# COLD Brew: Distilling Graph Node Representations with Incomplete or Missing Neighborhoods

Wenqing Zheng $^{1,2}$  Edward W Huang $^1$ , Nikhil Rao $^1$ , Sumeet Katariya $^1$ , Zhangyang Wang $^{1,2}$ , Karthik Subbian $^1$ 

<sup>1</sup>Amazon <sup>2</sup>The University of Texas at Austin {wenqzhen, ewhuang, nikhilsr, katsumee, wzhangwa, ksubbian}@amazon.com

# **ABSTRACT**

Graph Neural Networks (GNNs) have achieved state of the art performance in node classification, regression, and recommendation tasks. GNNs work well when high-quality and rich connectivity structure is available. However, this requirement is not satisfied in many real world graphs where the node degrees have power-law distributions as many nodes have either fewer or noisy connections. The extreme case of this situation is a node may have no neighbors at all, called Strict Cold Start (SCS) scenario. This forces the prediction models to rely completely on the node's input features. We propose Cold Brew to address the SCS and noisy neighbor setting compared to pointwise and other graph-based models via a distillation approach. We introduce feature-contribution ratio (FCR), a metric to study the viability of using inductive GNNs to solve the SCS problem and to select the best architecture for SCS generalization. We experimentally show FCR disentangles the contributions of various components of graph datasets and demonstrate the superior performance of Cold Brew on several public benchmarks and proprietary e-commerce datasets. The source code for our approach is available at: https: //github.com/amazon-research/gnn-tail-generalization.

# 1 Introduction

Graph Neural Networks (GNNs) achieve state-of-the-art results across a wide range of tasks such as graph classification, node-classification, -regression, link prediction, and recommendation [1, 2, 3, 4, 5, 6]. GNNs rely on the principle of message passing to aggregate node features across multi-hop neighborhoods in order to learn aggregated representations. The success of modern GNN models relies on the presence of dense connections and high-quality neighborhoods. State-of-the-art GNNs [7, 8, 9, 10, 11, 12] benefit from efficient message-passing frameworks developed to best leverage (deep) neighborhood information to learn node representations. Other methods like the spectral diffusion [13, 14, 15, 16] and label propagation [17, 18] also require a non-empty and high-quality neighborhood per node to perform message passing. Even the inductive GNNs (e.g., [9]) learn a function of the node feature and the node neighborhood, requiring the neighborhood to be present during the inference time.

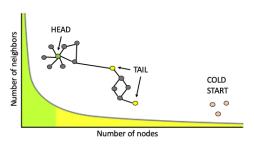
Most of the large-scale real-world graphs are power-law in nature, with a majority of the nodes having very few connections [19, 20, 21, 22]. In Figure 1 we conceptually show the long-tail distribution of such a graph and also empirically show this characteristics on several public datasets. In many information retrieval and recommender systems applications, there is another ubiquitous challenge: the *Strict Cold Start* (SCS) [23, 20], wherein some "nodes" will have no edges in the graph. For instance, in most of the public and proprietary datasets we used in the experimentation we have anywhere between 3% to 6% isolated nodes with no neighbors. In these cases, existing GNNs fail to perform due to sparsity or absence of neighborhood.

In this paper, we develop GNN models that can achieve *truly inductive* capabilities: one can learn effective node embeddings for "orphaned" nodes in a graph. This capability is

important to fully realize the potential of large-scale GNN models on modern, industrialsized datasets with very long tails and nodes with no neighbors in the graph. To this end,

we adopt the teacher-student knowledge distillation procedure [24, 25] and propose Cold Brew to distill the knowledge of a GNN teacher into a multilayer perceptron (MLP) student. The Cold Brew framework boils down to addressing two key questions: (1) how we efficiently distill the teacher's knowledge for the sake of tail and coldstart generalization, and (2) how a student can make use of this knowledge. We answer these two question by learning a latent node-wise embedding using knowledge distillation, which both avoid "over-smoothness" [26, 27, 28] and could discover the the neighborhoods upon their absence. We discuss everything else in detail in the following sections. Note that in contrast to traditional knowledge distillation [29], our aim is not to train a simpler student model to perform as well as the more complex teacher. Instead, we aim to train a student model that is better than the teacher, and generalizes to samples in the same graph where the teacher will be ineffective.

To help select the cold-start-friendly model architectures, we develop a metric called Feature-Contribution Ratio (FCR) that disentangles the graph data into node features and the neighborhood structure. We then build submodules for



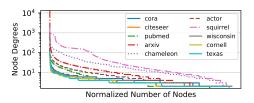


Figure 1: **Top:** Graphs may have a power-law ("long-tail") distribution, with a large fraction of nodes (yellow) having few to no neighbors. **Bottom:** The long-tail distribution is often the case in real-world datasets, and a GNN depending on the node neighborhood will not generalize to the tail/cold-start nodes.

each part and search for the best architecture. Besides selecting the optimal model architecture, we leverage FCR to provide a measure of importance of the node feature compared to the neighborhood structure, quantifying the difficulty of learning truly inductive GNNs. We summarize our key contributions as follows:

- To generalize better to tail and SCS nodes, we design the Cold Brew framework to distill a GNN teacher into an MLP student. We improve over GNN models by adding the node-wise Structural Embedding (SE) to the Cold Brew's teacher GNN to strengthen the expressiveness of the teacher GNN model. We designed a novel mechanism for the MLP student to discover the "latent/virtual neighborhoods" when they are missing, and perform message passing as its teacher model does.
- We propose **Feature-Contribution Ratio** (FCR): a new metric for graph datasets that quantifies the contribution of node features w.r.t. the adjacency structure in the dataset for a specific downstream task. FCR indicates the difficulty in generalizing to tail and cold-start nodes in a given dataset. We also leverage FCR as a principled "screen process" to select the best model architecture for both the GNN teacher and the MLP student in Cold Brew.
- Through extensive experiments on several public datasets as well as a proprietary ecommerce graph dataset, we validate the effectiveness of Cold Brew in cold-start generalization. We further uncover the contribution ratio of node features in node prediction tasks with FCR.

### 1.1 PROBLEM SETUP

GNNs effectively learn the representations of two components in graph data: they process *node features* by distributed node-wise transformations and process *adjacency structure* by localized neighborhood aggregations. For the first component, GNNs apply shared feature transformations to all nodes regardless of the neighborhoods, while for the second component, GNNs use permutation-invariant aggregators to collect neighborhood information.

We take the node classification problem in this paper for ease of exposition, and the proposed method can be trivially adapted to semi-supervised/unsupervised settings. We denote the graph data of interest by  $\mathcal G$  with node set  $\mathcal V$ ,  $|\mathcal V|=N$ . Each node possesses a  $d_{in}$ -dimensional feature and a  $d_{out}$ -dimensional label (either  $d_{out}$  classes or a continuous vector in the case of regression). Let  $\mathbf X^0 \in \mathbb R^{N \times d_{in}}$  and  $\mathbf Y \in \mathbb R^{N \times d_{out}}$  be the matrices of node features and labels, respectively. Let  $\mathcal N_i$  be the neighborhood of node  $i \in [N]$ . As is common with modern, large-scale graphs,  $|\mathcal N_i|$  is small for several nodes in the graph, which we refer to as tail nodes. For a number of nodes,  $|\mathcal N_i| = 0$ , and we refer to these nodes as cold-start nodes.

