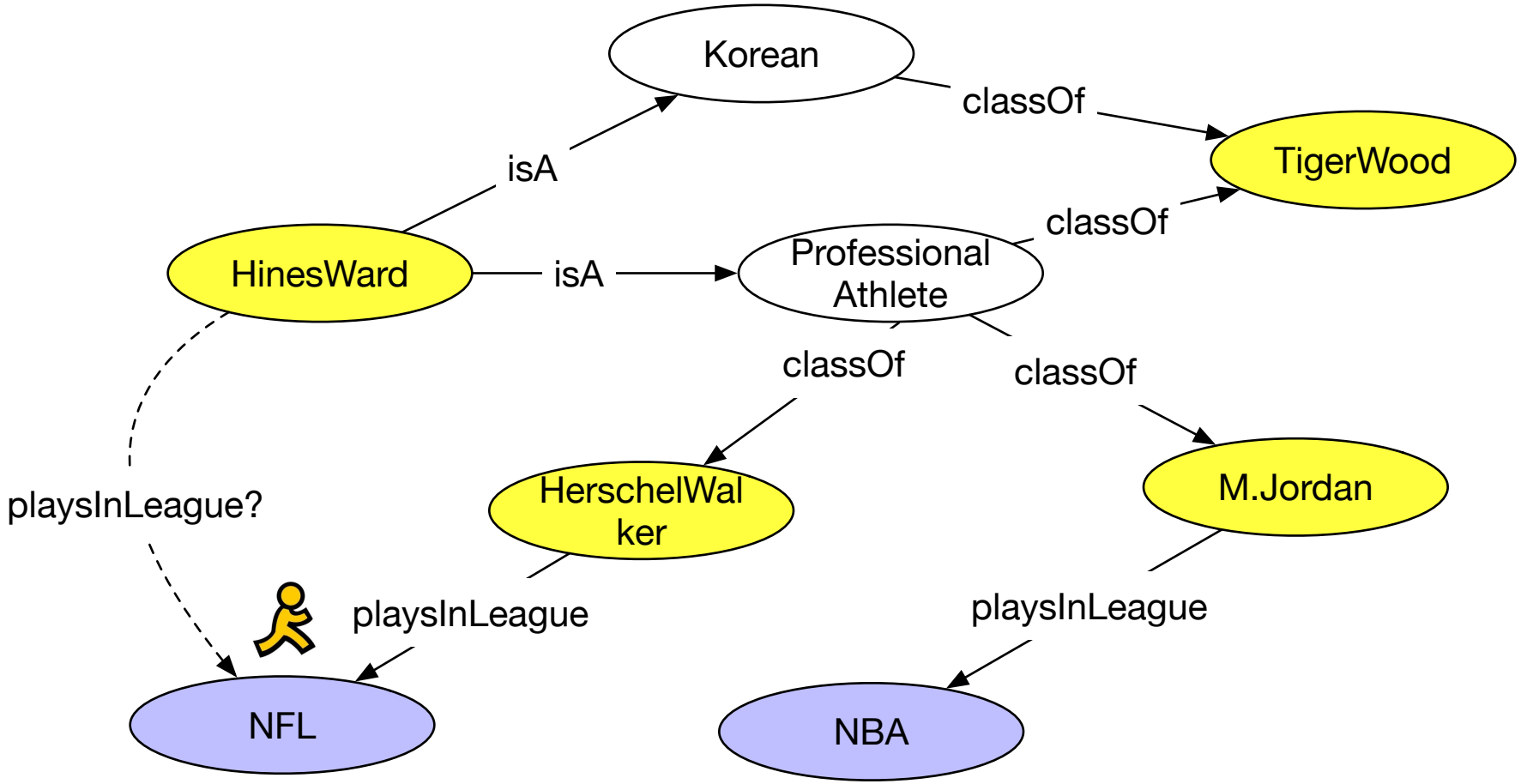

What's the probability that Hines Ward plays in NFL? 1/2 * 1/3

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Link Prediction with Random Walks

- Instead of doing random walks, we can constrain them following the links established by some rules we can mine from the graph

$$isA(x_1, c) \wedge classOf(c, x_2) \wedge playsInLeague(x_2, l) \rightarrow playsInLeague(x_1, l)$$

- We can group the rules by the predicate in the head (e.g. *playInLeague)*, and perform many random walks to estimate the probabilities with some training triples

