A Collective Learning Framework to Boost GNN Expressiveness

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Abstract

Graph Neural Networks (GNNs) have recently been used for node and graph classification tasks with great success, but GNNs model dependencies among the attributes of nearby neighboring nodes rather than dependencies among observed node labels. In this work, we consider the task of inductive node classification using GNNs in supervised and semi-supervised settings, with the goal of incorporating label dependencies. Because current GNNs are not universal (i.e., most-expressive) graph representations, we propose a general collective learning approach to increase the representation power of any existing GNN. Our framework combines ideas from collective classification with self-supervised learning, and uses a Monte Carlo approach to sampling embeddings for inductive learning across graphs. We evaluate performance on five real-world network datasets and demonstrate consistent, significant improvement in node classification accuracy, for a variety of state-of-the-art GNNs.

1. Introduction

Graph Neural Networks (GNNs) have recently shown great success at node and graph classification tasks (Kipf & Welling, 2016; Hamilton et al., 2017; Luan et al., 2019). GNNs have been applied in both transductive settings (where the test nodes are embedded in the training graph) and inductive settings (where the training and test graphs are disjoint). However, GNN methods focus on modeling dependencies among the observed attributes and the local graph structure around a node. And despite their success, existing GNNs have known shortcomings: they are not universal (most-expressive) graph representations (Morris et al., 2019; Murphy et al., 2019; Xu et al., 2018). That is, GNNs are not expressive enough for some node classification tasks. At the same time, a large body of work in relational learning has focused on strengthening poorly-expressive (i.e., local) classifiers in relational models (e.g., relational logistic regression, naive Bayes, decision trees (Neville et al., 2003a)) through collective classification, which have been shown to improve classification performance, particularly in semi-supervised learning over partially labeled graphs (Xiang & Neville, 2008; Koller et al., 2007; Pfeiffer III et al., 2015).

In this work, we empirically investigate our hypothesis that, by explicitly incorporating label dependencies among neighboring nodes—akin to how collective classification improves not-so-expressive classifiers—it is possible to devise an add-on training and inference procedure that can improve the expressiveness of existing GNNs, for both semi-supervised and supervised node classification tasks. However, dependencies among the node labels in a partially labeled graph are not straightforward to incorporate into GNNs, these require a redesign of how GNNs are trained.

Contributions. In this paper, we first show that collective classification is provably unnecessary if one can learn GNNs that are most-expressive. Then, because current GNNs are not most-expressive, we propose an add-on general collective classification framework for semi-supervised learning using GNNs, which our experiments show to consistently improve the node classification accuracy of a variety of state-of-the-art GNNs. Our framework uses a self-supervised learning procedure—via randomized input-masking—that is able to leverage true labels as input attributes. This is combined with a Monte Carlo approach to sampling embeddings, which encode global/joint information as local variability and facilitates inductive learning. Our approach is applicable for learning over partially labeled graphs, whether there are labels available in the test data or not.

2. Problem formulation

We consider the problem of inductive semi-supervised node classification, which takes as input a graph \(G^{(tr)} = (V^{(tr)}, E^{(tr)}), X^{(tr)}, Y^{(tr)}\) for training, where \(V^{(tr)}\) is a set of \(n^{(tr)}\) vertices, \(E^{(tr)} \subseteq V^{(tr)} \times V^{(tr)}\) is a set of edges with adjacency matrix \(A^{(tr)}\), \(X^{(tr)}\) is a \(n^{(tr)} \times p\) matrix containing node attributes as \(p\)-dimensional vectors, and \(Y^{(tr)}\) is a set of observed labels of a connected set of nodes \(V_L^{(tr)} \subseteq V^{(tr)}\), where \(V_L^{(tr)}\) is assumed to be a proper subset of \(V^{(tr)}\), noting
that $V^\text{(te)}_L = \emptyset$ is allowed. Let $Y^\text{(te)}_U$ be the unknown labels of nodes $V^\text{(te)}_U = V^\text{(te)} \setminus V^\text{(te)}_L$. The goal is to learn a joint model of $Y^\text{(te)}_U \sim P(Y^\text{(te)}_U | G^\text{(te)})$ and apply this same model to predict hidden labels $Y^\text{(te)}$ in another test graph $G^\text{(te)}$, i.e., $Y^\text{(te)}_U = \arg \max_{Y_U} P(Y_U | G^\text{(te)})$.

