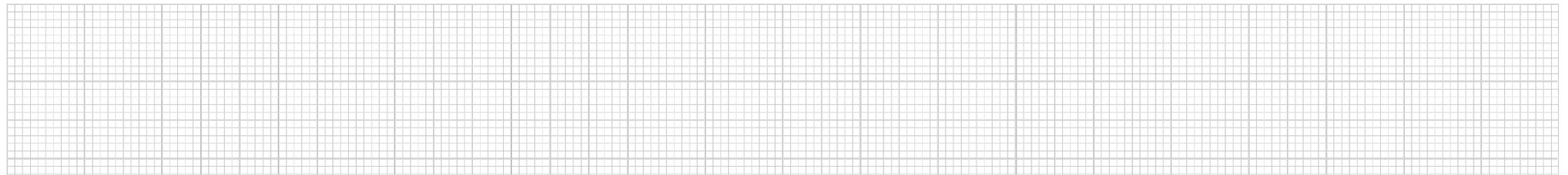




NeurIPS 2023:

Hyperbolic Graph Neural Networks at Scale: A Meta Learning Approach

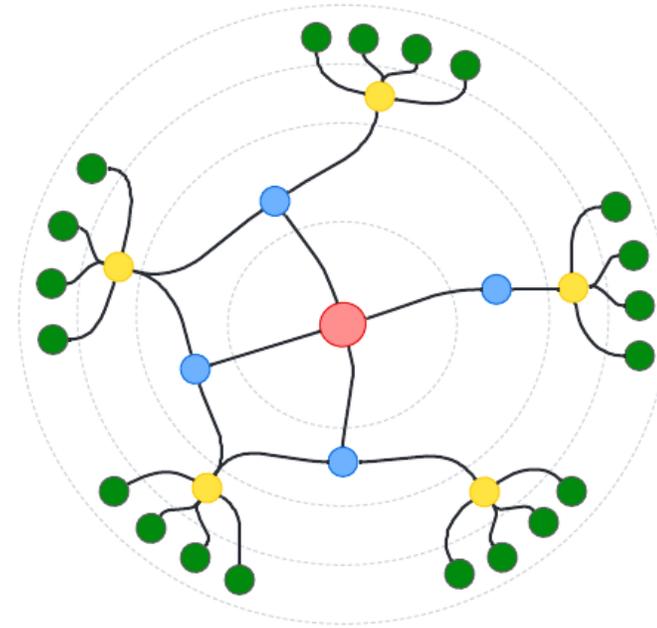
Authors: Nurendra Choudhary, Nikhil Rao, Chandan K. Reddy



Introduction

Scalable hyperbolic models

- In Euclidean Graphs, we depend on **local subgraph encodings** to scale over large graph datasets.
- In Hyperbolic Graphs, we are **not able to directly** apply this because the representations are relative to an **origin**.