Link Prediction with Random Walks

- Suppose we have *n* rules with *playsInLeague* has head. We can construct a feature vector of *n* elements and train a linear regression model with the objective function

$$score(e; s) = \sum_{P \in \boldsymbol{P}} h_{s,P}(e)\Theta_P$$ where $h_{s,P}(e)$represents the probability of reaching *e* from *s* following the path *p*

- The algorithm constructs one model per relation

Link Prediction with Random Walks

Evaluation

- Used NELL KG
- Relied on human assessment (5 humans, 75% agreement) on sample queries of the type R(x,?)
- If we look at the top-10 results, the method performs as good as a N-FOIL -- an inductive baseline
- If we move to the top-100 the results get significantly better

Link Prediction

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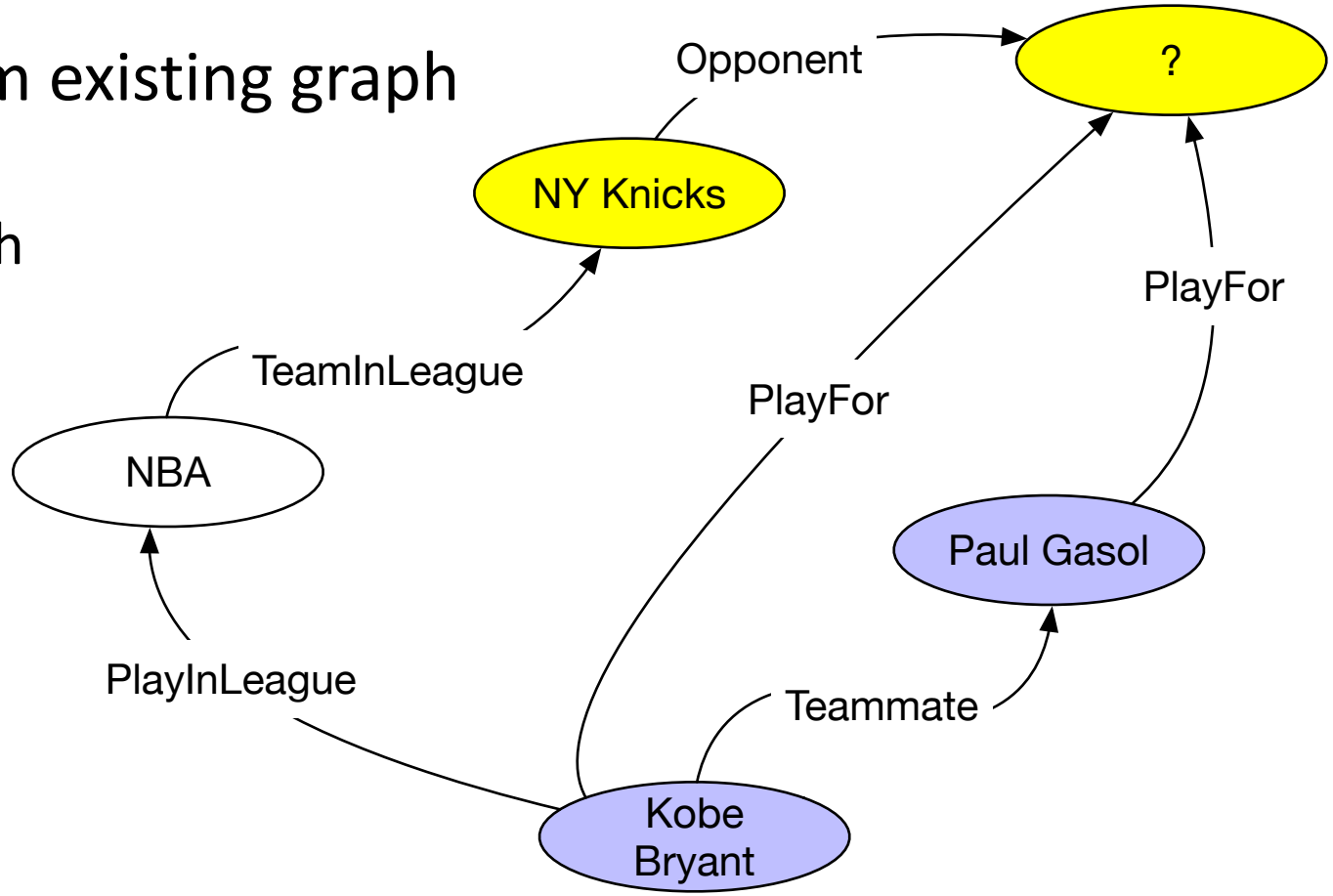
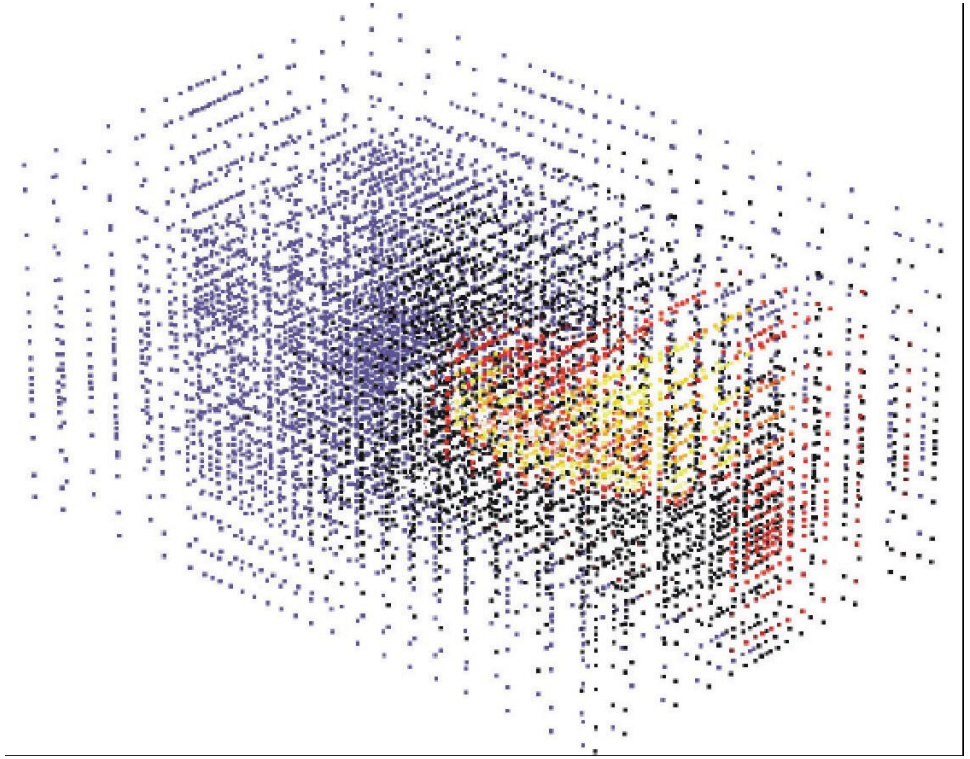


