NEURAL INFORMATION PROCESSING SYSTEMS

Zero-shot Transfer Learning within a Heterogeneous Graph via Knowledge Transfer Networks

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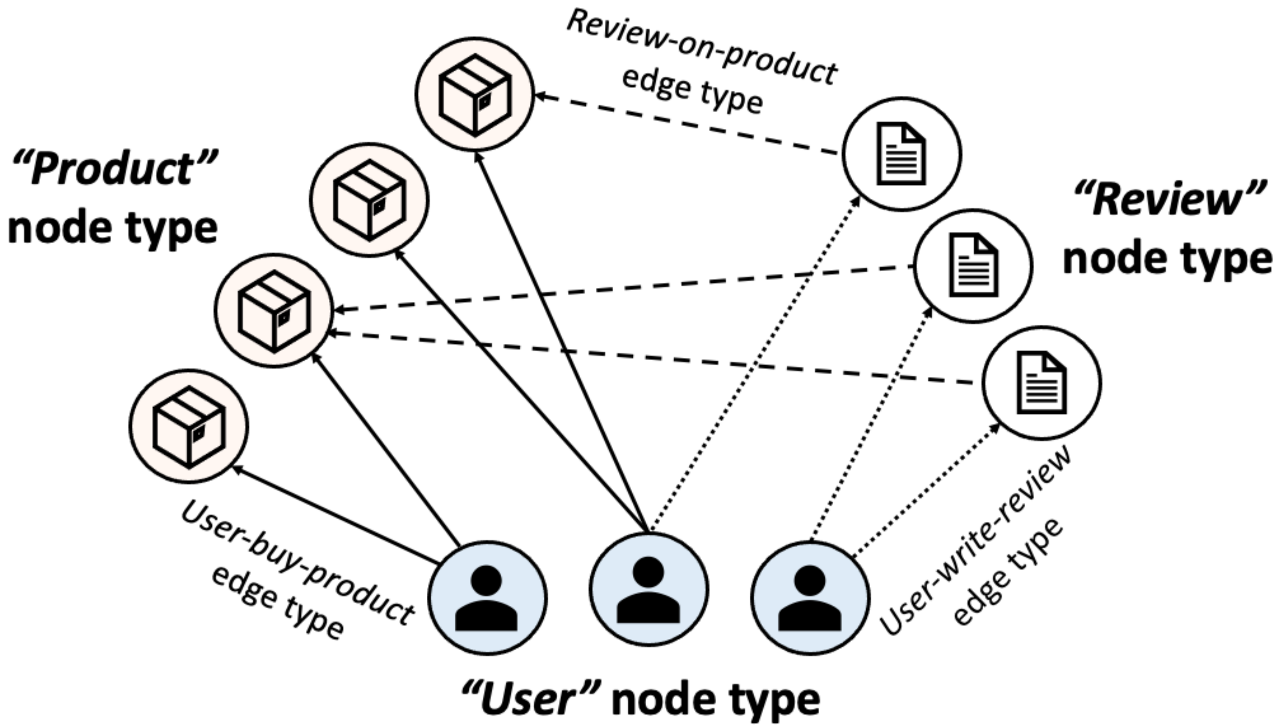
Heterogeneous Graphs (HG)

- Composed of multiple types of nodes and edges
- EX) e-commerce networks



Heterogeneous Graph Neural Networks (HGNNs)

- MPNNs for homogeneous graphs:

$$h_j^{(l)} = \alpha(\boxed{W^{(l)}} \cdot (\frac{1}{|\mathcal{E}(j)|} \sum_{e \in \mathcal{E}(j)} \boxed{M^{(l)}} \cdot \left(h_i^{(l-1)} \parallel h_j^{(l-1)}\right)))$$

Transformation parameters

Message-passing parameters

Heterogeneous Graph Neural Networks (HGNNs)

- MPNNs for homogeneous graphs:

$$h_j^{(l)} = \alpha\left(\boxed{W^{(l)}} \cdot \left(\frac{1}{|\mathcal{E}(j)|} \sum_{e \in \mathcal{E}(j)} \boxed{M^{(l)}} \cdot \left(h_i^{(l-1)} \,\|\, h_j^{(l-1)}\right)\right)\right)$$

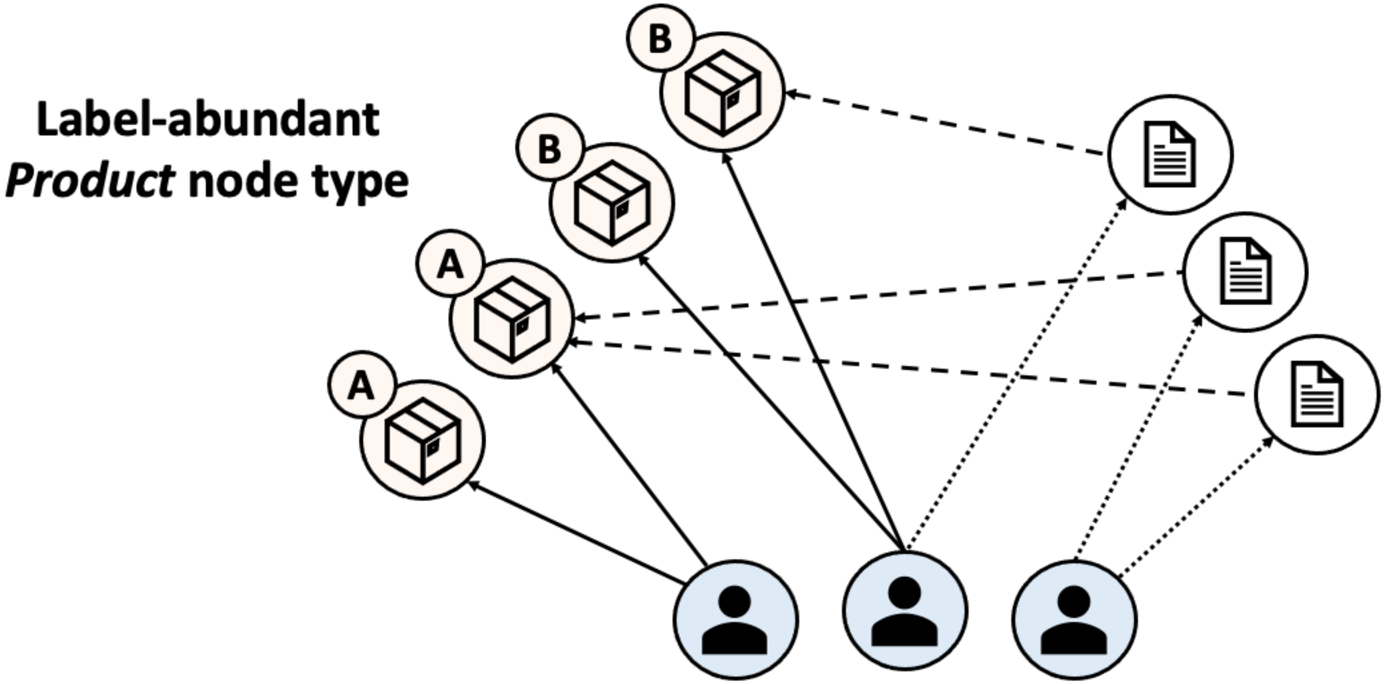
- H-MPNNs for heterogeneous graphs:

$$h_j^{(l)} = \alpha\left(\boxed{W_{\tau(j)}^{(l)}} \cdot \left(\big\|_{r \in \mathcal{R}} \frac{1}{|\mathcal{E}_r(j)|} \sum_{e \in \mathcal{E}_r(j)} \boxed{M_{\phi((i,j))}^{(l)}} \cdot \left(h_i^{(l-1)} \,\|\, h_j^{(l-1)}\right)\right)\right)$$

