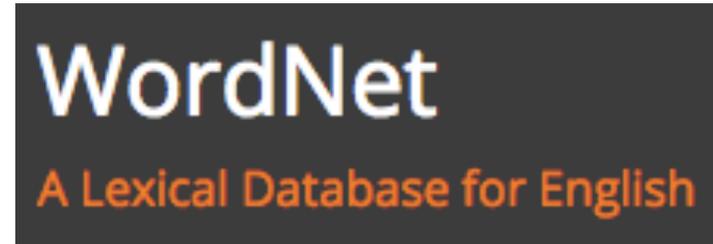


# **Multi-Hop Knowledge Graph Reasoning with Deep Reinforcement Learning**

**Richard Socher**

**Work by Victoria Lin et al.**

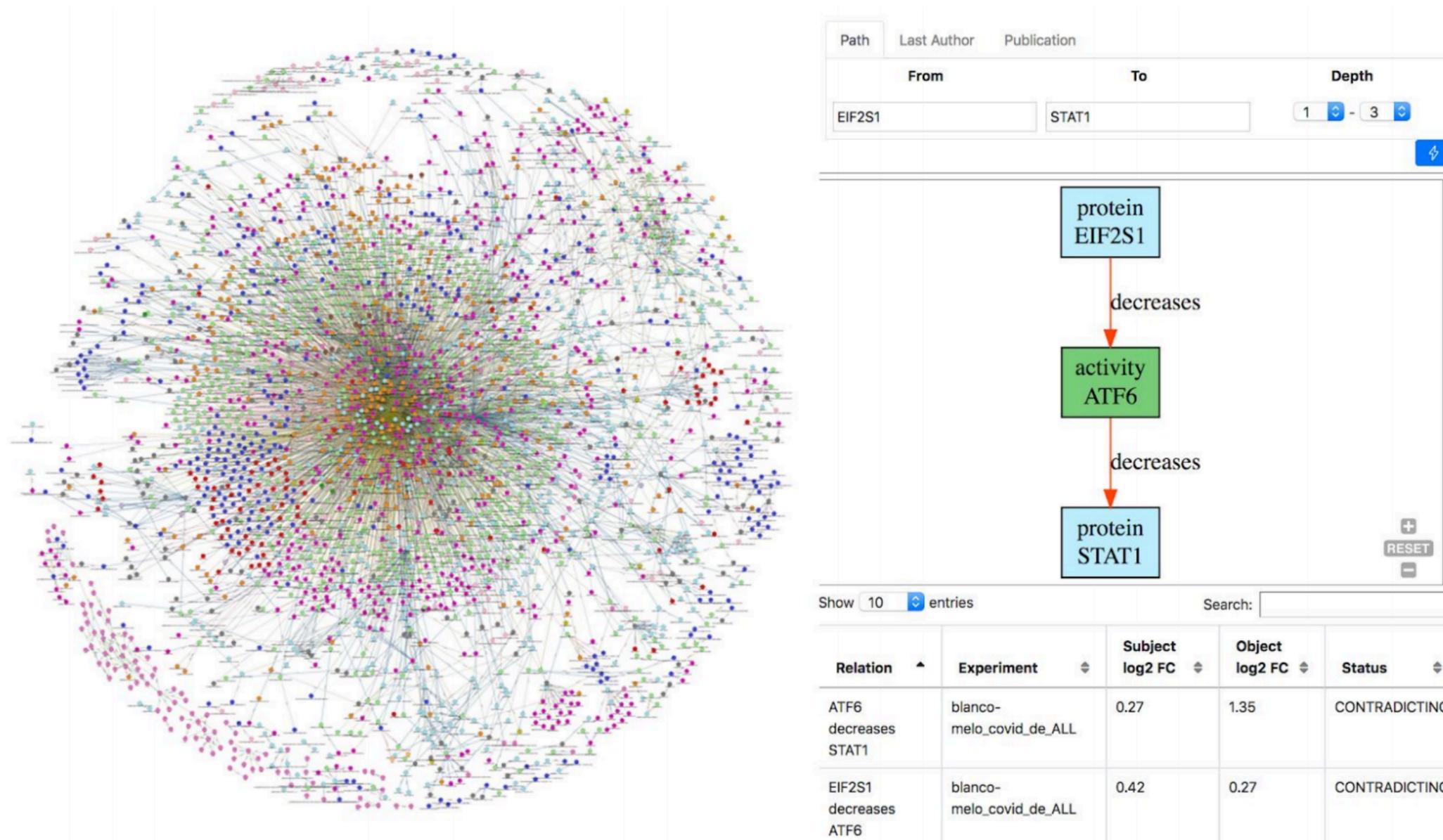
# Real-world Knowledge Graphs



Alibaba.com™



# Real-world Knowledge Graphs



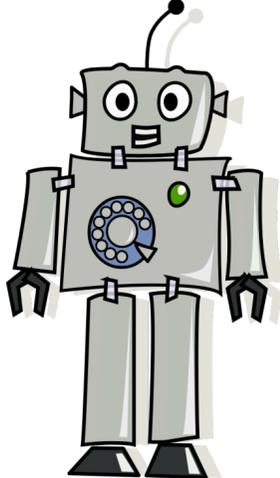
COVID-19 Knowledge Graph: a computable, multi-modal, cause-and-effect knowledge model of COVID-19 pathophysiology. (Domingo-Fernandez et. al. 2020)

# Chatbot

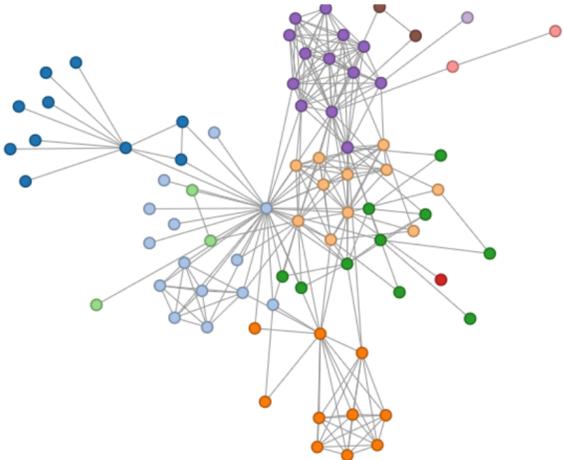
Text



Images



Knowledge Graph



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User

Which directors has Tom Hanks collaborated with?

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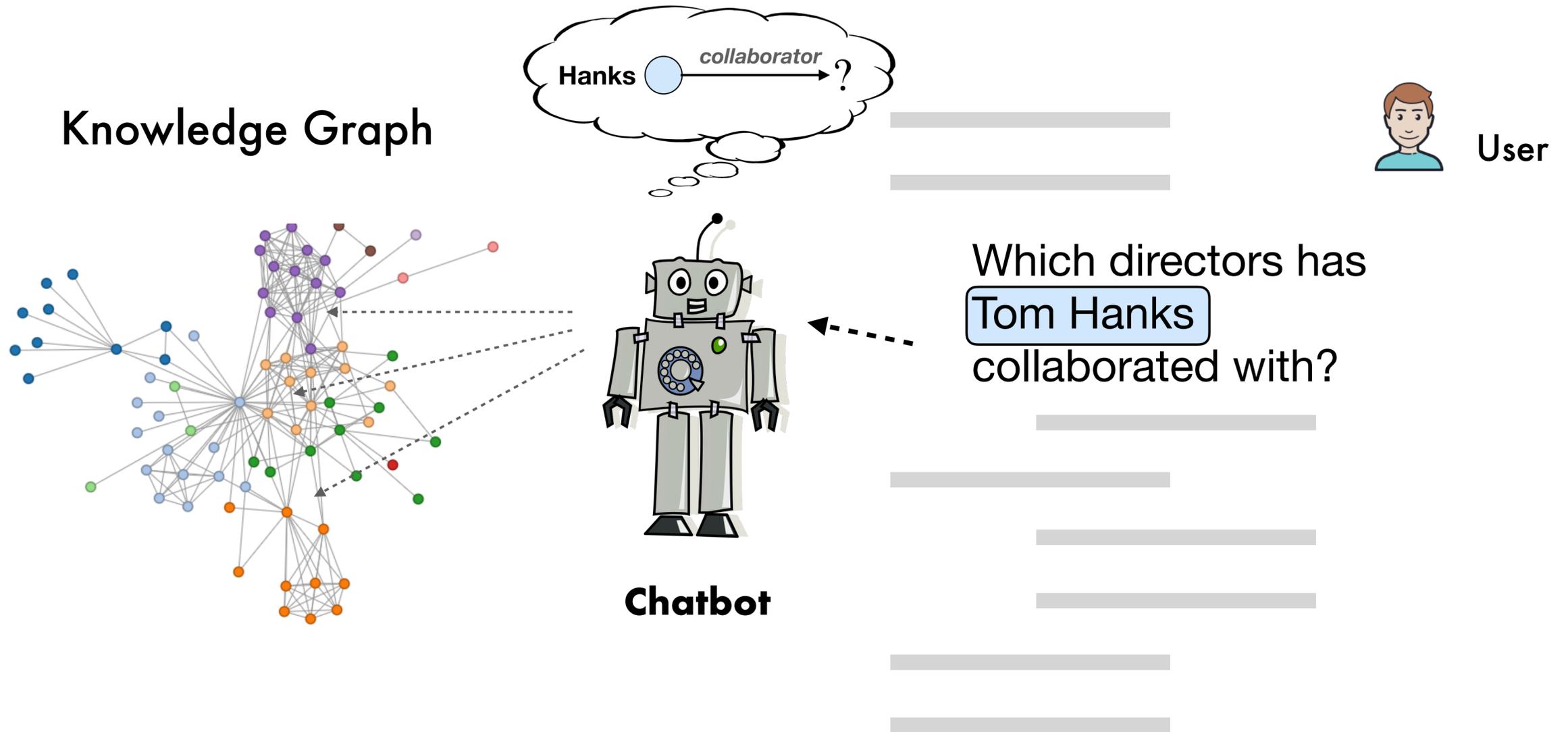
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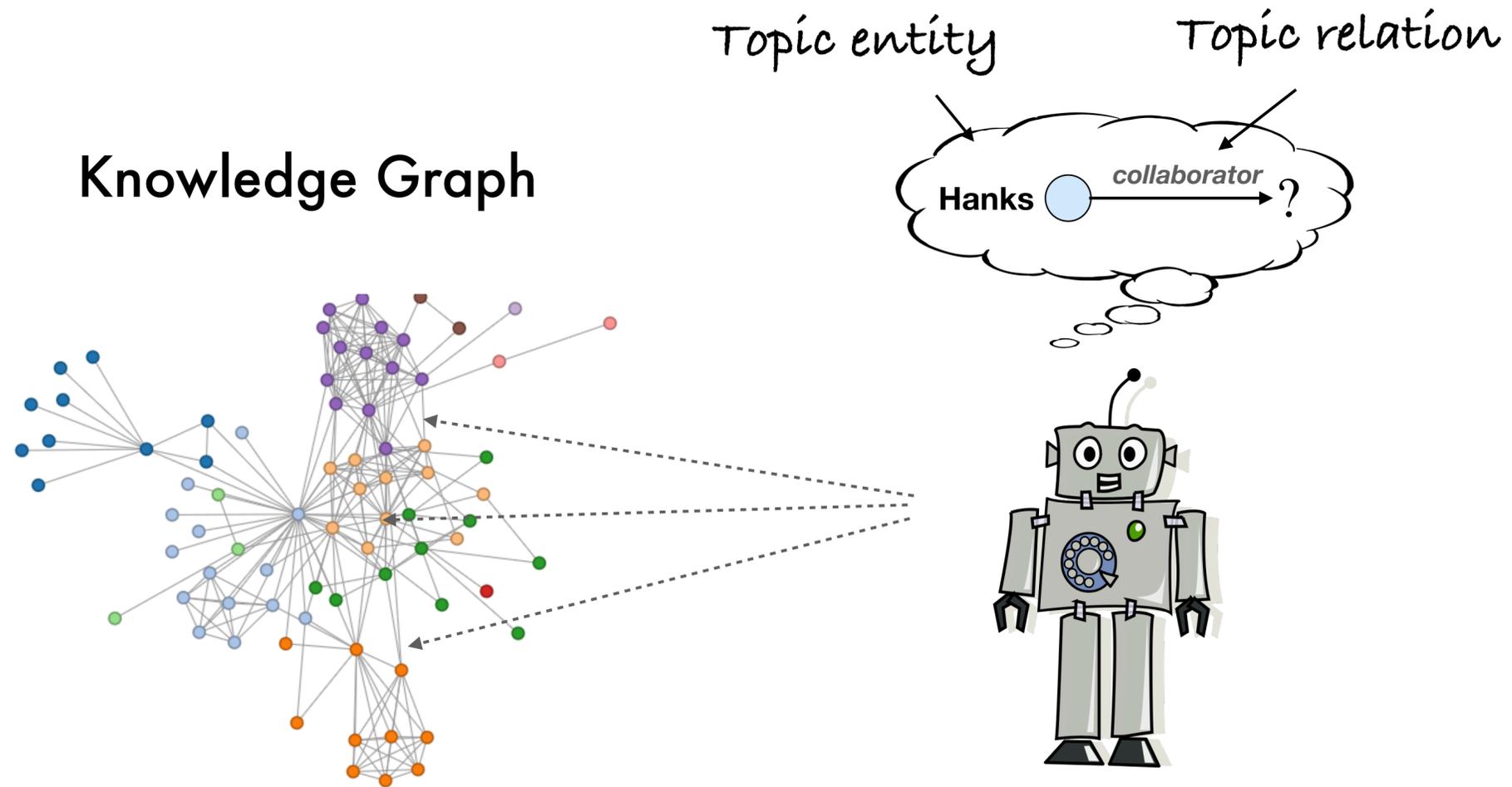
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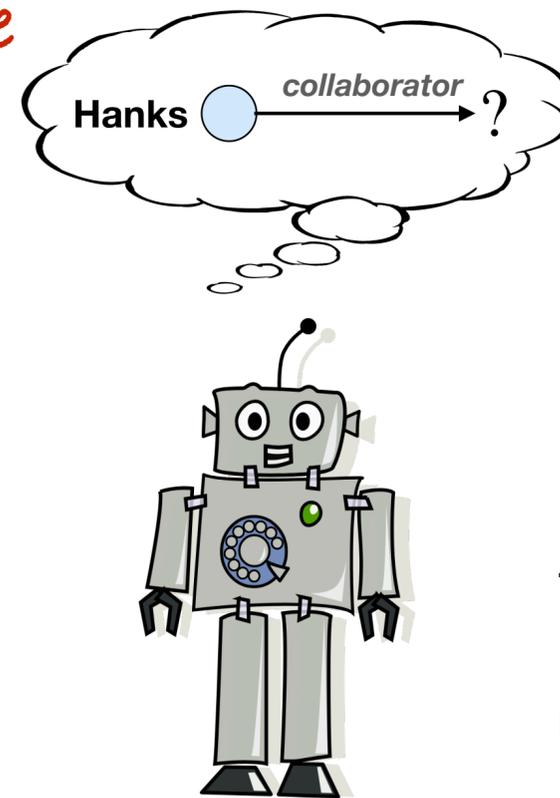
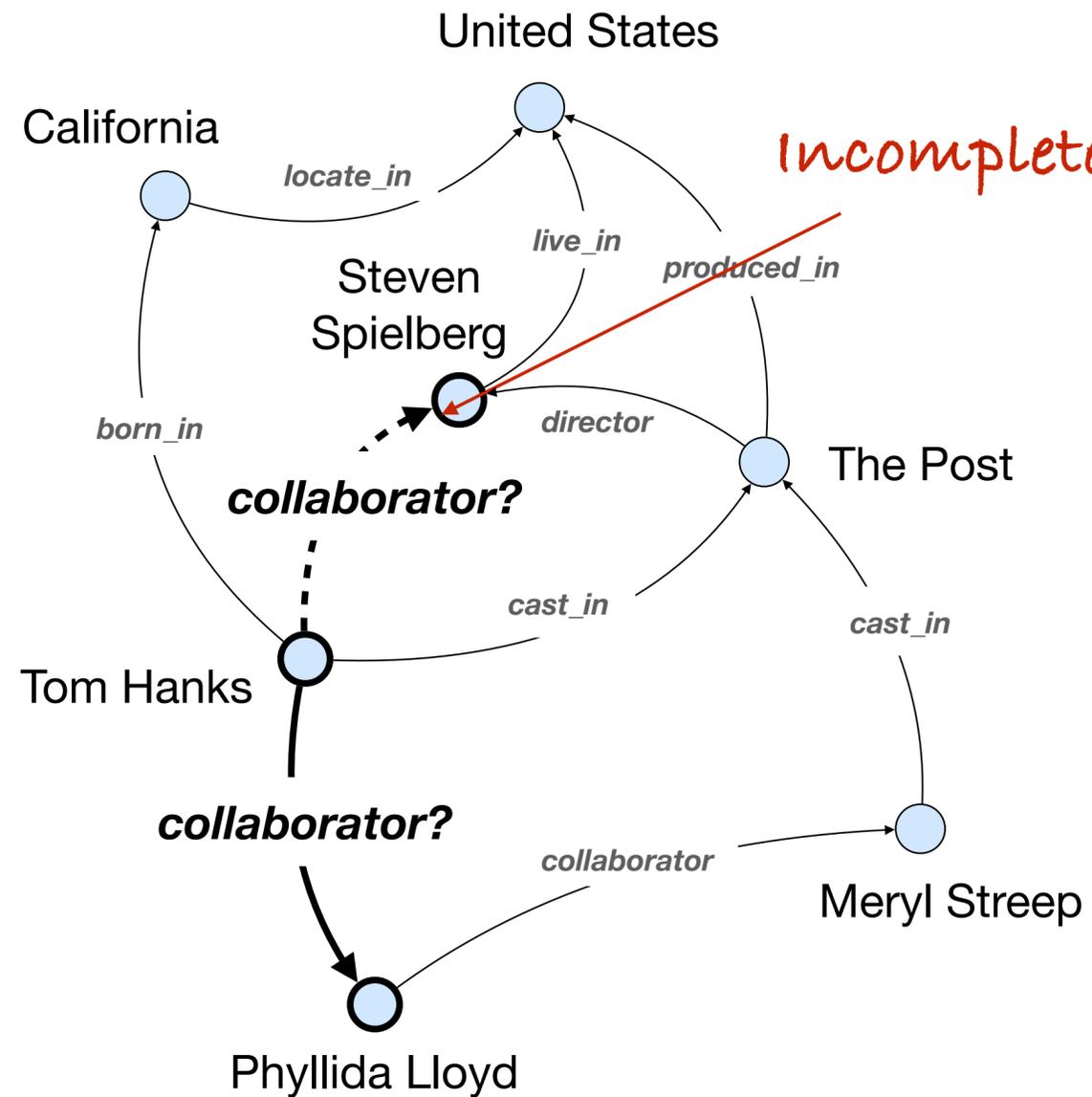
# Querying a Knowledge Graph



