### Learning to Propagate for Graph Meta-learning

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# Background



**Deep Neural Networks** 



Large Datasets



**Deep Neural Networks** 



Data with Privacy/Copyright Unseen/Rare Classes Data hard/costly to collect

# Background (cont.)



**Deep Neural Networks** 



Large Datasets



#### **Meta-Learning**

(Schmidhuber et al. '87, Bengio et al. '92)



Data with Privacy/Copyright Unseen/Rare Classes Data hard/costly to collect

## Background (cont.)

Meta-Learning: Learning how to learn



### Motivation

**Meta-Learning:** Learn the global **Examples of meta-learners** knowledge shared KNN Support Set [Snell et al., 2017] **Distance Metric** [Vinyals et al., 2016] by all learners/tasks **Initialization Point [Finn et al., 2017] Few Data Available** earn 50 Train 3 'earr **Meta-Learner Few Data Available** 

Graph Meta-Learning: learn to send message between learners/tasks on a graph









### Which kind of graph do we use ? How does graph relate to meta-learning?



**LEFT:** Visualization of the class prototypes produced by GPN (our model) for few-shot tasks and the associated graph.

**<u>RIGHT</u>**: GPN's propagation mechanism for one step: for each node, its neighbors pass messages (their prototypes) to it according to attention weight a, where a gate further choose to accept the message from the neighbors g+ or from the class itself g\*.

# Problem definition: graph meta-learning

We evaluate graph meta-learning methods on the tasks of few-shot classification



## **Gated Propagation Networks**



#### **Prototype propagation in GPN:**

in each step t+1, each class y aggregates prototypes from its neighbors (parents and children) by multi-head attention, and chooses between the aggregated message or the message from itself by a gate g.



1. **Initialize prototype:** We set the **initial prototype** for each class y by averaging over all the K-shot samples belonging to class y as in prototypical networks:

$$\boldsymbol{P}_{y}^{0} \triangleq \frac{1}{|\{(\boldsymbol{x}_{i}, y_{i}) \in \mathcal{D}^{T} : y_{i} = y\}|} \sum_{(\boldsymbol{x}_{i}, y_{i}) \in \mathcal{D}^{T}, y_{i} = y} f(\boldsymbol{x}_{i}).$$



#### 1. Initialize prototype

2. Aggregated messages from its neighbors: At step t, for each class y, we firstly compute the aggregated messages from its neighbors Ny by a dot-product attention module a(p, q), i.e.,

$$\boldsymbol{P}_{\mathcal{N}_y \to y}^{t+1} \triangleq \sum_{z \in \mathcal{N}_y} a(\boldsymbol{P}_y^t, \boldsymbol{P}_z^t) \times \boldsymbol{P}_z^t, \ a(p,q) = \frac{\langle h_1(p), h_2(q) \rangle}{\|h_1(p)\| \times \|h_2(q)\|}$$



1. Initialize prototype

2. Aggregated messages from its neighbors

3. **Apply a gate:** We apply a **gate** g to make decisions of whether accepting messages from its neighbors or message from itself, i.e.

$$\boldsymbol{P}_{y}^{t+1} \triangleq g\boldsymbol{P}_{y \to y}^{t+1} + (1-g)\boldsymbol{P}_{\mathcal{N}_{y} \to y}^{t+1}$$

$$g = \frac{\exp[\gamma \cos(\boldsymbol{P}_y^0, \boldsymbol{P}_{y \to y}^{t+1})]}{\exp[\gamma \cos(\boldsymbol{P}_y^0, \boldsymbol{P}_{y \to y}^{t+1})] + \exp[\gamma \cos(\boldsymbol{P}_y^0, \boldsymbol{P}_{\mathcal{N}_y \to y}^{t+1})]}$$



1. Initialize prototype

2. Aggregated messages from its neighbors

#### 3. Apply a gate

#### Note:

To capture different types of relation and jointly use them for propagation, we combine the results of k attentive and gated propagation modules with untied parameters.

$$P_y^{t+1} = \frac{1}{k} \sum_{i=1}^{k} P_y^{t+1}[i]$$



1. Initialize prototype

2. Aggregated messages from its neighbors

#### 3. Apply a gate

4. The **final prototype** is given as the weighted sum of the initial prototype and the refined prototype:

$$\boldsymbol{P}_{y} \triangleq \lambda \times \boldsymbol{P}_{y}^{0} + (1-\lambda) \times \boldsymbol{P}_{y}^{\mathcal{T}}$$

# **Training Strategy**

Generating training tasks by subgraph sampling: random sampling and snowball sampling.
Random sampling captures strongly-related classes
Snowball sampling captures weakly-related classes

- Building propagation pathways by maximum spanning tree Only propagate through the most related / close classes according to cosine similarity