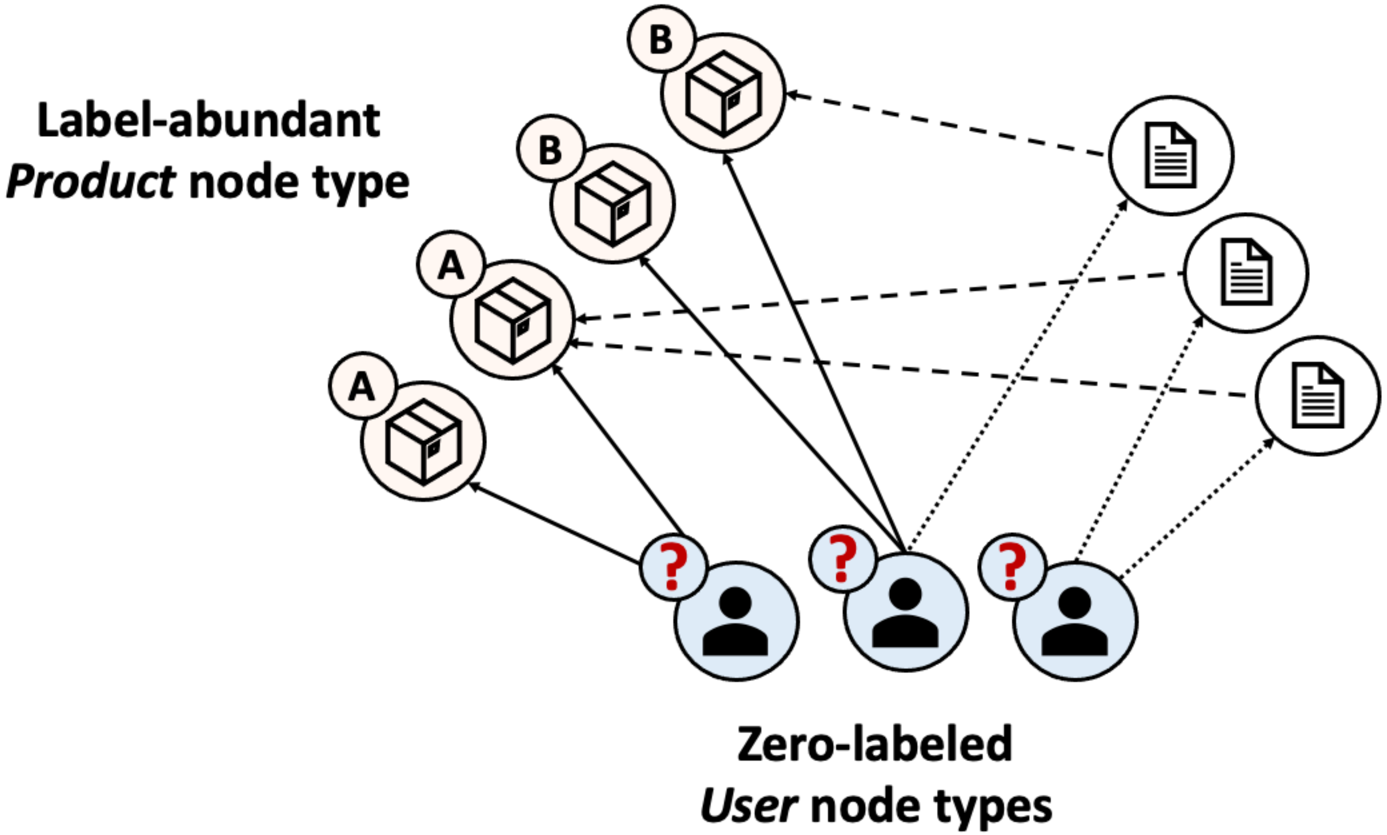
Node-type-specific transformation parameters