# Reason over Discrete Entities

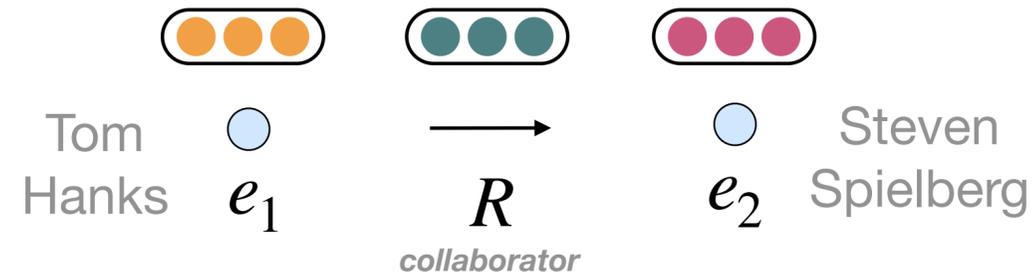


# Reason over Discrete Entities



The answer "Steven Spielberg" cannot be directly retrieved from the KG

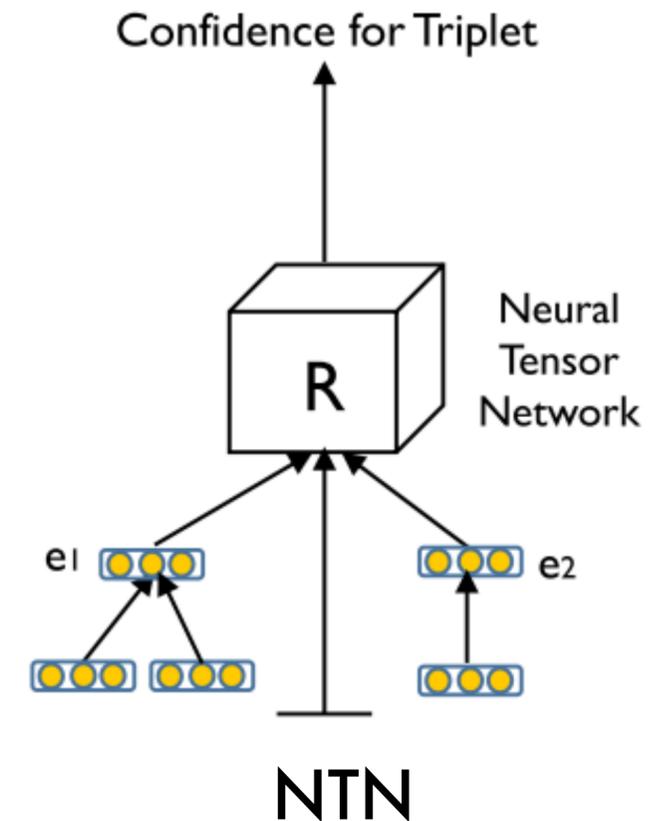
# Knowledge Graph Embeddings



Highly accurate & Efficient

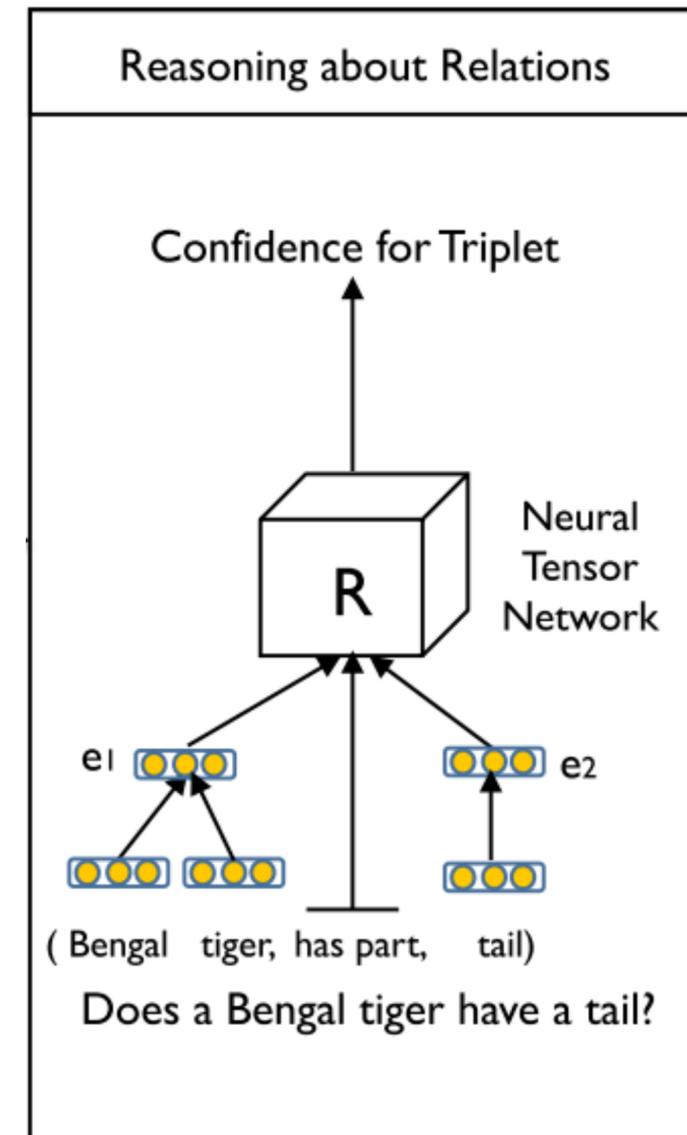
	Acc
WordNet	86.2
Freebase	90.0

Tab 1. NTN KB fact inference performance on the WordNet and Freebase benchmarks (Socher et. al. 2013)

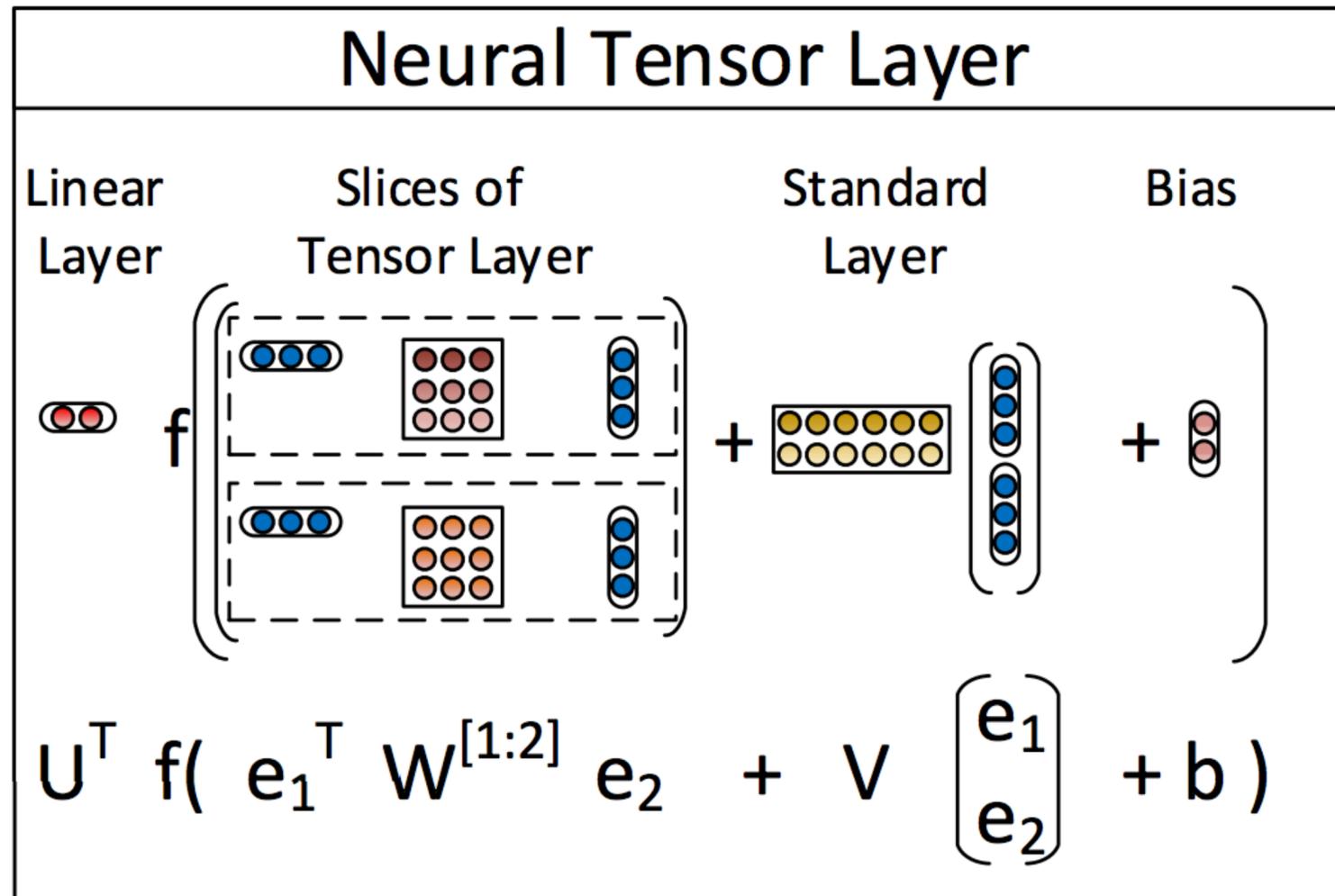


# Neural Tensor Network

Contribution 1: Neural Tensor Networks (NTNs) for relation classification

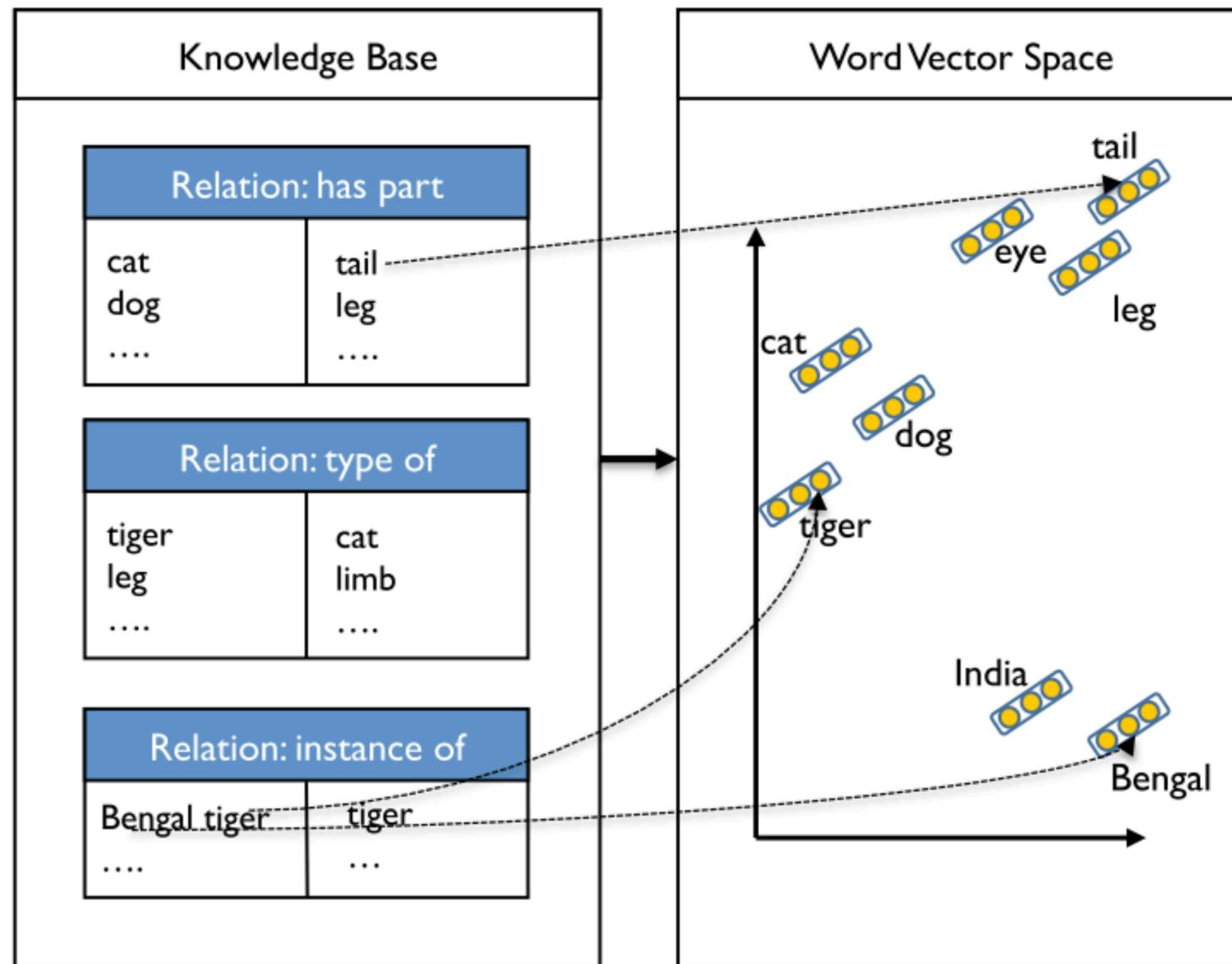


# Neural Tensor Network



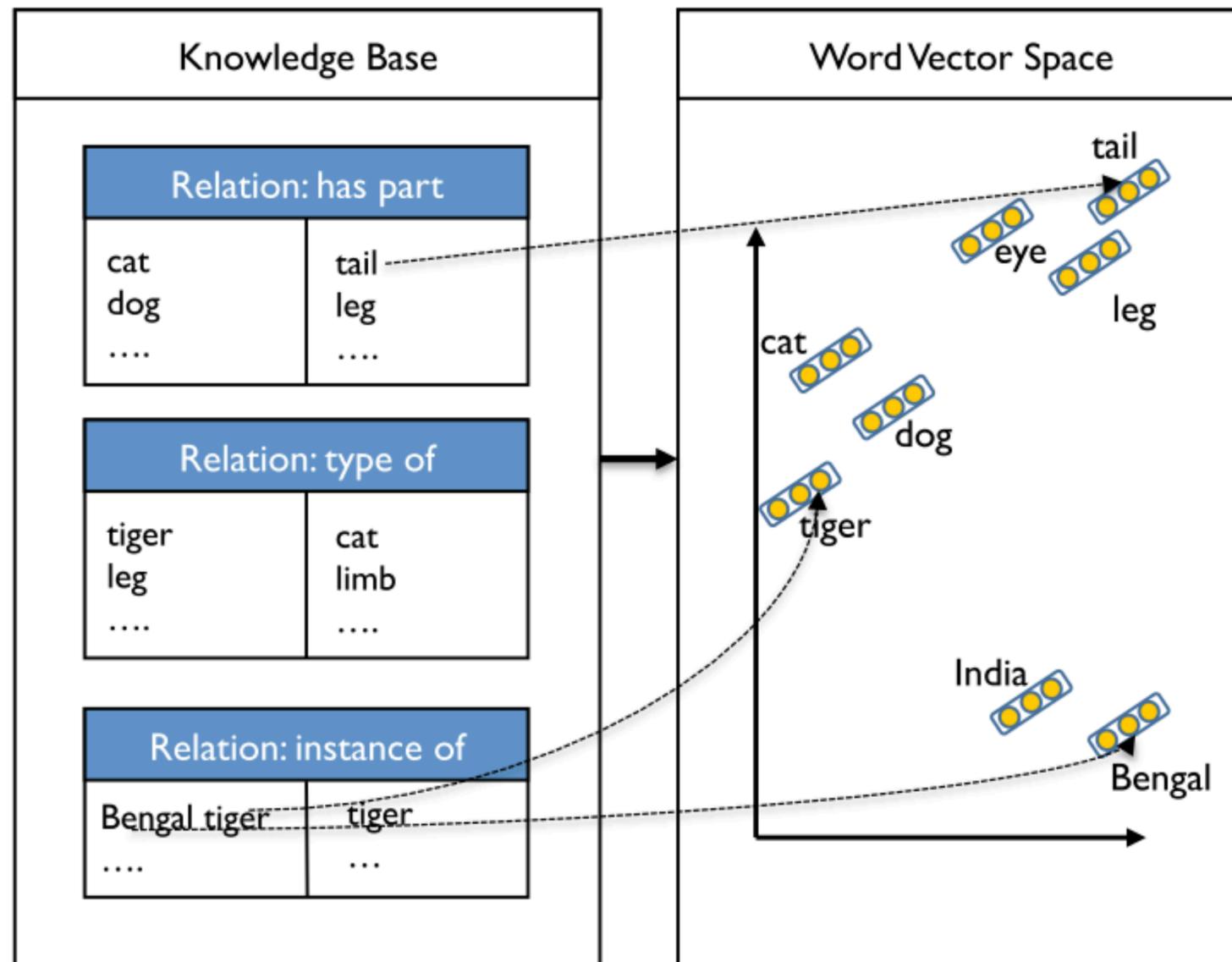
$$g(e_1, R, e_2) = u_R^T f \left( e_1^T W_R^{[1:k]} e_2 + V_R \begin{bmatrix} e_1 \\ e_2 \end{bmatrix} + b_R \right)$$