In this work, we explore two different classification tasks. The first task considers an unlabeled test graph $G^\text{(te)} = (V^\text{(te)}, E^\text{(te)}, X^\text{(te)}_V, Y^\text{(te)}_L)$. In this case, the goal is to predict the labels for all nodes $Y^\text{(te)}_U = Y^\text{(te)}$. The task of predicting node labels when no labels are available in test data sounds like a fully supervised learning task, rather than a semi-supervised task, but it is not. Although it has a similar description to supervised learning node classification tasks (e.g., (Hamilton et al., 2017)), fully supervised approaches do not fully exploit dependencies between observed labels of instances that are connected in the training data. Specifically, there is a measurable difference—in terms of information content—between having the known training labels $Y^\text{(tr)}_L$ connected in $G^\text{(tr)}$ or spread out through the graph. In the latter case, it is unlikely that labeled examples are connected, and thus it will be difficult to learn label dependencies. If the known labels are connected in training, and GNNs could exploit their dependencies through semi-supervised learning, that would further improve their representation power.

The second task is a more traditional semi-supervised learning task that considers a partially labeled test graph $G^\text{(te)} \text{partial} = (V^\text{(te)}, E^\text{(te)}, X^\text{(te)}_V, Y^\text{(te)}_L, Y^\text{(te)}_U)$.

In this case, the goal is to predict the hidden labels $Y^\text{(te)}_U = Y^\text{(te)} \setminus Y^\text{(te)}_L$ conditioned on the observed labels in the graph. Here, it is clear that exploiting the dependencies among connected labeled instances could improve representation power.

We denote the above tasks (A) semi-supervised learning with unlabeled test data and (B) semi-supervised learning with partially-labeled test data. In this work we explore variants of both tasks.

**Graph neural networks and semi-supervised learning tasks:** Broadly, GNNs can perform semi-supervised learning over partially labeled graphs by propagating feature information throughout the graph. However, in training, existing GNN models ignore the dependency of node labels by assuming conditional independence among node labels and factoring the joint distribution of labels as

$$ P(Y_U | X, Y_L, A) = \Pi_{v \in V_L} P(y_v | X, Y_L, A). $$

Hence, when $Y_L = \emptyset$, the above equation corresponds to unlabeled test data; otherwise, $Y_L \neq \emptyset$, the above equation corresponds to partially labeled test data.

Specifically, GNN models learn a node representation $Z$ that minimizes the negative log-likelihood loss. The model then makes predictions based on $Z$, i.e., $\forall v \in V$, where maybe $Y_L = \emptyset$, $Z_v = \text{GNN}(X, Y_L, A; \Theta)_v$, $P(y_v | X, Y_L, A) = \sigma(WZ_v + b)_{y_v}$, where $Z_v$ is the representation for node $v$, $\sigma(\cdot)$ is the softmaximum activation, and $\Theta, W$ and $b$ are model parameters. Therefore, current GNNs will infer the label distribution $P(y_v | X, Y_L, A)$ for each node $v \in V$ independently. While here we have described a function that conditions on an arbitrary label set $Y_L$ to illustrate GNN’s conditional independence assumptions, it is not yet described how to actually incorporate the partial labels into the embedding function. We will address this challenge in Section 3.2.

**Inductive collective classification:** Conventional relational machine learning (RML) developed methods to learn joint models from labeled graphs (Lu & Getoor, 2003; Neville & Jensen, 2000)

$$ P(Y_U | X, A) $$

To achieve this, many of the methods use pseudolikelihood estimation and consider a Markov assumption—every node $v_i \in V$ is considered conditionally independent of the rest of the network given its Markov Blanket ($\text{MB}(v_i)$). For undirected graphs, this is often simply the set of the immediate neighbors of $v_i$.

