

# Double Equivariance for Inductive Link Prediction for Both New Nodes and New Relation Types

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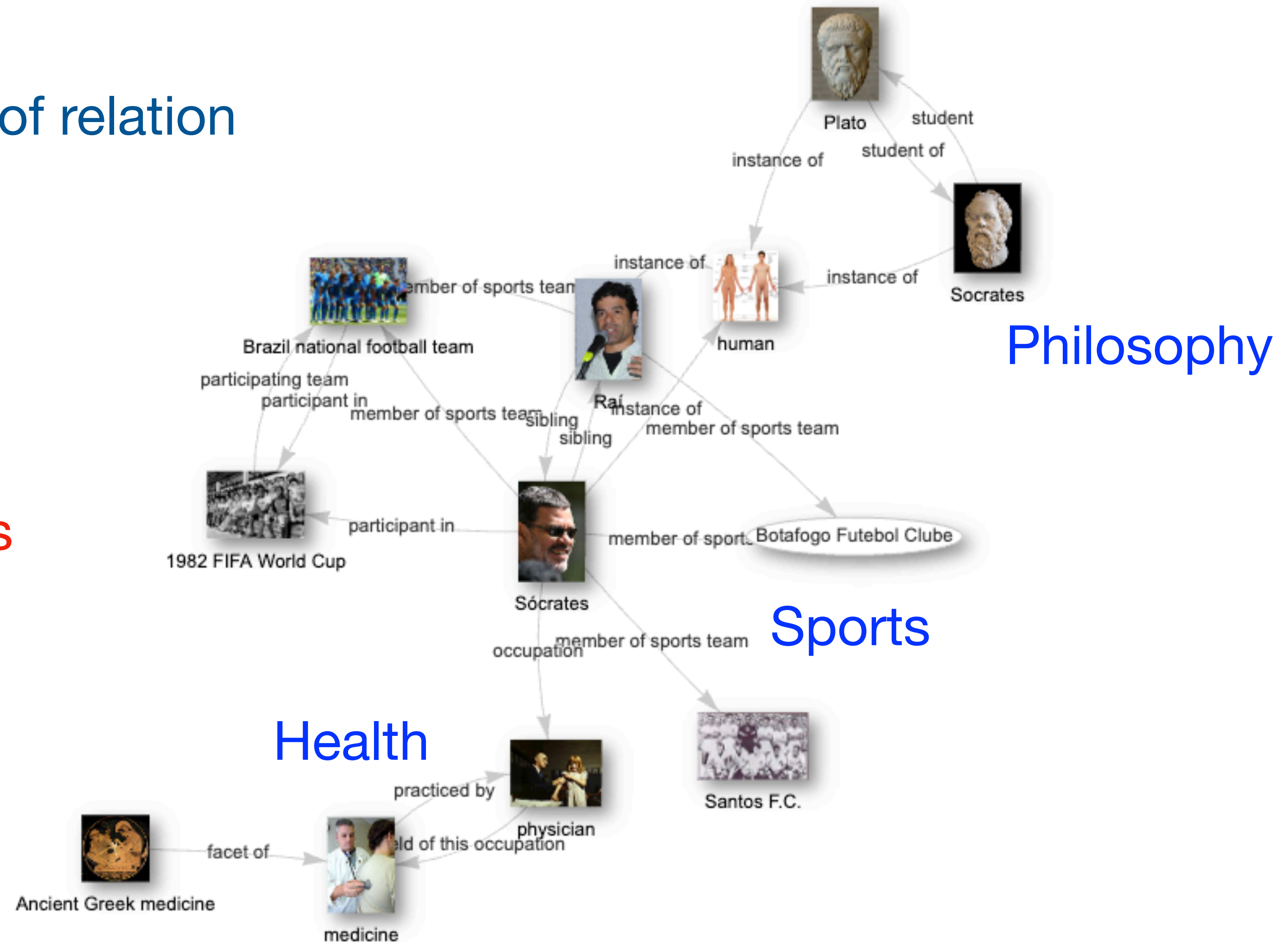
\*Equal Contribution