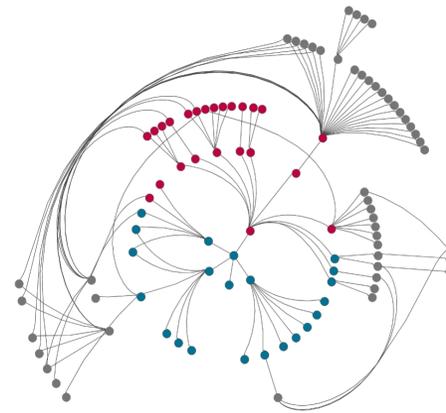


Hyperbolic Embeddings

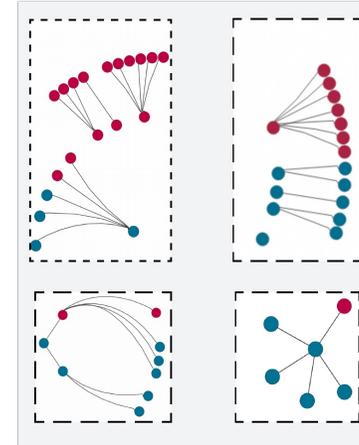
Our Solution: H-GRAM

Key Ideas

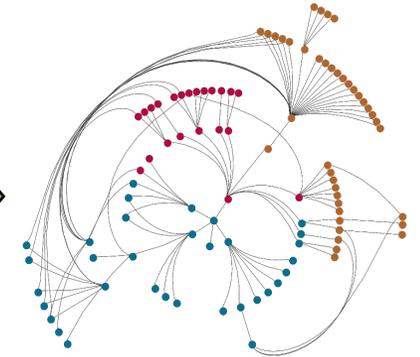
- It can be theoretically shown that one can **move the origin to local subgraphs** with a **bounded information loss**.



Generic graph with labeled samples (**red** and **blue**) and unlabeled samples (**silver**).



Meta learning structure priors on the labeled local partitions of the graph.

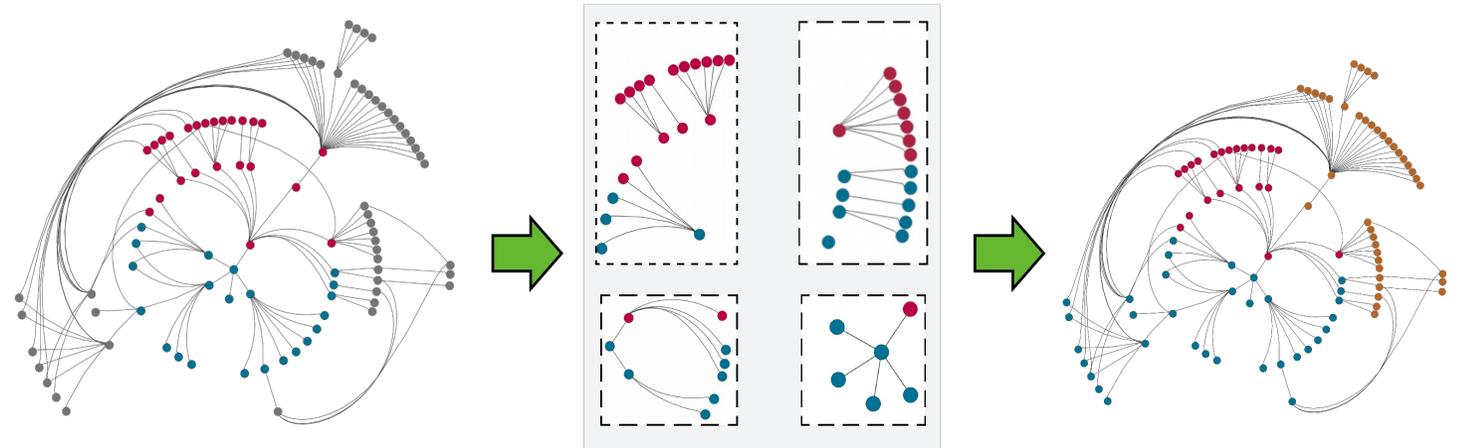


Utilize the meta information for faster learning over new nodes, edges and labels (**yellow** in this case).