Given the Markov blanket assumption, RML methods typically use a local conditional model (e.g., relational Naive Bayes (Neville et al., 2003b), relational logistic regression (Popescul et al., 2002)) to learn and infer labels within the network. The pseudolikelihood objective considers the nodes in a labeled subgraph $G_L$, where the labels of all neighbors are known:

$$ O = \sum_{v \in V^\text{(tr)}_L} \log P(y^\text{(tr)}_v | \text{MB}(v), X^\text{(tr)}, A^\text{(tr)}) $$

The key difference between Equation (2) and the GNNs objective in Equation (1): the RML model is conditioned on the labels $Y$ even when there are no observed labels in the test data, i.e., even when $Y^\text{(te)}_L = \emptyset$. When the model is applied to make predictions in an unlabeled graph, joint (i.e., collective) inference methods such as variational inference or Gibbs sampling must be applied in order to use the conditionals from Equation (2). This combines the local conditional probabilities with global inference to estimate the joint distribution over the unlabeled vertices, e.g.:

$$ P(Y_U | Y_L, X) \approx Q(Y_U) = \Pi_{v_i \in V_U} Q_i(y) $$

where each component $Q_i(y)$ is iteratively updated.

Alternatively, a Gibbs sampler iteratively draws a label from the corresponding conditional distributions of the unlabeled
vertices:
\[ y_v \sim P(y_v|Y_{MB(v)}, Y_L, X, A), \forall v \in V. \]

Note that for conventional RMLs, we assume a fully labeled (sub)network for learning, thus \( Y_{MB(v)} \) only includes known labels, i.e., \( v_j \in V_L \).

**Transductive collective classification:** For transductive settings, where the goal is to learn and predict within a partially labeled graph, RML methods have considered semi-supervised formulations (Koller et al., 2007; Xiang & Neville, 2008; Pfeiffer III et al., 2015) to model the joint probability distribution:
\[ P(Y_U|Y_L, X, A) \]

In this case RML methods use both collective learning and collective inference procedures for semi-supervised learning. For example Expectation Maximization (EM) (Xiang & Neville, 2008; Pfeiffer III et al., 2015), iterative updates the parameter estimates by utilizing the expected values of the unlabeled examples to relearn the parameters.

For instance, the PL-EM algorithm (Pfeiffer III et al., 2015) optimizes the pseudolikelihood

**E-Step:** evaluate \( P(Y_U^{(tr)}|Y_L^{(tr)}, X^{(tr)}, A^{(tr)}, \Theta_{t-1}) \)

**M-Step:** learn \( \Theta_t \):
\[ \Theta_t = \arg \max_{\Theta} \sum_{Y_U^{(tr)} \in \Gamma_U} P(Y_U^{(tr)}|Y_L^{(tr)}, X^{(tr)}, A^{(tr)}, \Theta_{t-1}) \times \sum_{v \in V^{(tr)}} \log P(y_v^{(tr)}|Y_{MB(v)}^{(tr)}, X^{(tr)}, A^{(tr)}, \Theta_t) \]

**Is collective classification able to better represent target label distributions than graph representations like GNNs?**

The answer to the above question is yes and no. Theorem 1 shows that a most-expressive GNNs (Murphy et al., 2019; Maron et al., 2019; Srinivasan & Ribeiro, 2019) would not be able to benefit from any collective classification method.

**Theorem 1 (Collective classification can be unnecessary).** Consider the task of predicting node labels when no labels are available in test data. Let \( \Gamma^*(v, G) \) be a most-expressive representation of node \( v \in V \) in graph \( G \). Then, for any collective inference procedure predicting the class label of \( v \in V \), there exists a classifier that takes \( \Gamma^*(v, G) \) as input and predicts the label of \( v \) with equal or higher accuracy.

The proof of Theorem 1 is in the Appendix. However, since state-of-the-art GNNs are not most-expressive, collective classification could help improve the expressiveness of GNNs. This leads to the key hypothesis of this work Hypothesis 1, which we validate empirically by extensive experimentation in Section 4.

**Hypothesis 1.** Since current Graph Neural Networks (e.g. GCN, GraphSAGE) cannot produce most expressive graph representation, collective learning should be able to improve the accuracy of node classification by producing a more expressive graph representation.