A traditional GNN learns representations for the  $i^{th}$  node at the  $l^{th}$  layer as a function of the node representation itself and its neighborhoods' representations, at the  $(l-1)^{th}$  layer:

$$x_i^l := f\left(\{x_i^{l-1}\}, \{x_i^{l-1}\}_{j \in \mathcal{N}_i}\right) \tag{1}$$

where  $f(\cdot)$  is a general function that applies node-wise transformation on node  $x_i^{l-1}$  and aggregates information of its neighborhood  $\{x_j^{l-1}\}_{j\in\mathcal{N}_i}$  to obtain the final node representation. Given i's input features  $x_i^0$  and its neighborhood  $\mathcal{N}_i$ , one can use (1) to obtain its representation and predict  $y_i$ , making these models inductive.

We are interested in improving the performance of these GNNs on a set of tail and cold-start nodes, where  $\mathcal{N}_i$  for node i is either unreliable or absent. In these cases, applying (1) will yield a suboptimal node representation, since  $\{x_j^{l-1}\}_{j\in\mathcal{N}_i}$  will be unreliable or empty at inference time.

# 2 Related Work

GNNs learn by aggregating neighborhood information to learn node representations [7, 8, 9, 10, 11, 12]. Inductive variants of GNNs such as GraphSAGE [9] require initial node features as well as the neighborhood information of each node to learn the representation. Most works on improving GNNs have focused on learning better aggregation functions, and methods that can work when the neighborhood is absent or noisy have not been sufficiently exploited, except two very recent or concurrent works [30, 31].

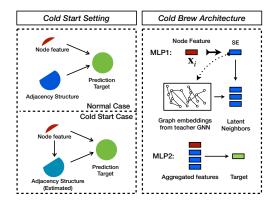
In the context of cold start, [19] and [20] employ a transfer learning approach. [24] proposes a knowledge distillation for GNN, while [25] proposes a self-distillation approach. In all the above cases, the models need full knowledge of the neighbors of the cold-start nodes in question and do not address the case of noisy or missing neighborhoods. Another possible solution is to directly train an MLP that only take node features. [30] proposes to learn graph embeddings with only node-wise MLP, while using contrastive loss to regularize the graph structure. However, in order to train it with contrastive loss, the training process still relies on neighbor information, and we show through experiments that such approach does not generalize well to tail and cold start nodes.

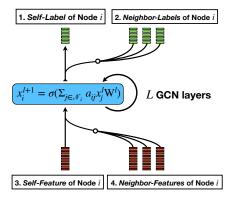
Some previous works have studied the relation between node feature similarity and edge connections and studied their influence on the selection of appropriate graph models. [32] proposed the homophily metric that categorizes the graphs into assortative and disassortative classes. [16] dissected the feature propagation steps of linear GCNs from a perspective of continuous graph diffusion and analyzed why linear GCNs fail to benefit from more propagation steps. [33] further studied the influence of homophily on model selection and proposed a non-local GNN. Compared with the homophily metric, our proposed FCR quantifies the contribution ratio of node features w.r.t. the adjacency structure. With FCR, one can not only assess the loss of performance for orphaned nodes (through the difference of MLP and GNN) but also obtain the most suitable configuration of the GNN model through a parameter-searching procedure when computing FCR.

# 3 STRICT COLD START GENERALIZATION

We now address the problem of generalization to the tail and cold-start nodes, where the neighborhood information is missing/noisy (Section 1). A naive baseline is to train an MLP to map node features to labels. However, such method disregards all graph information, and we show via our Feature-

<sup>&</sup>lt;sup>1</sup>For example, a user with only one movie watched or an item with too few purchases.





(a) The teacher-student knowledge distillation of the (b) Four GNN Atomic Components in deciding Cold Brew framework under the cold start setting.

GNN's output, which are used for FCR analysis.

Figure 2: (a): The proposed Cold Brew framework under the cold start setting: when the adjacency structure is missing (no explicit neighborhood), Cold Brew's student model learns to discover the latent neighborhood, and infer the target embedding from the node feature and the estimated neighbors. The "SE" in blue color is the structural embedding, learned by Cold Brew's teacher GNN. (b): Four atomic components of node i in deciding its embeddings learned by the GNN. Our proposed FCR metric disentangles them into two models: the MLP that only considers Part 1 and Part 3, and label propagation that only considers Part 1 and Part 2.

Contribution Ratio and other experimental results that for most assortative graph datasets, the node-wise MLP approach is suboptimal.

The key idea of our framework is the following: the GNN maps node features into a d-dimensional embedding space, and since the number of nodes N is usually much bigger than the embedding dimensionality d, we end up with an overcomplete set for this space using the embeddings as the basis. This implies the possibility that any node representation can be cast as a linear combination of  $K \ll N$  existing node representations. Our aim will be to train a student model that can accurately discover the combination of the best K existing node embeddings of a target isolated node. We call this procedure  $latent/virtual\ neighborhood\ discovery$ , which is equivalent to using MLPs to "mimic" the node representations learned by the teacher GNN.

We adopt the knowledge distillation procedure [24, 25] to improve the quality of the learned embeddings for tail and cold-start nodes. We use a teacher GNN model to embed the nodes onto a low-dimensional manifold by utilizing the graph structure. Then, the job of the student is to learn a mapping from the node features to this manifold without knowledge of the graph that the teacher has. We further aim to let the student model generalize to SCS cases where the teacher model fails, beyond just mimicking the teacher as standard knowledge distillation does.

# 3.1 THE TEACHER MODEL OF COLD BREW: STRUCTURAL EMBEDDING GNN

Consider a graph  $\mathcal{G}$ . For a Graph Convolutional Network with L layers, the l-th layer transformation can be written as<sup>2</sup>:  $\mathbf{X}^{(l+1)} = \sigma(\tilde{\mathbf{A}}\mathbf{X}^{(l)}\mathbf{W}^{(l)})$ , where  $\tilde{\mathbf{A}}$  is the normalized adjacency matrix,  $\tilde{\mathbf{A}} = \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$ ,  $\mathbf{D}$  is the diagonal degree matrix and  $\mathbf{A}$  is the adjacency matrix.  $\mathbf{X}^{(l)} \in \mathbb{R}^{N \times d_1}$  is the node representations in the l-th layer,  $\mathbf{W}^{(l)} \in \mathbb{R}^{d_1 \times d_2}$  is the feature transformation matrix, where the values of  $d_1/d_2$  depend on layer l:  $(d_1, d_2) = (d_{in}, d_{hidden})$  for l = 0,  $(d_{hidden}, d_{hidden})$  for  $1 \le l \le L - 2$ , and  $(d_{hidden}, n_{classes})$  for l = L - 1.  $\sigma(\cdot)$  is the nonlinear functions applied to each layer, (e.g. ReLU).  $Norm(\cdot)$  refers to an optional batch or layer normalization.

GNNs typically suffer from oversmoothing [26, 27, 28], making all the node representations similar to each other. This is harmful not only for the GNN itself, but also to the student model that looks to mimic the GNN. Inspired by the positional encoding in Transformers [34], we train the teacher GNN to additionally learn a set of node embeddings which we term the **Structural Embedding** (**SE**).

<sup>&</sup>lt;sup>2</sup>Compared to Equation (1), multiplication by  $\tilde{A}$  plays the role of aggregating both  $\{x_i\}$  and  $\{x_i\}_{i \in \mathcal{N}_i}$ .

SE learns to incorporate additional information (such as node labels in the case of semi supervised learning) through gradient backpropagation. The existence of SE avoids the oversmoothing issue in GNNs: the transformations applied to different nodes are no longer the same for each nodes, since the SE of each node is different, which is part of the feature transformation function. Note that this could be of independent interest to practitioners who train and study GNNs.