# Anatomy of a *Knowledge Graph*

- Nodes = entities
- Edge type = type of relation

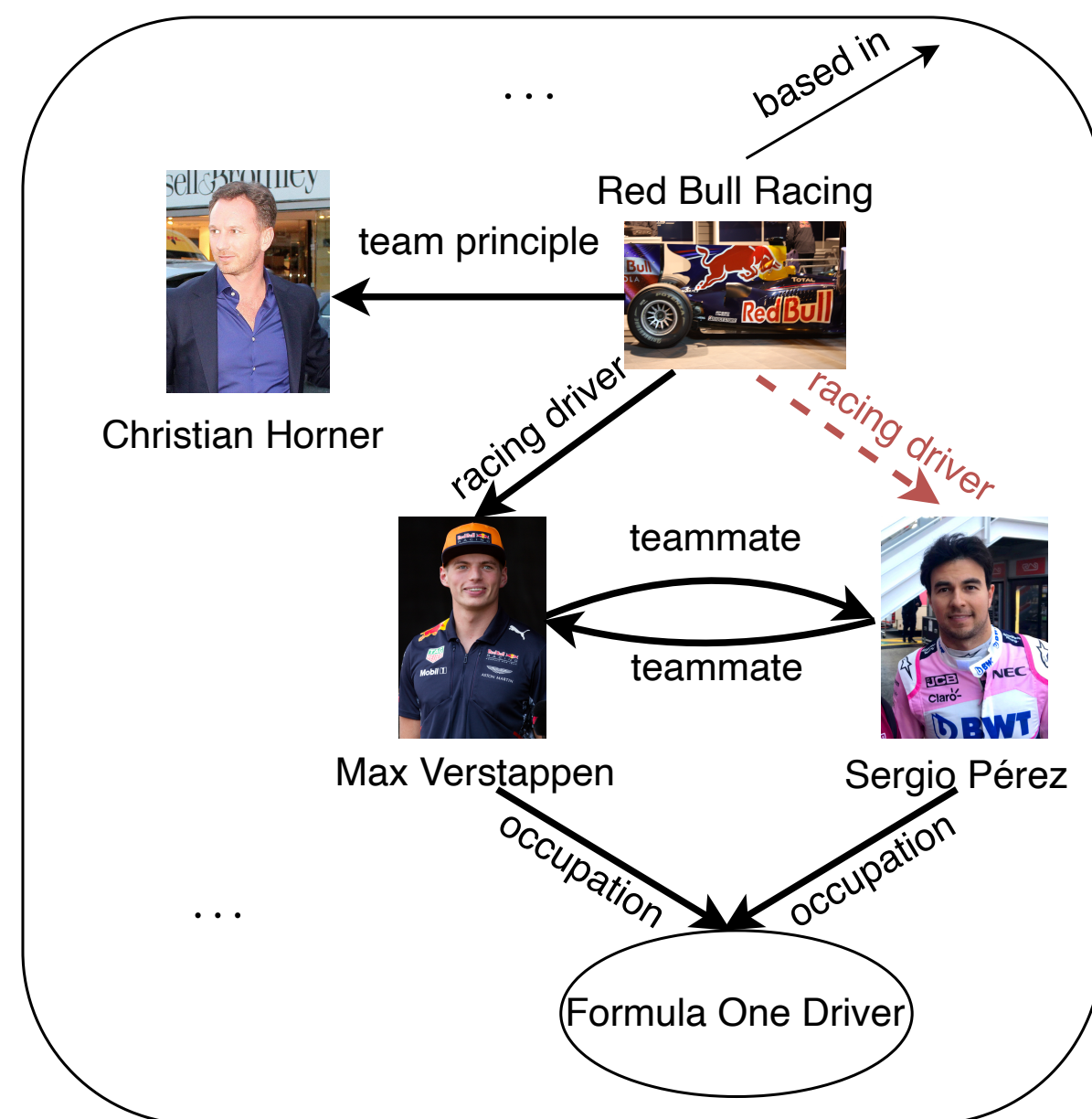
Wikipedia's knowledge graph has **multiple domains**