Link Prediction with Tensors

- **Definition:**
  - **1**-dimension array: vector
  - **2**-dimension array: matrix
  - **3 or more-dimensions** array: tensor

Multiple binary relations can be expressed naturally as a three-way tensor



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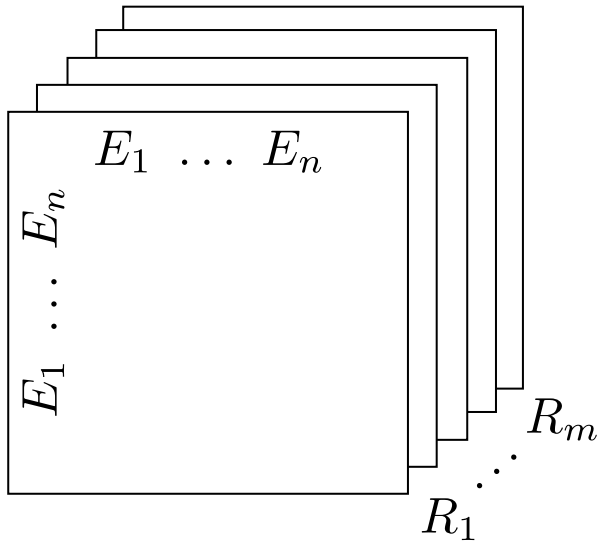
Link Prediction with Tensors

- Tensors are well-studied data structures in Machine Learning [1]
- Suppose our knowledge graph has *m* relations and *n* entities
- We can assign two *modes (=ways)* to the entities and one *mode* to the relations
- The entries of the tensor are 1 when a relation between two entities exists. Otherwise, the value is 0