Specifically, for each layer  $l, 0 \le l \le L - 1$ , the Structural Embedding is a learnable matrix  $\mathbf{E}^{(l)}$ , and the SE-GNN layer forward pass can be written as:

$$\mathbf{X}^{(l+1)} = \sigma\left(\tilde{\mathbf{A}}\left(\mathbf{X}^{(l)}\mathbf{W}^{(l)} + \mathbf{E}^{(l)}\right)\right), \mathbf{X}^{(l)} \in \mathbb{R}^{N \times d_1}, \mathbf{W}^{(l)} \in \mathbb{R}^{d_1 \times d_2}, \mathbf{E}^{(l)} \in \mathbb{R}^{N \times d_2}$$
(2)

**Remark 1:** Note that SE is not the same as the bias term in traditional feature transformation  $\mathbf{X}^{(l+1)} = \sigma\left(\tilde{A}\left(\mathbf{X}^{(l)}\mathbf{W}^{(l)} + \mathbf{b}^{(l)}\right)\right)$ , where for the bias  $\mathbf{b} \in \mathbb{R}^{N \times d_2}$  the rows are copied/shared across all nodes. In contrast, we have a different structural embedding for every node.

**Remark 2:** SE is also unlike traditional label propagation (LP) [35, 36, 37]. LP encodes label information through iterating  $\mathbf{E}^{(t+1)} = (1-\alpha)\mathbf{G} + \alpha\tilde{\mathbf{A}}\mathbf{E}^{(t)}$ , where  $\mathbf{G}$  is a one-hot encoding of ground truth for training node classes and zeros for test nodes, and  $0 < \alpha < 1$  is the portion of mixture at each iteration.

SE-GNN enables node i to learn to encode the self and neighbors' label information<sup>3</sup> into its own node embedding through  $\tilde{A}$ . We use the Graph Convolutional Networks [7], combined with other building blocks proposed in recent literature including: (1) initial/dense/jumping connections; and (2) batch/pair/node/group normalization, as the backbone of Cold Brew's teacher GNN. More details are described in Appendix A. We also apply a regularization term to the loss function, yielding the following loss function:

$$loss = CE(\mathbf{X}_{train}^{(L)}, \mathbf{Y}_{train}) + \eta \|\mathbf{E}\|_{2}^{2}$$
(3)

where  $\mathbf{X}_{train}^{(L)}$  is the model's embedding at the L-th layer, which is exactly the model's output,  $CE(\mathbf{X}_{train}^{(L)}, \mathbf{Y}_{train})$  is the Cross Entropy between the model output  $\mathbf{X}_{train}^{(L)}$  and the ground truth  $\mathbf{Y}$  on the training set, and  $\eta$  is the coefficient (grid-searched for different datasets in practice). The Cross-Entropy loss can be replaced by any other appropriate loss depending on the task.

# 3.2 THE STUDENT MLP MODEL OF COLD BREW

We design the student to be composed of two MLP modules. Given a target node, the first MLP module imitates the node embeddings generated by the GNN teacher. Next, given any node, we find a set of virtual neighbors of that node from the graph. Finally, the second MLP attends to both the target node and the virtual neighborhood and transforms them into the embeddings of interest.

Suppose we would like to obtain the embedding of an potentially isolated target node i, given only its feature  $\mathbf{x}_i$ . From the teacher GNN, at each layer l, we have access to two sets of node embeddings:  $\mathbf{X}^{(l)}\mathbf{W}^{(l)}$  and  $\mathbf{E}^{(l)}$ . Denote  $\bar{\mathbf{E}}$  as the desired embeddings that the teacher GNN pass over to the student MLP. We offer two options for  $\bar{\mathbf{E}}$ : it can be the final output of the teacher GNN, in this case,  $\bar{\mathbf{E}} \in \mathbb{R}^{N \times d_{out}} := \mathbf{X}^{(L)}$ , or optionally, it can be the concatenation of all intermediate results of the teacher GNN, similar to [38]:  $\bar{\mathbf{E}} \in \mathbb{R}^{N \times (d_{hidden}*(L-1)+d_{out})} := \mathbf{X}^{(L)} \bigcup_{l=0}^{L-1} (\mathbf{E}^{(l)} + \mathbf{X}^{(l)}\mathbf{W}^{(l)})$ , where  $\bigcup$  is the concatenation of matrices at the feature dimension (second dimension).  $\bar{\mathbf{E}}$  acts as the target for the first MLP module and the input to the second MLP module.

The first MLP learns a mapping from the input node features  $\mathbf{X}^{(0)}$  to  $\bar{\mathbf{E}}$ , that is  $\xi_1: \mathbf{x}_i^{(0)} \to e_i$  for node  $i, e_i = \bar{\mathbf{E}}[i,:]$ . Then, we discover the virtual neighborhood by applying an attention-based aggregation of the existing embeddings in the graph, before linearly combining them:

$$\tilde{e}_i = softmax(\Theta_K(e_i\bar{\mathbf{E}}^\top))\bar{\mathbf{E}}$$
 (4)

<sup>&</sup>lt;sup>3</sup>This will be inferred in the case of labels missing.

where  $\Theta_K(\cdot)$  is the top-K hard thresholding operator: for  $z \in \mathbb{R}^{1 \times N}$ :  $[\Theta_K(z)]_j = z_j$  if  $z_j$  is among the top-K largest elements of z, and  $\Theta_K(z)_j = -\infty$  otherwise. Finally, the second MLP learns a mapping  $\xi_2 : [\mathbf{x}_i, \mathbf{e}_i] \to \mathbf{y}_i$ , where  $\mathbf{y}_i = \mathbf{Y}[i, :]$  is the ground truth for node i.

Equation (4) first selects K nodes from the N nodes that the teacher GNN was trained on via the hard thresholding operator.  $\tilde{e_j}$  is then a linear combination of K node <sup>4</sup> embeddings. Thus, every sample whether or not seen previously while training the GNN can be represented as a linear combination of these representations. The MLP  $\xi_2(\cdot)$  maps this representation to the final target of interest. Thus, we decompose every node embedding as a linear combination of an (overcomplete) basis.

The training of  $\xi_1(\cdot)$  is by minimizing the mean squared error over the non-isolated node in the graph (mimicing the teacher's embeddings), and the training of  $\xi_2(\cdot)$  is by minimizing the cross entropy (for node classification task) or mean squared error (for node regression task) on the training split of the tail and isolated part of the graph. An illustration of SE-MLP's inference procedure for the isolated nodes is shown in Fig. 2. When the number of nodes is large, the ranking procedure involved in  $\Theta_K(\cdot)$  can be pre-computed after training the first part and before training the second part.

#### 3.3 MODEL INTERPRETATION FROM A LABEL SMOOTHING PERSPECTIVE

We cite Theorem 1 in [36]: Suppose that the latent ground-truth mapping from node features to node labels is differentiable and L-Lipschitz. If the edge weights  $a_{ij}$  approximately smooth  $\mathbf{x}_i$  over its immediate neighbors with error  $\epsilon_i$ , i.e.,  $\mathbf{x}_i = \frac{1}{d_{ii}} \sum_{j \in \mathcal{N}} a_{ij} \mathbf{x}_j + \epsilon_i$ , then the  $a_{ij}$  also approximately smooth  $y_i$  to bound within error  $|y_i - \frac{1}{d_{ii}} \sum_{j \in \mathcal{N}_i} a_{ij} y_j| \leq L||\epsilon||_2 + o(\max_{j \in \mathcal{N}_i} (||\mathbf{x}_j - \mathbf{x}_i||_2))$ , where  $o(\cdot)$  denotes a higher order infinitesimal.