Edge-type-specific message-passing parameters

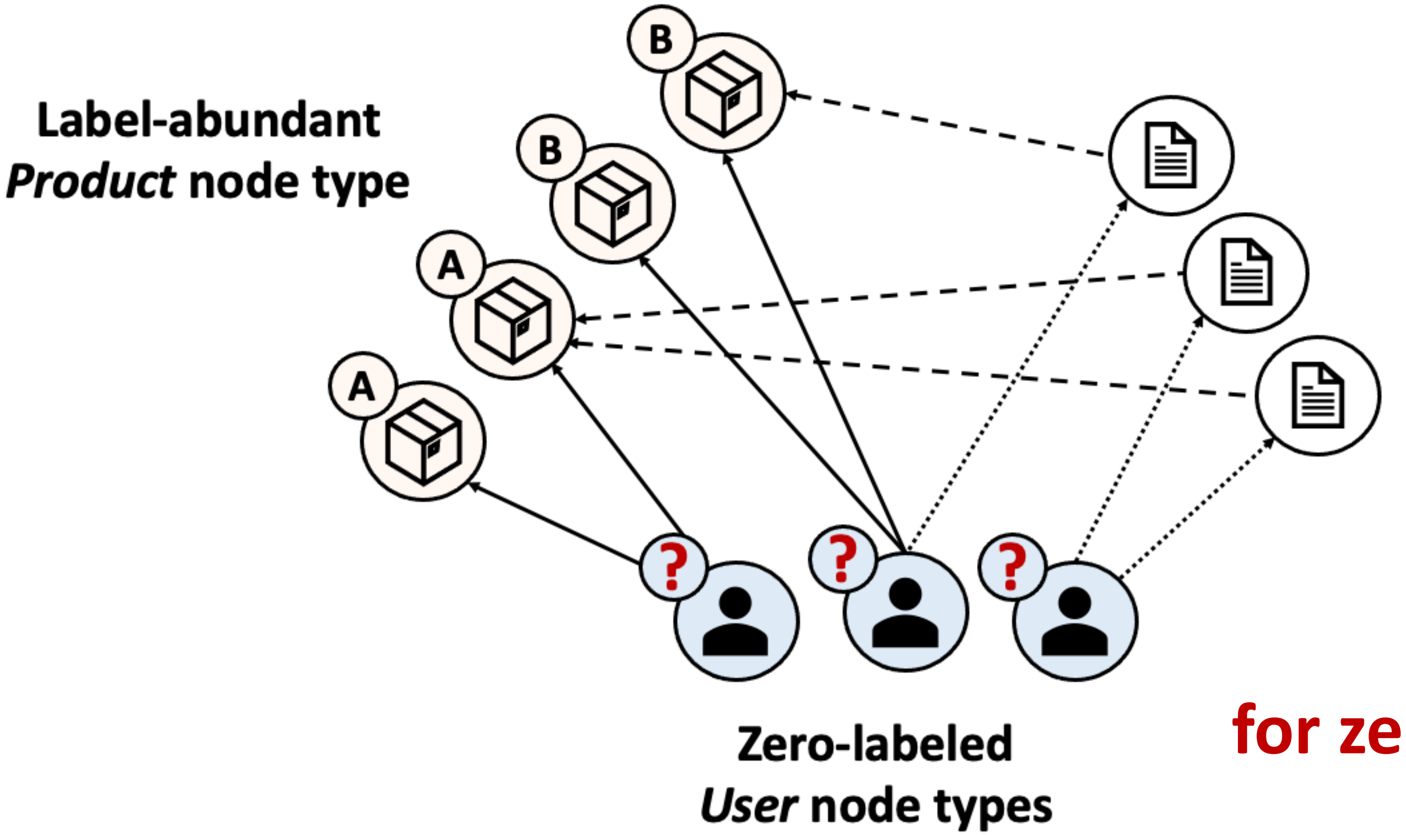
Label imbalance between node types



Label imbalance between node types

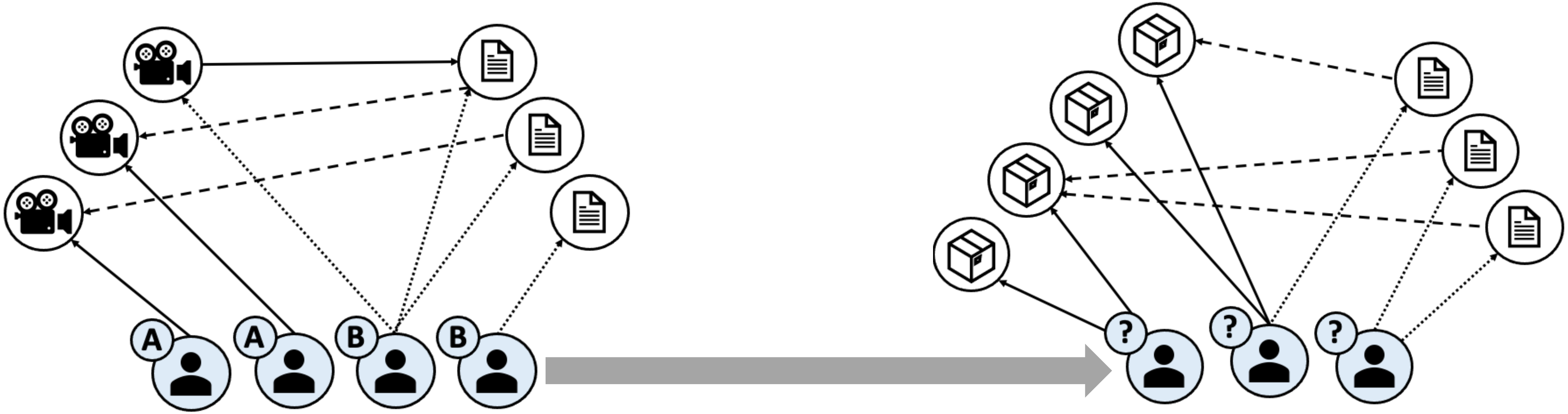


Label imbalance between node types



How can we train a HGNN model for zero-labeled node types?

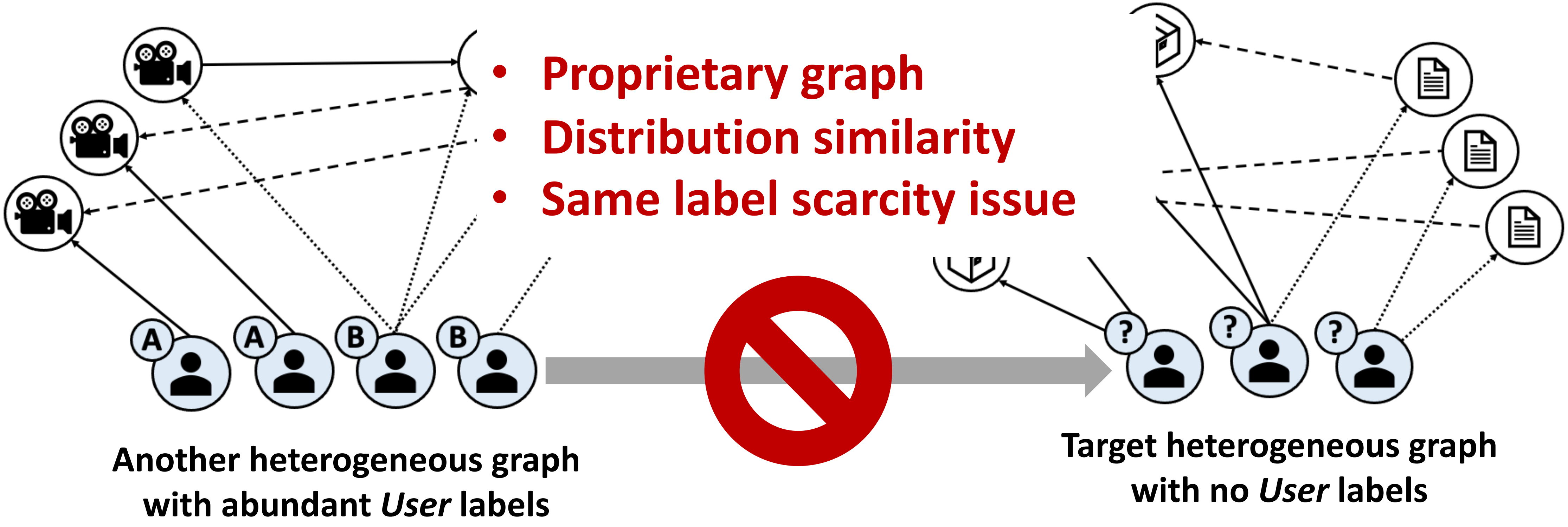
Previous approach:
Graph-to-Graph Transfer Learning



Another heterogeneous graph with abundant *User* labels

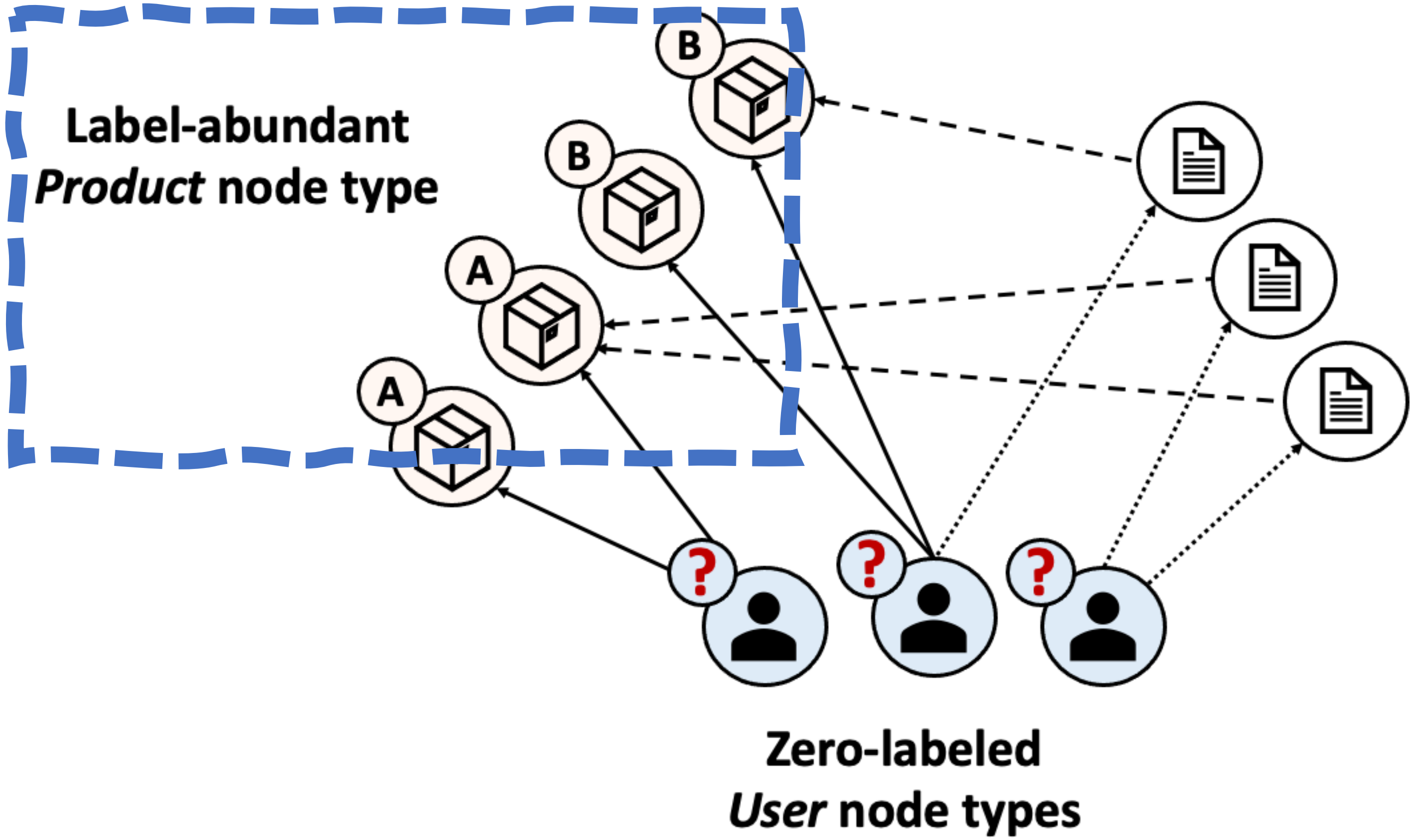
Target heterogeneous graph with no *User* labels