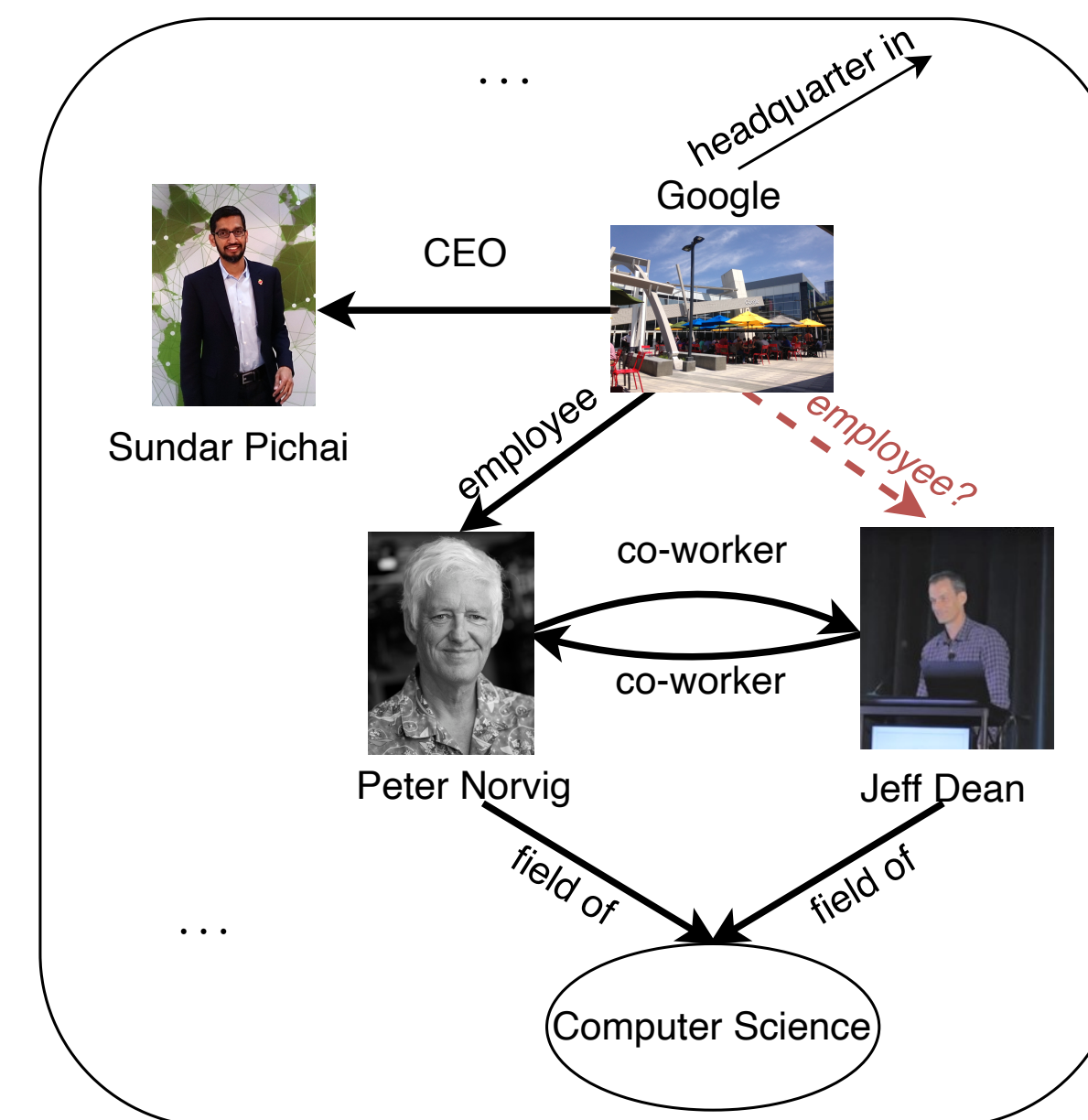
# Transferability over Multiple Domains?

- Can we transfer the relational patterns we learn in Sports to **zero-shot** predict relations in Organizations?

