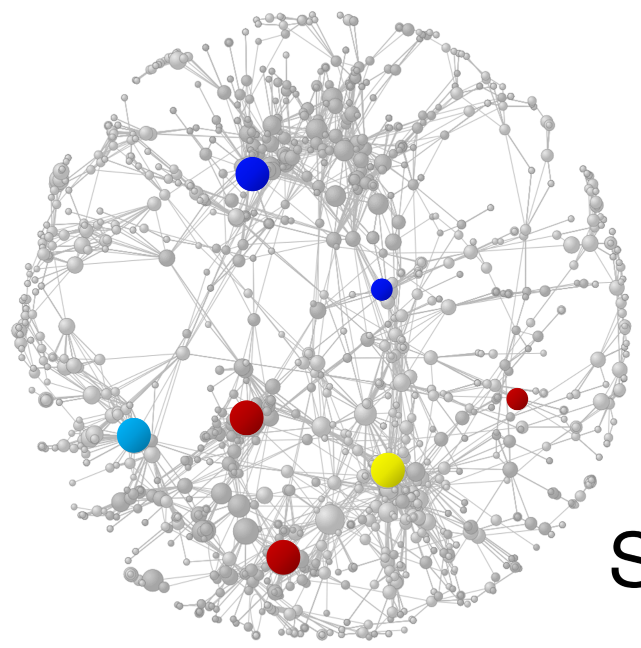
# Graph Meta Learning via Local Subgraphs

*How to adapt to a never-before-seen graph or a label set with only a handful of labels?*

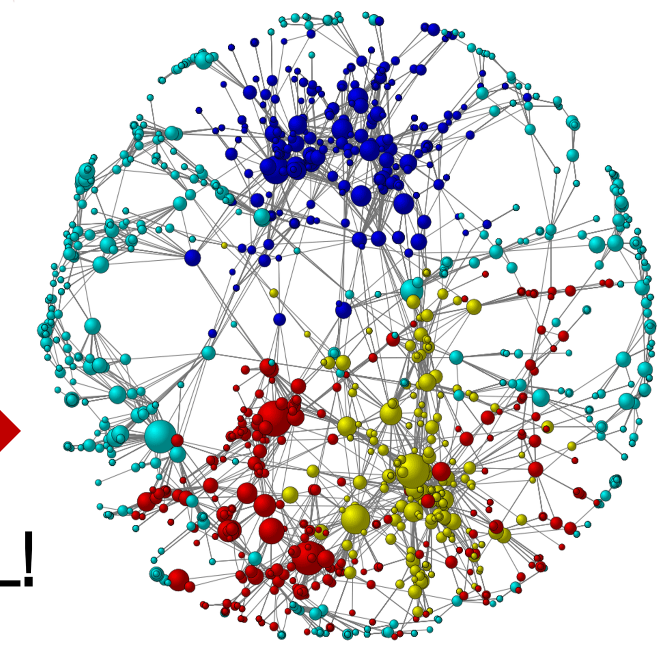
Kexin Huang, Marinka Zitnik kexinhuang@hsph.harvard.edu, marinka@hms.harvard.edu

HARVARD UNIVERSITY

NEURAL INFORMATION PROCESSING SYSTEMS



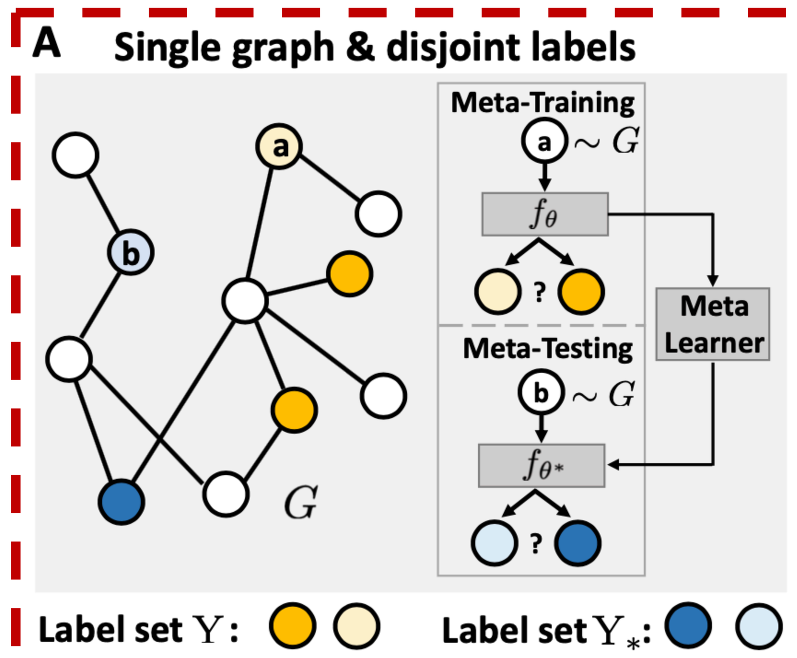
Graph Few-shot Learning?