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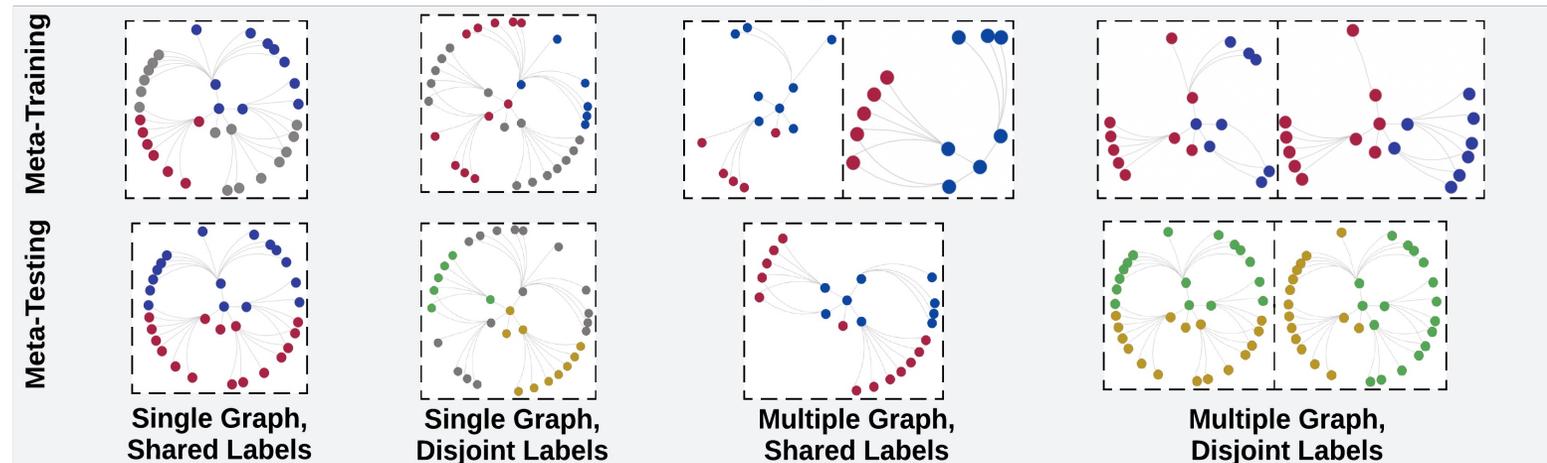
Graph Sections

- It can be theoretically shown that one can **move the origin to local subgraphs** with a **bounded information loss**.
- Divide the graph into subgraphs and note **four possible scenarios**:
 - Single Graph, Shared Labels
 - Single Graph, Disjoint Labels
 - Multiple Graph, Shared Labels
 - Multiple Graph, Disjoint Labels



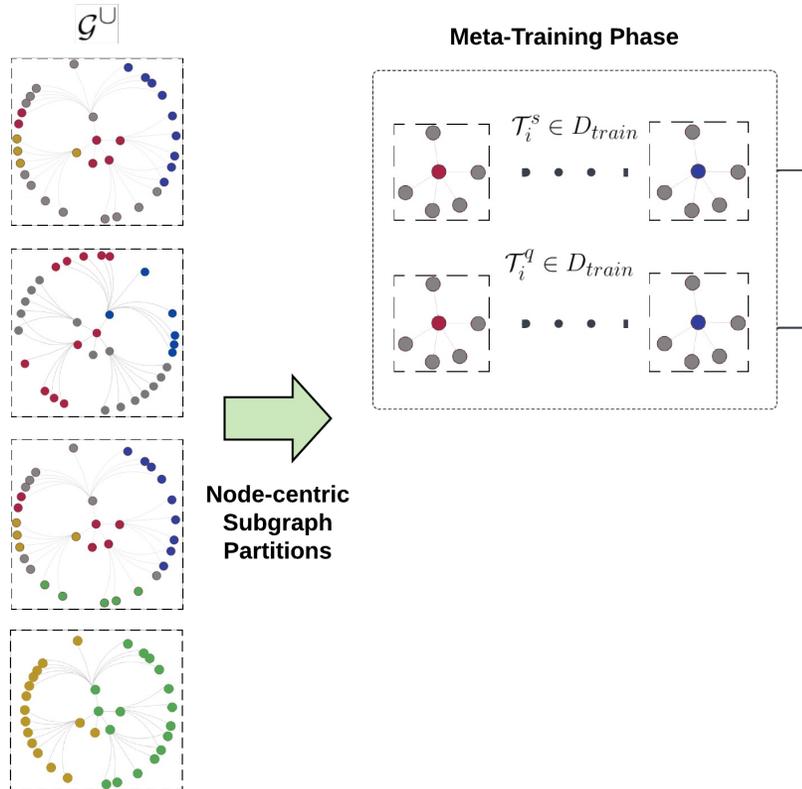
Generic graph with labeled samples (red and blue) and unlabeled samples (silver). Meta learning structure priors on the labeled local partitions of the graph.