Train data: Sports



Test data: Organizations



Change in domain

Unseen entities and relation types

# New Benchmark: WikiTopics

- A benchmark for pre-training, zero-shot transferability
- Sampled from WikiData-5M<sup>1</sup>
- Domains have different entities and non-overlapping relation types

Domain KG index	Abbreviation	Description
T1	Art	Art and Media Representation
T2	Award	Award Nomination and Achievement
T3	Edu	Education and Academia
T4	Health	Health, Medicine, and Genetics
T5	Infra	Infrastructure and Transportation
T6	Loc	Location and Administrative Entity
T7	Org	Organization and Membership
T8	People	People and Social Relationship
T9	Science	Science, Technology, and Language
T10	Sport	Sport, and Game Competition
T11	Tax	Taxonomy and Biology

	#Nodes	# Relations	#Triplets (Obv.)	#Triplets (Qry.)	Avg. Deg.
Art	10000	45	28023	3113	6.23
Award	10000	10	25056	2783	5.57
Edu	10000	15	14193	1575	3.15
Health	10000	20	15337	1703	3.41
Infra	10000	27	21646	2405	4.81
Loc	10000	35	80269	8918	17.84
Org	10000	18	30214	3357	6.71
People	10000	25	58530	6503	13.01
Sci	10000	42	12516	1388	2.78
Sport	10000	20	46717	5190	10.38
Tax	10000	31	19416	2157	4.32

[1] Wang, Xiaozhi, et al. "KEPLER: A unified model for knowledge embedding and pre-trained language representation." *Transactions of the Association for Computational Linguistics* 9 (2021): 176-194.