- E.g. (2,3,1) = 1 if $R_1(e_2,e_3)$ exists in the KG

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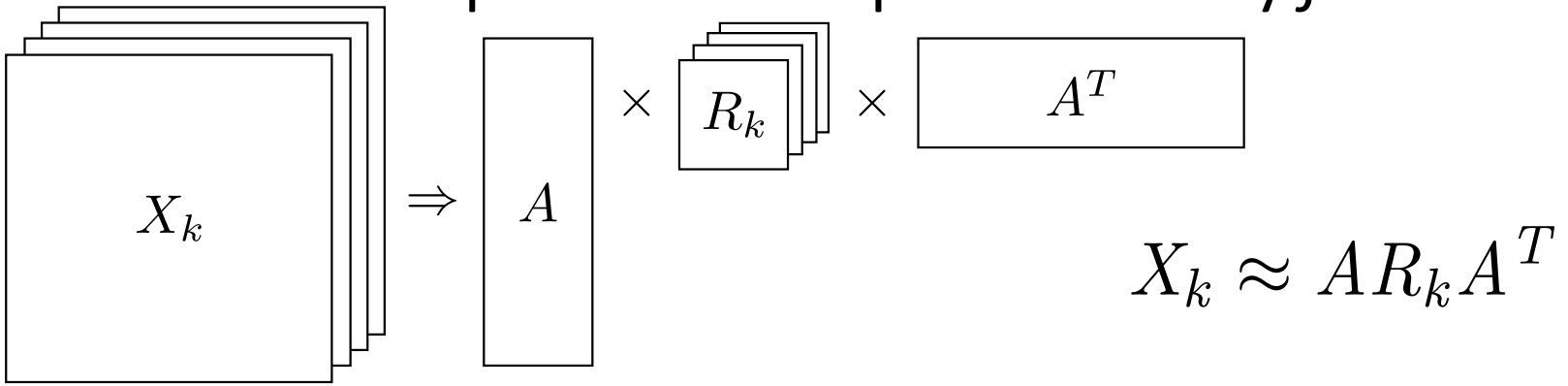
[1] T. Kolda and B. Bader, "Tensor Decompositions and Applications," *SIAM Rev.*, vol. 51, no. 3, pp. 455–500, Aug. 2009.

Link Prediction with Tensors

- **RESCAL [1]** is a method that performs link predictions by *factorizing* the tensor



$$X_k \approx A R_k A^T$$

- **Let** *n* be the number of entities and *r* the number of dimensions
- **A** is a *nxr* matrix that represents the *global* entity-latent-components
- $\mathbf{R_k}$ is a asymmetric *rxr* matrix that specifies the interaction of the latent components per predicate

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[1] M. Nickel, V. Tresp, and H.-P. Kriegel, "A Three-Way Model for Collective Learning on Multi-Relational Data," in *Proceedings of the 28th International Conference on Machine Learning (ICML-11)*, ACM, 2011, pp. 809–816.

Link Prediction with Tensors

The factorization is translated as an optimization problem

$$\min_{A,R_k} loss(A, R_k) + reg(A, R_k)$$

where *loss* is the loss function

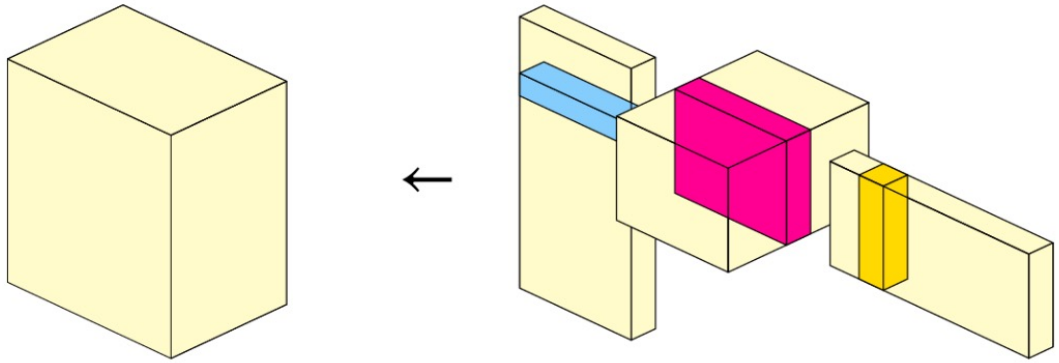
$$loss(A, R_k) = \frac{1}{2} \sum_k \|\mathcal{X}_k - A R_k A^T\|_F^2$$

and *reg* is the regularization function

$$reg(A, R_k) = \frac{1}{2} \lambda \left(\|A\|_F^2 + \sum_k \|R_k\|_F^2 \right)$$