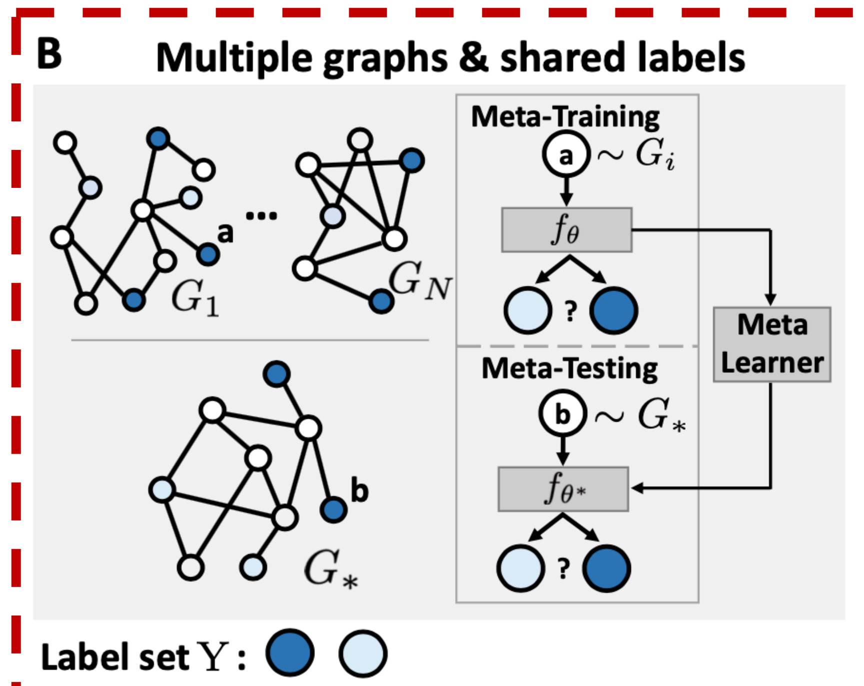
SOTA GNNs: FAIL!

Learning from related tasks? Obtain the learning ability to quickly adapt using a few data (meta learning)!

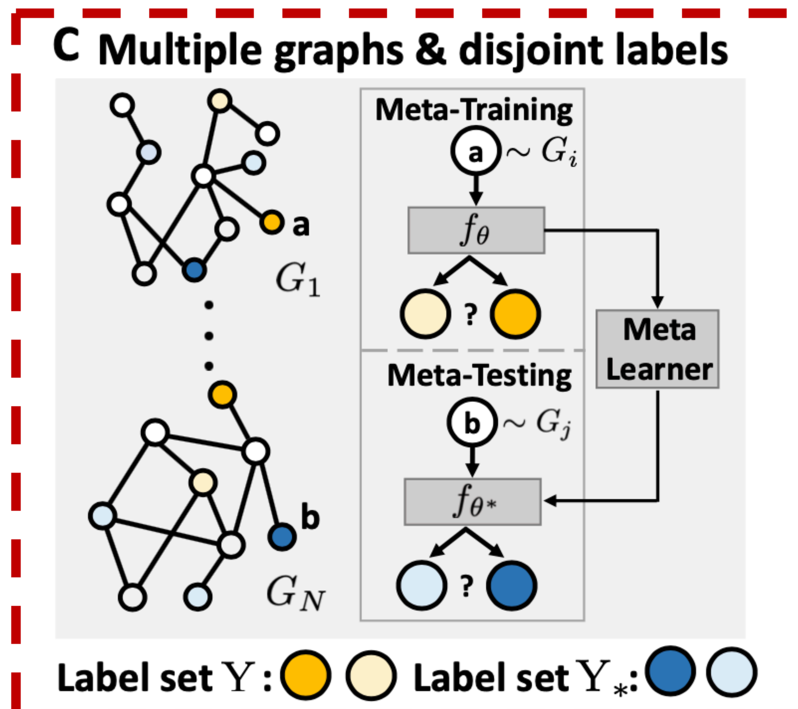
## Graph Meta Learning Problems




Meta-learner classifies unseen label set by observing other label sets in the same graph.