# Theory: A new notion of *Symmetry* in Knowledge Graphs

entity permutations

relation permutations

For any KG  $\mathbf{A}$

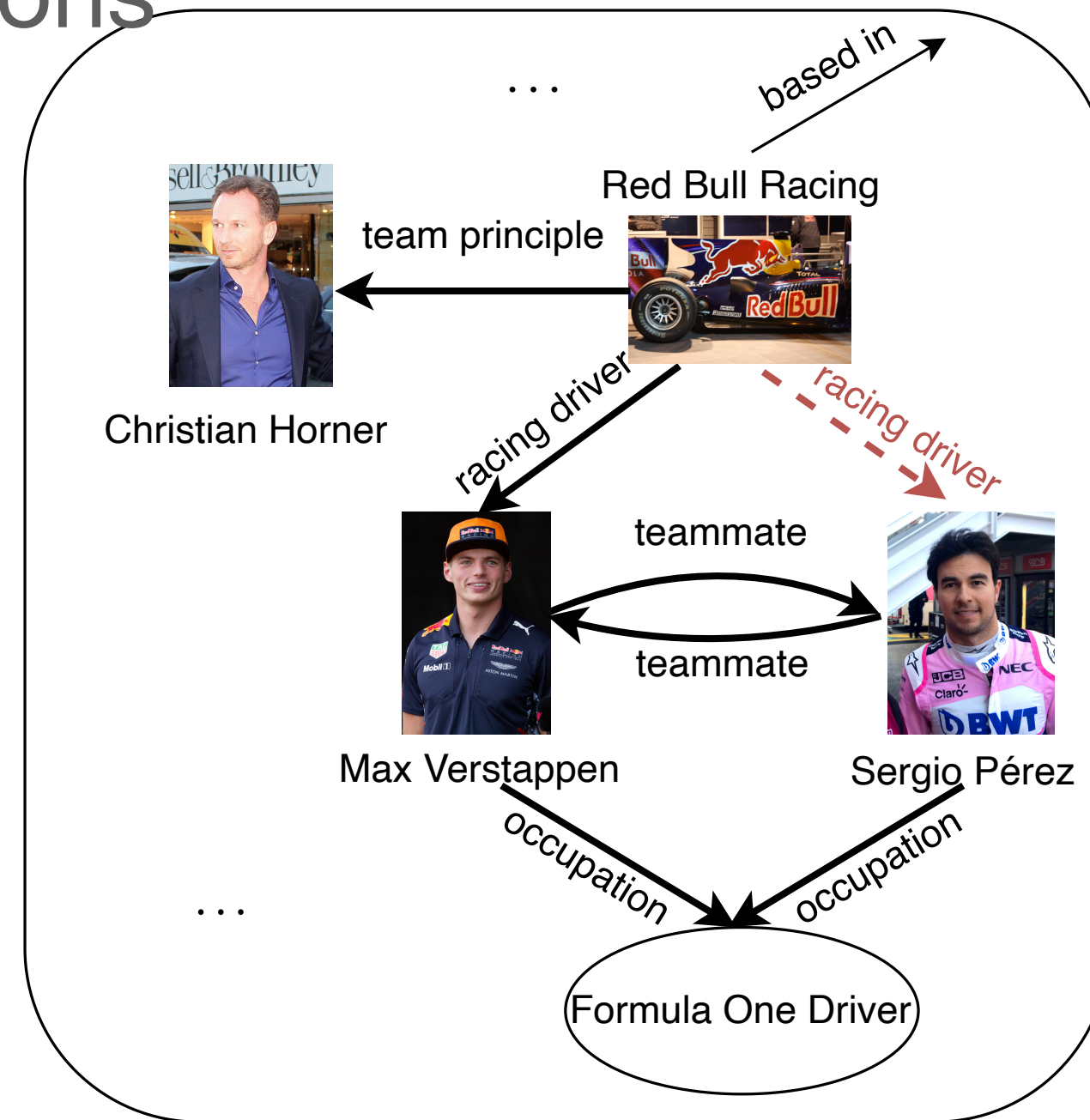
1.  $\mathbf{A} \neq \mathbf{A}'$ , and

2.  $\exists \pi_e \in \mathcal{S}_n, \exists \pi_r \in \mathcal{S}_m,$

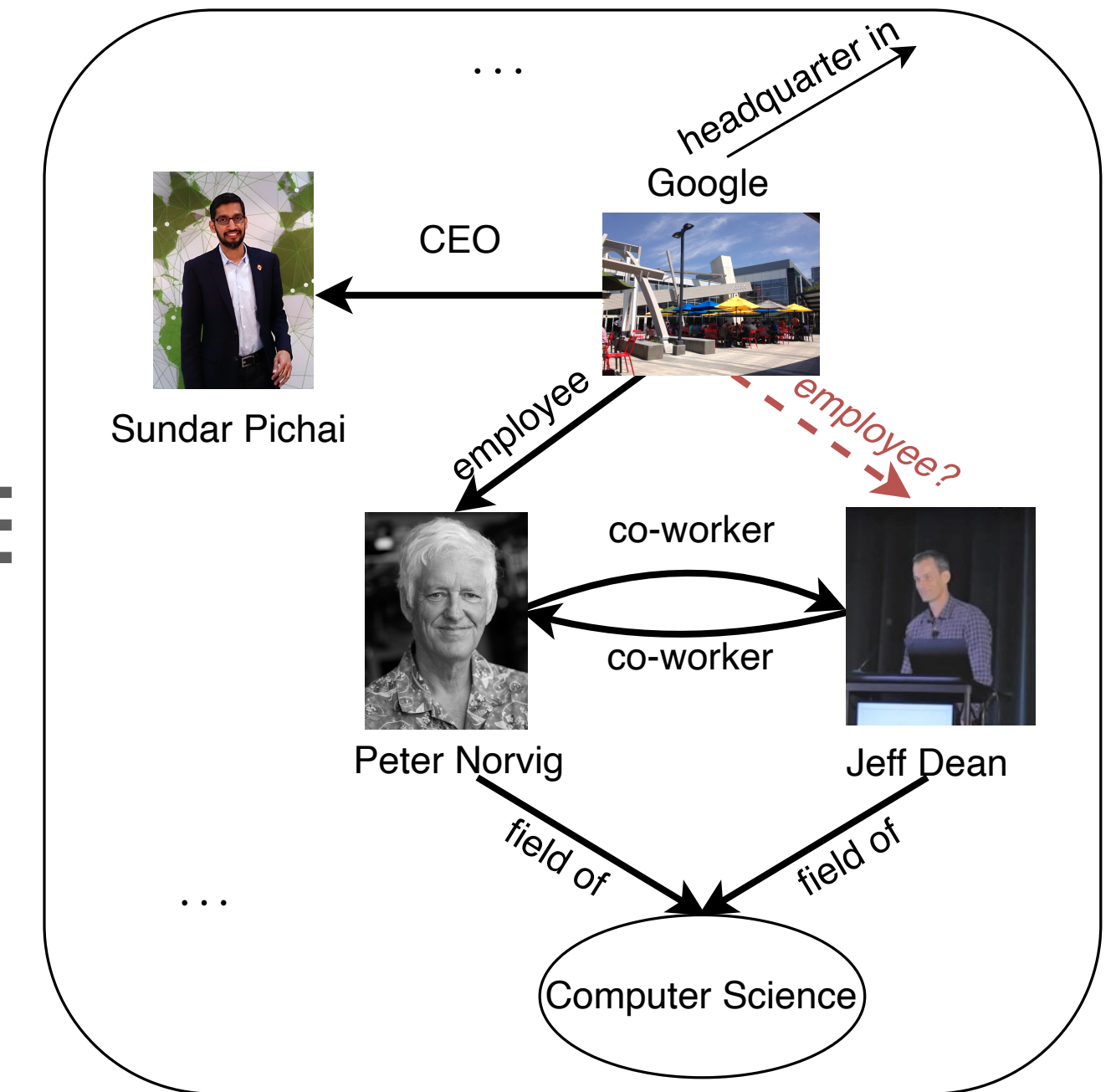
$$\mathbf{A}' = \pi_e \circ \pi_r \circ \mathbf{A}$$