Previous approach:
Graph-to-Graph Transfer Learning

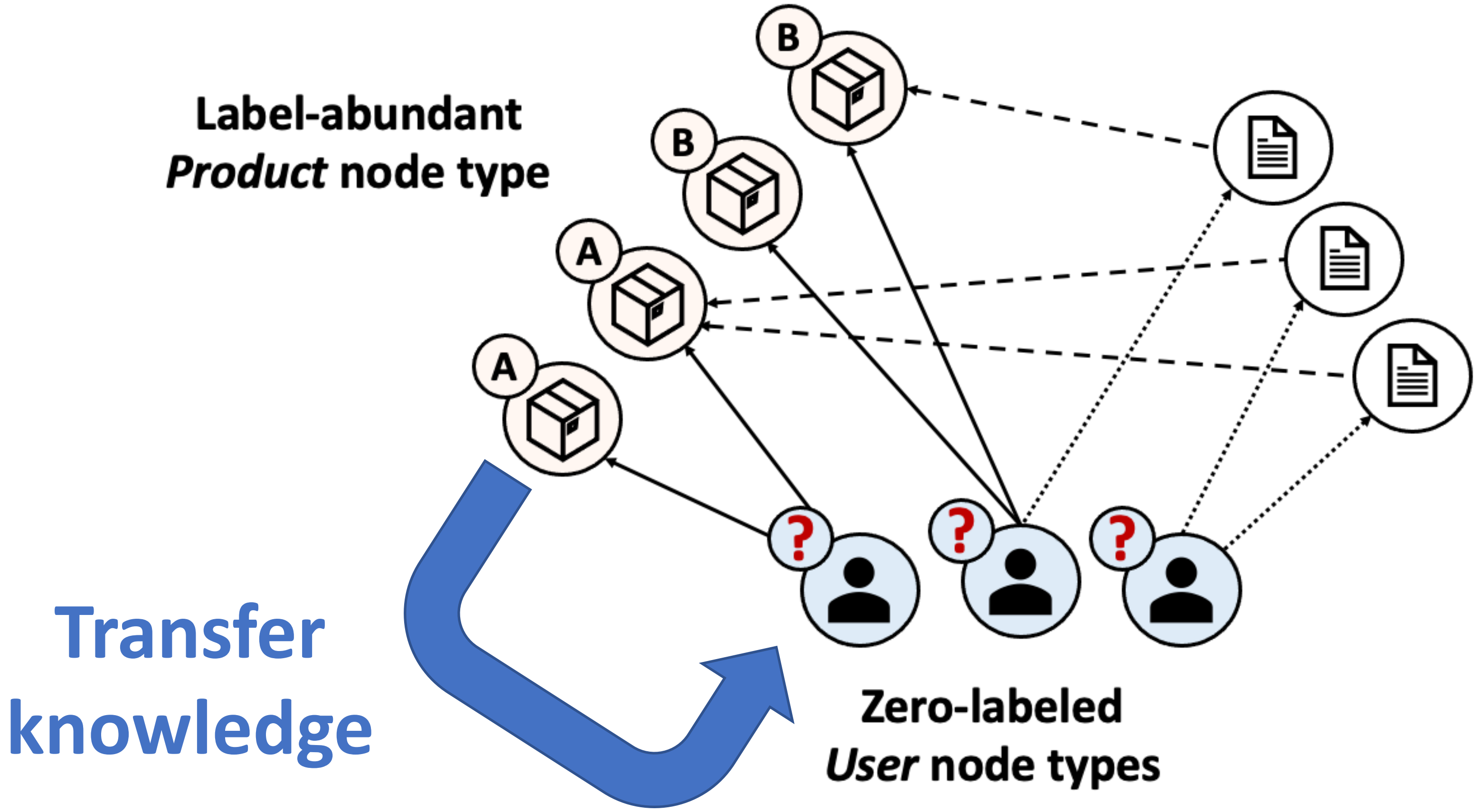


- Proprietary graph
- Distribution similarity
- Same label scarcity issue

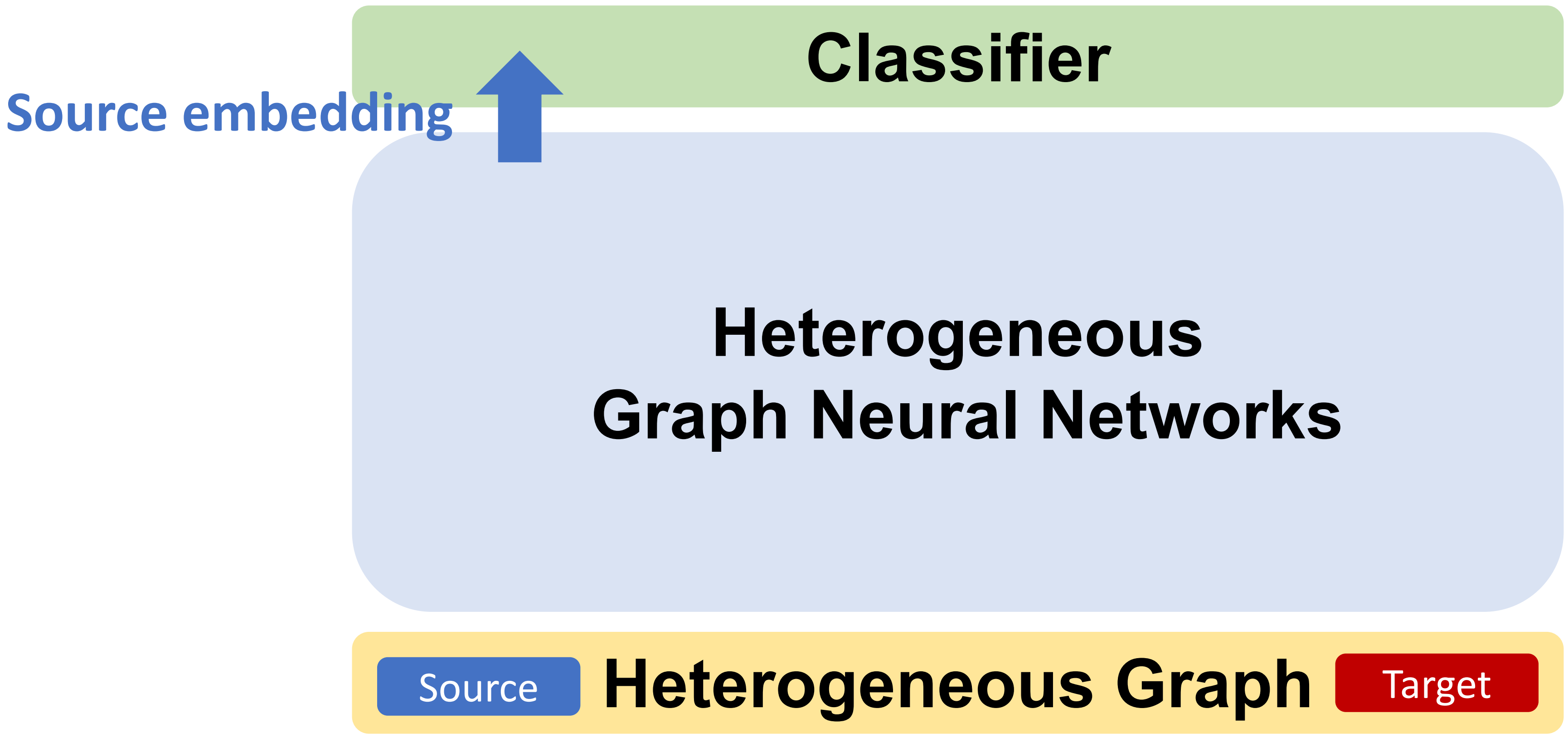
Transfer Learning within a Heterogeneous Graph