# Neural Tensor Network



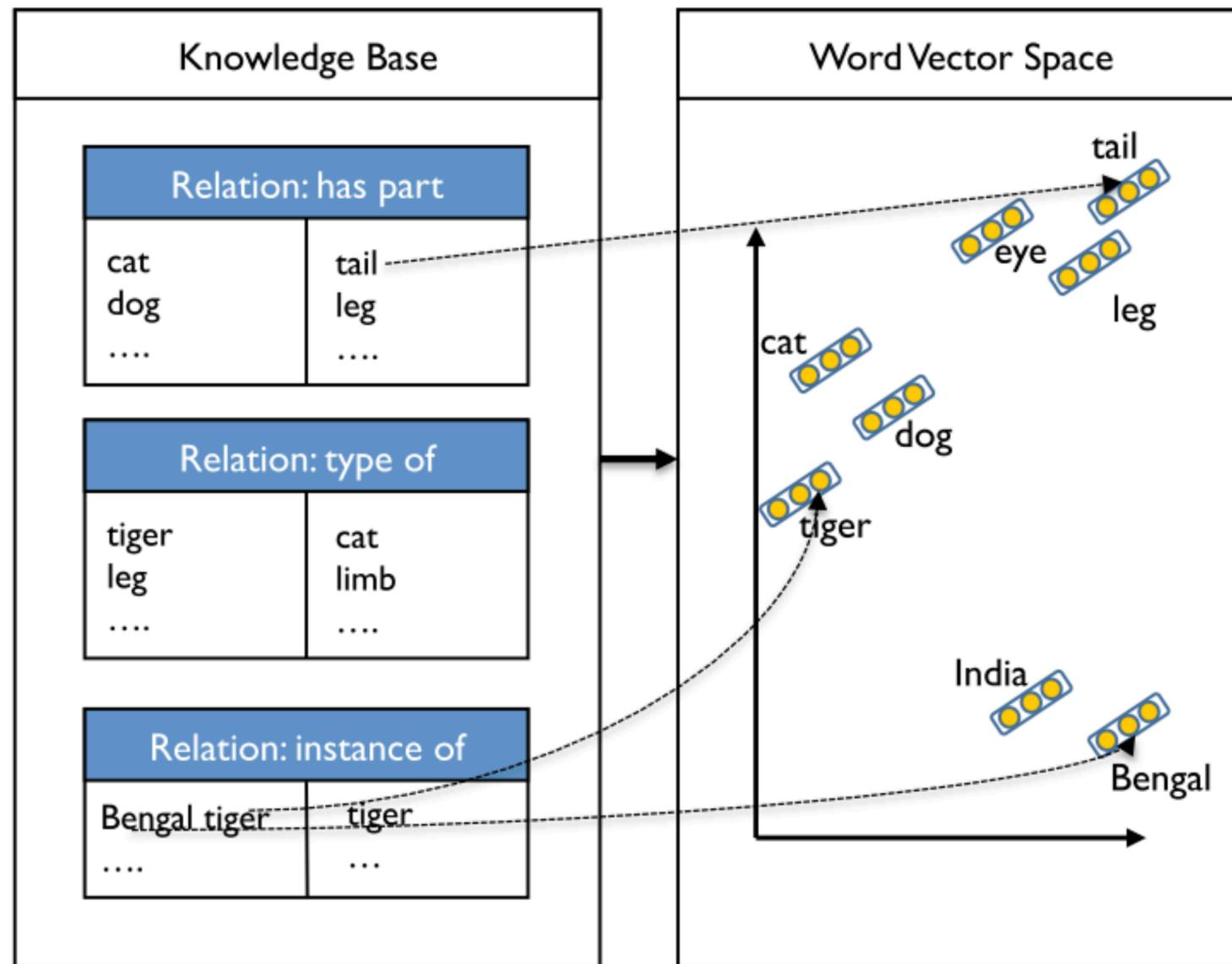
**Contribution 2: Compositional Representation of Knowledge Base Entities**

# Neural Tensor Network



$$v_{\text{Bengal tiger}} = 0.5(v_{\text{Bengal}} + v_{\text{tiger}})$$

# Neural Tensor Network



**Contribution 3: Initialize entity word vectors using those pre-trained on large unlabeled text**

# Neural Tensor Network

## Training Objective

# training triples

# randomly sampled corrupted triples

$\Omega = \mathbf{u}, \mathbf{W}, \mathbf{V}, \mathbf{b}, \mathbf{E}$

$$J(\Omega) = \sum_{i=1}^N \sum_{c=1}^C \max \left( 0, 1 - g \left( T^{(i)} \right) + g \left( T_c^{(i)} \right) \right) + \lambda \|\Omega\|_2^2$$

Correct triple

Corrupted triple

$$T_c^{(i)} = (e_1^{(i)}, R^{(i)}, e_c)$$

# Neural Tensor Network

## Experiments

Dataset	#R.	# Ent.	# Train	# Dev	# Test
Wordnet	11	38,696	112,581	2,609	10,544
Freebase	13	75,043	316,232	5,908	23,733

Model	WordNet	Freebase	Avg.
Distance Model	68.3	61.0	64.7
Hadamard Model	80.0	68.8	74.4
Single Layer Model	76.0	85.3	80.7
Bilinear Model	84.1	87.7	85.9
Neural Tensor Network	<b>86.2</b>	<b>90.0</b>	<b>88.1</b>

# Neural Tensor Network

## Experiments

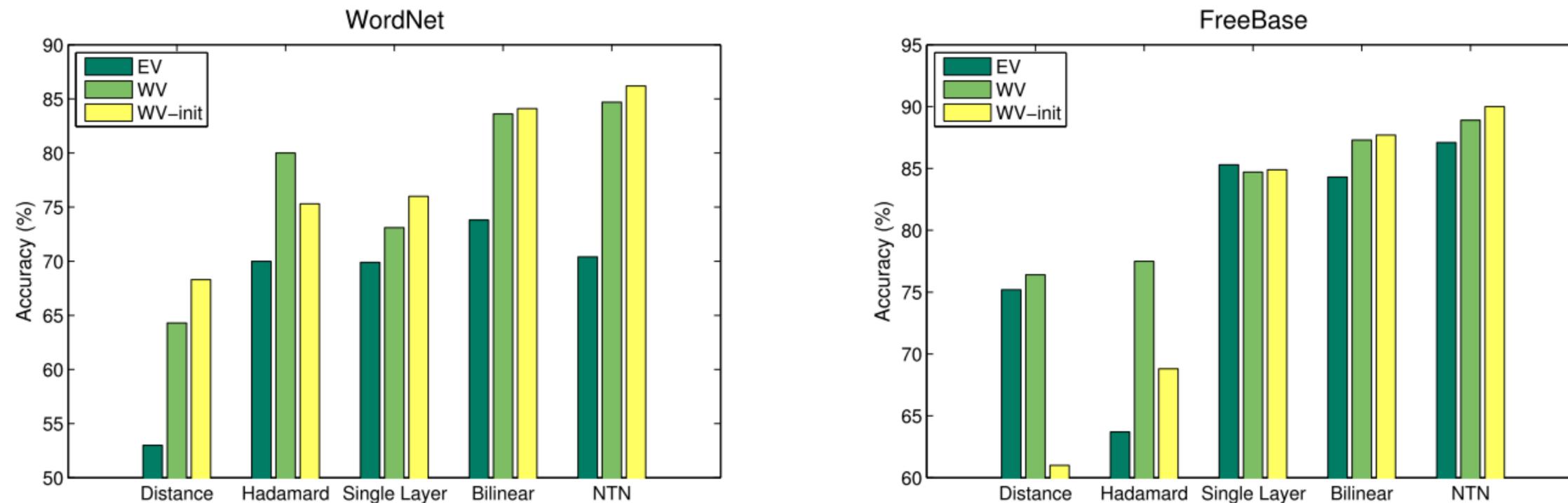
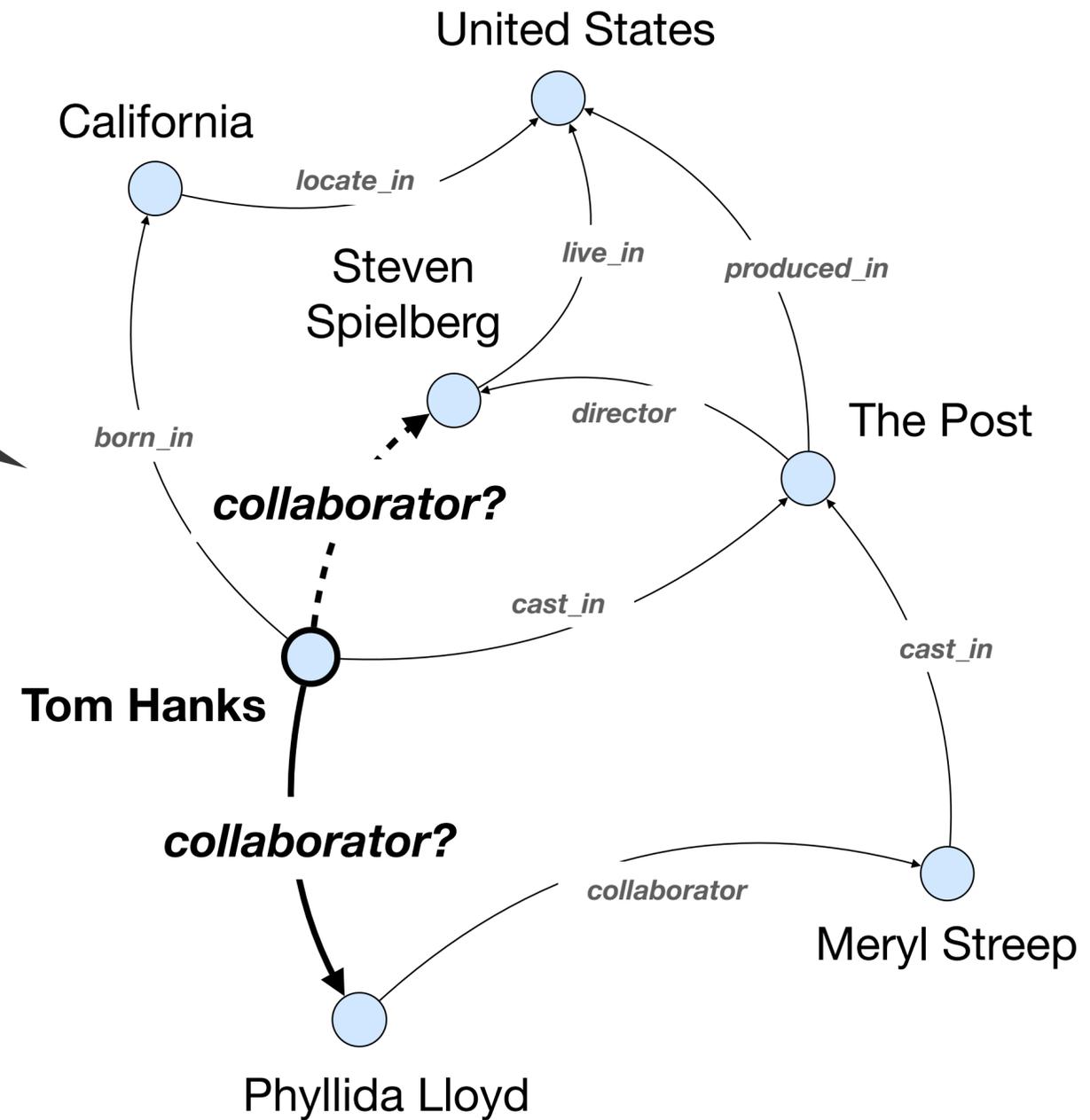


Figure 4: Influence of entity representations. **EV**: entity vectors. **WV**: randomly initialized word vectors. **WV-init**: word vectors initialized with unsupervised semantic word vectors.

# Multi-Hop Reasoning Models

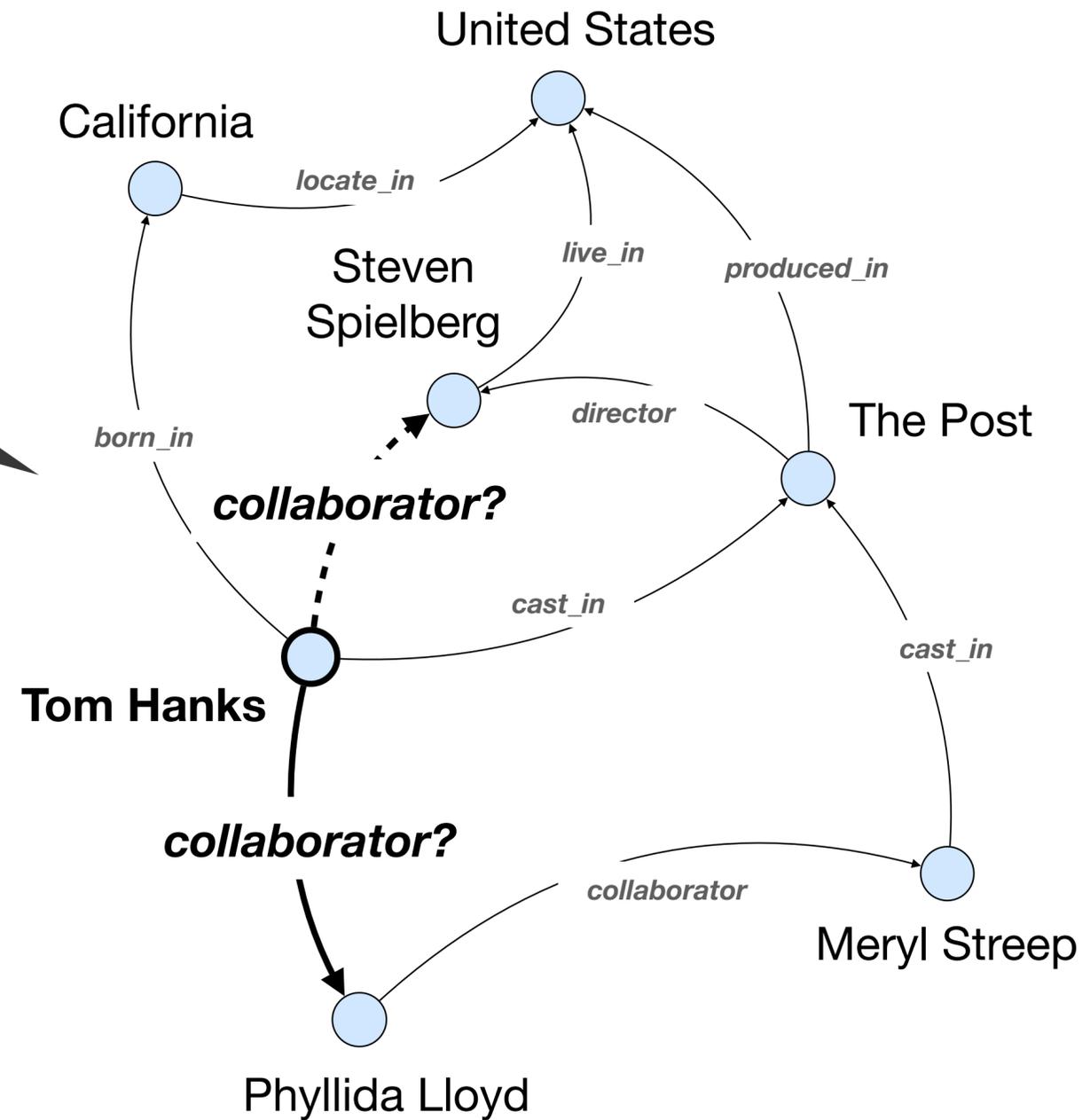
Reasoning over discrete structures



Which directors has Tom Hanks collaborated with?

# Multi-Hop Reasoning Models

Sequential decision making

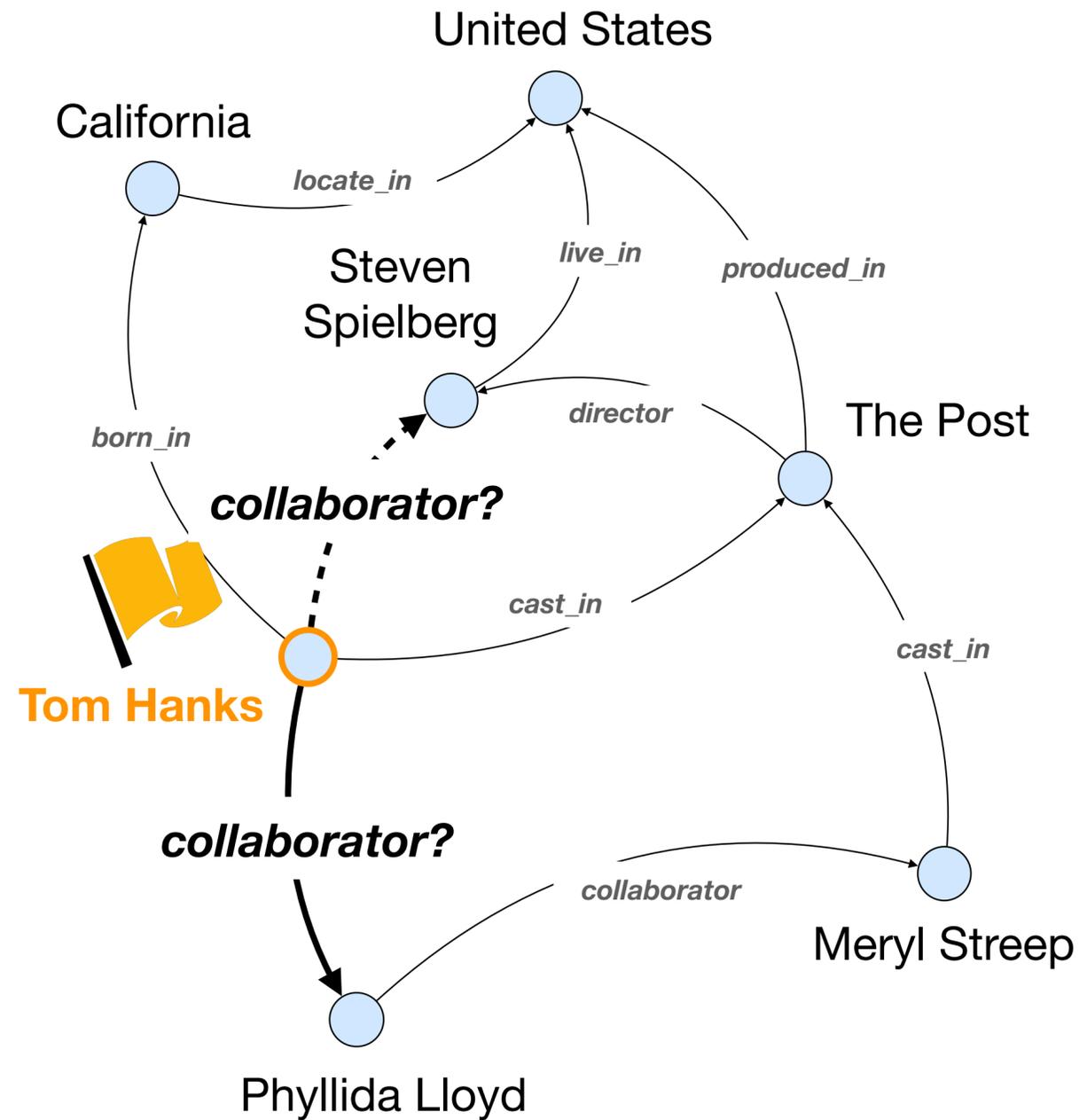


Which directors has Tom Hanks collaborated with?