Why? Because current GNNs only propagate node attributes and not observed label information, they are not able to pay attention to the relationship between node attributes, the graph topology, and label dependencies. By including label information as input, the GNNs will be able to incorporate more information, while they try to model the joint label distribution.

In Section 3, we propose a self-supervised approach to incorporate what we denote as collective learning into GNNs. We develop methods for both task A and task B: for test graphs with and without observed labels.

### 3. Proposed framework: Collective Learning with GNNs

In this section, we outline MCC-GNN. It is a general framework to incorporate any GNN, and combines self-supervised learning and Monte Carlo embedding sampling to improve inductive learning on partially labeled graphs. We start by describing an implementation for task A and then add some adjustments to address task B.

#### 3.1. Collective learning with unlabeled test data

Given a partially labeled training graph \( G^{(tr)} = (V^{(tr)}, E^{(tr)}, X^{(tr)}, Y^{(tr)}) \) and an unlabeled test graph \( G^{(te)} = (V^{(te)}, E^{(te)}, X^{(te)}) \), the goal of the inductive node classification task is to train a joint model on \( G^{(tr)} \) to learn \( P(Y|G^{(tr)}) \) and apply it to \( G^{(te)} \).

| Notation | Description |
|----------|-------------|
| \( G^{(tr)} \) | training graph |
| \( (y^{(tr)}_L, y^{(tr)}_M) \) | labeled nodes and labels in training graph |
| \( (y^{(tr)}_{in}, y^{(tr)}_{out}) \) | nodes with true labeled used as model input |
| \( (y^{(te)}_{in}, y^{(te)}_{out}) \) | test graph |
| \( (y^{(te)}_L, y^{(te)}_M) \) | labeled nodes and labels in test graph |
| \( \hat{Y} \) | prediction of all vertices at iteration \( t \) |

Table 1. Table of Notations

**No test labels: Bootstrapping the predicted input labels.** Following Hypothesis 1, we propose Monte Carlo Collective Learning GNNs (MCC-GNN), which includes label information as input to GNNs to produce a more expressive representation. Assume we have label predictions \( \hat{Y}^{(t-1)} = \{y_v^{(t-1)}\}_{v \in V} \) at the \( t \)-th step of our algorithm. At iteration \( t \), the MCC-GNN model parameters are updated by considering \( \hat{Y}^{(t-1)} \) as part of the input attributes, and the graph representation is an average over the samples of
where $\sigma(\cdot)$ is the softmax activation function, $V_{L}^{(tr)}$ are the nodes with observed labels in the training data, and $X^{(te)}$ is again node attribute matrix in the training data. Suppose we use $K$ input samples, then the time/space complexity of the MCC-GNN is $K$ times the time/space complexity of the corresponding GNN model as we have to compute $K$ embeddings at each gradient step.

**Obtaining $\hat{Y}^{(t−1)}$.** In iteration $t$, we use the MCC-GNN model parameter $\Theta_{t−1}$ to obtain

$$Z_{u}^{(t−1)} = \mathbb{E}_{\hat{Y}^{(t−1)}} \left[ \text{GNN}(X^{(tr)}, \hat{Y}^{(t−1)}, A^{(tr)}; \Theta_{u}) \right]. \quad (3)$$

The optimization then becomes

$$\theta_{t}, W_{t}, b_{t} = \arg \min_{\theta, W, b} \sum_{v \in V_{L}^{(tr)}} \log (\sigma(W_{v}Z_{v}^{(t)} + b))_{y^{(v)}}, \quad (4)$$

where $\sigma(\cdot)$ is the softmax activation function, $V_{L}^{(tr)}$ are the nodes with observed labels in the training data, and $X^{(te)}$ is again node attribute matrix in the training data. Suppose we use $K$ input samples, then the time/space complexity of the MCC-GNN is $K$ times the time/space complexity of the corresponding GNN model as we have to compute $K$ embeddings at each gradient step.