This theorem indicates that the errors of the label predictions are determined by the difference of the features after neighborhood aggregation: if  $\epsilon_i$  is large, then the error in the label prediction is also large, and vice versa. However, with structural embedding, each node i also learns an independent embedding  $\bar{\mathbf{E}}[:,i]$  during the aggregation, which changes  $\frac{1}{d_{ii}} \sum_{j \in \mathcal{N}} a_{ij} \mathbf{x}_j + \epsilon_i$  into  $\frac{1}{d_{ii}} \sum_{j \in \mathcal{N}} a_{ij} \mathbf{x}_j + \bar{\mathbf{E}}[:,i] + \epsilon_i$ . Deduced from this theorem, the structural embedding  $\bar{\mathbf{E}}$  is important for the teacher model: it allows higher flexibility and expressiveness in learning the residual difference between nodes, and hence the error  $\epsilon_i$  can be are lowered if  $\bar{\mathbf{E}}$  is properly learned.

From this theorem, one can also see the necessity of introducing neighborhood aggregations like the Cold Brew's student model. If one directly applies MLP models without neighborhood aggregation, the  $\epsilon_i$  turns out to be non-negligible, leading to higher losses in the label predictions. However, Cold Brew introduced the neighborhood aggregation mechanism, so that the second part of the student MLP takes over the aggregation of neighborhood generated by the first MLP. Therefore, Cold Brew eliminates the above residual error even in the absence of the actual neighborhood.

# 4 MODEL SELECTION AND GRAPH COMPONENT DISENTANGLEMENT WITH FEATURE-CONTRIBUTION RATIO

We now discuss Feature Contribution Ratio (FCR): a metric to quantify the difficulty of learning representations under the truly inductive cold start case, and a hyperparameter optimization approach to select the best suitable model architecture that helps tail and cold start generalization.

As conceptually illustrated in Figure 2, there are four atomic components contributing to the learned embedding of node i in the graph: 1. the label of i (self-label); 2. the label of neighbors of i (neighbor-labels); 3. the features of i (self-feature); 4. the features of neighbors of i (neighbor-features). To quantize the SCS generalization difficulty, we divide these four components into two submodules to disentangle the contributions of the node features with respect to the adjacency structure of the graph dataset, and quantize it based on the assumption that the SCS generalization difficulty is propotional to the contribution ratio of the node features.

We posit that a submodule that learns accurate node representations must include the node's (self) label, so that training can be performed via backpropagation. What remains is to use the label

 $<sup>^4</sup>$ We abuse terminology here since E contains node and structural embeddings from multiple layers

with other atomic components to construct two specialized models that each make use of only the node features or the adjacency structure. For the first submodule, we build an MLP that maps the self-features to self-labels, ignoring any neighborhood information present in the dataset. For the second submodule, we adopt a Label Propagation (LP) method [17]<sup>5</sup> to learn representations from self- and neighbor-labels. This model ignores any node feature information.

With the above two submodules, we introduce the Feature-Contribution Ratio (FCR) that characterizes the relative importance of the node features and the graph structure. Specifically, for graph dataset  $\mathcal{G}$ , we define the contribution of a submodule to be the *residual performance* of the submodule compared to a full-fledged GNN (e.g., Equation (1)) using both the node feature as well as the adjacency structure. Denote  $z_{MLP}, z_{LP}$ , and  $z_{GNN}$  as the performance of the MLP submodule, LP submodule, and the full GNN on the test set, respectively. If  $z_{MLP} \ll z_{GNN}$ , then  $FCR(\mathcal{G})$  is small and the graph structure is important, and noisy or missing neighborhood information will hurt model performance. Based on this intuition, we build SCR as:

$$\delta_{MLP} = z_{GNN} - z_{MLP}, \quad \delta_{LP} = z_{GNN} - z_{LP} \tag{5a}$$

$$FCR(\mathcal{G}) = \begin{cases} \frac{\delta_{LP}}{\delta_{MLP} + \delta_{LP}} \times 100\% & z_{MLP} \le z_{GNN} \\ 1 + \frac{|\delta_{MLP}|}{|\delta_{MLP}| + \delta_{LP}} \times 100\% & z_{MLP} > z_{GNN} \end{cases}$$
 (5b)

**Interpreting FCR values.** For a particular graph  $\mathcal{G}$ , if  $0\% \leq FCR(\mathcal{G}) < 50\%$ , it means  $z_{GNN} > z_{LP} > z_{MLP}$ , and the neighborhood information in  $\mathcal{G}$  is mainly responsible for the GNN achieving good performance. If  $50\% \leq FCR(\mathcal{G}) < 100\%$ , then  $z_{GNN} > z_{MLP} > z_{LP}$ , the node features contribute more to the GNN's performance. If  $FCR(\mathcal{G}) \geq 100\%$ , then  $z_{MLP} > z_{GNN} > z_{LP}$ , and the node aggregation in GNNs can actually lead to reduced performance compared to pointwise models. This case usually happens for some disassortative graphs (the majority of neighborhoods hold different labels than the center node), e.g. as observed by [33].

Integrate FCR as a tool to design teacher and student models. For some graph datasets and models, the SCS generalization can be challenging without neighborhood information (i.e,  $z_{GNN} > z_{LP} > z_{MLP}$ ). We hence consider FCR as a principled "screening process" to select model architectures for both teacher and student, that own the best inductive bias for SCS generalization.

To achieve this, during the computation of FCR, we perform exhaustive grid search of the architectures (residual connection types, normalization, hidden layers, etc.) for the MLP, LP, and GNN modules, and pick the best-performing variant. Detailed definition of the search space can be found in Appendix A. We treat this grid search procedure as a special case of architecture selection and hyperparameter optimization for Cold Brew. We observe that FCR is able to identify the GNN and MLP architectures that are particularly friendly for SCS generalization, improving our method design.

In experiments, we observe that different model configurations are favored by different datasets, and we use the found optimal teacher GNN and student MLP architectures to perform Cold Brew. More detailed discussions will be presented in section 5.3

# 5 EXPERIMENTS AND DISCUSSION

In this section, we first evaluate the FCR for several commonly used graph datasets to ascertain how well GNNs trained on them can generalize to tail and cold-start nodes. We also compare it to the the graph homophility metric  $\beta$  proposed in [32]. Next, we apply Cold Brew to these datasets and compare its generalization ability to baseline graph-based as well as purely pointwise models on these datasets. We also show results on proprietary industry datasets.

#### 5.1 Datasets and Splits

We first detail the datasets used in this paper. We perform studies on several open-source datasets, together with four proprietary datasets. The proprietary E-commerce datasets, E-comm 1/2/3/4, refers to graphs subsampled from anonymized logs of an e-commerce store. They are sampled so as to not reflect the actual raw traffic distributions, and results are provided with respect to a baseline model for these datasets. The different datasets refer to different product subsets, and the labels indicate

<sup>&</sup>lt;sup>5</sup>We ignore the node features and use the label logits as explained in [17].

product categories that we wish to determine. Node features are text embeddings obtained from a fine-tuned BERT model. We show FCR values for the public datasets and exhaustively evaluate the proposed Cold Brew as well as several baselines for five public datasets and the proprietary datasets. The statistics of the datasets are summarized in Table 1.

We create specific training and test splits of the datasets in order to specifically study the generalization ability of Cold Brew to tail and cold-start nodes. In the following tables, the *head* data corresponds to the top 10% highest degree nodes in the graph, and the subgraph that they induce. The *tail* data corresponds to the 10% nodes in the graph with lowest (non-zero) degree, and the subgraph that they induce. All the zero degree nodes are in the *isolation* data. For datasets that don't have isolated nodes, we manually remove edges from 10% lowest degree nodes. The *Overall* data refers to the training/test splits without distinguishing head/tail/isolation.