# Multi-Hop Reasoning Models

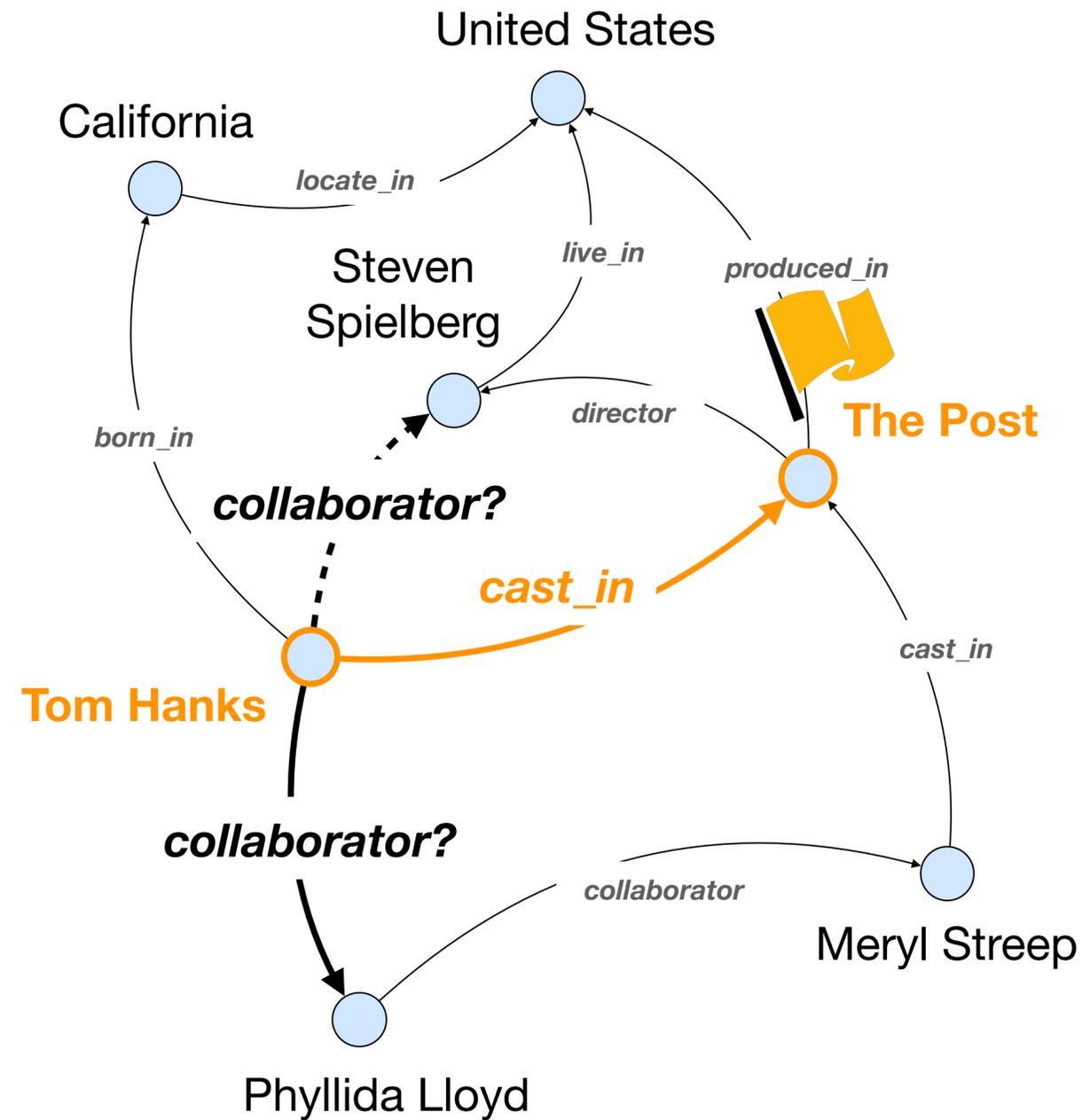
- Tom Hanks

Topic entity



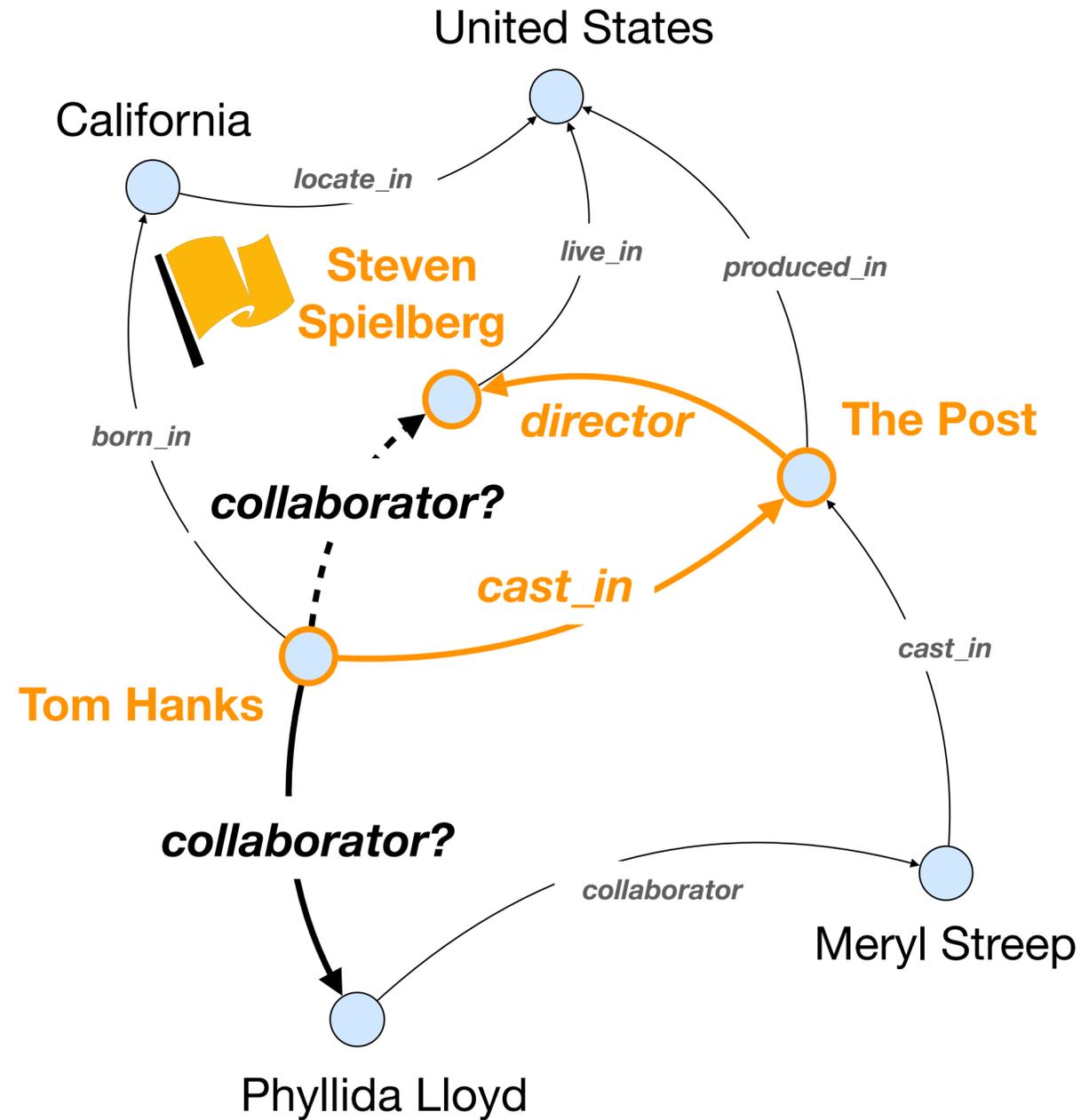
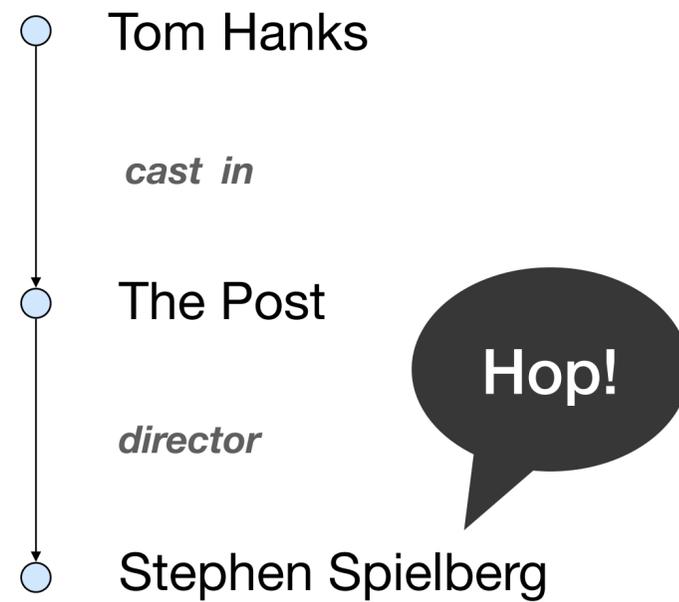
Which directors has Tom Hanks collaborated with?

# Multi-Hop Reasoning Models



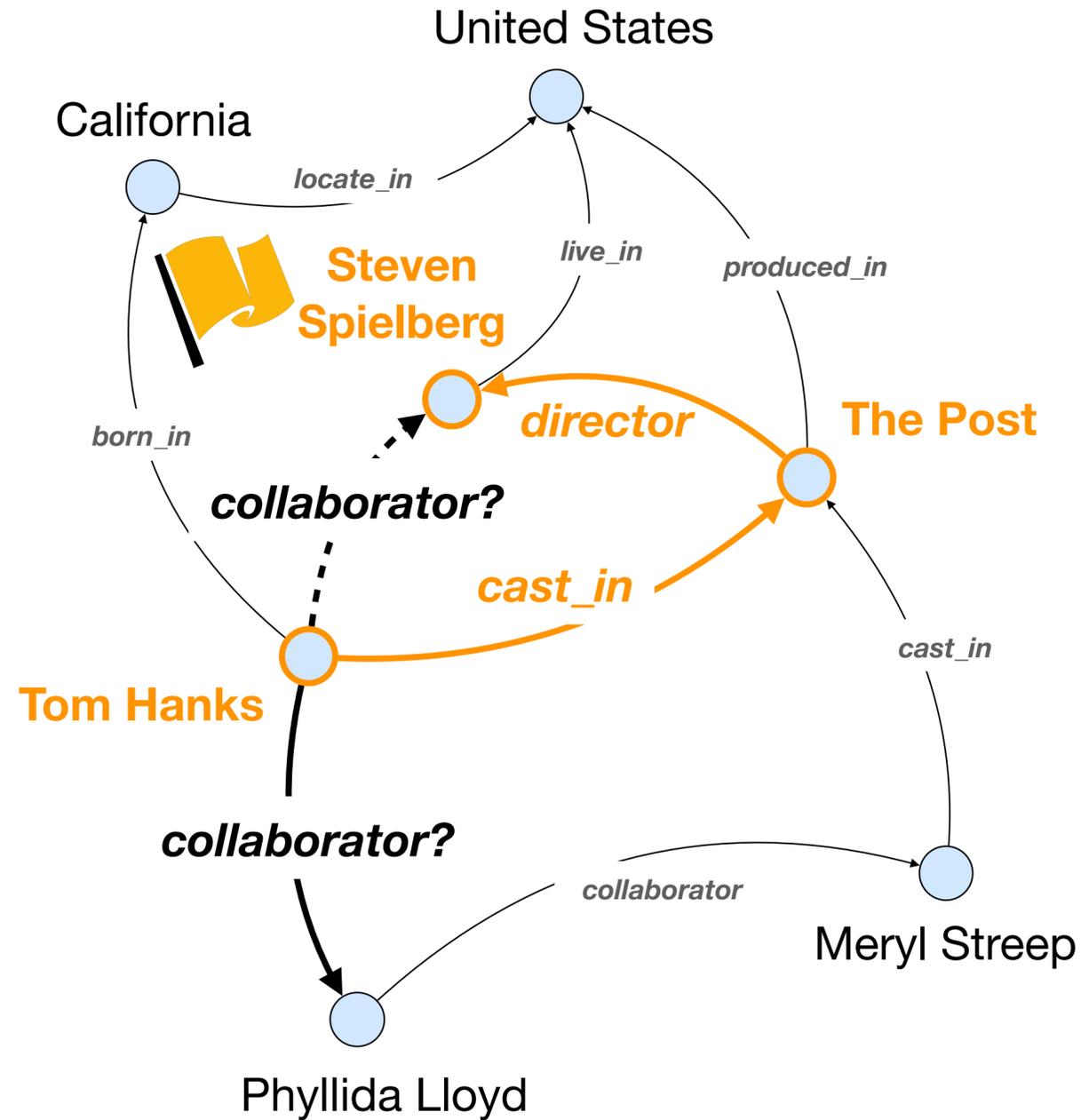
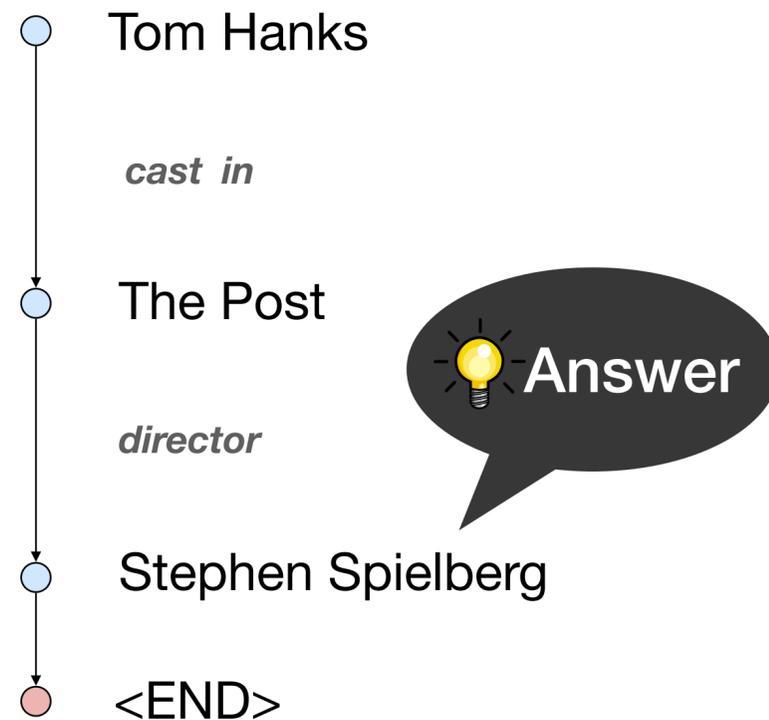
Which directors has Tom Hanks collaborated with?

# Multi-Hop Reasoning Models



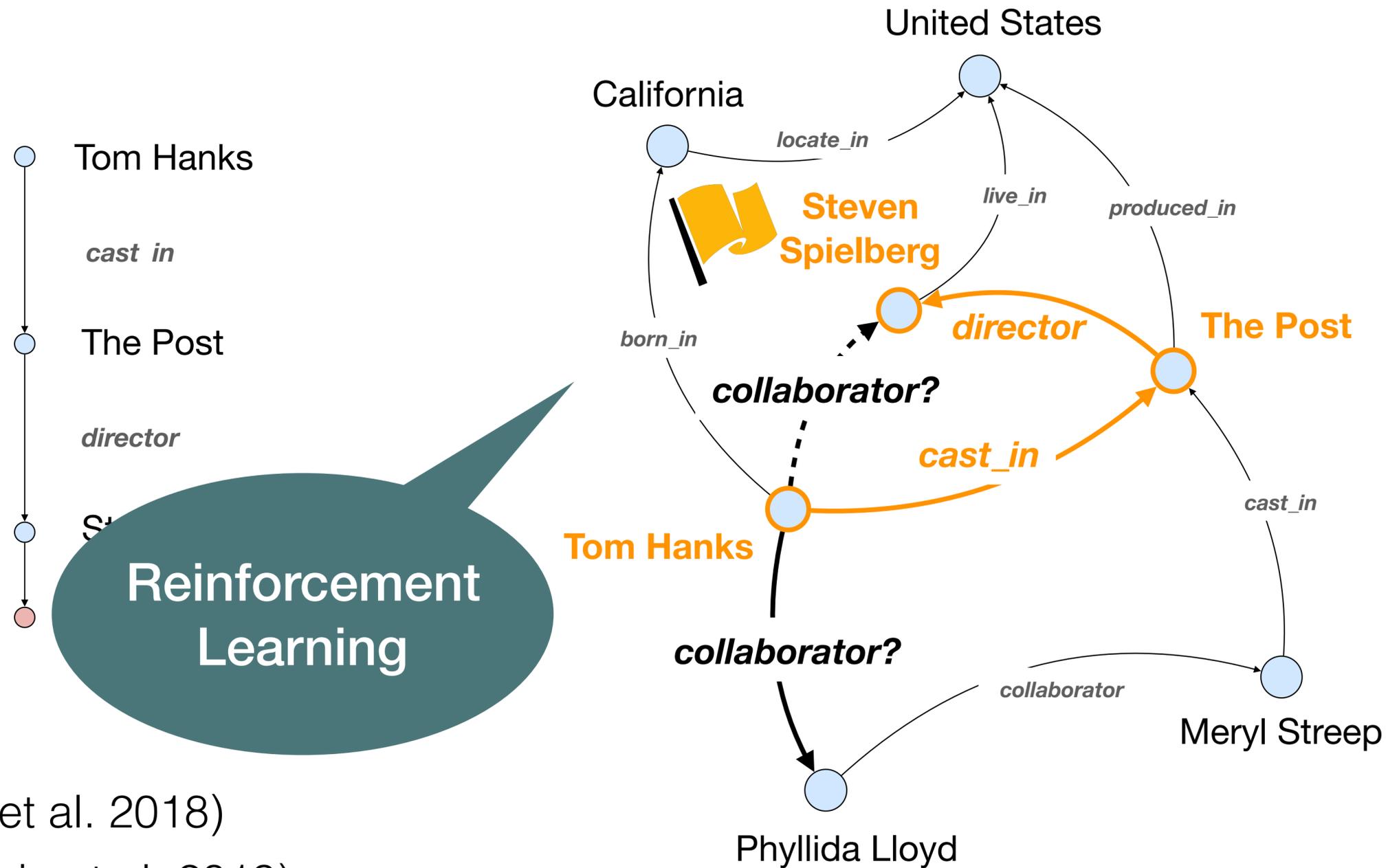
Which directors has Tom Hanks collaborated with?

# Multi-Hop Reasoning Models



Which directors has Tom Hanks collaborated with?