Utilize the meta information for faster learning over new nodes, edges and labels (yellow in this case).



Our Solution: H-GRAM

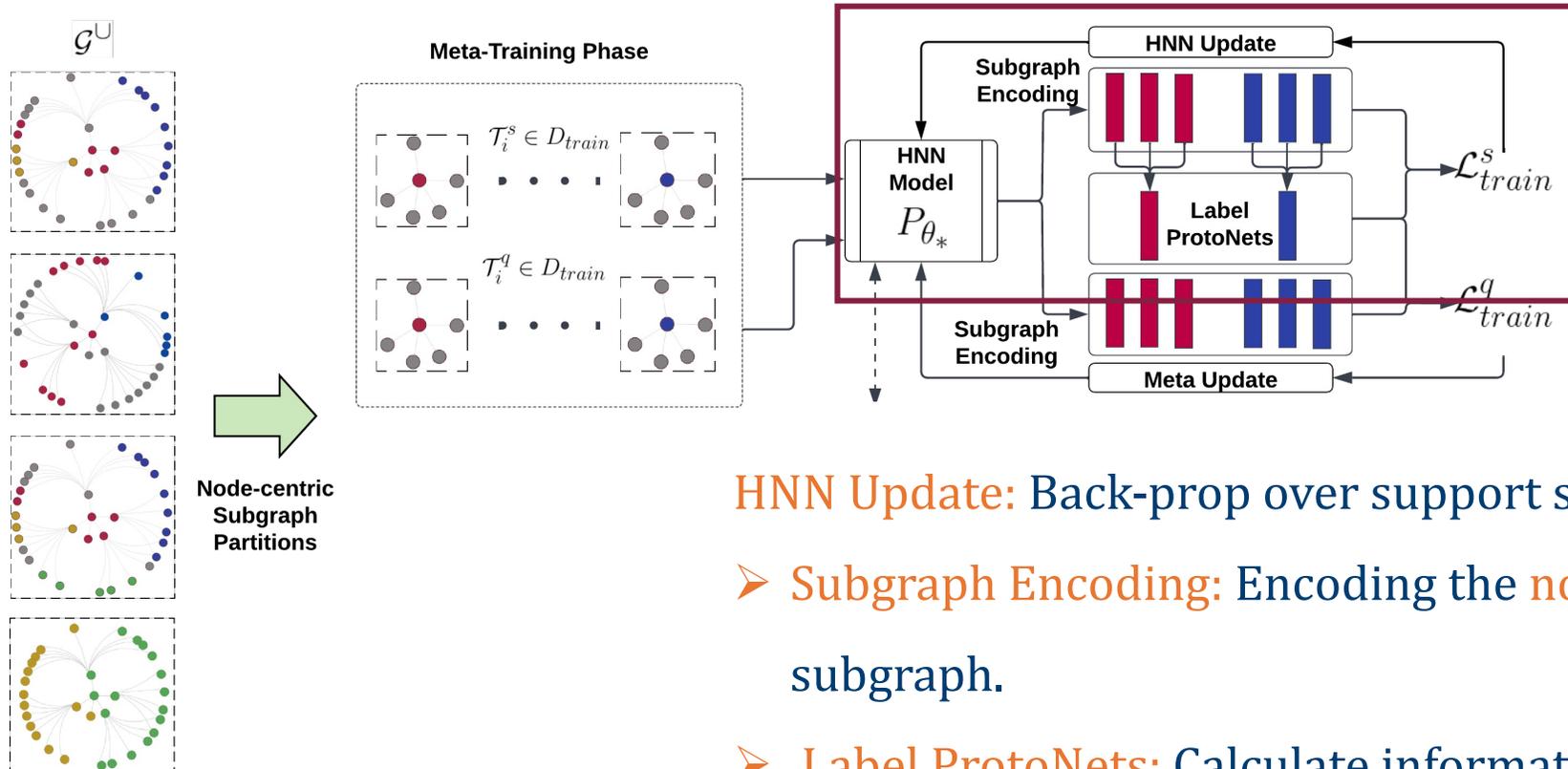
Meta-learning: Handling the Graph Sections