Stats.	Cora	Citeseer	Pubmed	Arxiv	Chameleon	E-comm1	E-comm2	E-comm3	E-comm4
Num. of Nodes	2708	3327	19717	169343	2277	4918	29352	319482	793194
Num. of Edges	13264	12431	108365	2315598	65019	104753	1415646	8689910	22368070
Max Degree	169	100	172	13161	733	277	1721	4925	12452
Mean Degree	4.90	3.74	5.50	13.67	28.55	21.30	48.23	27.20	28.19
Median Degree	4	3	3	6	13	10	21	15	14
Isolated Nodes %	3%	3%	3%	3%	3%	6%	5%	5%	6%

Table 1: The statistics of datasets selected for evaluations.

### 5.2 FCR EVALUATION

In Table 2, the top half presented the FCR results together with the homophily metric  $\beta$  in [32] (Equation 6). The below half uncovered the different prediction quality for the head and the tail nodes. As can be seen from the table, as an indicator of the tail generalization difficulty, FCR differs among datasets, and is negatively correlated with the homophily metric (with pearson correlation coefficient -0.76). The evaluations on more datasets (including the datasets where FCR > 100%) are presented in Appendix B.

$$\beta(\mathcal{G}) = \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} \frac{\text{the number of } v \text{'s direct neighbors that have the same labels as } v}{\text{the number of } v \text{'s directly connected neighbors}} \times 100\%$$
 (6)

	Cora	Citeseer	Pubmed	Arxiv	Chameleon
GNN	86.96	72.44	75.96	71.54	68.51
MLP	69.02	56.59	73.51	54.89	58.65
Label Propagation	78.18	45.00	67.8	68.26	41.01
FCR %	32.86 %	63.39 %	76.91%	16.45%	73.61%
$\beta(\mathcal{G})$ %	83%	71%	79%	68%	25%
head-tail(GNN)	4.44	23.98	11.71	5.9	0.24
head-isolation(GNN)	31.01	33.09	15.21	28.81	1.55

Table 2: Above half: FCR and its components,  $\beta$  metric are added as a reference; below half: the performance difference of GNN on the head/tail and head/isolation splits. Here the "head/tail/isolation" means the 10% most connected, fewest connected, and isolated nodes in the graph.

### 5.3 EXPERIMENTAL RESULTS ON TAIL GENERALIZATION WITH COLD-BREW

In Table 3, we present the performances of the Cold Brew together with baselines on the tail and the isolation splits, across several different datasets. All models in the table are trained on the overall training subset, and are evaluated on the hold-out test subsets of tail and isolation splits (discussed in section 5.1). For the isolation split, the GNNs are evaluated with only self-loop (all other edges are non-existent/removed). The *GCN* refers to the the best configuration found through FCR-guided grid search (the search is performed over a range of hyperparameters, check Appendix A for details), without Structural Embedding. Correspondingly, GCN + SE refers to the best FCR-guided configuration with Structural Embedding, which is the default teacher model of Cold Brew. *GraphSAGE* refers to [9], *Simple MLP* refers to a simple node-wise MLP that has two hidden layers with 128 hidden dimensions, and *GraphMLP* refers to [30]. The results for E-commerce datasets are presented as relative improvements to the baseline (each value is the difference w.r.t. the value of the

Splits	Metrics/Models			Ope	n-Source I	Datasets	Proprietary Datasets				
Бриц				Citeseer	Pubmed	Arxiv	Chameleon	E-comm1	E-comm2	E-comm3	E-comm4
	GNNs	GCN 2 layers GraphSAGE	58.02 66.02	47.09 51.46	71.50 69.87	44.51 47.32	57.28 59.83	+3.89	+4.81	+5.24	+0.52
Isolation	MLPs	Simple MLP GraphMLP	68.40 65.00	<b>53.26</b> 52.82	65.84 71.22	51.03 51.10	60.76 <b>63.54</b>	+5.89 +6.27	+9.85 +9.46	+5.83 + <b>5.99</b>	+6.42 +7.37
	Cold Brew	GCN + SE 2 layers Student MLP	58.37 <b>69.62</b>	47.78 53.17	<b>73.85</b> 72.33	45.20 <b>52.36</b>	60.13 62.28	+0.27 +7.56	+0.76 +11.09	-0.50 +5.64	+1.22 +9.05
	GNNs	GCN 2 layers GraphSAGE	84.54 82.82	<b>56.51</b> 52.77	74.95 73.07	67.74 63.23	58.33 61.26	-3.82	- -3.07	- -2.87	-6.42
Tail	MLPs	Simple MLP GraphMLP	70.76 70.09	54.85 55.56	67.21 71.45	52.14 52.40	50.12 52.84	-0.37 -0.33	+1.74 +1.64	-0.13 <b>+1.27</b>	-0.45 +0.80
j	Cold Brew	GCN + SE 2 layers Student MLP	<b>84.66</b> 71.80	56.32 54.88	<b>75.33</b> 72.54	<b>68.11</b> 53.24	<b>60.80</b> 51.36	+0.85 +0.32	+0.44 +3.09	-0.60 -0.18	+1.10 +2.09

Table 3: The performance comparisons on the isolation and tail splits of different datasets. The full comparisons on head/tail/isolation/overall data are in the Appendix B. GCN+SE 2 layers is Cold Brew's teacher model. The Cold Brew outperforms GNN and other MLP baselines, and achieves the best performance on the isolation splits as well as some tail splits.

Splits	Metrics/Models		Ope	n-Source I	)atasets		Proprietary Datasets				
		Cora	Citeseer	Pubmed	Arxiv	Chameleon	E-comm1	E-comm2	E-comm3	E-comm4	
Overall	GCN 64 layers	40.04	23.66	75.65	65.53	58.14	-5.49	-6.59	-6.13	-3.57	
	GCN + SE 64 layers	<b>74.23</b>	<b>46.80</b>	<b>78.12</b>	<b>69.28</b>	<b>59.88</b>	<b>-1.71</b>	<b>-2.92</b>	<b>-3.29</b>	<b>-0.06</b>	
Head	GCN 64 layers	46.46	49.84	85.89	67.53	67.16	-5.60	-6.24	-6.05	-3.16	
	GCN + SE 64 layers	<b>87.38</b>	<b>71.18</b>	<b>86.81</b>	<b>71.35</b>	<b>69.63</b>	<b>-1.78</b>	<b>-2.17</b>	<b>-2.79</b>	<b>-0.35</b>	
Tail	GCN 64 layers	45.14	24.42	71.89	63.91	56.48	-3.85	-3.62	-3.84	<b>-1.14</b>	
	GCN + SE 64 layers	<b>79.56</b>	<b>36.52</b>	<b>74.88</b>	<b>65.19</b>	<b>61.73</b>	<b>-2.42</b>	-2.52	<b>-3.68</b>	-1.23	
Isolation	GCN 64 layers	39.97	22.12	68.57	40.03	57.60	-4.66	-4.63	-4.93	<b>-1.89</b>	
	GCN + SE 64 layers	<b>40.33</b>	<b>24.53</b>	<b>71.22</b>	<b>41.18</b>	<b>60.13</b>	- <b>3.08</b>	- <b>3.02</b>	<b>-4.00</b>	-2.32	

Table 4: The comparisons of Cold Brew's GCN and the traditional GCN for deep layers. When the number of layers is large, Cold Brew's GCN retained good performance while traditional GCN without SE suffers from the "over-smoothess" and degrades. Even for shallow layer, Cold Brew's GCN is better than traditional GCN.