# Multi-Hop Reasoning Models



MINERVA (Das et al. 2018)

MINERVA+RS (Lin et al. 2019)

# Multi-Hop Reasoning Models

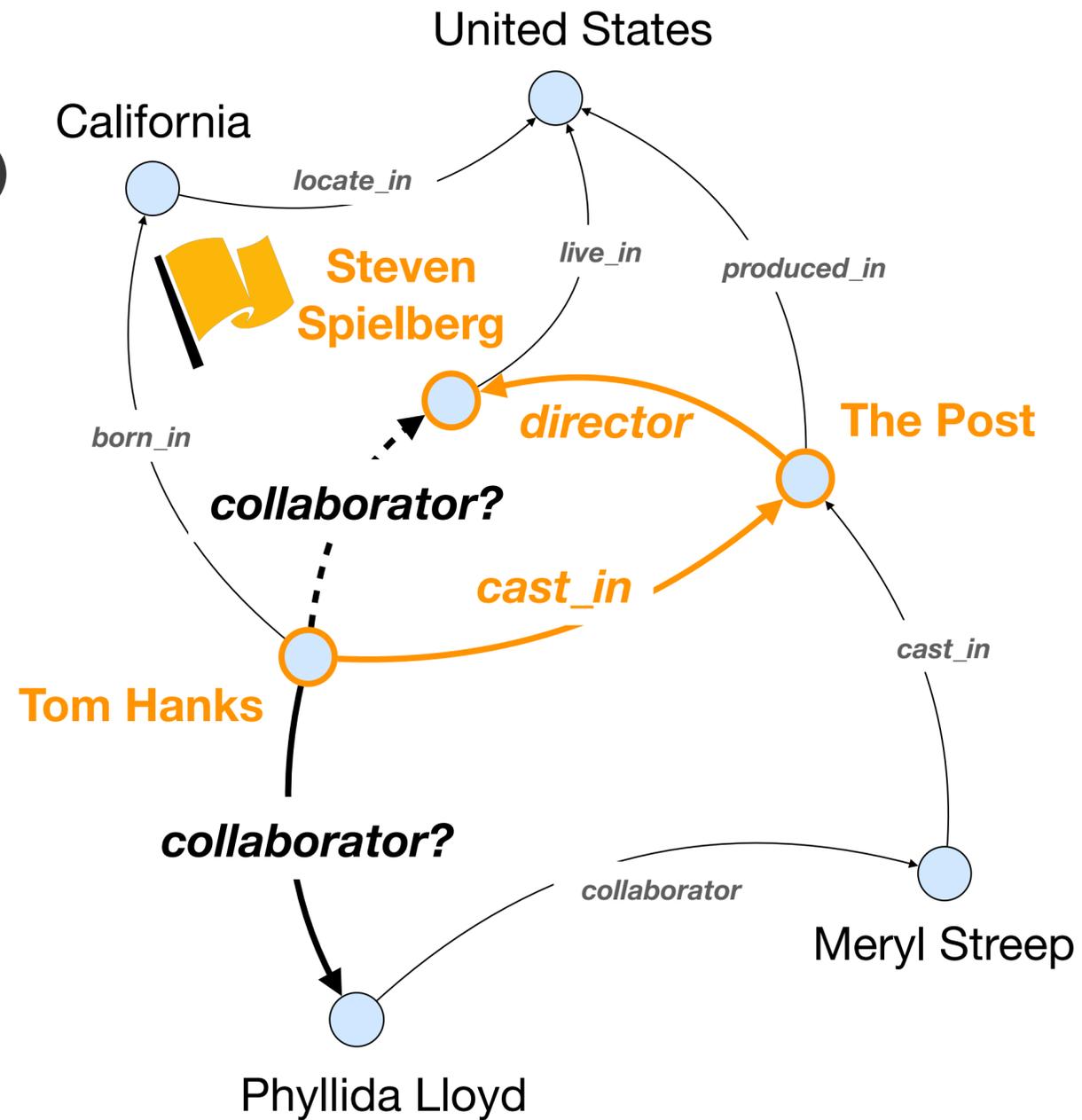


Interpretable

Competitive Accuracy

	MRR
MINERVA	0.825
MINERVA+RS	0.94

Tab 2. MINERVA and MINERVA + Reward Shaping fact inference performance on the UMLS benchmark dataset (Das et. al. 2018; Lin et. al 2018)



# Reinforcement Learning Framework

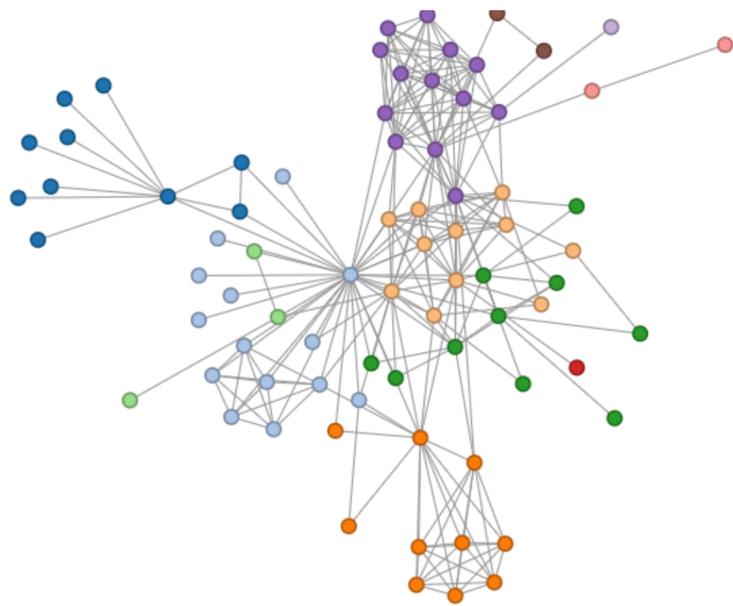
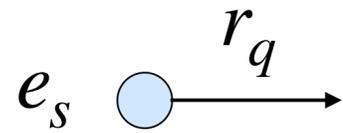
Environment

State

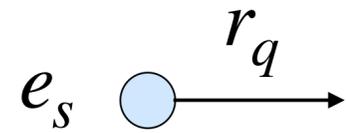
Action

Transition

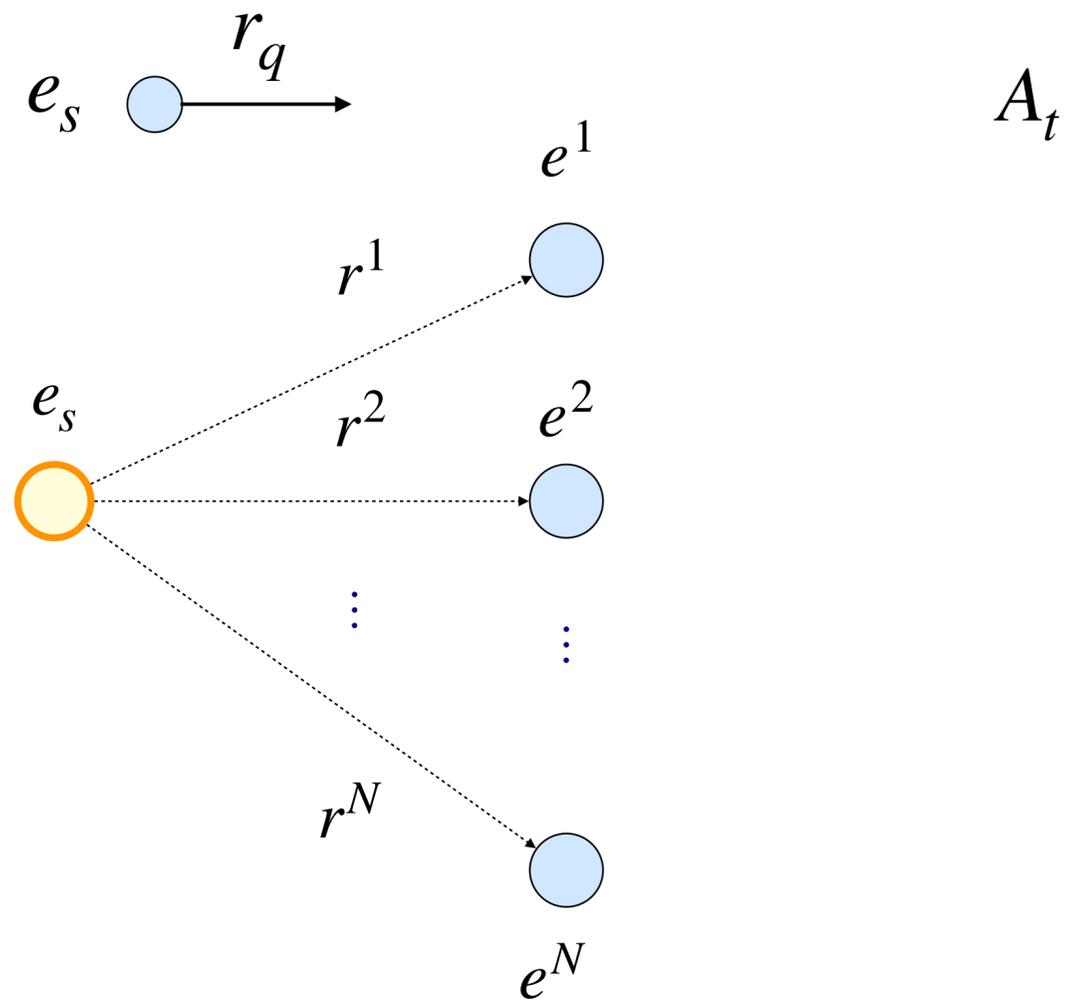
Reward



# Reinforcement Learning Framework



# Reinforcement Learning Framework



# Reinforcement Learning Framework

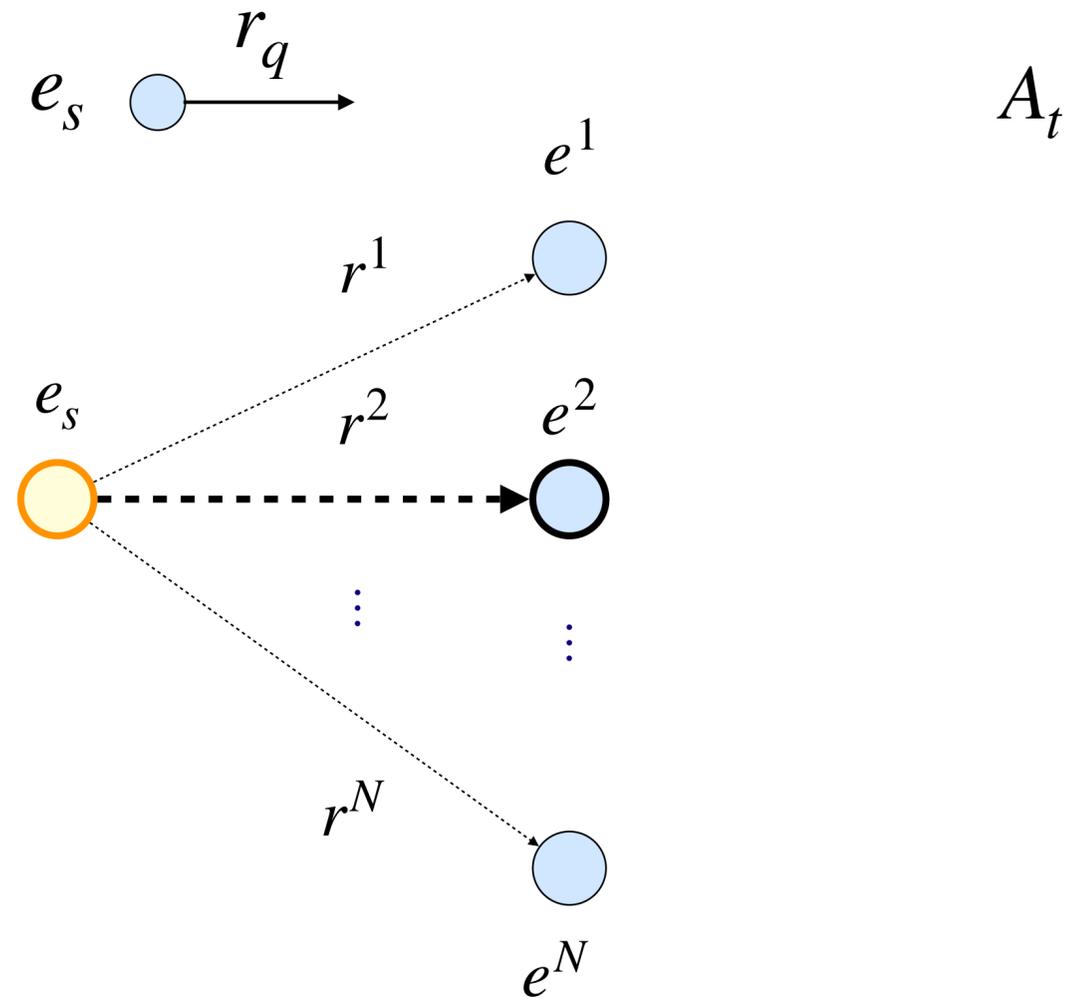
Environment

State

Action

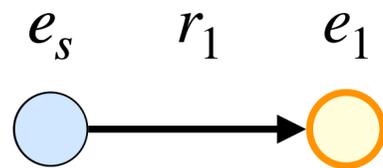
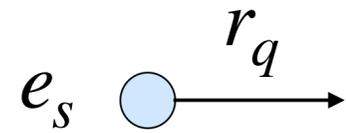
Transition

Reward

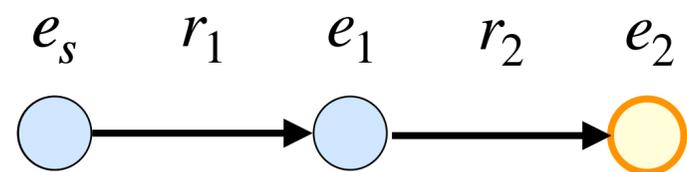
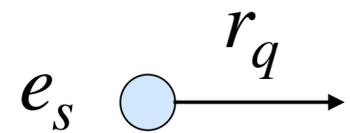


Action space: All nodes with incoming edges from  $e_s$  in the graph

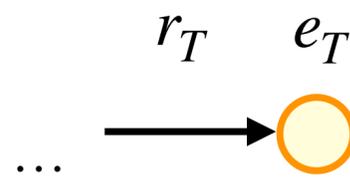
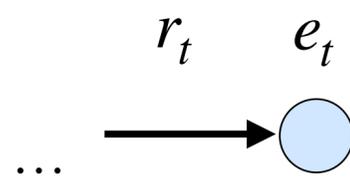
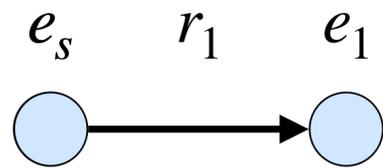
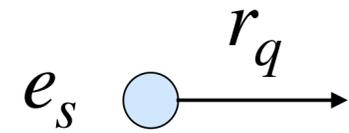
# Reinforcement Learning Framework