- In the case of Multiple Graphs or Disjoint Labels, we need to rely on **Meta-learning** for **knowledge transfer** between different subgraphs.
- In Meta-learning, we partition the problem into;
 - **Meta-training**: only training samples
 - **Meta-testing**: few training samples

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Model Architecture: Local HNN update



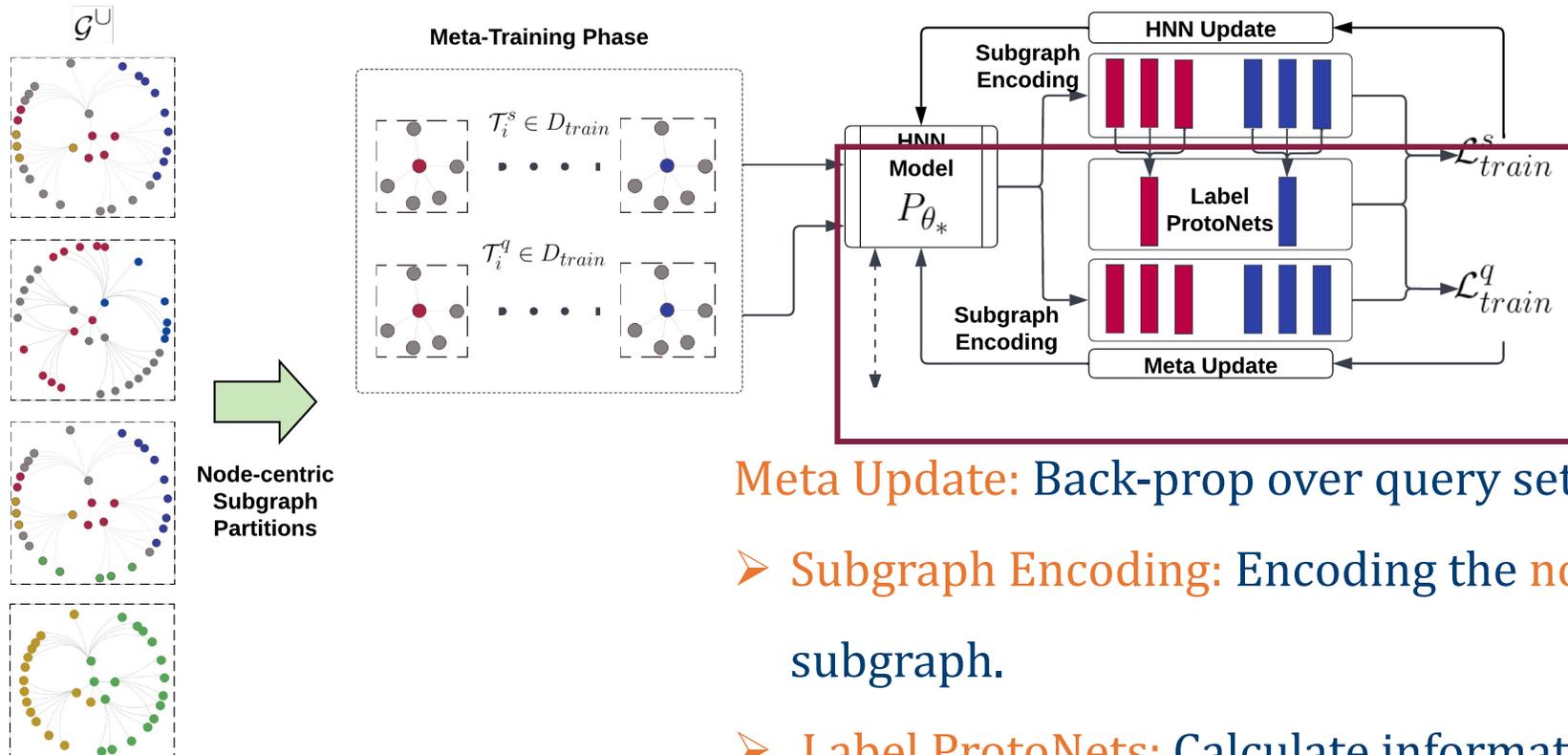
HNN Update: Back-prop over support set.