GCN 2 layers on same dataset of the same split), and we do not disclose the absolute numbers due to proprietary reasons.

As shown in Table 3, Cold Brew's student MLP improves accuracy on isolated nodes by up to +11% on the E-commerce datasets and +2.4% on open source datasets. Cold Brew's student model handles isolated nodes much better, and it teacher GNN also achieves better performance in the tail split, compared to all other models. Especially, when compared with GraphMLP, Cold Brew's student MLP shows consistently better performance in most datasets. This can be explained from their different mechanisms: GraphMLP encodes graph knowledge implicitly in the learned weights, while Cold Brew explicitly attends to neighborhoods, even when it is absent. More detailed comparisons can be found in Appendix B.

There are other interesting observations. First, if the FCR is high (such as Pubmed), then for this dataset the MLP-type models tend to outperform GNN-type models in all splits. Regardless of FCR, for almost all datasets, the MLP-type models outperform the GNN-type models on the isolation split, and a few on the tail split, while the GNN-type models are superior in other splits. Second, the proposed structural embeddings imply a tantalizing potential to alleviate the over-smoothness [26, 27, 28] and bottleneck [39] issues observed in deep GCN models. As shown in table Table 4, Cold Brew's GCN (GCN + SE) significantly outperformed the traditional GCN on 64 layers: the former has 34% test accuracy higher on Cora, 23% higher on Citeseer and similar on others.

Indeed, the improvement over isolation and tail splits (especially the isolation split) comes with a cost: we observed a performance drop for the student MLP model on the head and several other datasets' tail splits, compared with the naive GCN model. The full performance on other splits are listed in the appendix as a reference. However, the cold-brew specifically targets at the challenging strict cold start issues, as a new compelling alternative for in these cases. Meanwhile in the non-cold-start cases, the traditional GCN models can still be used to obtain good performance. Note that, even on the head splits, the proposed GNN teacher model of Cold Brew still outperformed traditional GNN models. We hence consider as promising future work to adaptively switch between using Cold Brew teacher and student models, based on the current node connectivity degree and tailedness.

# 5.4 VISUALIZATION

Figure 3 visualizes the last-layer embeddings of different models after t-SNE dimensionality reduction. In the figure, colors denotes node labels and all nodes are marked as dots, with isolation subset

nodes additionally marked with 'x's and the tail subset additionally marked with triangles. Although the GCN model did a decent job in separating different classes, a significant portion of the tail and isolation nodes fall into wrong class clusters. Cold Brew's MLP is much better discriminative in the tail and isolation splits.

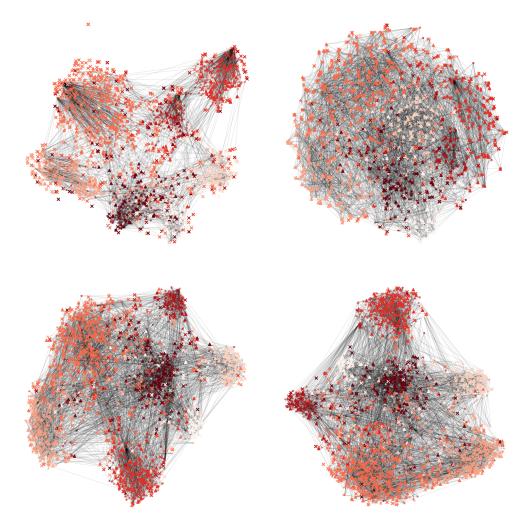


Figure 3: The top two subfigures: the last layer embeddings of GCN and Simple MLP, the bottom two subfigures: the last layer embeddings of GraphMLP and Cold Brew's student MLP. All embeddings are projected to 2D with t-SNE. Cold Brew's MLP has the fewest isolated nodes that are misplaced into wrong clusters.

# 6 Conclusion

In this paper, we studied the problem of generalizing GNNs to the tail and strict cold start nodes, whose neighborhood information is noisy or missing. We proposed a teacher-student knowledge distillation procedure to better generalize to the isolated nodes. We added an independent set of structural embeddings in GNN layers to to alleviate node over-smoothness, and also proposed a virtual neighbor discovery step for the student model to attend to estimated neighborhood nodes. We additionally established FCR, a metric for quantifying the difficulty of truly inductive representation learning, to optimize our method design. Experiments demonstrated the consistently superior performance of our proposed framework, on several common benchmarks as well as proprietary datasets.

# REFERENCES

- [1] Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and S Yu Philip. A comprehensive survey on graph neural networks. *IEEE transactions on neural networks and learning systems*, 32(1):4–24, 2020.
- [2] Palash Goyal and Emilio Ferrara. Graph embedding techniques, applications, and performance: A survey. *Knowledge-Based Systems*, 151:78–94, 2018.
- [3] Mahdi Kherad and Amir Jalaly Bidgoly. Recommendation system using a deep learning and graph analysis approach. *arXiv preprint arXiv:2004.08100*, 2020.
- [4] Shakila Shaikh, Sheetal Rathi, and Prachi Janrao. Recommendation system in e-commerce websites: A graph based approached. In 2017 IEEE 7th International Advance Computing Conference (IACC), pages 931–934. IEEE, 2017.
- [5] Nitai B Silva, Ren Tsang, George DC Cavalcanti, and Jyh Tsang. A graph-based friend recommendation system using genetic algorithm. In *IEEE congress on evolutionary computation*, pages 1–7. IEEE, 2010.
- [6] Jiani Zhang, Xingjian Shi, Shenglin Zhao, and Irwin King. Star-gcn: Stacked and reconstructed graph convolutional networks for recommender systems. arXiv preprint arXiv:1905.13129, 2019.
- [7] Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. *arXiv preprint arXiv:1609.02907*, 2016.
- [8] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. Graph attention networks. *arXiv preprint arXiv:1710.10903*, 2017.
- [9] William L Hamilton, Rex Ying, and Jure Leskovec. Inductive representation learning on large graphs. *arXiv preprint arXiv:1706.02216*, 2017.
- [10] Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? *arXiv preprint arXiv:1810.00826*, 2018.
- [11] Felix Wu, Amauri Souza, Tianyi Zhang, Christopher Fifty, Tao Yu, and Kilian Weinberger. Simplifying graph convolutional networks. In *International conference on machine learning*, pages 6861–6871. PMLR, 2019.
- [12] Johannes Klicpera, Aleksandar Bojchevski, and Stephan Günnemann. Predict then propagate: Graph neural networks meet personalized pagerank. *arXiv preprint arXiv:1810.05997*, 2018.
- [13] Thorsten Joachims. Transductive learning via spectral graph partitioning. In *Proceedings of the 20th International Conference on Machine Learning (ICML-03)*, pages 290–297, 2003.
- [14] Kamalika Chaudhuri, Fan Chung, and Alexander Tsiatas. Spectral clustering of graphs with general degrees in the extended planted partition model. In *Conference on Learning Theory*, pages 35–1. JMLR Workshop and Conference Proceedings, 2012.
- [15] Yilin Zhang and Karl Rohe. Understanding regularized spectral clustering via graph conductance. *arXiv preprint arXiv:1806.01468*, 2018.
- [16] Yifei Wang, Yisen Wang, Jiansheng Yang, and Zhouchen Lin. Dissecting the diffusion process in linear graph convolutional networks. *arXiv* preprint arXiv:2102.10739, 2021.
- [17] Qian Huang, Horace He, Abhay Singh, Ser-Nam Lim, and Austin R Benson. Combining label propagation and simple models out-performs graph neural networks. *arXiv* preprint *arXiv*:2010.13993, 2020.
- [18] Xiaojin Zhu. Semi-supervised learning with graphs. Carnegie Mellon University, 2005.
- [19] Bowen Hao, Jing Zhang, Hongzhi Yin, Cuiping Li, and Hong Chen. Pre-training graph neural networks for cold-start users and items representation. In *Proceedings of the 14th ACM International Conference on Web Search and Data Mining*, pages 265–273, 2021.
- [20] Hao Ding, Yifei Ma, Anoop Deoras, Yuyang Wang, and Hao Wang. Zero-shot recommender systems. *arXiv preprint arXiv:2105.08318*, 2021.
- [21] Xuan Nhat Lam, Thuc Vu, Trong Duc Le, and Anh Duc Duong. Addressing cold-start problem in recommendation systems. In *Proceedings of the 2nd international conference on Ubiquitous information management and communication*, pages 208–211, 2008.