we say  $\mathbf{A} \equiv \mathbf{A}'$  are **symmetric**

Train: Sports



Test: Organizations

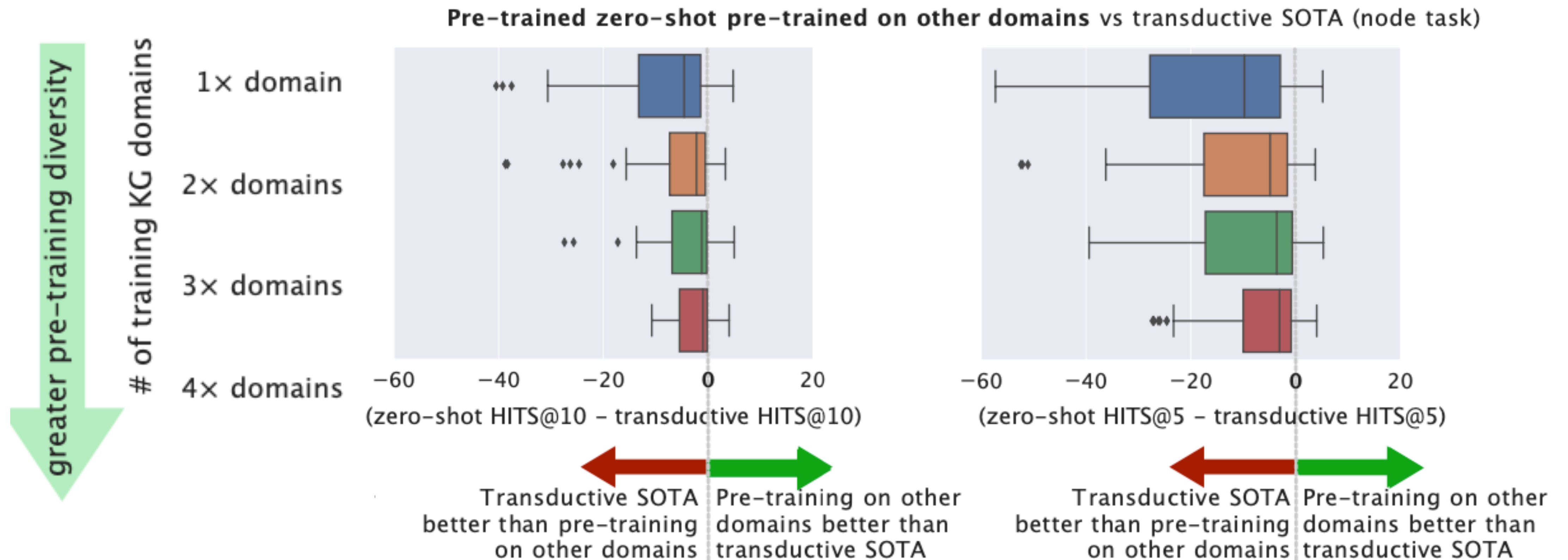


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**Key result: Double equivariant neural networks can provably and sufficiently perform zero-shot domain transfer**