➤ **Subgraph Encoding:** Encoding the node-centric subgraph.

➤ **Label ProtoNets:** Calculate informative continuous label prototypes.

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Model Architecture: Meta-Update

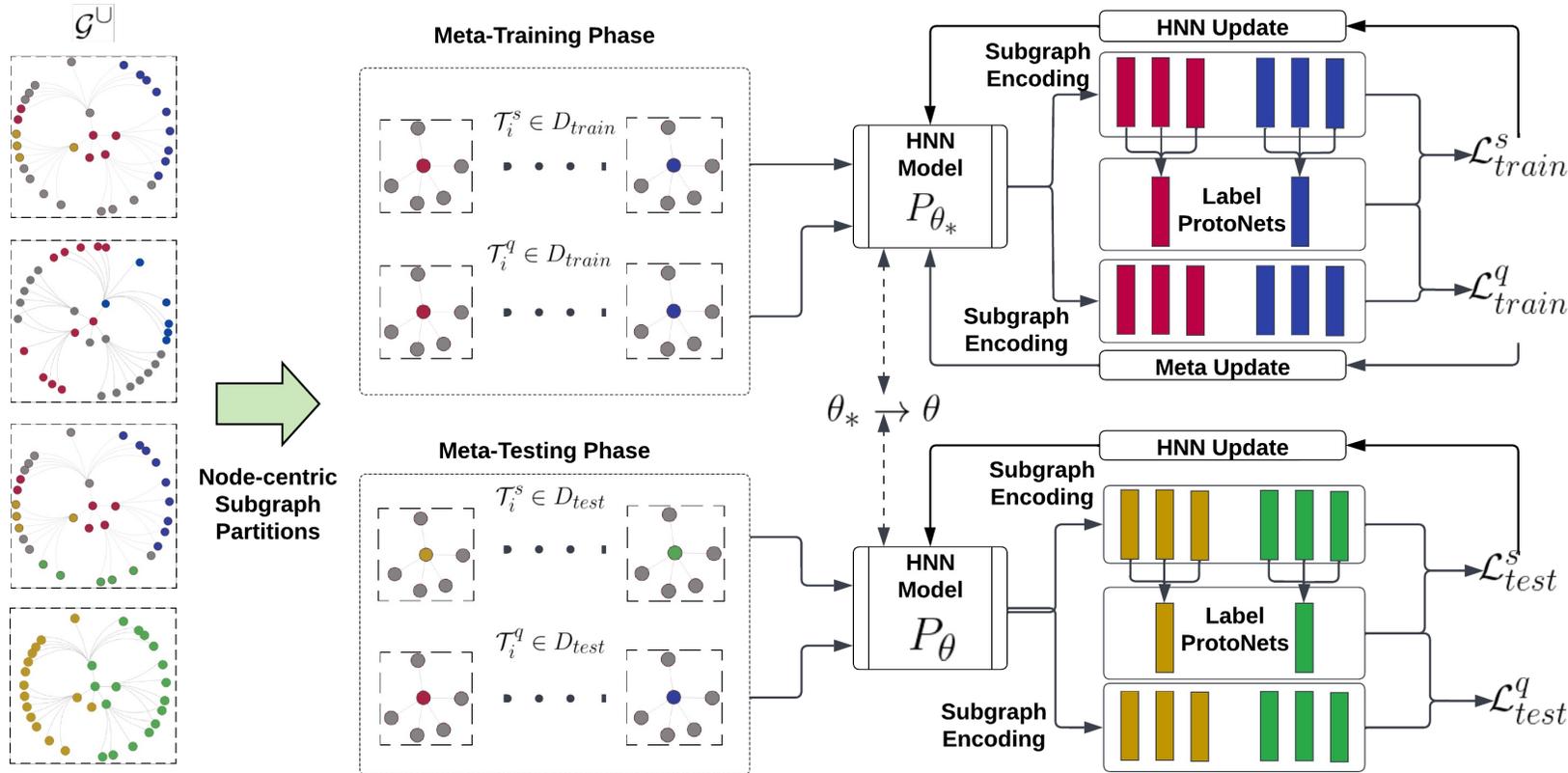


Meta Update: Back-prop over query set.