- [22] Yuanfu Lu, Yuan Fang, and Chuan Shi. Meta-learning on heterogeneous information networks for cold-start recommendation. In *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pages 1563–1573, 2020.
- [23] Jingjing Li, Mengmeng Jing, Ke Lu, Lei Zhu, Yang Yang, and Zi Huang. From zero-shot learning to cold-start recommendation. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 33, pages 4189–4196, 2019.
- [24] Cheng Yang, Jiawei Liu, and Chuan Shi. Extract the knowledge of graph neural networks and go beyond it: An effective knowledge distillation framework. In *Proceedings of the Web Conference* 2021, pages 1227–1237, 2021.
- [25] Yuzhao Chen, Yatao Bian, Xi Xiao, Yu Rong, Tingyang Xu, and Junzhou Huang. On self-distilling graph neural network. arXiv preprint arXiv:2011.02255, 2020.
- [26] Kenta Oono and Taiji Suzuki. Graph neural networks exponentially lose expressive power for node classification. In *International Conference on Learning Representations*, 2020.
- [27] Qimai Li, Zhichao Han, and Xiao-Ming Wu. Deeper insights into graph convolutional networks for semi-supervised learning. In *Thirty-Second AAAI Conference on Artificial Intelligence*, 2018.
- [28] Hoang NT and Takanori Maehara. Revisiting graph neural networks: All we have is low-pass filters. *arXiv preprint arXiv:1905.09550*, 2019.
- [29] Geoffrey Hinton, Oriol Vinyals, and Jeff Dean. Distilling the knowledge in a neural network. *arXiv preprint arXiv:1503.02531*, 2015.
- [30] Yang Hu, Haoxuan You, Zhecan Wang, Zhicheng Wang, Erjin Zhou, and Yue Gao. Graph-mlp: Node classification without message passing in graph. *arXiv preprint arXiv:2106.04051*, 2021.
- [31] Shichang Zhang, Yozen Liu, Yizhou Sun, and Neil Shah. Graph-less neural networks: Teaching old mlps new tricks via distillation. *arXiv preprint arXiv:2110.08727*, 2021.
- [32] Hongbin Pei, Bingzhe Wei, Kevin Chen-Chuan Chang, Yu Lei, and Bo Yang. Geom-gcn: Geometric graph convolutional networks. *arXiv preprint arXiv:2002.05287*, 2020.
- [33] Meng Liu, Zhengyang Wang, and Shuiwang Ji. Non-local graph neural networks. *arXiv preprint* arXiv:2005.14612, 2020.
- [34] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. In *Advances in neural information processing systems*, pages 5998–6008, 2017.
- [35] Ahmet Iscen, Giorgos Tolias, Yannis Avrithis, and Ondrej Chum. Label propagation for deep semi-supervised learning. In *Proceedings of the IEEE/CVF Conference on Computer Vision* and Pattern Recognition, pages 5070–5079, 2019.
- [36] Hongwei Wang and Jure Leskovec. Unifying graph convolutional neural networks and label propagation. *arXiv preprint arXiv:2002.06755*, 2020.
- [37] Qian Huang, Horace He, Abhay Singh, Ser-Nam Lim, and Austin R Benson. Combining label propagation and simple models out-performs graph neural networks. *arXiv* preprint *arXiv*:2010.13993, 2020.
- [38] Adriana Romero, Nicolas Ballas, Samira Ebrahimi Kahou, Antoine Chassang, Carlo Gatta, and Yoshua Bengio. Fitnets: Hints for thin deep nets. *arXiv preprint arXiv:1412.6550*, 2014.
- [39] Uri Alon and Eran Yahav. On the bottleneck of graph neural networks and its practical implications. *arXiv* preprint arXiv:2006.05205, 2020.
- [40] Guohao Li, Matthias Muller, Ali Thabet, and Bernard Ghanem. Deepgcns: Can gcns go as deep as cnns? In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pages 9267–9276, 2019.
- [41] Ming Chen, Zhewei Wei, Zengfeng Huang, Bolin Ding, and Yaliang Li. Simple and deep graph convolutional networks. *arXiv preprint arXiv:2007.02133*, 2020.
- [42] Hongwei Zhang, Tijin Yan, Zenjun Xie, Yuanqing Xia, and Yuan Zhang. Revisiting graph convolutional network on semi-supervised node classification from an optimization perspective. *arXiv* preprint arXiv:2009.11469, 2020.

- [43] Guohao Li, Chenxin Xiong, Ali Thabet, and Bernard Ghanem. Deepergen: All you need to train deeper gens. *arXiv preprint arXiv:2006.07739*, 2020.
- [44] Sitao Luan, Mingde Zhao, Xiao-Wen Chang, and Doina Precup. Break the ceiling: Stronger multi-scale deep graph convolutional networks. *arXiv preprint arXiv:1906.02174*, 2019.
- [45] Keyulu Xu, Chengtao Li, Yonglong Tian, Tomohiro Sonobe, Ken-ichi Kawarabayashi, and Stefanie Jegelka. Representation learning on graphs with jumping knowledge networks. In *International Conference on Machine Learning*, pages 5453–5462. PMLR, 2018.
- [46] Meng Liu, Hongyang Gao, and Shuiwang Ji. Towards deeper graph neural networks. In *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pages 338–348, 2020.
- [47] Sergey Ioffe and Christian Szegedy. Batch normalization: Accelerating deep network training by reducing internal covariate shift. *ICML*, 2015.
- [48] Lingxiao Zhao and Leman Akoglu. Pairnorm: Tackling oversmoothing in gnns. *arXiv preprint* arXiv:1909.12223, 2019.
- [49] Kuangqi Zhou, Yanfei Dong, Kaixin Wang, Wee Sun Lee, Bryan Hooi, Huan Xu, and Jiashi Feng. Understanding and resolving performance degradation in graph convolutional networks. *arXiv preprint arXiv:2006.07107*, 2020.
- [50] Chaoqi Yang, Ruijie Wang, Shuochao Yao, Shengzhong Liu, and Tarek Abdelzaher. Revisiting "over-smoothing" in deep gcns. *arXiv* preprint arXiv:2003.13663, 2020.
- [51] Kaixiong Zhou, Xiao Huang, Yuening Li, Daochen Zha, Rui Chen, and Xia Hu. Towards deeper graph neural networks with differentiable group normalization. *Advances in Neural Information Processing Systems*, 33, 2020.

#### A SEARCH SPACE DETAILS

In the computation of FCR, we include a search space of model hyperparameters for GNN, MLP and LP, in order to find the best suitable configurations for distillation.