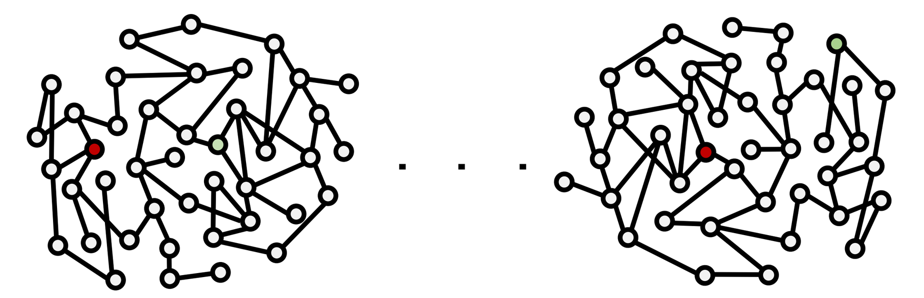

Meta-learner learns unseen graph by learning from other graphs with the same label set




Meta-learner classifies unseen label set by learning from other label sets across multiple graphs.

## How to design good graph meta-learners?

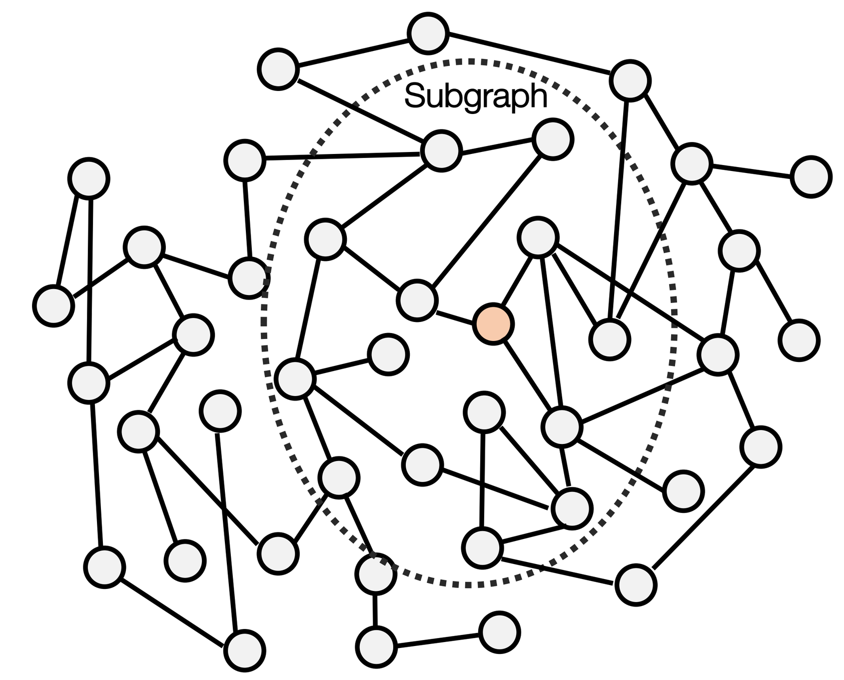
### Status Quo



1st Graph 1,000th Graph