- Subgraph Encoding: Encoding the node-centric subgraph.
- Label ProtoNets: Calculate informative continuous label prototypes.
- Aggregate over a task and meta update.

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Model Architecture: Meta-learning



Meta Testing:

➤ HNN Updates: Few-shot over support set of test data.

Prediction over query set of test data for final evaluation.

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Evaluation: Experiments

1. Performance of H-GRAM
2. Challenging Few-shot Settings
3. Time Comparison and Ablation Study

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Dataset and Baselines

1. **Datasets:** Synthetic Cycle graph and Synthetic Barabási-Albert graph, ogbn-arxiv, Tissue-PPI, FirstMM-DB, Fold-PPI, Tree-of-Life, Cora, PubMed, and Citeseer.
2. **Baselines:** Meta-Graph, Meta-GNN, FS-GIN, FS-SGC, ProtoNet, MAML, HMLP, HGCN, and HAT.
3. **Evaluation:** Accuracy of Node Classification and Link Prediction

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Performance on Graph Tasks

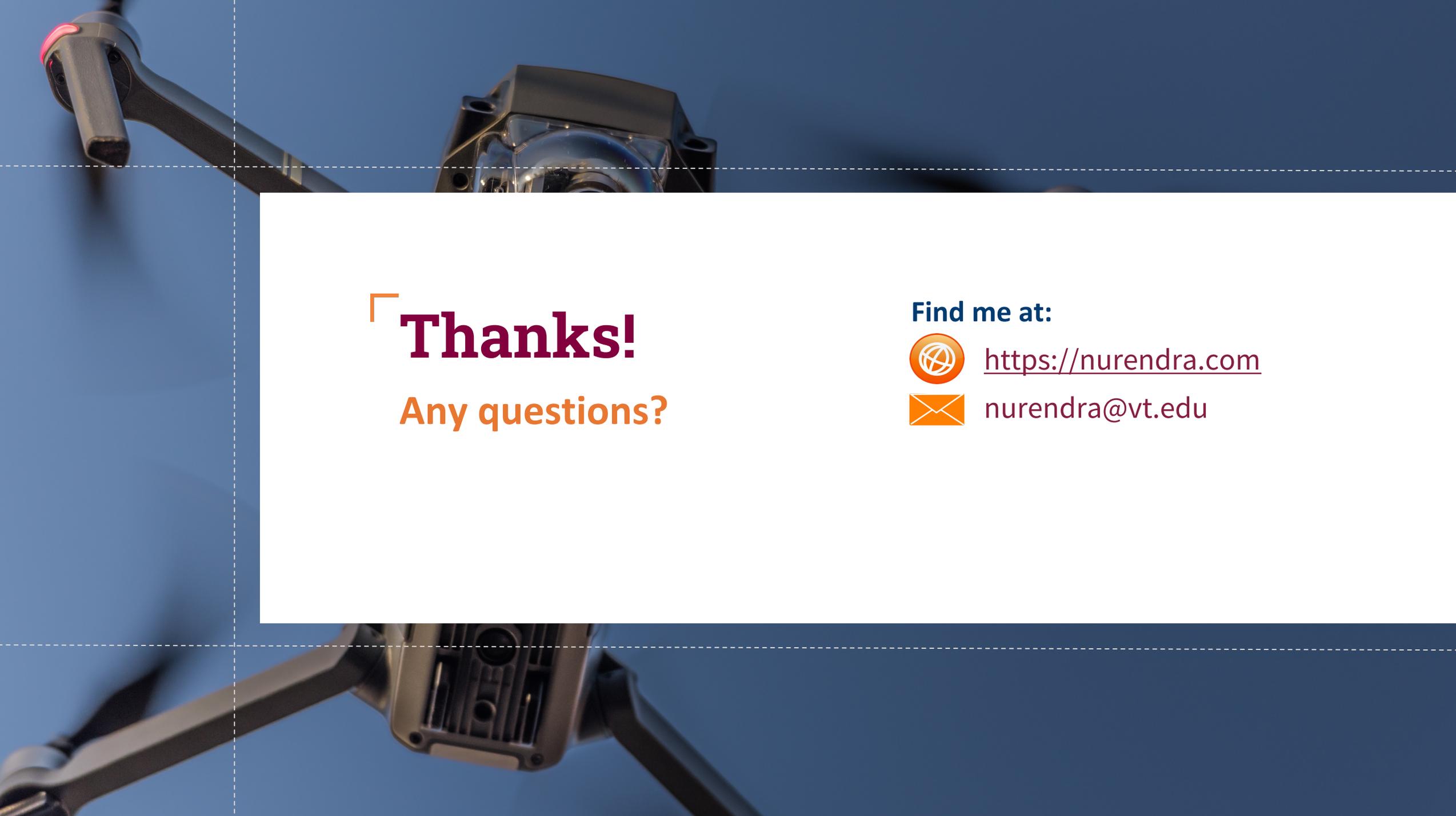
| Task | Node Classification | | Node Classification | | Node Classification | | Node Classification | | | Link Prediction | |
|------------|---------------------|---------|---------------------|---------|---------------------|---------|---------------------|------------|----------|-----------------|--------------|
| Setup | SG,DL | | MG,SL | | MG,DL | | SG,DL | MG,SL | MG,DL | MG,SL | MG,SL |
| Dataset | Syn. Cycle | Syn. BA | Syn. Cycle | Syn. BA | Syn. Cycle | Syn. BA | ogbn-arxiv | Tissue-PPI | Fold-PPI | FirstMM-DB | Tree-of-Life |