We note that a self-supervised learning approach is critical for GNN methods to incorporate label dependencies and move towards collective classification. This is because the input to GNNs is typically the full graph $G^{(0)}$. If we included the observed labels directly $Y_{L}^{(te)}$ in the input, then it would be trivial to learn a model that optimized Equation (1). Instead, we can apply a mask to some of the labels so they do not appear in $Y_{L}^{(te)}$ and we can optimize over the masked set. In this way, the model is trained to explore different parts of the graph by applying random masks.

**Self-supervised MCC-GNN.** Given two partially labeled graphs $G^{(tr)} = (V^{(tr)}, E^{(tr)}, X^{(tr)}, Y^{(tr)}_{L})$ and $G^{(te)} = (V^{(te)}, E^{(te)}, X^{(te)}, Y^{(te)}_{L})$, the goal is to learn a model that estimates the label distribution conditioning on node attributes $X$ and some true labels $Y_{L}$ on the training graph $G^{(tr)}$, and apply the learned model to the test graph $G^{(te)}$ with true labels $Y_{L}^{(te)}$.

We find that given the label prediction $\hat{Y}$, the semi-supervised collective learning recursion in Equation (4) is ripe for self-supervision. To this end, we apply a mask to some of the observed training labels $Y_{L}^{(tr)}$. The unmasked $Y_{L}^{(tr)}$ labels replace the predicted labels $\hat{Y}^{(t−1)}$ in Equation (3). And the masked $Y_{L}^{(te)}$ labels and their respective nodes now become the target of the optimization in Equation (4).

The self-supervised mask is randomly sampled from a set of masks $M$ at every gradient step. In this way, the model is trained to explore different label correlations in the graph through these random masks.

### 3.2. Collective learning with partially labeled test data

**Self-supervised learning and collective classification.** In semi-supervised collective classification, algorithms typically only estimate labels for $Y_{L}$ in the E-step. Thus, optimization (in the M-step) only incorporates the impact of collective inference over the unknown portion of the graph. In order to learn more robust models, we may also want to consider self-supervised learning, where we mask part of the labeled input, to ensure that collective inference is able to reproduce the correct labeling over labeled portions of the graph.

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the model, we design a self-supervised learning procedure with random label masking. In each stochastic gradient descent step, we randomly sample a binary mask $M \sim \text{Uniform}(M)$ from a set of masks, where $M$ is a $|V| \times 1$ binary (0-1) vector. By applying the mask on the observed labels $Y^{(t)}_L$, this set is effectively partitioned into two parts, i.e. $Y^{(t)}_L \rightarrow \{Y^{(t)}_m, Y^{(t)}_o\}$, where true labels $Y^{(t)}_m = Y^{(t)}_L \odot M$ are used as input to MCC-GNN, and $Y^{(t)}_o = Y^{(t)}_L \odot \overline{M}$ are used as optimization target, where $\overline{M} := 1 - M$ is the bitwise negated vector of $M$.

We now rewrite Equations (3) and (4) using the sampled mask $M$. At iteration $t$, the MCC-GNN model parameters are updated by considering both $Y^{(t)}_m \odot M$, $Y^{(t-1)}$ as part of the input attributes. Given a mask $M$, the graph representation is an average over the samples of $Y^{(t-1)}$, changing Equation (3) to:

$$Z_v^{(t)}(M) = \mathbb{E}_{Y^{(t-1)}}[\text{GNN}(X^{(t-1)}_L, Y^{(t)}_m \odot M, Y^{(t-1)} \odot \overline{M}, A^{(t)}; \Theta_v)].$$ (5)

Then, the optimization in Equation (4) becomes

$$\Theta_v, W_t, b_t = \arg \min_{\Theta_v, W_t, b_t} \mathbb{E}_M \left[ -\sum_{v \in V_L^{(t-1)}} \overline{M}_v \log \sigma(W Z_v^{(t)}(M) + b)_{y^{(t)}_v} \right],$$ (6)

where, again, $\sigma(\cdot)$ is the softmax activation function, $Y^{(t)}_v$ are the nodes with observed labels in the training data, and $X^{(t)}_L$ is again node attribute matrix in the training data.