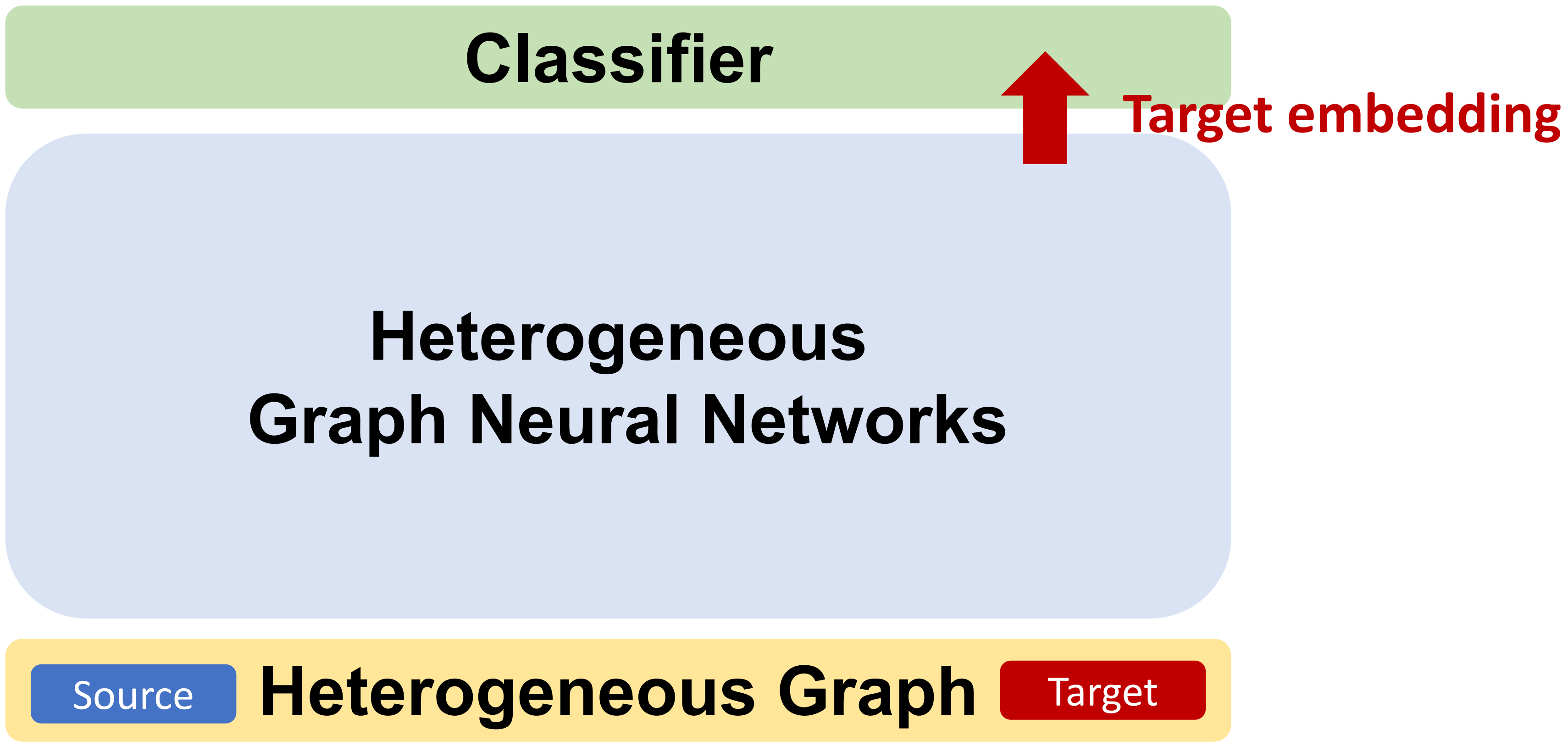
Transfer Learning within a Heterogeneous Graph



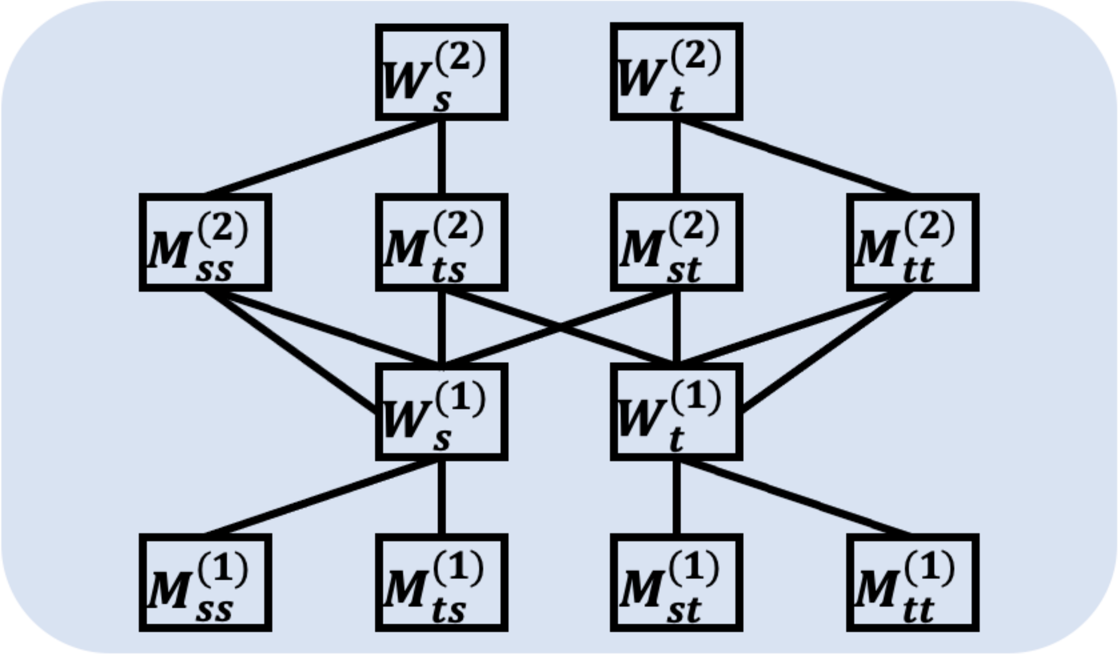
Is this problem challenging?



Is this problem challenging?



Distinct Feature Extractors in HGNNs



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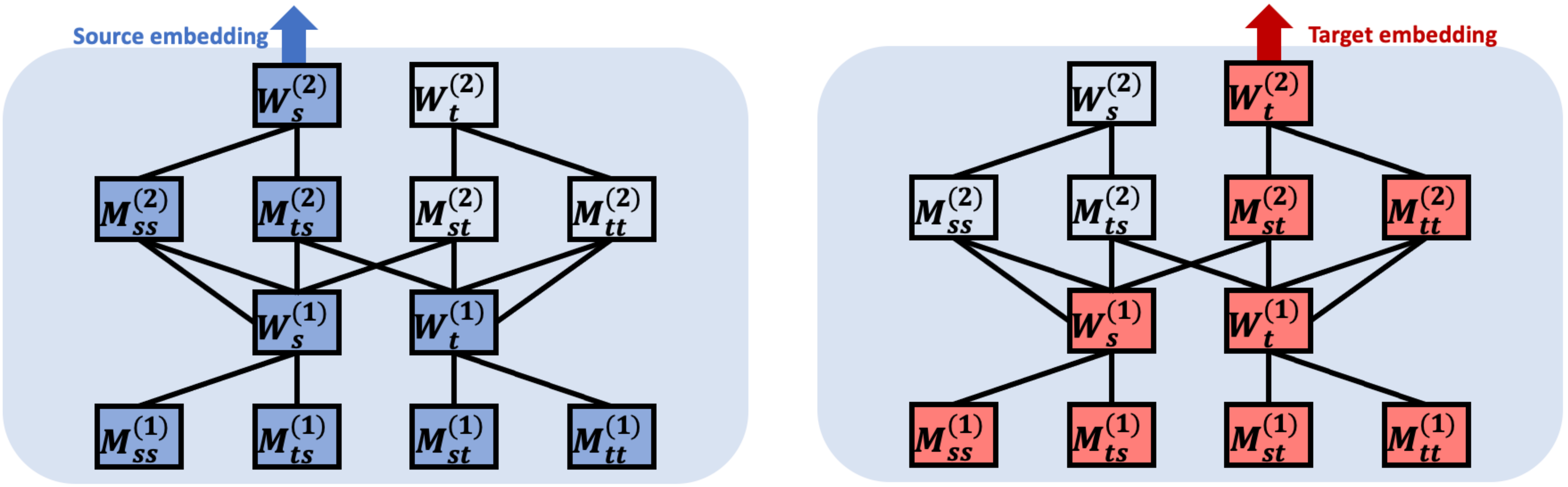
Distinct Feature Extractors in HGNNs