# Reinforcement Learning Framework

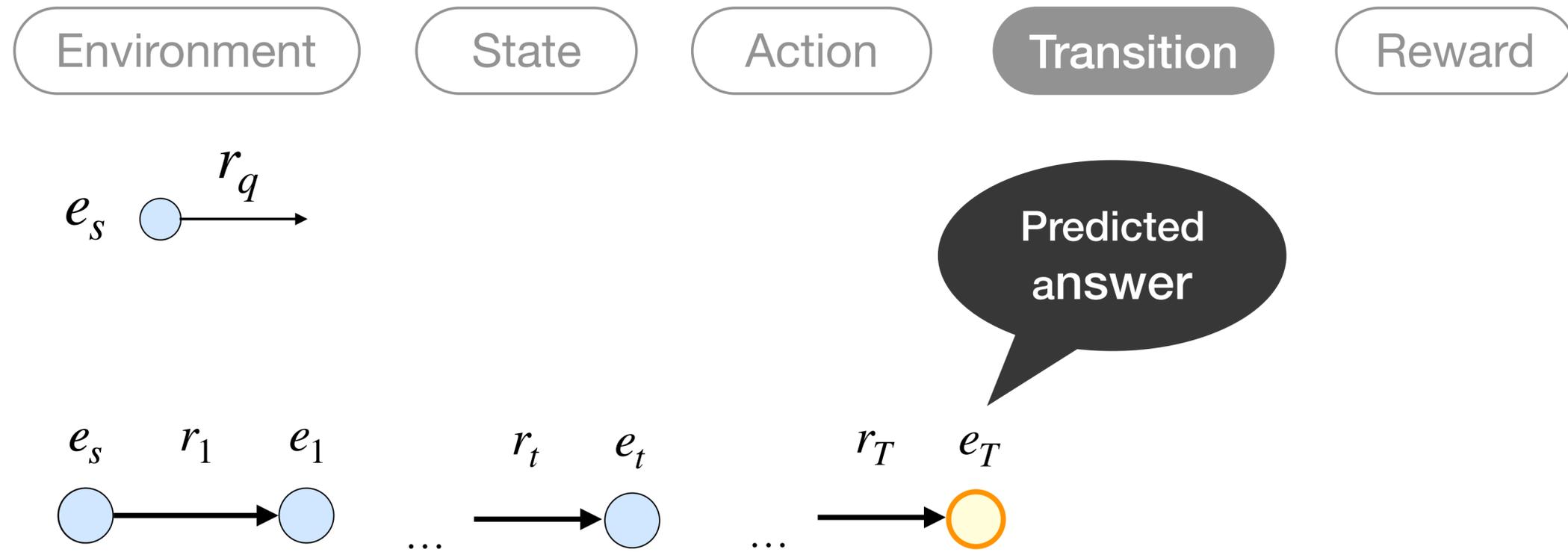


# Reinforcement Learning Framework

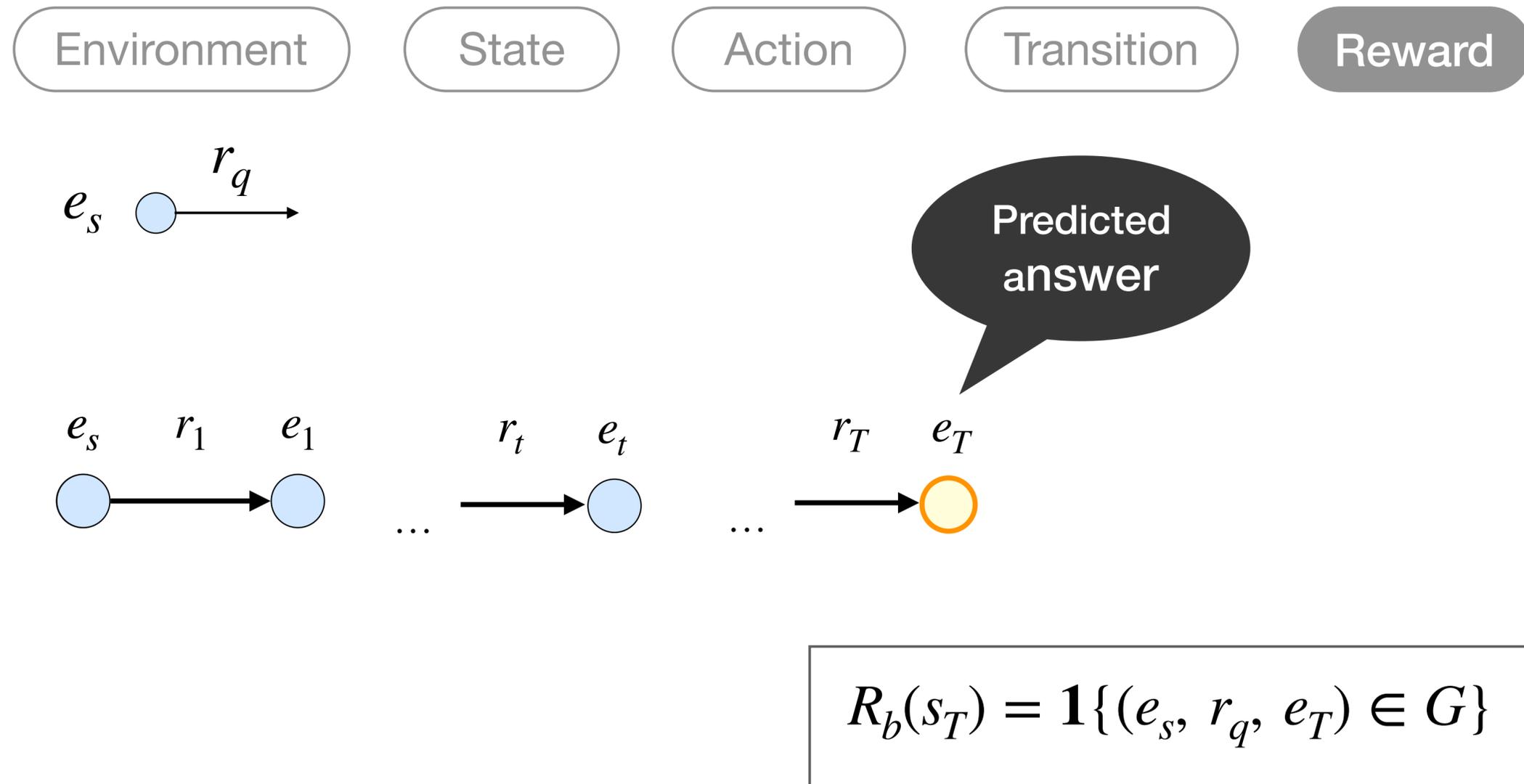


Max #  
steps

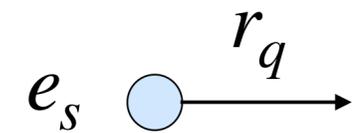
# Reinforcement Learning Framework



# Reinforcement Learning Framework

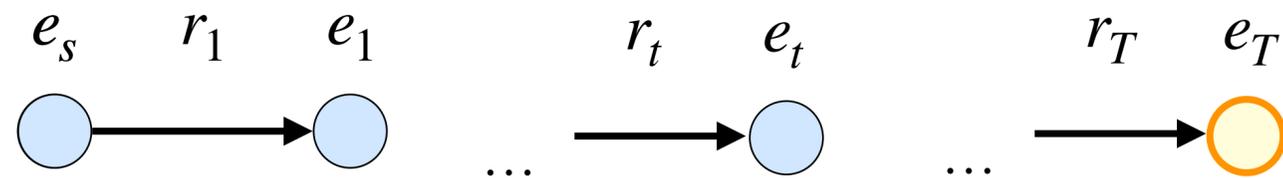


# Reinforcement Learning Framework



Policy gradient

Learn **which action to choose** given a state



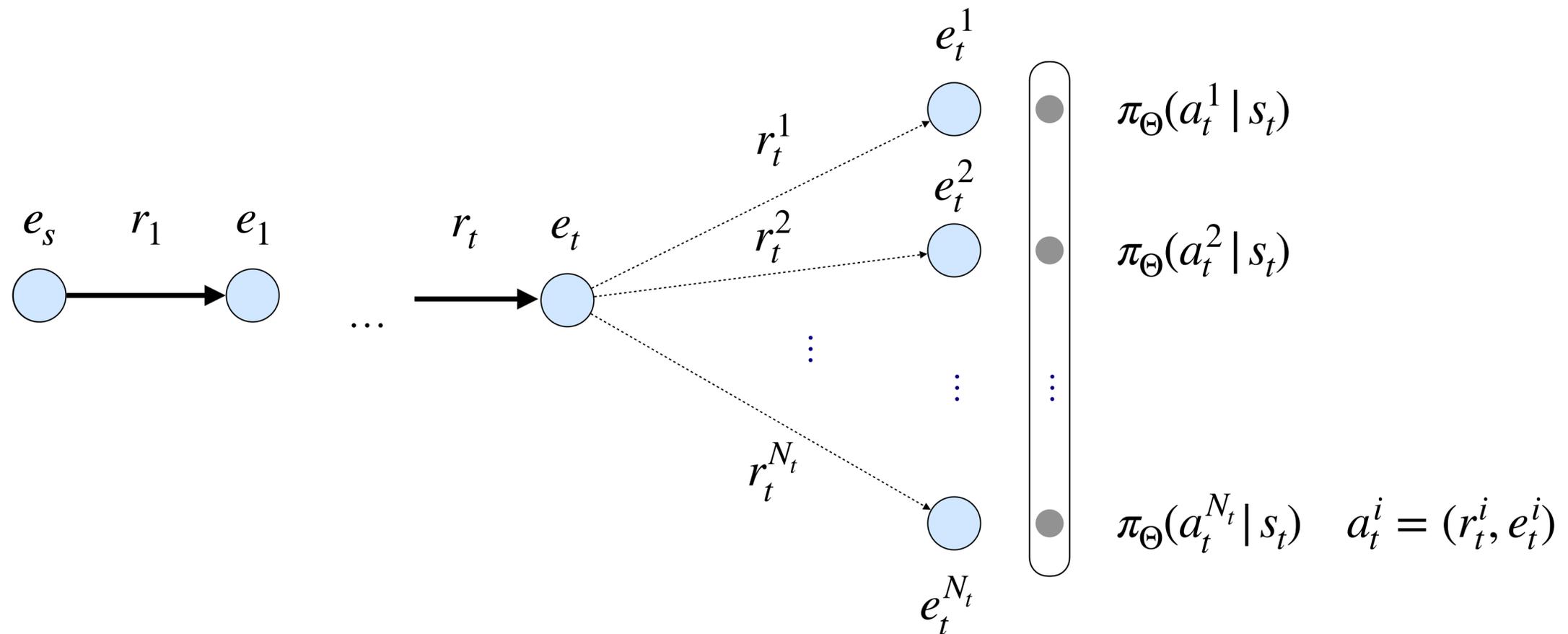
$$R_b(s_T) = \mathbf{1}\{(e_s, r_q, e_T) \in G\}$$

# Policy Gradient

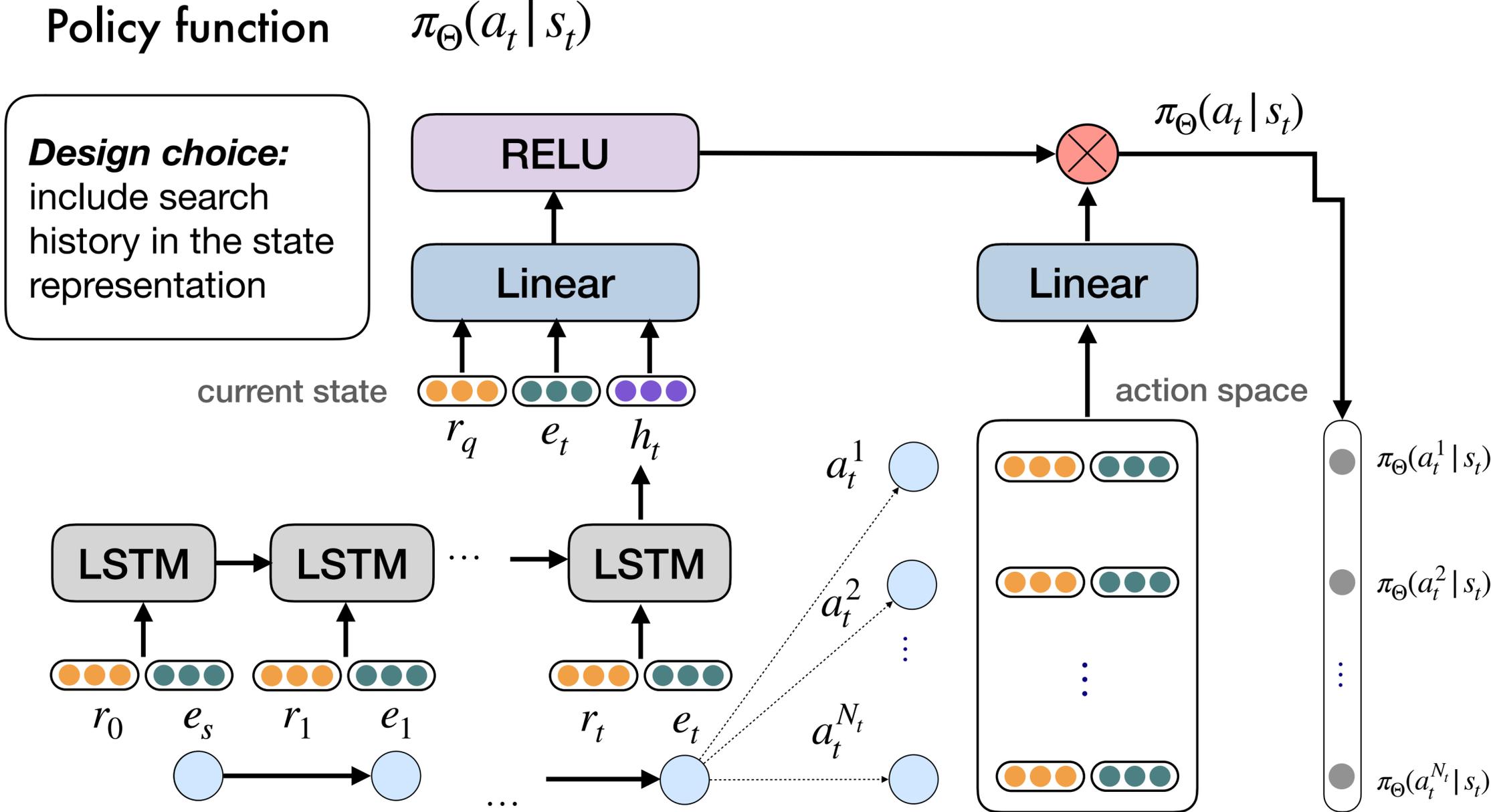
Policy function

$$\pi_{\Theta}(a_t | s_t)$$

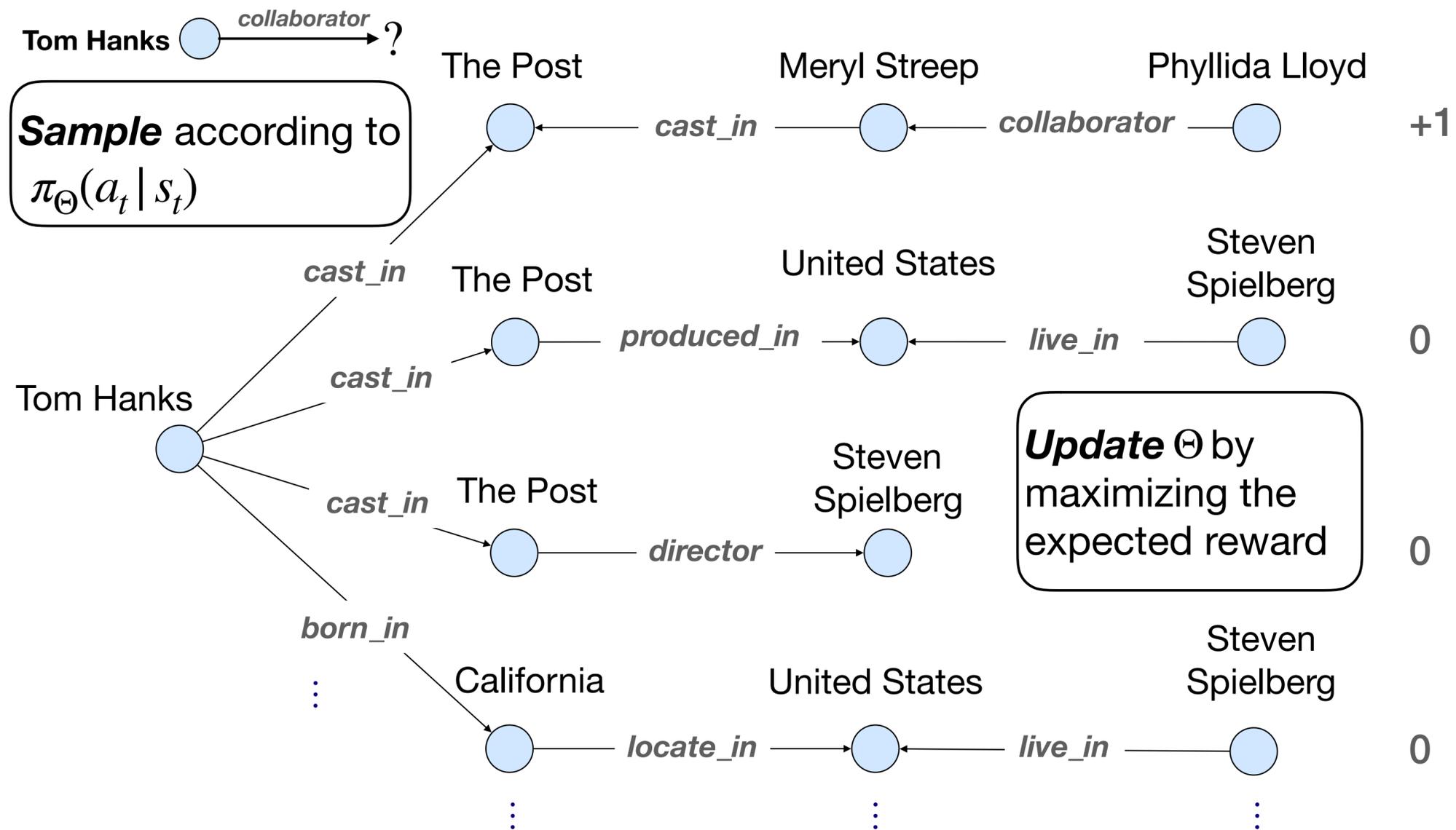
**Probability** of choosing an action given the current state