**Stochastic optimization of Equation (6).** In order to optimize Equation (6), we first need to compute unbiased estimates for $\{Z_v^{(t)}\}_{v \in V}$ in Equation (5) and an unbiased estimate of the expectation over $M$ in Equation (6).

First, an unbiased estimate of the expectation over $M$ can lead to a proper Robbins-Monro stochastic optimization procedure (Robbins & Monro, 1951), since we can obtain unbiased (low-variance) estimates of the gradient of the loss function by simply sampling a new mask $M \sim \text{Uniform}(M)$ at each gradient step.

Second, we can compute an unbiased estimate of $\{Z_v^{(t-1)}\}_{v \in V}$ in Equation (5) at each gradient step, by sampling multiple label assignments $Y^{(t-1)}_1, \ldots, Y^{(t-1)}_K$ (one-hot encoded), $K > 1$, and feeding them to GNNs and use the average of the generated node embeddings, much like the procedure in Section 3.1.

To obtain an initial label prediction $\hat{Y}^{(0)}$ and start the recursion, we use only the true labels as input to MCC-GNN, replacing the $Y^{(t-1)}$ in Equation (5) with zero matrix. Same random masking procedure is applied. The whole iterative process is visualized in Figure 1.

# Nodes

$\begin{array}{l|ccccc}
\text{Dataset} & \# \text{Nodes} & \# \text{Attributes} & \# \text{Classes} & \# \text{Test} \\
\hline
\text{Cora} & 2708 & 1433 & 7 & 1000 \\
\text{Pubmed} & 19717 & 500 & 3 & 1000 \\
\text{Friendster} & 43880 & 644 & 5 & 6251 \\
\text{Facebook} & 4556 & 3 & 2 & 1000 \\
\text{Protein} & 12679 & 29 & 2 & 2376 \\
\end{array}$

Table 2. Dataset statistics

## 4. Experiments

### 4.1. Datasets

We use five datasets for evaluation. The dataset statistics are shown in Table 2, and the descriptions are as follows:

- **Cora** and **Pubmed** are benchmark datasets for node classification tasks from (Sen et al., 2008). They are citation networks with nodes representing publications and edges representing citation relation. Node attributes are bag-of-word features of each document, and the predicted label is the corresponding research field.

- **Facebook** (Yang et al., 2017) is social network of Facebook users from Purdue university, where nodes represent users and edges represent friendship. The features of the nodes are: religious views, gender and whether the users hometown is in Indiana. The predicted labels is political view.

- **Friendster** (Teixeira et al., 2019) is social network. Nodes represent users and edges represent friendship. The node attributes include numerical features (e.g number of photos posted, etc) and categorical features (e.g. gender, college, music interests, etc), encoded as binary one-hot features. The node labels represent one of the five age groups: 0-24, 25-30, 36-40, 46-50 and over 50. This version of the graph contain 40K nodes, 25K of which are labeled.

- **Protein** is a collection of protein graphs from (Borgwardt et al., 2005). Each node is labeled with a functional role of the protein, and has a 29 dimensional feature vector. We use 85 graphs with an average size of 150 nodes.

### 4.2. Experiment Setup

To conduct inductive learning tasks, we have to properly split the graphs into labeled and unlabeled parts. For datasets containing only one graph (Cora, Pubmed, Facebook and Friendster), we randomly sample a connected component to be $V_L^{(in)}$, and then sample a test set ($V_T$) from the remainder nodes ($V_U$). To make partially-labeled test data available, we sample another connected component as $V_L^{(te)}$ with the same size as $V_L^{(in)}$. The nodes are sampled to guarantee that there is no overlapping between any two sets of $V_L^{(in)}$, $V_L^{(te)}$ and $V_T$. Here $G^{(in)}$ and $G^{(te)}$ have the same graph structure but with different labeled nodes.
For the protein dataset, as we have 85 disjoint graphs, we randomly choose 51 (60%) graphs for training, 17 (20%) graphs for validation and the remaining 17 (20%) graphs for testing. To simulate semi-supervised learning settings, we mask out 50% of true labels on the training graphs. For the tasks with partially-labeled test data, we randomly select 50% of the nodes in the test graphs as labeled nodes, and test on the remaining 50% nodes. We run five trials for all the experiments, and in each trial we randomly split the nodes/graphs as described.