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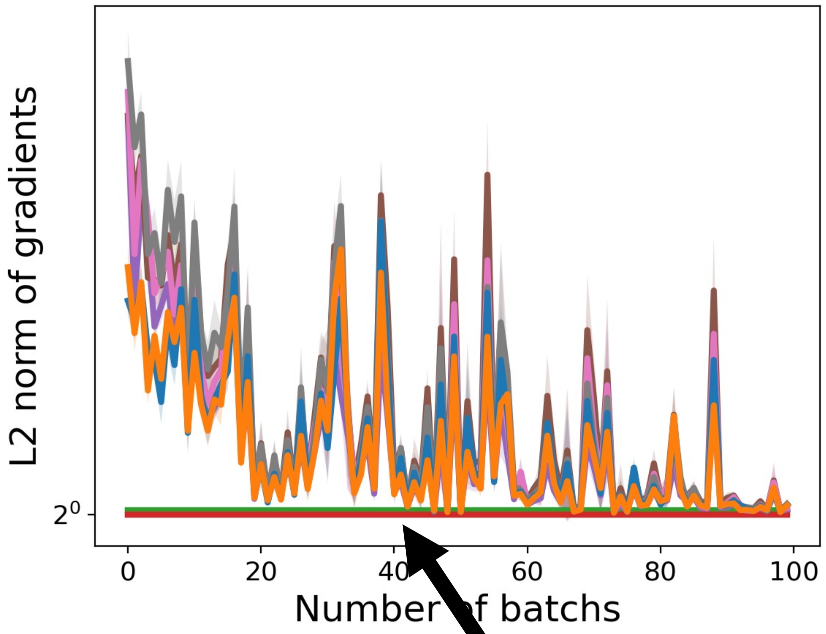
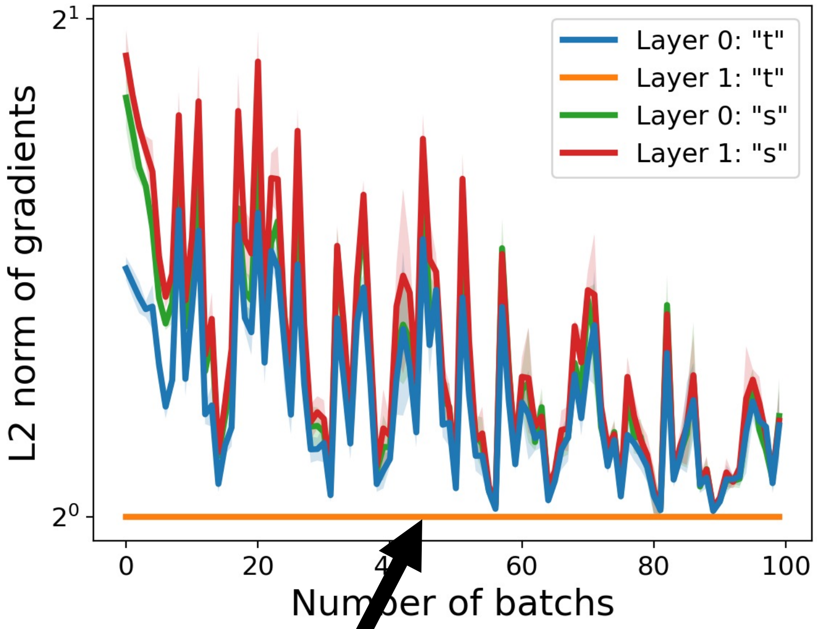
Distinct Feature Extractors in HGNNs





Small or no gradients
for target-type parameters

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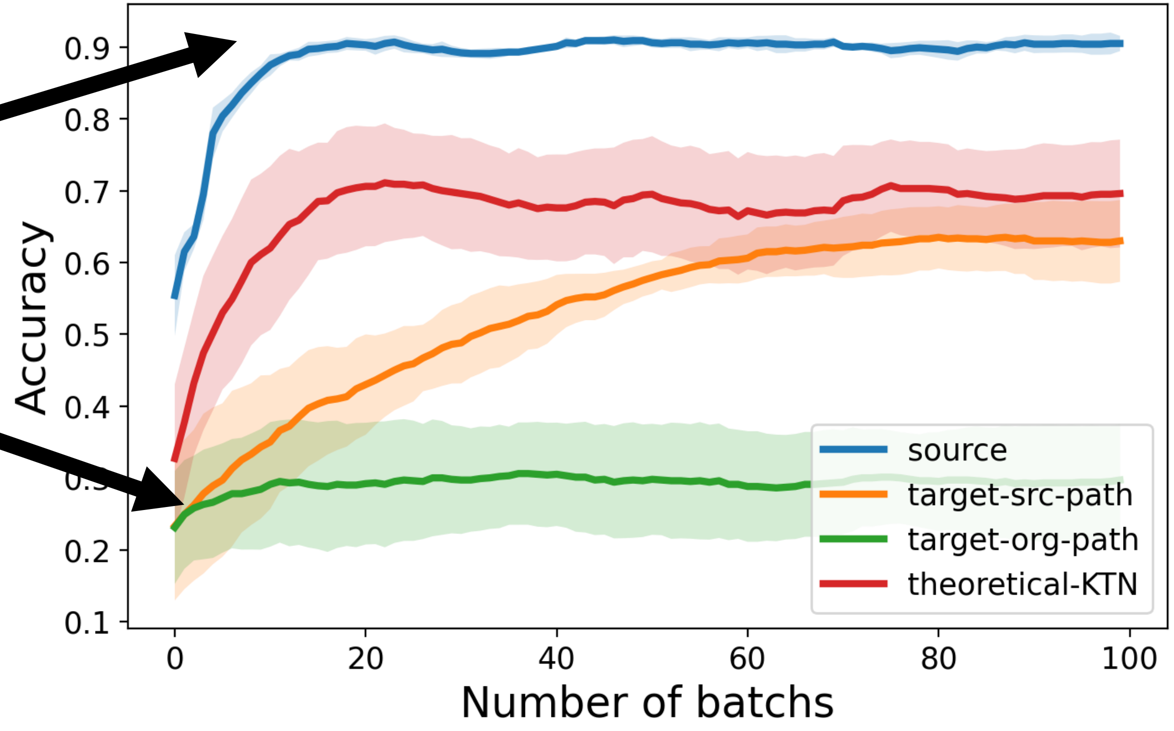
Distinct Feature Extractors in HGNNs