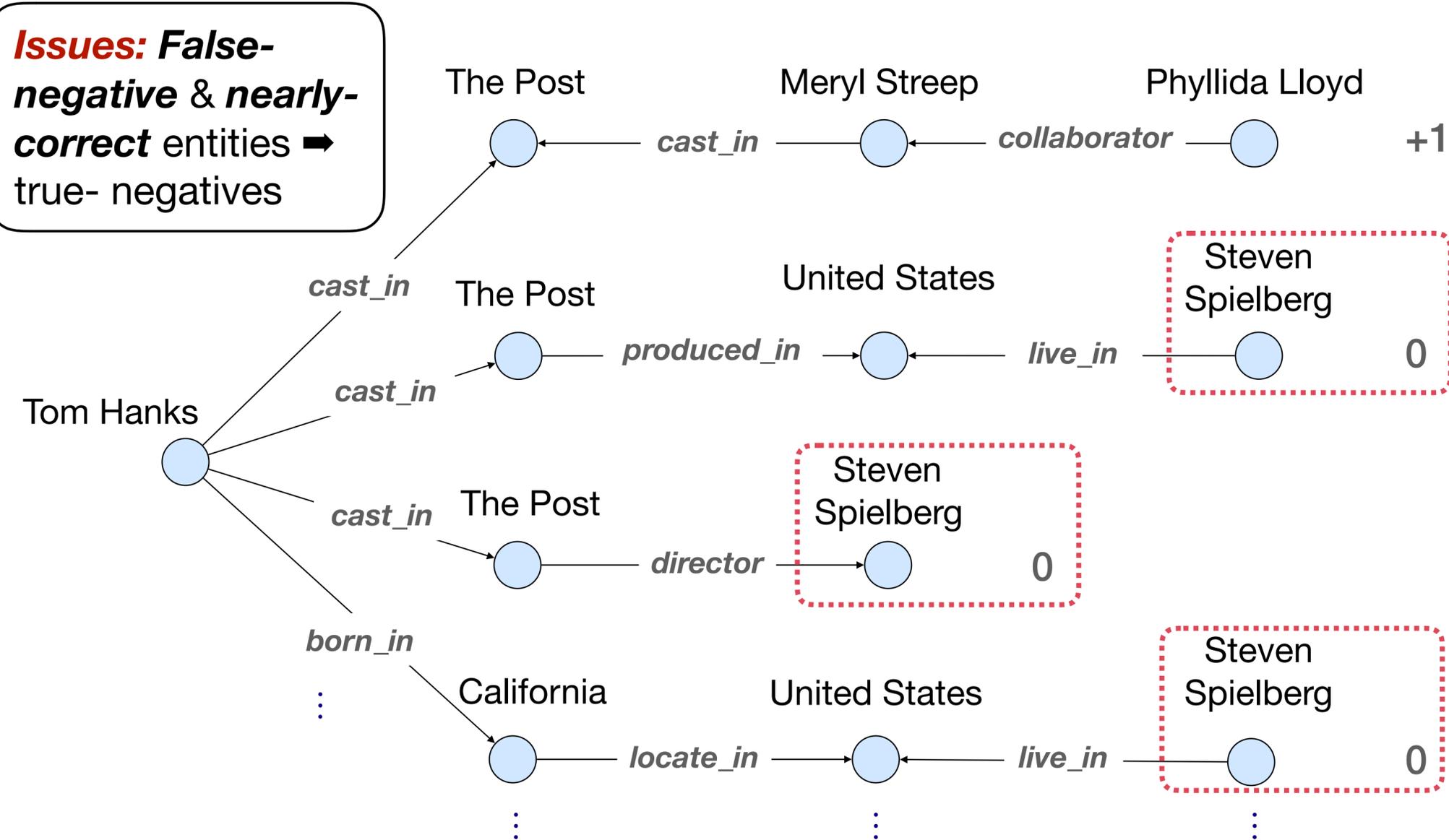
# Policy Gradient



# REINFORCE Training



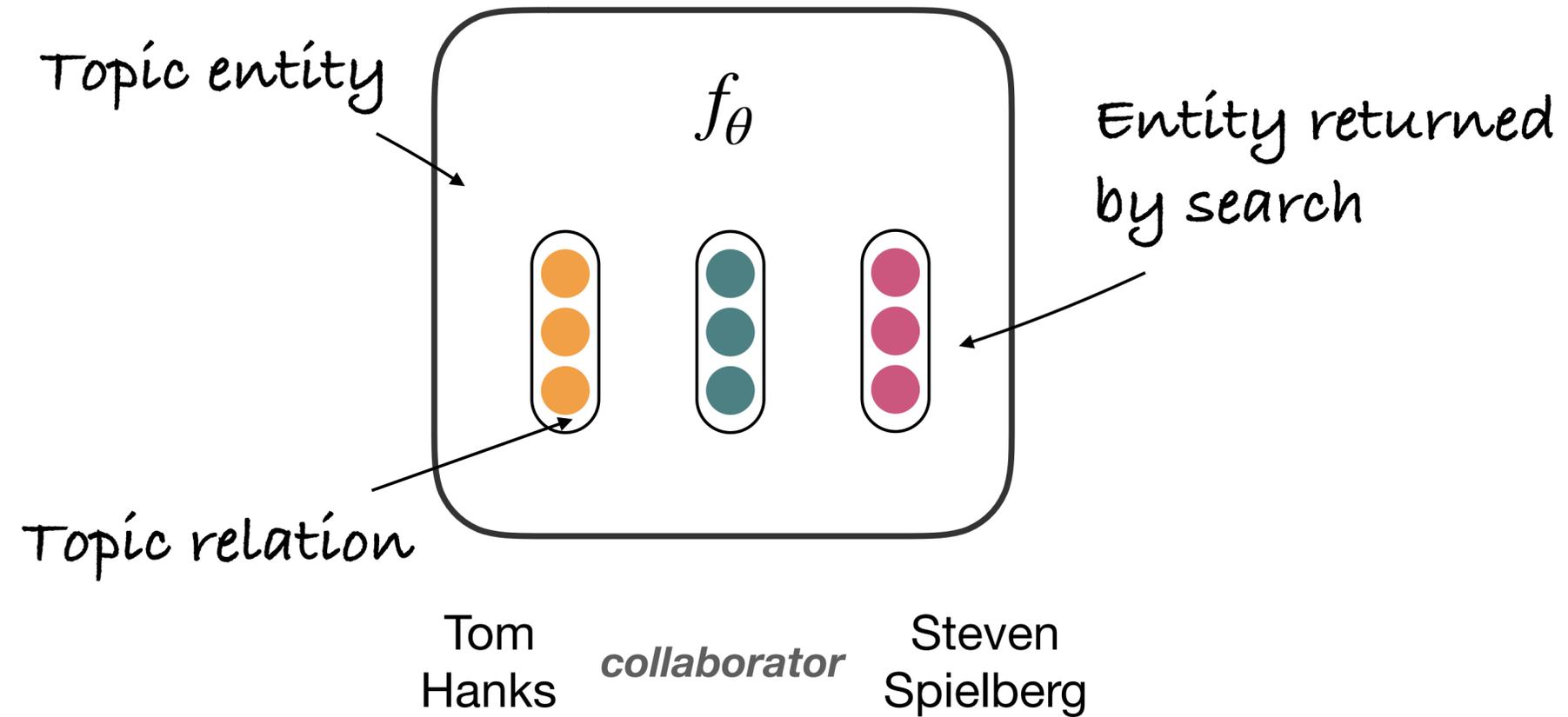
# REINFORCE Training



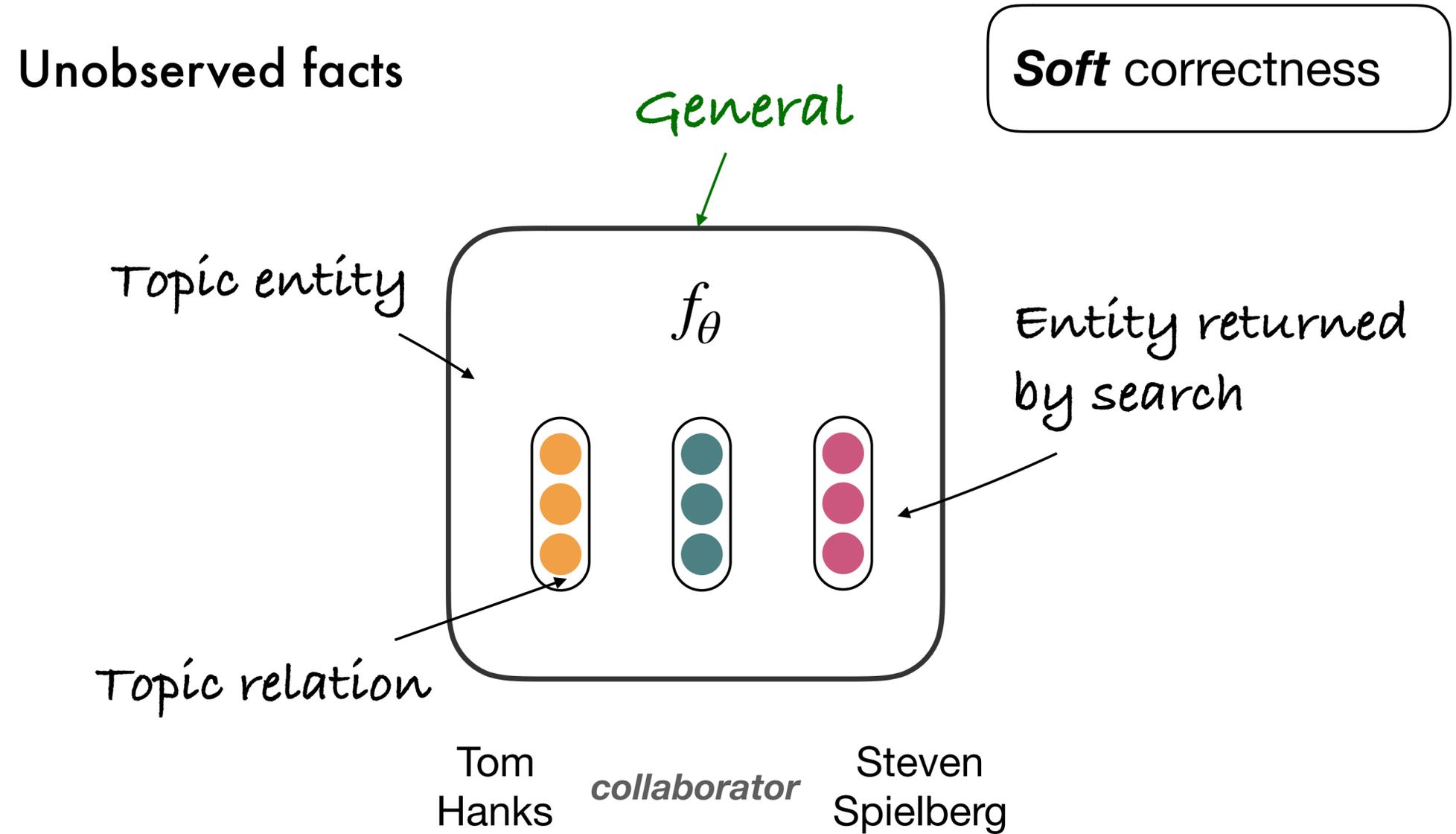
# Reward Shaping

Unobserved facts

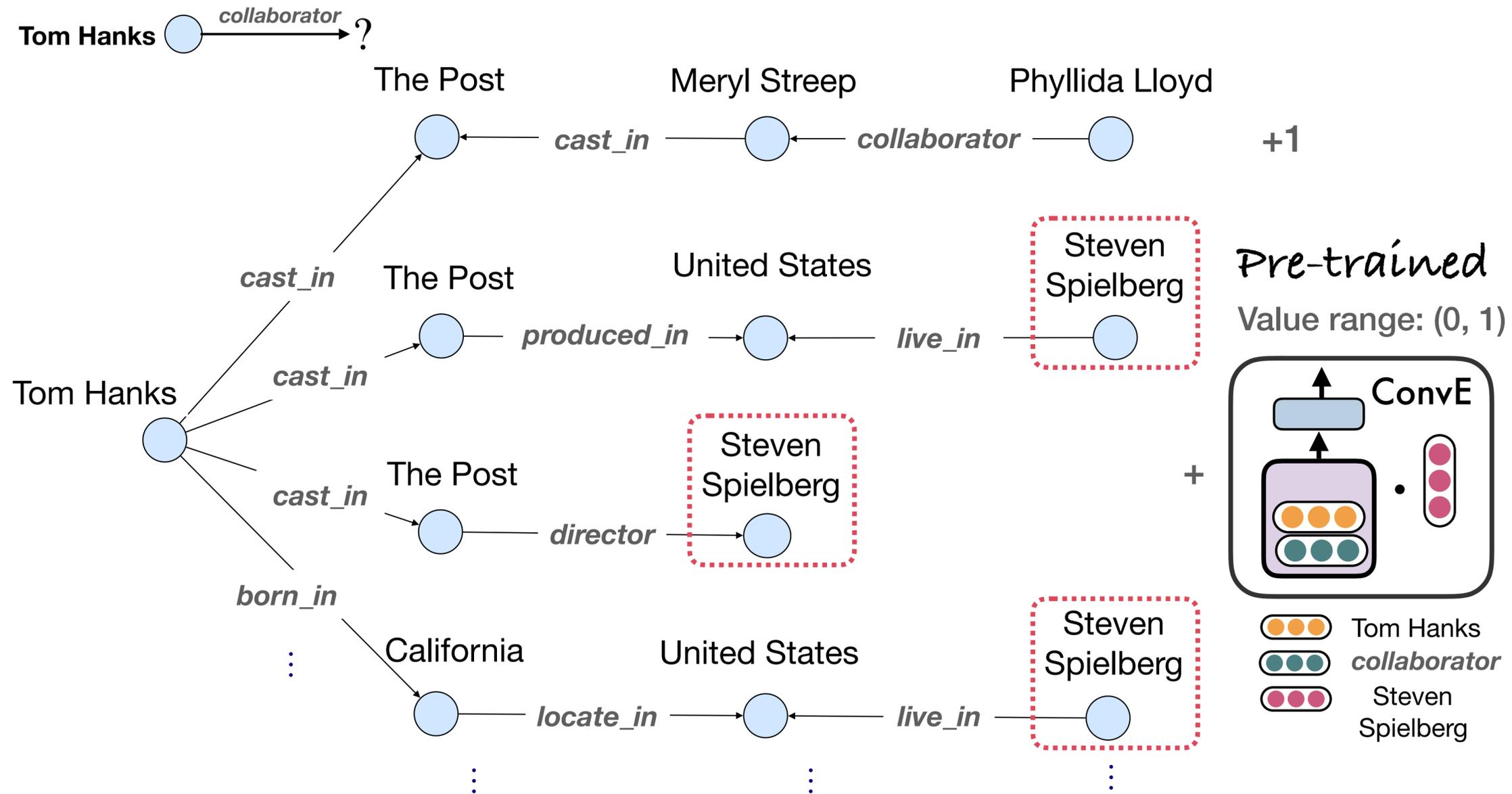
**Soft** correctness



# Reward Shaping



# Reward Shaping



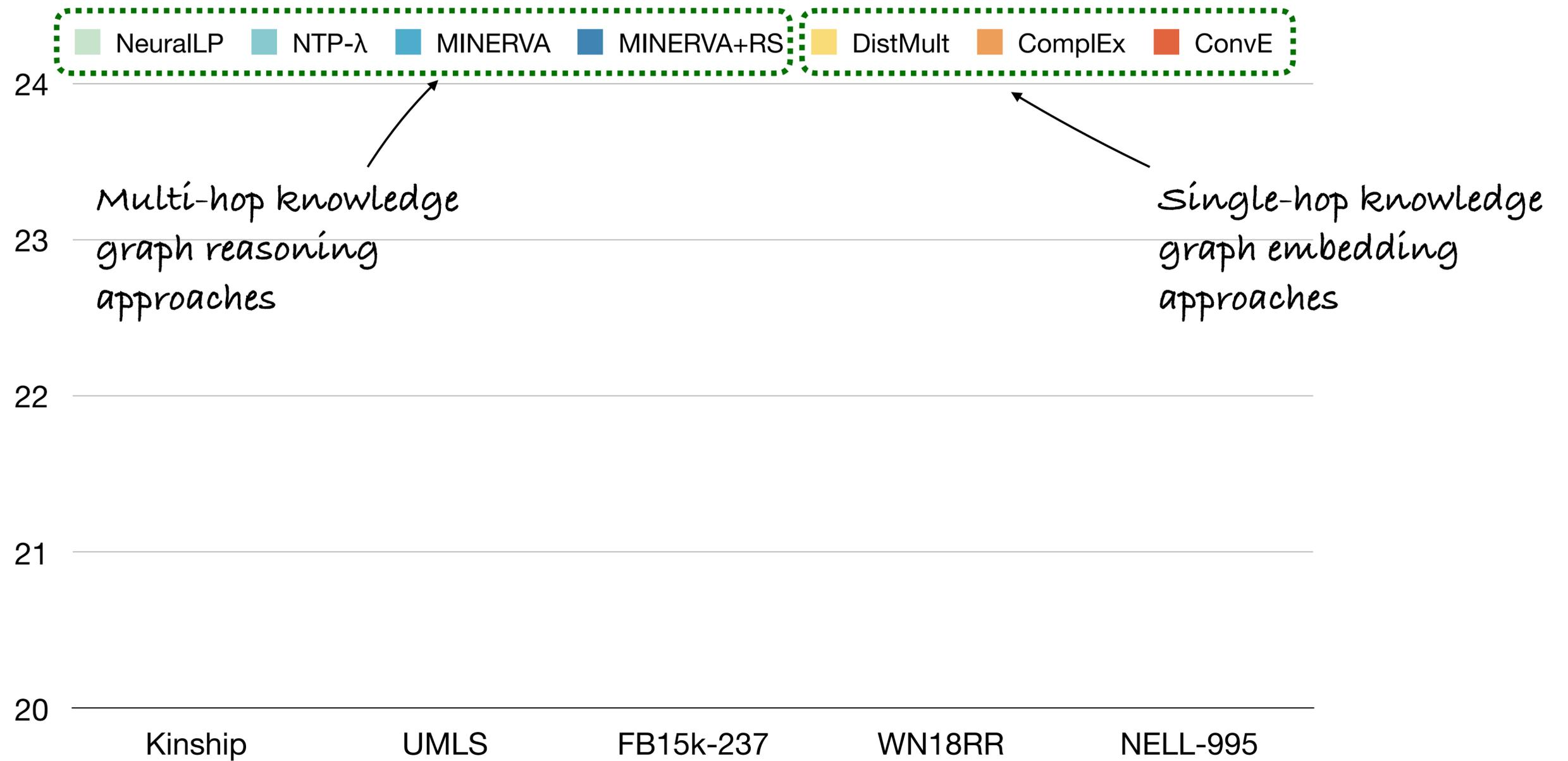
# Experiment Setup

## KG Benchmarks

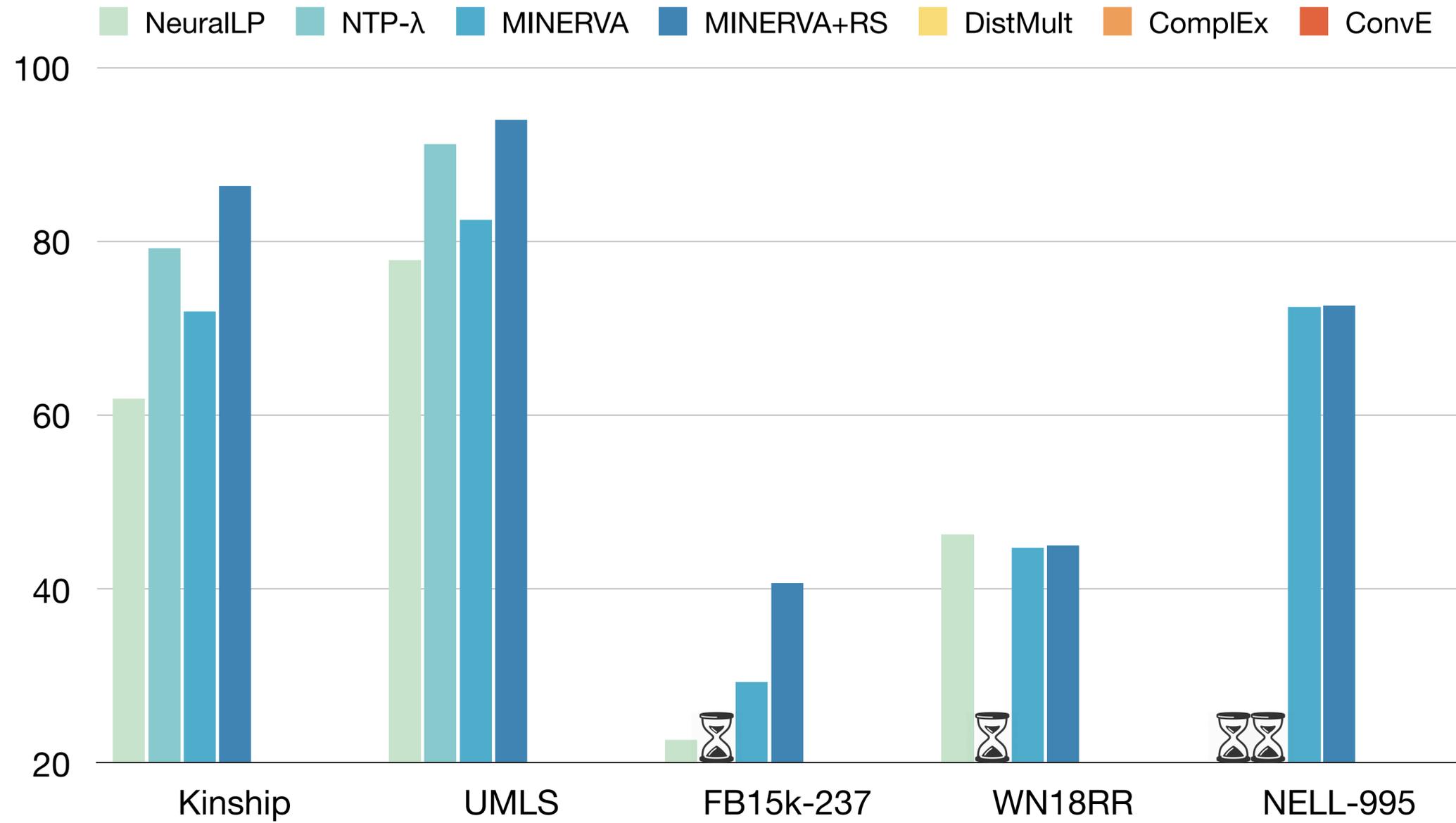
Name	# Ent.	# Rel.	# Fact	# Degree Avg	# Degree Median
Kinship	104	25	8,544	85.15	82
UMLS	135	46	5,216	38.63	28
FB15k-237	14,505	237	272,115	19.74	14
WN18RR	40,945	11	86,835	2.19	2
NELL-995	75,492	200	154,213	4.07	1