As our method can be applied to any GNN model structure, we trained three GNNs as examples:

- GCN (Kipf & Welling, 2016) which includes two graph convolutional layers. Here we implemented an inductive variant of the original GCN model for our tasks.

- Supervised GraphSage (Hamilton et al., 2017) (denoted by GS) with Mean pooling aggregator. We use sample size of 5 for neighbor sampling.

- Truncated Krylov GCN (Luan et al., 2019) (denoted by TK), a recent GNN model that leverages multi-scale information in different ways and are scalable in depth. The TK-GCN has stronger expressive power and achieved state-of-the-art performance on node classification tasks. We implemented Snowball architecture which achieved comparable performance with the other truncated Krylov architecture in according to the original paper. In our implementation, we use 10 layers.

For each of GNNs, we compare its baseline performance (on its own) to the performance we achieve using it for collective learning in MCC-GNN. For a fair comparison, the baseline GNN and MCC-GNN are trained with the same model parameters, e.g. model depth, hidden dimensions, learning rate, early-stopping procedures. For unlabeled test data, we directly compare to the initial prediction obtained by GNN, which is used by MCC-GNN as input attributes. For partially labeled test data, the baseline GNN is trained with labeled set $V_L^{(tr)}$. As GNNs cannot take labels as input, $Y_L^{(te)}$ is not be used.

In addition, we also compare to three relational classifiers, ICA (Lu & Getoor, 2003), PL-EM (Pfeiffer III et al., 2015) and GMNN (Qu et al., 2019). The first two models apply collective learning and inference with simple local classifiers. Naive Bayes for PL-EM and Logistic regression for ICA. GMNN is the state-of-the-art collective model with GNNs, which uses two GCN models to model label dependency and node attribute dependency respectively. All the three models take true labels in their input, thus we use $Y_L^{(tr)}$ for training and $Y_L^{(te)}$ for testing.

We report the average accuracy score and standard error of five trials for the baseline models, and compute the absolute improvement of accuracy of our method over the corresponding base GNN. The only exception is on Friendster dataset. As the labels are highly imbalanced, we report the balanced accuracy score. Numbers in bold represent significant improvement over the baseline GNN based on a paired t-test ($p < 0.05$), and numbers with * is the best performing method in each column.

### 4.3. Results

The performance of all the models on node classification task is shown in Table 3 (task A with unlabeled test data) and Table 4 (task B with partially-labeled test data). Our proposed MCC-GNN is denoted as +CL (for Collective Learning) in the results and our model performance is shown in shaded area.

#### 4.3.1. UNLABELED TEST DATA

**Comparison with base GNN models** Table 3 shows that our method is able to improve the corresponding non-collective GNN models for all the three model architectures (i.e. GCN, GraphSage and TK-GCN). Although all the models have large variances over multiple trials — which is because different parts of the graphs are being trained and tested on in different trials, our model consistently improves the baseline GNN. The results from a paired t-test comparing the performance of our method and the corresponding non-collective GNN shows that the improvement is almost always significant (marked as bold), with two exceptions on Pubmed and Friendster. Comparing the gains on different datasets, our method achieved smaller gains on Friendster. This is because the Friendster graph is much more sparse than all other graphs (e.g. edge density of Friendster is 1.5e-4 and edge density of Cora is 1.44e-3 (Teixeira et al., 2019)), which makes it hard for any model to propagate label information and capture the dependency.

Moreover, comparing the improvement over GCN and TK-GCN, we can observe that in general our method adds more gains to GCN performance, and the difference is more obvious on Cora and Pubmed. For example, with 3% labeled data, our method when combining with GCN has an average of 62.9% improvement over GCN, 23.5% improvement over GraphSage, and 9.6% improvement over TK-GCN. This is in line with our assumption Hypothesis 1 that collective inference can help GNNs produce a more expressive representation. As GCN is provably less expressive than TK-GCN (Luan et al., 2019), there is a larger room to increase its expressiveness.