For GNN model, we take GCN as a backbone and performed grid search over the number of hidden layers, whether it has structural embedding or not, the type of residual connection, and the type of normalization. For the number of hidden layers, we considered 2, 4, 8, 16, 32, and 64. For the types of residual connections, we include: (1) connecting to the last layer [40, 27], (2) initial connection connecting to the initial layer [41, 12, 42], (3) dense connection connecting to all the preceding layers [40, 27, 43, 44], and (4) jumping connection combining all all the preceding layers only at the final graph convolutional layer [45, 46]. For the types of normalizations, we grid search over: batch normalization (BatchNorm) [47], pair normalization (PairNorm) [48], node normalization (NodeNorm) [49], mean normalization (MeanNorm) [50], and differentiable group normalization (GroupNorm) [51].

For the architecture design for Cold Brew's MLP, we conducted hyperparameter search over the number of hidden layers, the existence of residual connection, the hidden dimensions, and the optimizers. The number of hidden layers is searched over (2, 8, 16, 32). The number of hidden dimensions is searched over (128, 256). The optimizer is searched over (Adam(lr=0.001) Adam(lr=0.005), Adam(lr=0.002), SGD(lr=0.005))

For the Label Propagation, we conducted hyperparameter search over number of propagations, propagation matrix type, and the mixing coefficient  $\alpha$  [17]. The number of propagations is searched over (10, 20, 50, 100, 200). The propagation matrix type is searched over adjacency matrix or normalized Laplacian matrix. The mixing coefficient  $\alpha$  is searched over (0.01, 0.1, 0.5, 0.9, 0.99).

The best GCN, MLP, and LP configurations are reported in Tables 5, 6, and 7, respectively.

# B THE PERFORMANCE ON ALL SPLITS OF THE DATA

The performance evaluations on all splits are listed in Table 8.

The FCR evaluation on more datasets are presented in Fig 9.

Dataset	Best GCN								
	Num layers	whether has SE	residual type	normalization type					
Cora	2 layer	has structural embedding	no residual	PairNorm					
Citeseer	2 layer	has structural embedding	no residual	PairNorm					
Pubmed	16 layer	has structural embedding	initial connection	GroupNorm					
Arxiv	4 layer	has structural embedding	initial connection	GroupNorm					
Chameleon	2 layer	has structural embedding	initial connection	BatchNorm					

Table 5: Best GCN configurations

Dataset	Best MLP								
	hidden layers	residual connection	hidden dimensions	optimizer					
Cora	2 layer	no residual	128	Adam(lr=0.001)					
Citeseer	4 layer	no residual	128	Adam(lr=0.001)					
Pubmed	2 layer	no residual	256	Adam(lr=0.02)					
Arxiv	2 layer	no residual	256	Adam(lr=0.001)					
Chameleon	2 layer	no residual	256	Adam(lr=0.001)					

Table 6: Best MLP configurations

Dataset	Best LP								
	number of propagation	propagation matrix type	mixing coefficient						
Cora	50	Laplacian matrix	0.1						
Citeseer	100	Laplacian matrix	0.01						
Pubmed	50	Adjacency matrix	0.5						
Arxiv	100	Laplacian matrix	0.5						
Chameleon	50	Laplacian matrix	0.1						

Table 7: Best Label Propagation configurations

Table 8: The performance comparisons on different splits of different datasets.

Splits	Me	trics/Models	I	Ope	n-Source I	atasets		Proprietar	ry Datasets		
орию				Citeseer	Pubmed	Arxiv	Chameleon	E-comm1	E-comm2	E-comm3	E-comm4
	GNNs	GCN 2 layers GraphSAGE	58.02 66.02	47.09 51.46	71.50 69.87	44.51 47.32	57.28 59.83	+3.89	- +4.81	- +5.24	+0.52
Isolation	MLPs	Simple MLP GraphMLP	68.40 65.00	<b>53.26</b> 52.82	65.84 71.22	51.03 51.10	60.76 <b>63.54</b>	+5.89 +6.27	+9.85 +9.46	+5.83 + <b>5.99</b>	+6.42 +7.37
	Cold Brew	GCN + SE 2 layers Student MLP	58.37 <b>69.62</b>	47.78 53.17	<b>73.85</b> 72.33	45.20 <b>52.36</b>	60.13 62.28	+0.27 +7.56	+0.76 +11.09	-0.50 +5.64	+1.22 +9.05
	GNNs	GCN 2 layers GraphSAGE	84.54 82.82	<b>56.51</b> 52.77	74.95 73.07	67.74 63.23	58.33 61.26	-3.82	- -3.07	-2.87	- -6.42
Tail	MLPs	Simple MLP GraphMLP	70.76 70.09	54.85 55.56	67.21 71.45	52.14 52.40	50.12 52.84	-0.37 -0.33	+1.74 +1.64	-0.13 +1.27	-0.45 +0.80
	Cold Brew	GCN + SE 2 layers Student MLP	<b>84.66</b> 71.80	56.32 54.88	<b>75.33</b> 72.54	<b>68.11</b> 53.24	<b>60.80</b> 51.36	+0.85 +0.32	+0.44 +3.09	-0.60 -0.18	+1.10 +2.09
	GNNs	GCN 2 layers GraphSAGE	88.68 87.75	80.37 74.81	85.79 86.94	73.35 70.85	67.49 62.08	-4.26	- -4.17	- -3.50	- -7.46
Head	MLPs	Simple MLP GraphMLP	74.33 72.45	72.00 69.83	89.00 89.00	56.34 56.65	60.82 62.44	-16.74 -15.96	-18.10 -18.08	-16.73 -15.33	-16.51 -15.41
	Cold Brew	GCN + SE 2 layers Student MLP	<b>89.39</b> 74.53	<b>80.76</b> 72.33	87.83 <b>90.33</b>	<b>74.01</b> 57.41	70.56 61.28	+1.11 -15.28	<b>+0.47</b> -17.42	-0.39 -17.02	<b>+1.28</b> -15.41
	GNNs	GCN 2 layers GraphSAGE	84.89 80.90	70.38 66.21	78.18 76.73	71.50 68.33	59.30 70.02	-3.09	- -3.86	-2.58	- -5.48
Overall	MLPs	Simple MLP GraphMLP	69.02 71.87	56.59 68.22	73.51 82.03	54.89 53.81	58.65 57.67	-12.69 -12.26	-12.86 -12.01	-12.68 -10.80	-13.16 -11.41
	Cold Brew	GCN + SE 2 layers Student MLP	<b>86.96</b> 72.36	<b>72.44</b> 67.54	79.03 <b>82.00</b>	<b>71.92</b> 54.94	<b>68.51</b> 59.07	+0.65 -11.25	-0.24 -11.51	-0.77 -11.55	<b>+1.43</b> -11.21

	Cora	Citeseer	Pubmed	Arxiv	Cham.	Squ.	Actor	Cornell	Texas	Wisconsin
GNN	86.96	72.44	75.96	71.54	68.51	31.95	59.79	65.1	61.08	81.62
MLP	69.02	56.59	73.51	54.89	58.65	38.51	37.93	86.26	83.33	85.42
Label Propagation	78.18	45.00	67.8	68.26	41.01	22.85	29.69	32.06	52.08	40.62
FCR %	32.86 %	63.39 %	76.91%	16.45%	73.61%	141.91%	57.93%	139.04%	171.2 %	108.48 %
$\beta(\mathcal{G})$ %	83%	71%	79%	68%	25%	22%	24%	11%	6%	16%
head - tail(GNN)	4.44	23.98	11.71	5.9	0.24	-6.51	2.22	-4.37	-11.26	-33.92
head-isolation(GNN)	31.01	33.09	15.21	28.81	1.55	-4.85	22.61	-18.68	-24.62	-29.23

Table 9: Above half: FCR and its components,  $\beta$  metric are added as a reference; below half: the performance difference of GNN on the head/tail and head/isolation splits.