Decreasing  
connectivity

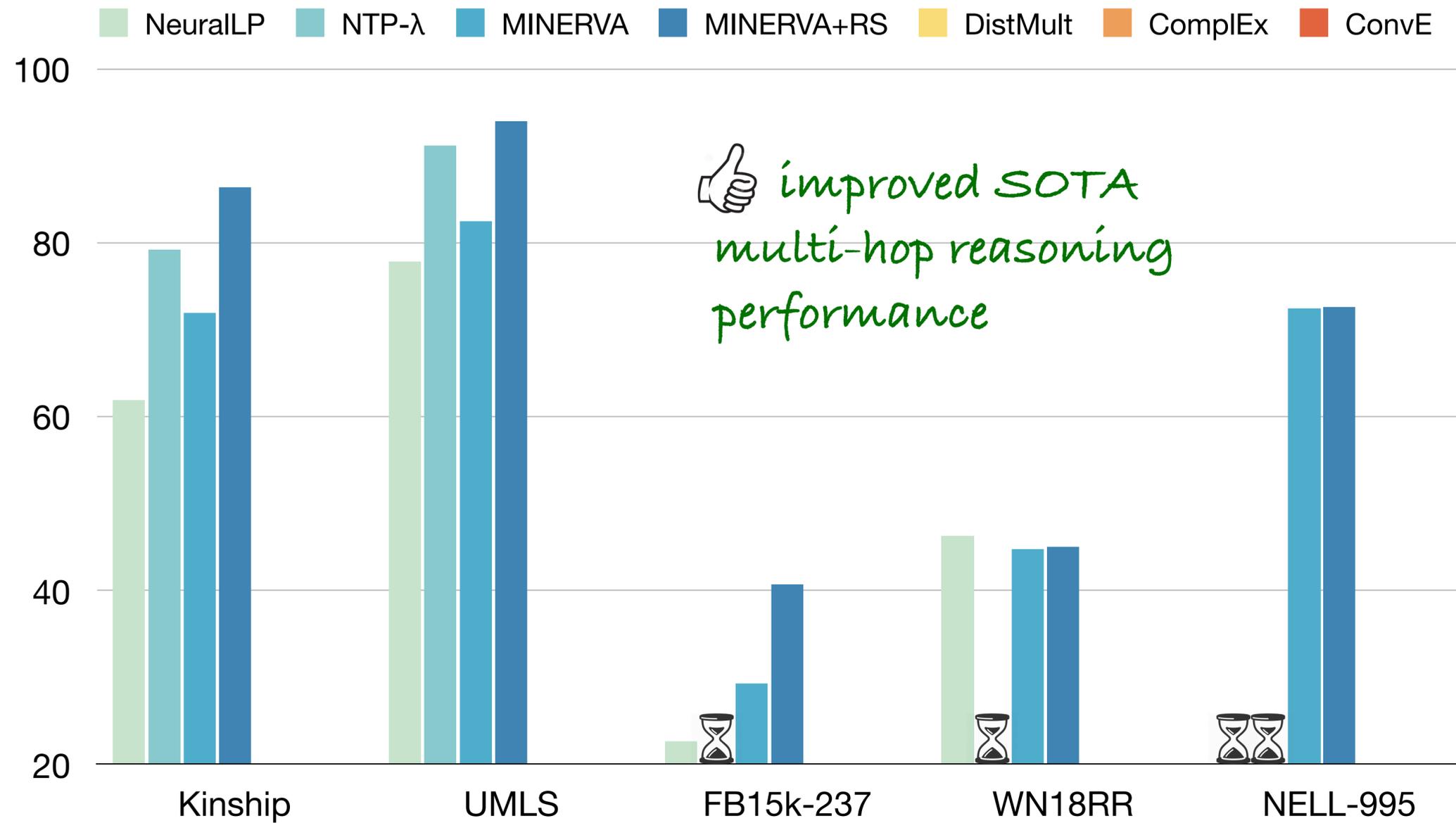
# Main Results



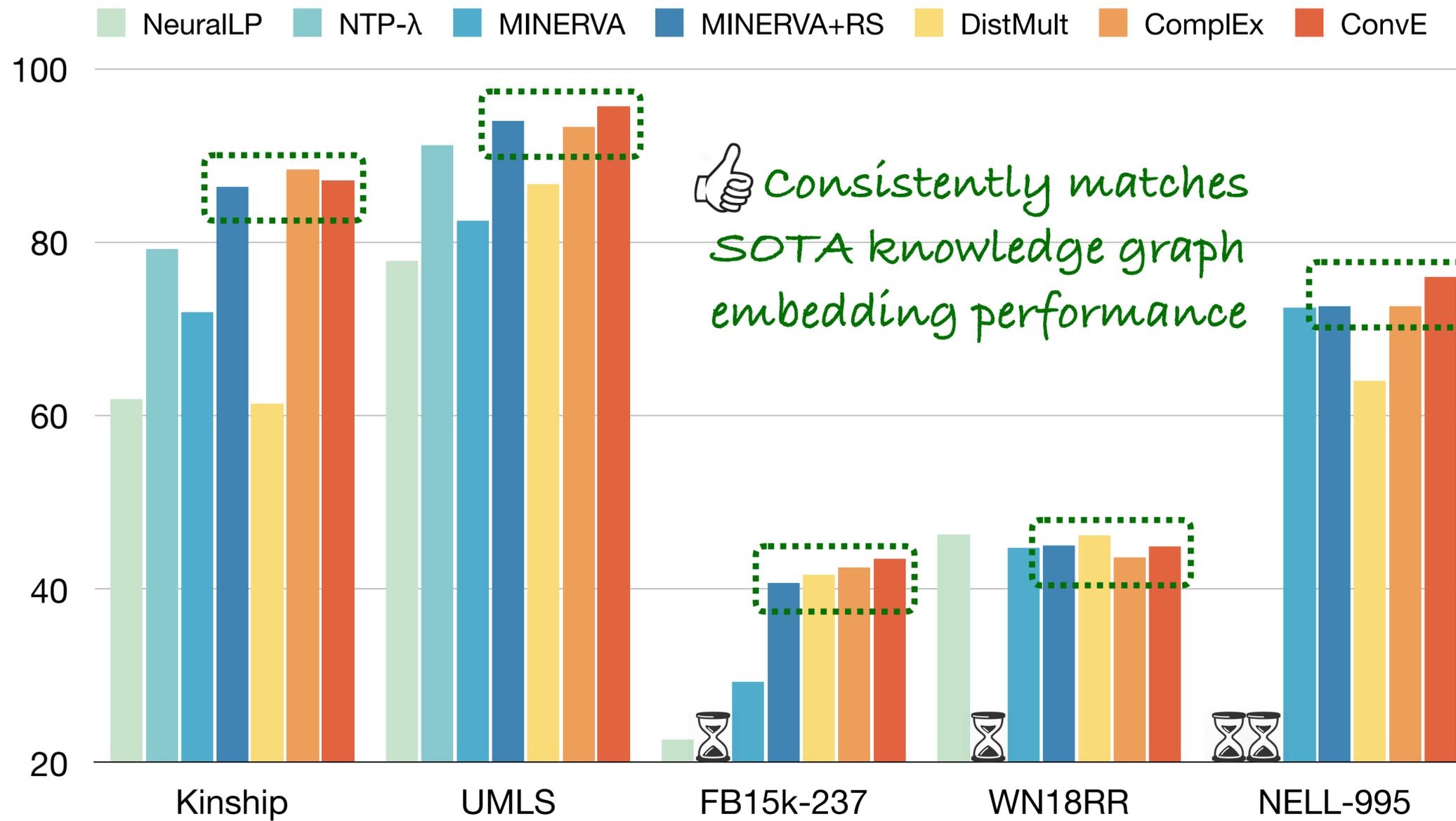
# Main Results



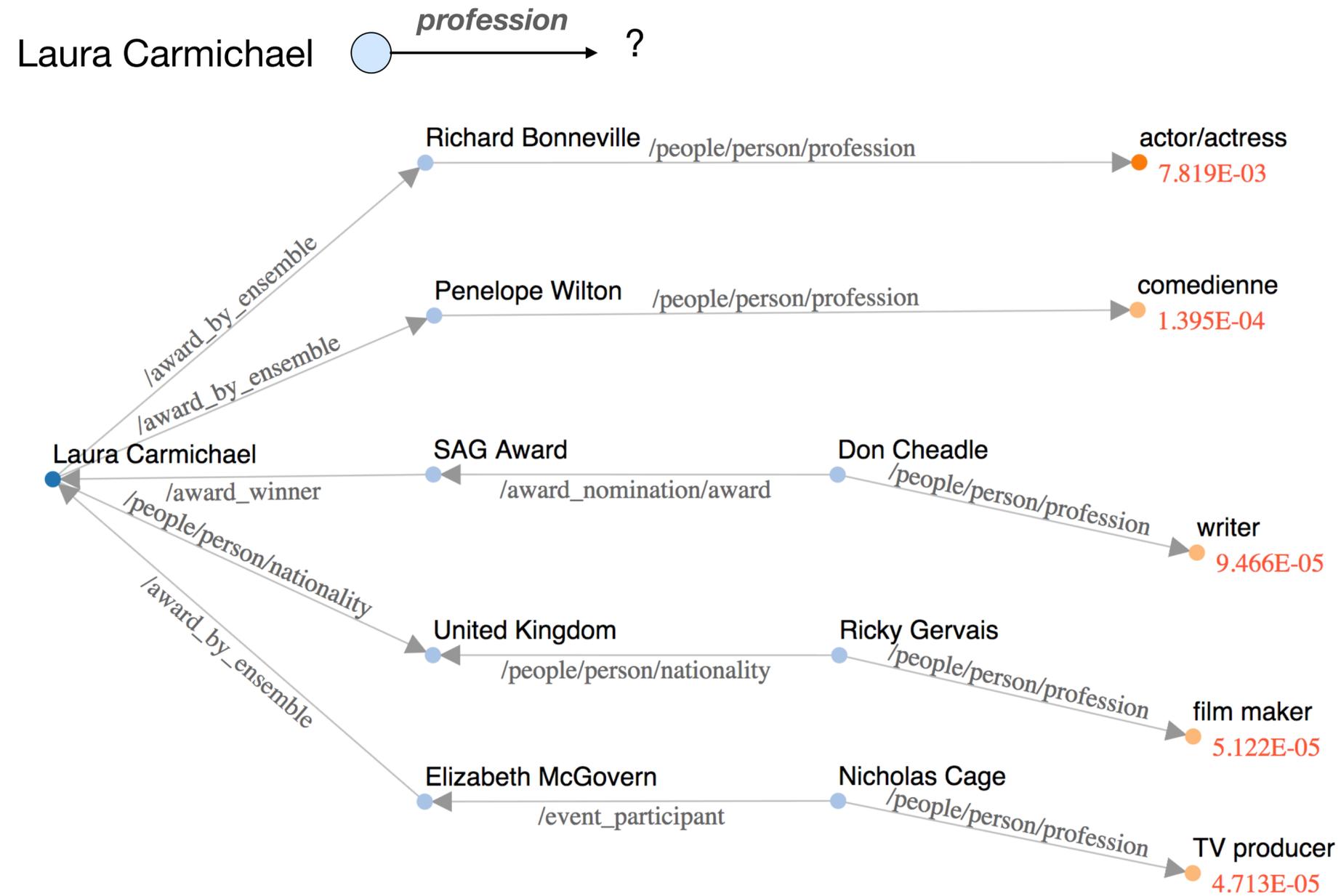
# Main Results



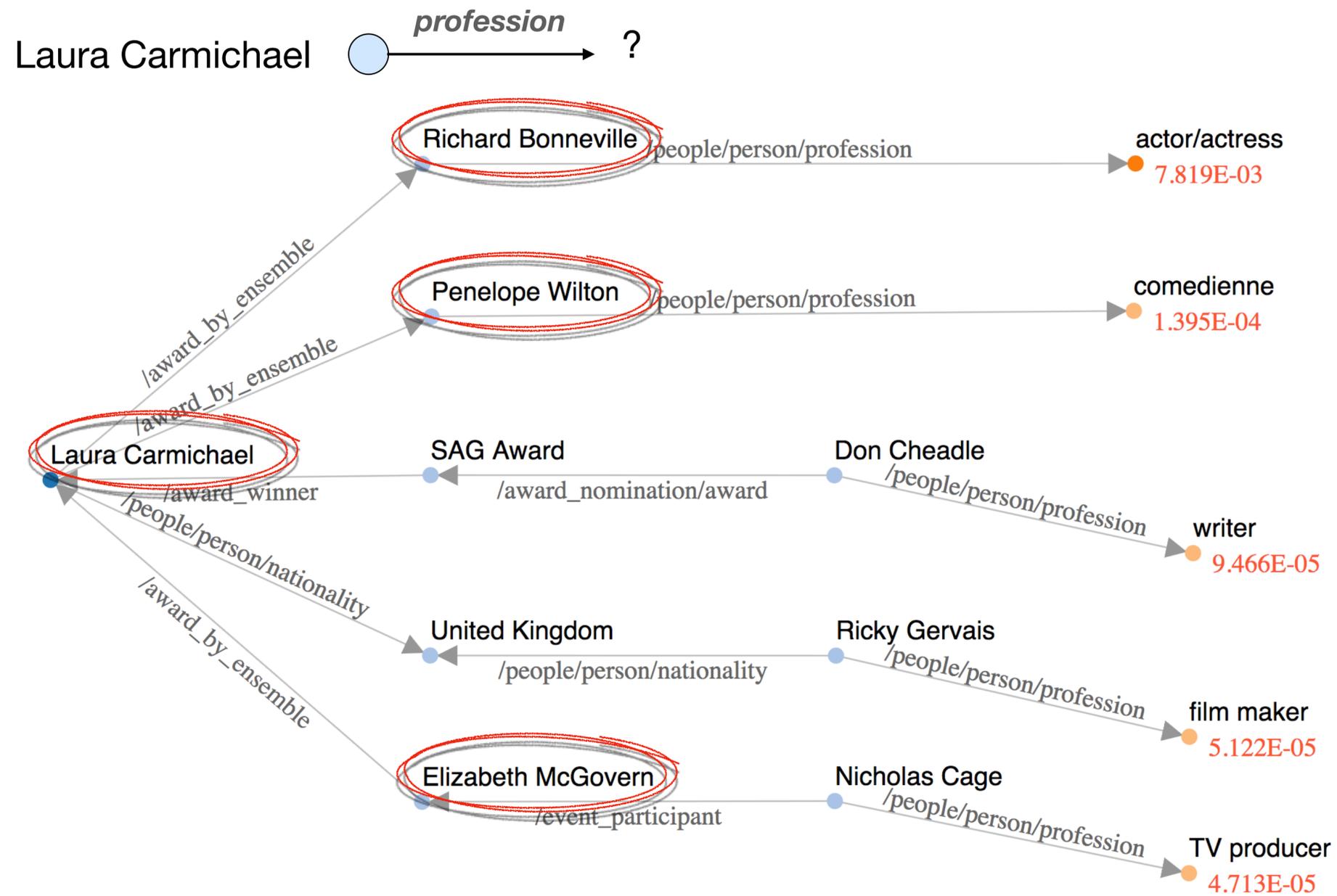
# Main Results



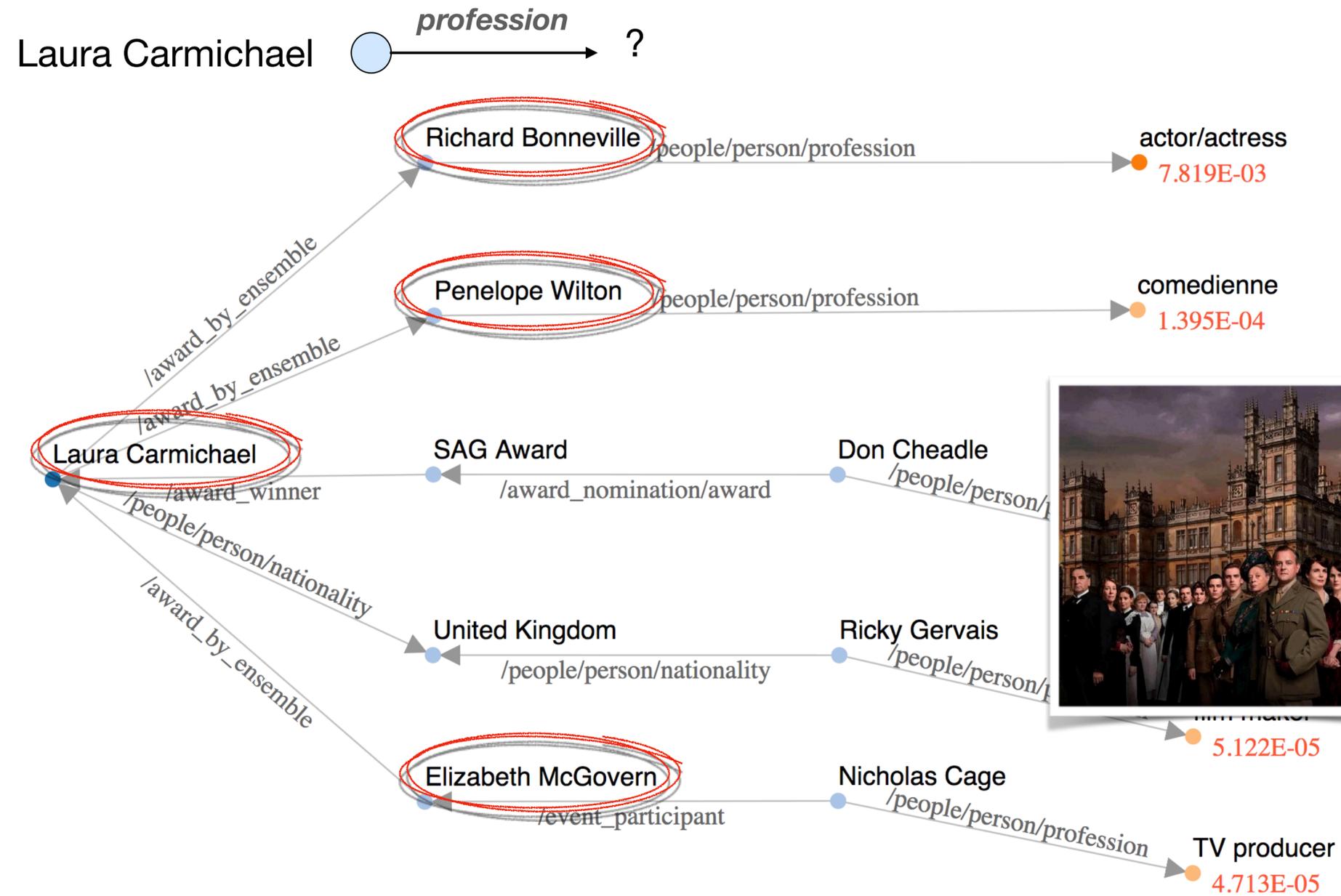
# Interpretable Results



# Interpretable Results



# Interpretable Results



# Take-aways

- Practical knowledge graphs are incomplete and require automatic completion
- KG embeddings are effective approaches for recovering missing facts, but lack interpretability
- Multi-hop KG inference is interpretable but less accurate
- Multi-hop KG inference with embedding-based reward shaping combines the best of both approaches
- The method can potentially be extended to multi-hop reasoning over joint KG and text to better support downstream AI systems