| Meta-Graph | - | - | - | - | - | - | - | - | - | 0.719 | 0.705 |
| Meta-GNN | 0.72 | 0.694 | - | - | - | - | 0.273 | - | - | - | - |
| FS-GIN | 0.684 | 0.749 | - | - | - | - | 0.336 | - | - | - | - |
| FS-SGC | 0.574 | 0.715 | - | - | - | - | 0.347 | - | - | - | - |
| ProtoNet | 0.821 | 0.858 | 0.282 | 0.657 | 0.749 | 0.866 | 0.372 | 0.546 | 0.382 | 0.779 | 0.697 |
| MAML | 0.842 | 0.848 | 0.511 | 0.726 | 0.653 | 0.844 | 0.389 | 0.745 | 0.482 | 0.758 | 0.719 |
| G-META | 0.872 | 0.867 | 0.542 | 0.734 | 0.767 | 0.867 | 0.451 | 0.768 | 0.561 | 0.784 | 0.722 |
| H-GRAM | 0.883 | 0.873 | 0.555 | 0.746 | 0.779 | 0.888 | 0.472 | 0.786 | 0.584 | 0.804 | 0.742 |

Accuracy of H-GRAM compared to Euclidean baselines on Node Classification and Link Prediction

Our Solution: H-GRAM

Summary

- **Meta-learning** helps in learning meta-information from **local subgraphs** and generalizing it over the **global graph structure**.
- **H-GRAM** shows improved performance on different graph tasks compared to both **scalable Euclidean** methods and **non-scalable hyperbolic** methods.
- **H-GRAM** parallelizes well in a **multi-GPU** setup, thus providing a scalable formulation of **HNN models**.

A close-up, low-angle shot of a drone's camera and gimbal against a clear blue sky. The drone's arms and propellers are visible in the foreground, slightly out of focus. A white rectangular box is overlaid on the center of the image, containing text and contact information.

Thanks!

Any questions?

Find me at:



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