Poor target performance



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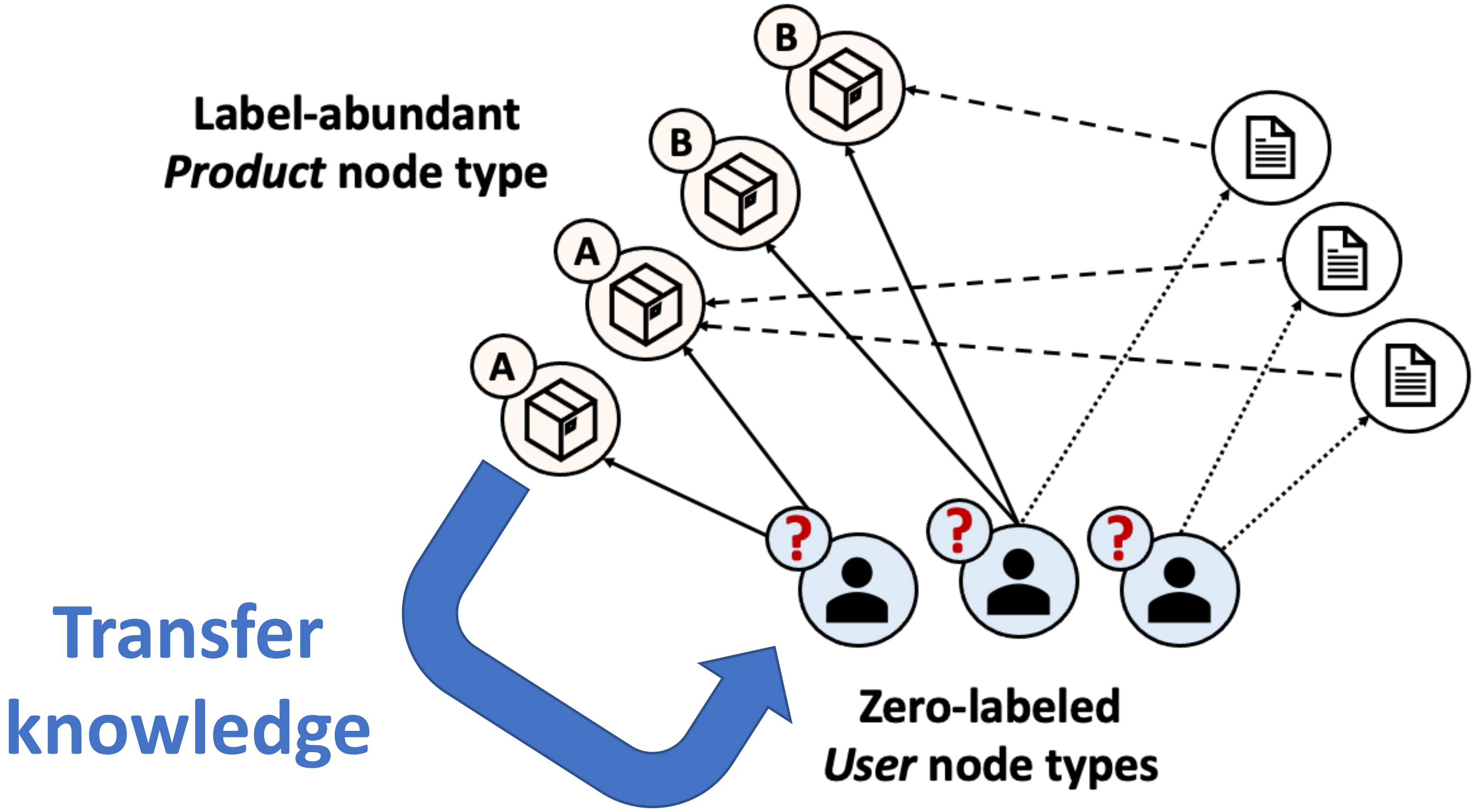
Then.. How can we solve this problem?



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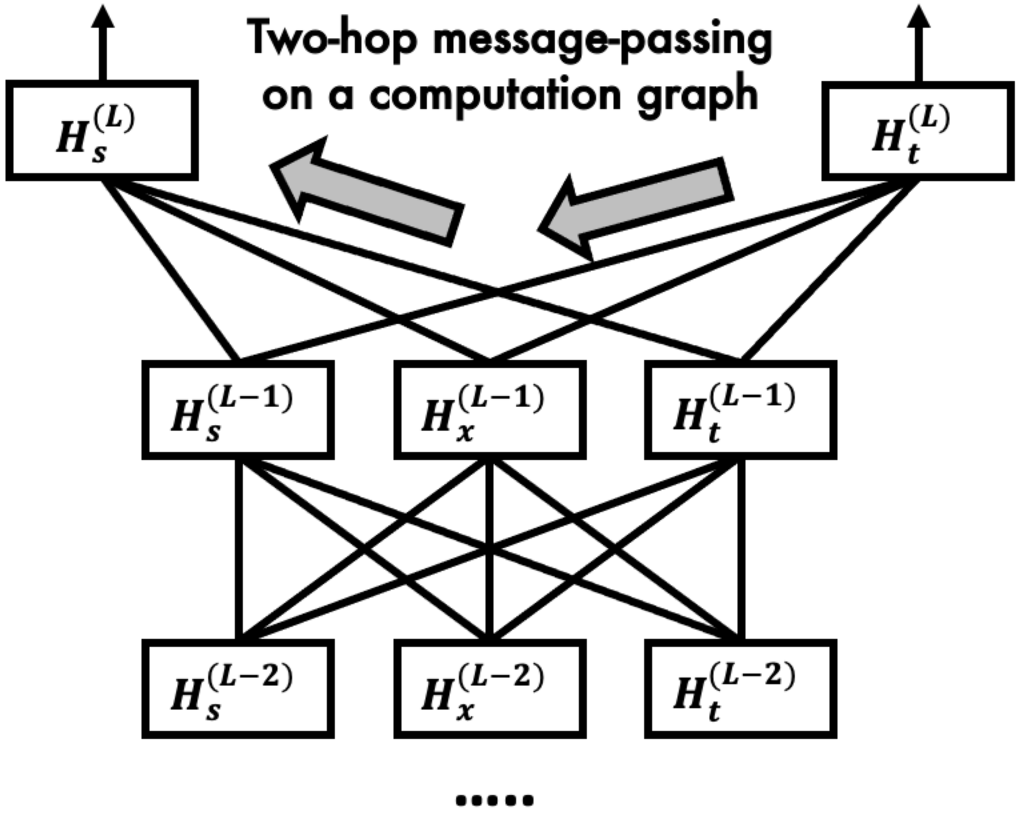
Hints: Relationship between Feature Extractors



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Theoretically-induced

Mapping Function between Feature Extractors

Theorem 1. *Given a heterogeneous graph* $\mathcal{G} = \{\mathcal{V}, \mathcal{E}, \mathcal{T}, \mathcal{R}\}$*. For any layer* $l > 0$*, define the set of* $(l-1)$-th *layer HMPNN parameters as*

$$\mathcal{Q}^{(l-1)} = \{M_r^{(l-1)} : r \in \mathcal{R}\} \cup \{W_t^{(l-1)} : t \in \mathcal{T}\}. \tag{9}$$

Let A *be the total* $n \times n$ *adjacency matrix. Then for any* $s, t \in \mathcal{T}$ *there exist matrices* $A^*_{ts} = a_{ts}(A)$ *and* $Q^*_{ts} = q_{ts}(\mathcal{Q}^{(l-1)})$ *such that*

$$H_s^{(l)} = A^*_{ts} H_t^{(l)} \boxed{Q^*_{ts}} \tag{10}$$

where $a_{ts}(\cdot)$ *and* $q_{ts}(\cdot)$ *are matrix functions that depend only on* s, t*.*

Hand-computed mapping functions

Proposed method:
Knowledge Transfer Networks (KTN)

$$\mathbf{t}_{\mathrm{KTN}}(H_t^{(L)}) = A_{ts} H_t^{(L)} \boxed{T_{ts}}$$

$$\mathcal{L}_{\mathrm{KTN}} = \left\| H_s^{(L)} - \mathbf{t}_{\mathrm{KTN}}(H_t^{(L)}) \right\|_2$$