#### - Curriculum learning

Early stage: train on traditional supervised learning tasks Later stage: train on few-shot learning tasks

# Training Strategy (Cont.)

**Algorithm 1** GPN Training **Input:**  $\mathcal{G} = (\mathcal{Y}, E)$ , memory update interval m, propagation steps  $\mathcal{T}$ , total episodes  $\tau_{total}$ ; 1: Initialization:  $\Theta^{cnn}, \Theta^{prop}, \Theta^{fc}, \tau \leftarrow 0;$ 2: for  $\tau \in \{1, \cdots, \tau_{total}\}$  do if  $\tau \mod m = 0$  then 3: 4: Update prototypes in memory by Eq. (3); 5: end if Draw  $\alpha \sim \text{Unif}[0, 1];$ 6: if  $\alpha < 0.9^{20\tau/\tau_t}$  then 7: Train a classifier to update  $\Theta^{cnn}$  with loss 8:  $\sum_{(\boldsymbol{x},y)\sim\mathcal{D}} -\log \Pr(y|\boldsymbol{x};\Theta^{cnn},\Theta^{fc});$ else 9: 10: Sample a few-shot task T as in Sec. 3.3; Construct MST  $\mathcal{Y}_{MST}^T$  as in Sec. 3.3; 11: For  $y \in \mathcal{Y}_{MST}^T$ , compute  $P_y^0$  by Eq. (3) if 12:  $y \in T$ , otherwise fetch  $P_y^0$  from memory; for  $t \in \{1, \cdots, \mathcal{T}\}$  do 13: For all  $y \in \mathcal{Y}_{MST}^T$ , concurrently update 14: their prototypes  $P_u^t$  by Eq. (4)-(6); end for 15: Compute  $P_y$  for  $y \in \mathcal{Y}_{MST}^T$  by Eq.(7); 16: Compute  $\log \Pr(y|\boldsymbol{x}; \Theta^{cnn}, \Theta^{prop})$  by 17: Eq. (2) for all samples (x, y) in task T; Update  $\Theta^{cnn}$  and  $\Theta^{prop}$  by minimizing 18:  $\sum -\log \Pr(y|x; \Theta^{cnn}, \Theta^{prop});$  $(x,y) \sim \mathcal{D}^T$ 19: end if 20: end for

### **Experimental Results**



Table 3: Validation accuracy (mean $\pm$ CI%95) on 600 test tasks achieved by GPN and baselines on *tiered*ImageNet-Close with few-shot tasks generated by **random sampling**.

Model	5way1shot	5way5shot	10way1shot	10way5shot	
Prototypical Net [23]	42.87±1.67%	62.68±0.99%	30.65±1.15%	$48.64 \pm 0.70\%$	
GNN [6]	$42.33 {\pm} 0.80\%$	59.17±0.69%	$30.50 {\pm} 0.57\%$	$44.33 {\pm} 0.72\%$	
Closer Look [3]	35.07±1.53%	$47.48 {\pm} 0.87\%$	$21.58 {\pm} 0.96\%$	$28.01 {\pm} 0.40\%$	
PPN [15]	$41.60{\pm}1.59\%$	$63.04{\pm}0.97\%$	$28.48{\pm}1.09\%$	$48.66 {\pm} 0.70\%$	
GPN	48.37±1.80%	$64.14{\pm}1.00\%$	33.23±1.05%	$50.50 {\pm} 0.70\%$	
GPN+	50.54±1.67%	65.74±0.98%	34.74±1.05%	51.50±0.70%	

tieredImageNet-Close

### 1~4 steps/hops between training classes and test classes

Table 4: Validation accuracy (mean $\pm$ CI%95) on 600 test tasks achieved by GPN and baselines on *tiered*ImageNet-Close with few-shot tasks generated by **snowball sampling**.

Model	5way1shot	5way5shot	10way1shot	10way5shot
Prototypical Net [23]	35.27±1.63%	52.60±1.17%	$26.08 \pm 1.04\%$	$41.48 {\pm} 0.76\%$
GNN [6]	36.50±1.03%	52.33±0.96%	$27.67 \pm 1.01\%$	$40.67 {\pm} 0.90\%$
Closer Look [3]	$34.07 \pm 1.63\%$	$47.48 {\pm} 0.87\%$	$21.02{\pm}0.99\%$	$33.70 {\pm} 0.44\%$
PPN [15]	36.50±1.62%	52.50±1.12%	$27.18 \pm 1.08\%$	40.97±0.77%
GPN	39.56±1.70%	54.35±1.11%	27.99±1.09%	42.50±0.76%
GPN+	$40.78{\pm}1.76\%$	55.47±1.41%	$\textbf{29.46}{\pm}\textbf{1.10\%}$	<b>43.76±0.74%</b>

### **Experimental Results**



tieredImageNet-Far

5~10 steps/hops between training classes and test classes

Table 5: Validation accuracy (mean $\pm$ CI%95) on 600 test tasks achieved by GPN and baselines on *tiered*ImageNet-**Far** with few-shot tasks generated by **random sampling**.