The calculation is performed using the Alternating-least Square algorithm (ALS)

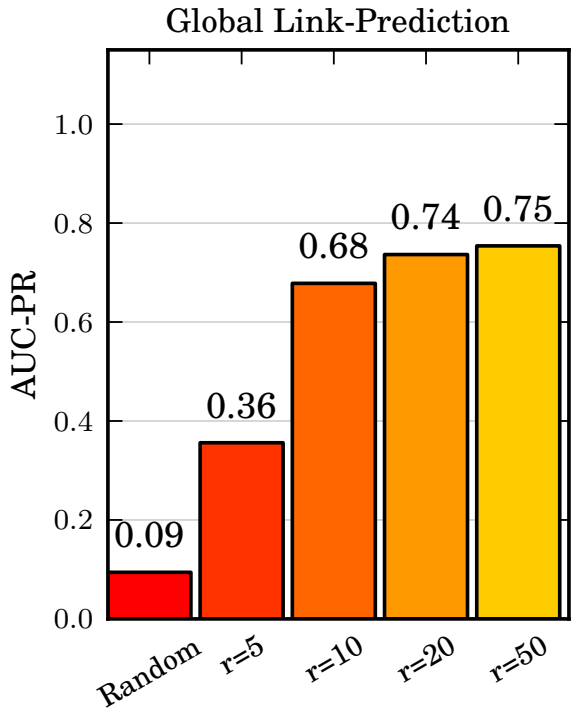
Link Prediction with Tensors



- **Basic procedure** of link prediction with RESCAL
  - **First,** we compute the "rank-reduced" factorization
  - **Second,** entries after reconstruction (i.e. $\hat{x}_{ijk} = \vec{a}_i^T R_k \vec{a}_j$) can be regarded as *confidence values* of the model that the corresponding triple exists

Factorizing YAGO

- As an experiment, the authors of [1] took a subset of YAGO of 2.6M entities and 64M facts
- Type of queries: p(?,o) over 38 relations



[1] M. Nickel, V. Tresp, and H.-P. Kriegel, “Factorizing YAGO: Scalable Machine Learning for Linked Data,” in *WWW*, 2012, pp. 271–280.

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Link Prediction with Tensors

- Collective learning is performed via the entities' latent-component representation
- **A** is an matrix that contains **embeddings** of the entities. We can use in a similar way as for word embeddings (word2vec)
- A major problem of RESCAL is that it has to learn a very large number of parameters (esp. R). Not so cheap to compute