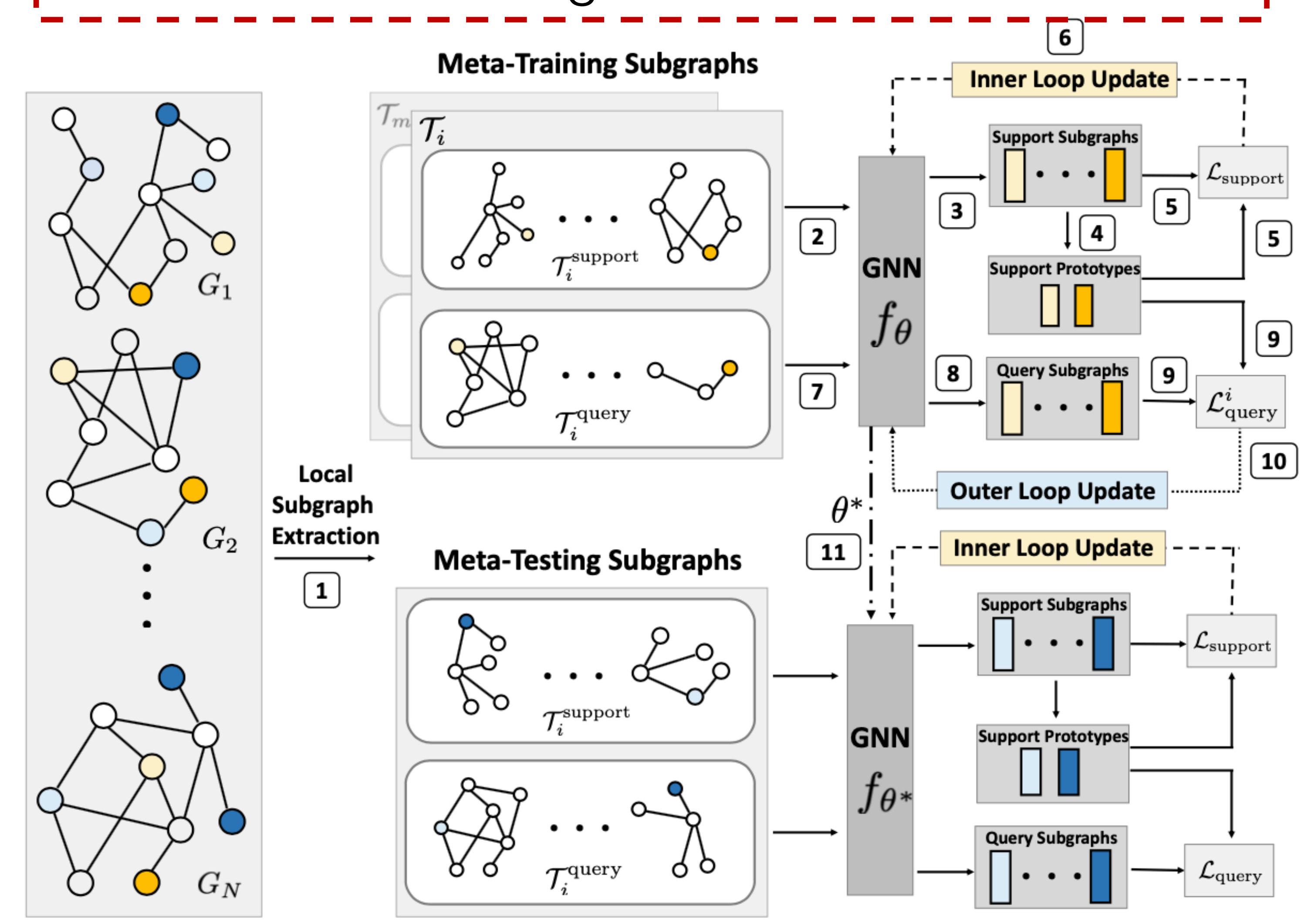
Propagate with ten labels in 1,000 graphs with millions of nodes?

### G-Meta



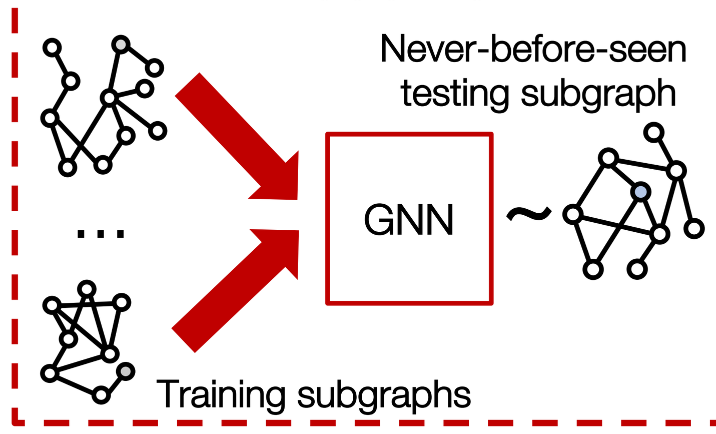

Extract Subgraphs around the few labels and apply GNN on each subgraph individually.

**Analysis**: Subgraph formulation 1. captures local graph structures; 2. preserves features; 3. allows metric learning on labels.