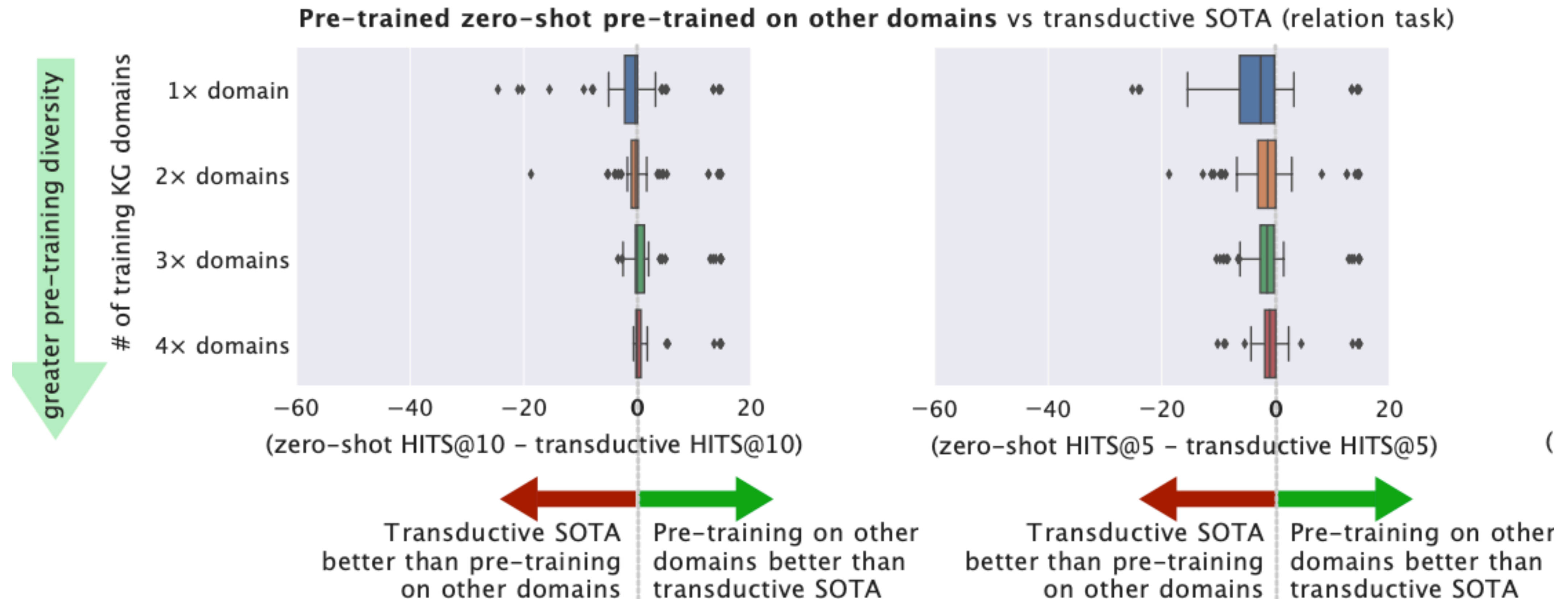
# ISDEA+: Transferability through double equivariance (2)

- Pre-train up to 4x domains, zero-shot test on new domain (no overlapping relations) to predict tail node (i,r,?)



# ISDEA+: Transferability through double equivariance (1)

- Pre-train up to 4x domains, zero-shot test on new domain (no overlapping relations) to predict relation (i,?,j)



# Summary and Q&A

- First **theoretical** definition of the task of **Doubly Inductive Link Prediction (zero-shot domain transfer)** in Knowledge Graphs
- Propose the theoretical concept of **double equivariant models**, sufficient to solve the task
- Develop a double equivariant model implementation, **ISDEA+** (details in poster)
- Introduce a novel zero-shot multi-domain KG benchmark: **WikiTopics**

**Thank you!**



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Scan for code  
& benchmarks