Link Prediction

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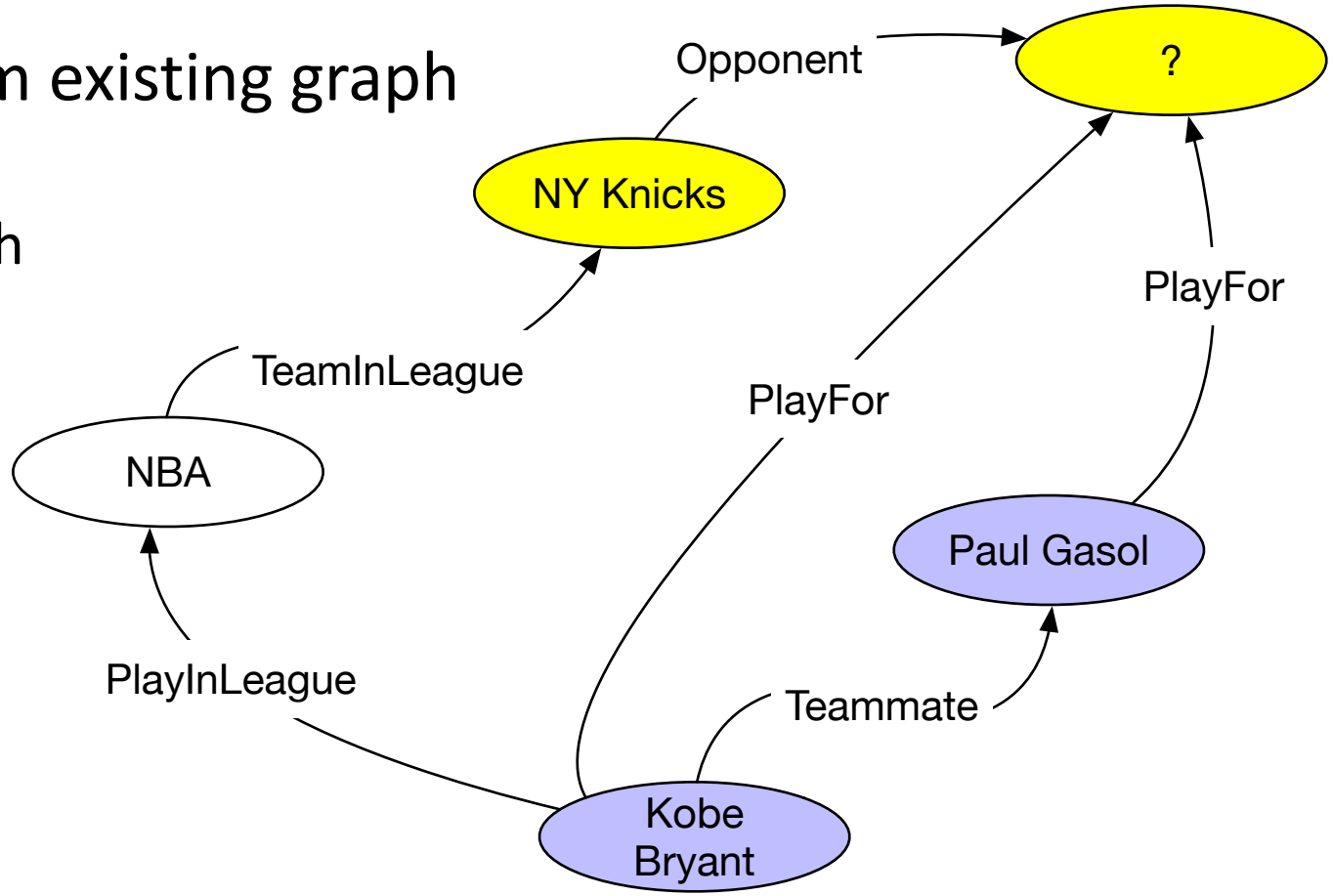

Latent-features model

- *RESCAL* is a latent-features model. Predictions are conditionally independent w.r.t. a given set of global latent features [1]
- Number of parameters in the RESCAL model = $rd^2 + nd$ where *d* = # dimensions, *n* = # entities, *r* = # relations
- Can we lower the number of parameters?

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[1] M. Nickel, K. Murphy, V. Tresp, and E. Gabrilovich, "A Review of Relational Machine Learning for Knowledge Graphs," *arXiv:1503.00759* 2015

Latent distance models

- Latent distance models are a subclass of latent feature models where the likelihood of links depends on the distance between the latent representation of the entities
- Consider one relation (e.g. *friendsOf*) and two entities (e.g. Mark and John)
  - $friendsOf(Mark, John) = d(\boldsymbol{e}_{mark}, \boldsymbol{e}_{john})$ where *d* is a arbitrary distance measure (e.g. Euclidean distance) [1]
- See the connection with word2vec?

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[1] P. D. Hoff, A. E. Raftery, and M. S. Handcock, "Latent space approaches to social network analysis," *Journal of the american Statistical association*, vol. 97, no. 460, pp. 1090–1098, 2002.

TransE

- **TransE** [1] is a latent distance model with less parameters than RESCAL
- Every entity and relation get a vector of *d* elements.
- The distance in TransE is: $d(\boldsymbol{e}_i + \boldsymbol{r}_k, \boldsymbol{e}_j)$ which reads as: "given an entity and a relation, what is the closest vertex to their sum?
- The model has $rd + nd$ parameters, much less than RESCAL

[1] A. Bordes, N. Usunier, A. Garcia-Duran, J. Weston, and O. Yakhnenko, "Translating Embeddings for Modeling Multi-relational Data," in *NIPS* 2013.