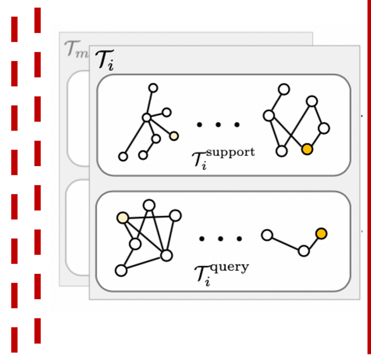



## Attractive Properties of G-Meta

### Inductive



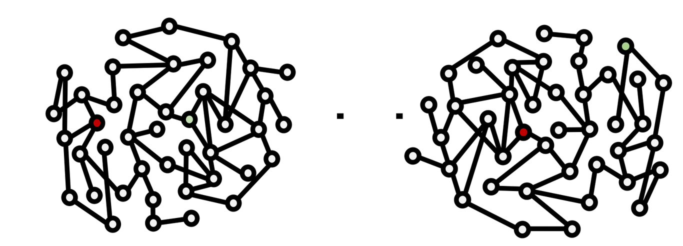

### Broadly Applicable



Subgraph formulation breaks the dependency across graphs and across label sets.

### Scalable

Suppose multiples graphs with millions of nodes and a 3-ways 3-shots task.



1st Graph 1,000th Graph

Status Quo: Majority of message-passing are wasted!

G-Meta: only use the local subgraphs of these 3 x 3 nodes for the task!

## Datasets

**Table 1:** Dataset statistics. Fold-PPI and Tree-of-Life are new datasets introduced in this study.

| | Dataset | Task | # Graphs | # Nodes | # Edges | # Features | # Labels |
|---|---|---|---|---|---|---|---|
| | Synthetic Cycle | Node | 10 | 11,476 | 19,687 | N/A | 17 |
| | Synthetic BA | Node | 10 | 2,000 | 7,647 | N/A | 10 |
| | ogbn-arxiv | Node | 1 | 169,343 | 1,166,243 | 128 | 40 |
| | Tissue-PPI | Node | 24 | 51,194 | 1,350,412 | 50 | 10 |
| | FirstMM-DB | Link | 41 | 56,468 | 126,024 | 5 | 2 |
| New! | Fold-PPI | Node | 144 | 274,606 | 3,666,563 | 512 | 29 |
| | Tree-of-Life | Link | 1,840 | 1,450,633 | 8,762,166 | N/A | 2 |

## Results

| Graph Meta-Learning Problem | Single graph Disjoint labels | Multiple graphs Shared labels | Multiple graphs Disjoint labels | Multiple graphs Shared labels | Multiple graphs Shared labels |
|---|---|---|---|---|---|
| Prediction Task | Node | Node | Node | Link | Link |
| Dataset | ogbn-arxiv | Tissue-PPI | Fold-PPI | FirstMM-DB | Tree-of-Life |
| G-META (Ours) | **0.451**±0.032 | **0.768**±0.029 | **0.561**±0.059 | **0.784**±0.028 | **0.722**±0.032 |
| Meta-Graph | N/A | N/A | N/A | 0.719±0.020 | 0.705±0.004 |
| Meta-GNN | 0.273±0.122 | N/A | N/A | N/A | N/A |
| FS-GIN | 0.336±0.042 | N/A | N/A | N/A | N/A |
| FS-SGC | 0.347±0.005 | N/A | N/A | N/A | N/A |
| KNN | 0.392±0.015 | 0.619±0.025 | 0.433±0.034 | 0.603±0.072 | 0.649±0.012 |
| No-Finetune | 0.364±0.014 | 0.516±0.006 | 0.376±0.017 | 0.509±0.006 | 0.505±0.001 |
| Finetune | 0.359±0.010 | 0.521±0.013 | 0.370±0.022 | 0.511±0.007 | 0.504±0.003 |
| ProtoNet | 0.372±0.017 | 0.546±0.025 | 0.382±0.031 | 0.779±0.020 | 0.697±0.010 |
| MAML | 0.389±0.021 | 0.745±0.051 | 0.482±0.062 | 0.758±0.025 | 0.719±0.012 |

- G-Meta can successfully learn in challenging, few-shot learning settings: up to 29.9 % over previous works and 16.3 % over other meta learning methods!
- G-Meta scales to large graphs: on our new Tree-of-Life dataset comprising of 1,840 graphs!

Project Website: zitniklab.hms.harvard.edu/projects/G-Meta GitHub: https://github.com/mims-harvard/G-Meta arXiv Paper: arxiv.org/abs/2006.07889