Model	5way1shot	5way5shot	10way1shot	10way5shot
Prototypical Net [23]	44.30±1.63%	61.01±1.03%	30.63±1.07%	47.19±0.68%
GNN [6]	$43.67 {\pm} 0.69\%$	59.33±1.04%	$30.17 {\pm} 0.47\%$	$43.00 \pm 0.66\%$
Closer Look [3]	$42.27 \pm 1.70\%$	$58.78 {\pm} 0.94\%$	$22.00 \pm 0.99\%$	32.73±0.41%
PPN [15]	$43.63 {\pm} 1.59\%$	$60.20{\pm}1.02\%$	$29.55{\pm}1.09\%$	$46.72 {\pm} 0.66\%$
GPN	47.54±1.68%	<b>64.20</b> ±1.01%	31.84±1.10%	48.20±0.69%
GPN+	<b>47.49</b> ±1.67%	$64.14{\pm}1.02\%$	$31.95{\pm}1.15\%$	<b>48.65±0.66%</b>

Table 6: Validation accuracy (mean $\pm$ CI%95) on 600 test tasks achieved by GPN and baselines on *tiered*ImageNet-**Far** with few-shot tasks generated by **snowball sampling**.

Model	5way1shot	5way5shot	10way1shot	10way5shot
Prototypical Net [23]	43.57±1.67%	62.35±1.06%	29.88±1.11%	$46.48 \pm 0.70\%$
GNN [6]	44.00±1.36%	$62.00 \pm 0.66\%$	$28.50 {\pm} 0.60\%$	46.17±0.74%
Closer Look [3]	38.37±1.57%	$54.64{\pm}0.85\%$	$30.40{\pm}1.09\%$	$33.72{\pm}0.43\%$
PPN [15]	42.40±1.63%	61.37±1.05%	28.67±1.01%	$46.02{\pm}0.61\%$
GPN	47.74±1.76%	63.53±1.03%	<b>32.94</b> ±1.16%	47.43±0.67%
GPN+	47.58±1.70%	63.74±0.95%	<b>32.68</b> ±1.17%	<b>47.44</b> ± <b>0.71</b> %

# **Ablation Studies**

Table 7: Validation accuracy (mean $\pm$ CI%95) for possible variants of GPN on *tiered*ImageNet-Close for 5-way-1-shot tasks. Original GPN's choices are in **bold** fonts. Details of the variants are given in Sec. 4.5.

Task SR-S	Gene S-S	ration R-S	Pr N→C	opaga CF→C	tion M C→C	<b>Iechan</b> C B→P	ism PM→P	Trai  AUX	ining MST	M-H	Model [ M-A	A-A	ACCURACY
	$\checkmark$	$\checkmark$	$\checkmark$					$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$		$\begin{array}{c} 46.20{\pm}1.70\% \\ 49.33{\pm}1.68\% \end{array}$
$\checkmark$				V	$\checkmark$	$\checkmark$	V	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$		$42.60 \pm 1.61\%$ $37.90 \pm 1.50\%$ $47.90 \pm 1.72\%$ $46.90 \pm 1.78\%$
$\checkmark$			$\checkmark$					$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$		41.87±1.72% 45.83±1.64%
$\checkmark$			$\checkmark$					$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$	49.40±1.69% 46.74±1.71%
$\checkmark$			$\checkmark$					$\checkmark$	$\checkmark$	$\checkmark$	$\checkmark$		<b>50.54</b> ±1.67%

# Visualization



Visualization of the class prototypes produced by GPN for few-shot tasks and the associated graph.







Prototypes **before** (top row) and **after GPN propagation** (bottom row) on tieredImageNet-Close by random sampling for 5-way-1-shot few-shot learning. The prototypes in top row equal to the ones achieved by prototypical network. Different tasks are marked by a different shape, and classes shared by different tasks are highlighted by non-grey colors.

It shows that GPN is capable to map the prototypes of the same class in different tasks to the same region. Comparing to the result of prototypical network, GPN is more powerful in relating different tasks.







# Takeaways

- A **novel problem**: Graph Meta-learning, which learns to send message between learners/tasks on a graph.
- A meta-learning method based "Learning to Propagate", where the propagation scheme on the graph is a metalearner.
- Two new benchmark datasets for the new problem and thorough experiments for comparison, ablation and visualization.

For more, refer our paper at <u>https://arxiv.org/abs/1909.05024</u>