TransE

Overview training

1. Create a vector of *d* elements for each entity $e \in E$ and $r \in R$
2. Take as input a set of triples $(h, l, t) \in S$ (*S* is our knowledge graph)
3. Minimize the function with stochastic gradient descent)

$$\mathcal{L} = \sum_{(h,\ell,t)\in S} \sum_{(h',\ell,t')\in S'_{(h,\ell,t)}} \left[\gamma + d(\boldsymbol{h}+\boldsymbol{\ell},\boldsymbol{t}) - d(\boldsymbol{h'}+\boldsymbol{\ell},\boldsymbol{t'})\right]_+$$

where

$$S'_{(h,\ell,t)} = \left\{(h',\ell,t)|h' \in E\right\} \cup \left\{(h,\ell,t')|t' \in E\right\}$$

TransE

Overview testing

1. Given an "unseen" triple $(h, l, t) \in S'$, we calculate $d(\boldsymbol{h} + \boldsymbol{l}, \boldsymbol{e}_v) for\ \ all\ \forall v \in E$ and rank the results
2. Then, we check the average position of *t* (mean rank) or whether *t* occurs in the top *k* positions (hits@k).
3. We can look at the position of t w.r.t. all other entities (*raw position)* or remove all the "answers" that are already explicit in the KB (*filtered position*)

TransE

- **Evaluation**

Dataset	WN				FB15k				FB1M	
Metric	Mean Rank		Hits@10 (%)		Mean Rank		Hits@10 (%)		Mean Rank	Hits@10 (%)
Eval. setting	*Raw*	*Filt.*	*Raw*	*Filt.*	*Raw*	*Filt.*	*Raw*	*Filt.*	*Raw*	*Raw*
Unstructured [2]	315	304	35.3	38.2	1,074	979	4.5	6.3	15,139	2.9
RESCAL [11]	1,180	1,163	37.2	52.8	828	683	28.4	44.1	-	-
SE [3]	1,011	985	68.5	80.5	273	162	28.8	39.8	22,044	17.5
SME(linear) [2]	545	533	65.1	74.1	274	154	30.7	40.8	-	-
SME(bilinear) [2]	526	509	54.7	61.3	284	158	31.3	41.3	-	-
LFM [6]	469	456	71.4	81.6	283	164	26.0	33.1	-	-
TransE	**263**	**251**	**75.4**	**89.2**	**243**	**125**	**34.9**	**47.1**	**14,615**	**34.0**

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TransE

Open problems: Negation

- In TransE, we create random triples to use as evidence
- However, the OWA does not allow to make such assumption
- Some approaches proposed to leverage the schema to create negative examples:
  - *Functional properties* => if <a> <bornIn> <b>, then <a> <bornIn> <c> where b!=c is surely false
  - Class hierarchies => if <p> has a range C, then we can pick an instance of a class D!=C to construct negative samples
- These approaches introduce biases and do not work well because some classes are too popular and will get only few negative examples

TransE

Open problems: Data sparsity

- Some relations appear only a few times to be properly trained.
- This is an open problem. There is not yet an effective solution for that.

TransE

Open problems: Lack of established evaluation methodology

- There is not a single metric that can be representative for the overall performance of the method
- Datasets are too different from each others. TransE returns very different results depending on the used KG
  - Freebase 74% (hit@10)
  - Wordnet 94%
  - YAGO 22%
- The latest research is focusing on trying to replicate reasoning (logical rules) using these models!

TransE

Open problems: Scalability

- Hogwild! [1] is a well-know technique to parallelize the learning of *sparse* models

Algorithm 1 HOGWILD! update for individual processors

1: **loop**
2: Sample e uniformly at random from E
3: Read current state x_e and evaluate $G_e(x_e)$
4: **for** $v \in e$ **do** $x_v \leftarrow x_v - \gamma G_{ev}(x_e)$
5: **end loop**

E: training set
x_e: parameters that relate to *e*
G: gradient of the loss function on *e*

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[1] B. Recht, C. Re, S. Wright, and F. Niu, "Hogwild: A lock-free approach to parallelizing stochastic gradient descent," in *Advances in Neural Information Processing Systems*, 2011, pp. 693–701.

TransE

Open problems: Scalability

- Hogwild! [1] is a well-know technique to parallelize the learning of *sparse* models.
- It can be trivially expanded to an arbitrary number of threads. It works only if the problem is *sparse*
- Are KG embeddings an example of a sparse problem? Preliminary evaluation indicate it is