Learnable mapping functions

Proposed method:
Knowledge Transfer Networks (KTN)

$$\mathbf{t}_{\mathrm{KTN}}(H_t^{(L)}) = A_{ts} H_t^{(L)} T_{ts}$$

$$\mathcal{L}_{\mathrm{KTN}} = \left\| H_s^{(L)} - \mathbf{t}_{\mathrm{KTN}}(H_t^{(L)}) \right\|_2$$

$$\underset{\mathbf{f},\ \mathbf{g},\ \mathbf{t}_{\mathrm{KTN}}}{min}\ \mathcal{L}_{\mathrm{CL}}(\mathbf{g}(\mathbf{f}(\mathcal{G}, \mathcal{X})_s), \mathcal{Y}_s) + \boxed{\lambda \left\| \mathbf{f}(\mathcal{G}, \mathcal{X})_s - \mathbf{t}_{\mathrm{KTN}}(\mathbf{f}(\mathcal{G}, \mathcal{X})_t) \right\|_2}$$

Knowledge transfer loss

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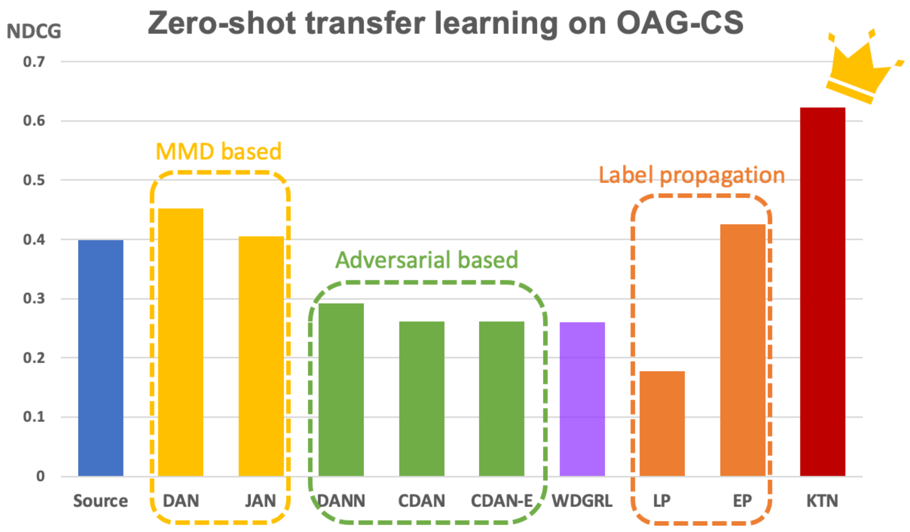
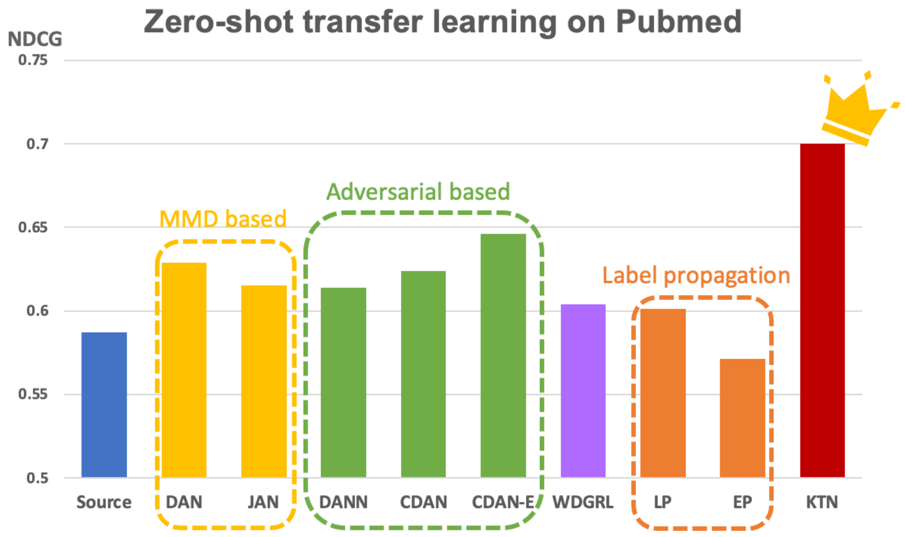
Experiment (1) Zero-shot Transfer Learning

- 18 different tasks
- 6 SOTA zero-shot transfer learning baselines
- 2 traditional label propagation baselines
- 73% higher in MRR





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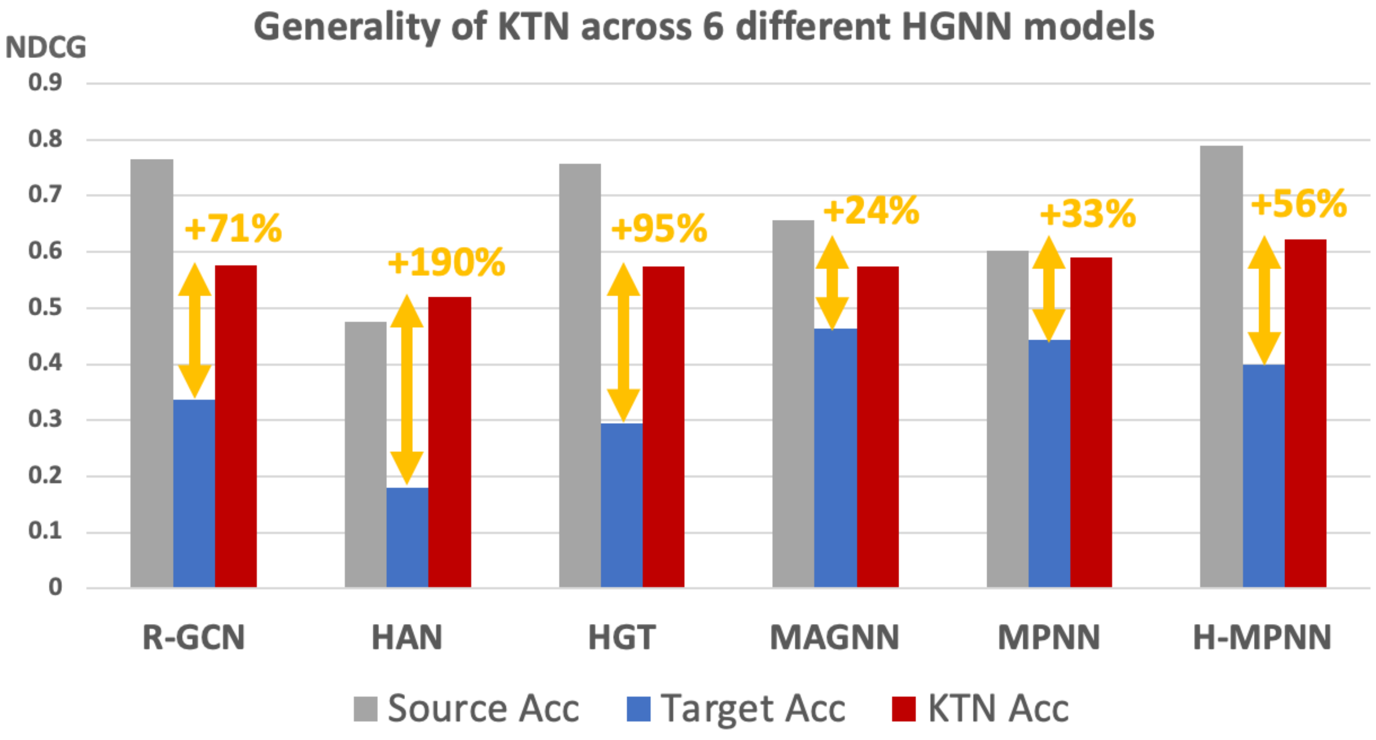
Experiment (2) Generality

- 6 different HGNN models
- 960% improvement



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Paper: www.minjiyoon.xyz/Paper/KTN.pdf
Code: https://github.com/minjiyoon/KTN

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