**Comparison with other relational classifiers** The two baseline non-GNN relational models, i.e. PL-EM and ICA generally perform worse than GNNs, with the only exception on Protein dataset. This could be because the two non-GNN models generally need a larger portion of labeled
Table 3. Node classification accuracy with unlabeled test data (%). Not to be compared with Table 4 due to the (required) different train and test data splits. Numbers in bold represent significant improvement in a paired t-test at the $p < 0.05$ level, and numbers with $^*$ is the best performing method in each column.

| # labels | Cora | Pubmed | Friendster | Facebook | Protein |
|----------|------|--------|------------|----------|---------|
| Random | 14.28 (0.00) | 14.28 (0.00) | 14.28 (0.00) | 20.00 (0.00) | 50.00 (0.00) |
| GCN (Kipf & Welling, 2016) | - | +6.29 (1.49) | +5.20 (1.12) | +5.18 (0.66) | +4.48 (2.33) | +3.30 (1.52) | +0.98 (0.23) | +0.81 (1.10) | +1.72 (0.48) | +1.22 (0.51) |
| GMNN (Pfeiffer III et al., 2015) | - | 50.69 (1.50) | 56.24 (2.08) | 66.08 (0.96) | 59.34 (3.47) | 64.37 (3.70) | 72.08 (1.87) | 28.10 (10.59) | 64.56 (0.92) | 73.85 (1.12) |
| TC (Lan et al., 2019) | - | +2.35 (0.50) | -2.78 (0.59) | -1.95 (0.45) | -1.48 (0.41) | -0.62 (0.21) | +0.65 (0.25) | +0.31 (0.15) | +2.38 (0.77) | +0.84 (0.12) |
| PL-EM (Pham et al., 2019) | - | 63.74 (2.61) | 70.01 (1.93) | 74.45 (0.34) | 61.13 (5.03) | 63.09 (5.57) | 75.46 (1.46) | 28.89 (10.16) | 67.63 (1.03) | 73.65 (1.69) |
| ICA (Lu & Getoor, 2003) | - | 20.70 (0.05) | 24.65 (0.38) | 30.46 (1.48) | 38.05 (4.85) | 44.85 (5.75) | 51.25 (3.06) | 23.26 (6.01) | 56.17 (7.42) | 78.46 (1.45) |
| GMNN (Pfeiffer III et al., 2019) | - | 26.20 (0.51) | 41.05 (0.50) | 49.51 (1.90) | 44.40 (1.92) | 45.62 (0.86) | 54.26 (2.09) | 25.14 (0.03) | 47.93 (6.04) | 84.88 (3.35) |
| PL-EM (Pham et al., 2019) | - | 49.05 (1.86) | 54.55 (1.15) | 67.16 (1.86) | 58.03 (3.62) | 62.50 (3.77) | 71.03 (4.54) | 22.20 (0.07) | 65.82 (1.30) | 76.75 (0.74) |

Set to train the weak local classifier, whereas GNNs utilize a neural network architecture as "local classifier”, which is better at representation learning by transforming and aggregating node attribute information. However, when the model is trained with a large training set (e.g. with 30% nodes on Protein dataset), modeling the label dependency becomes crucial.

For GMNN, the collective GNN model, it achieved better performance than its non-collective base model, i.e. GCN, and we can see that our model combining with GCN achieved comparable or slightly better results than GMNN. When combing with other more powerful GNNs, our model can easily out-perform it, e.g. on Cora, Pubmed and Facebook datasets, the TK-GCN performs better than GMNN and our method adds extra gains over TK-GCN.

4.3.2. Partially Labeled Test Data

Comparison to base GNN models Table 4 shows that our method again achieves consistent improvement over the corresponding non-collective GNNs. Comparing with unlabeled test data (task A), the gains are much larger with partially-labeled test data (task B). For example, when combining with GCN on Cora dataset, with unlabeled test data, the improvements of our method are 6.29%, 5.20% and 5.18% for various label rates, but with labeled test data, the improvements are 15.69%, 14.02% and 6.31%. This shows the importance of modeling label dependency especially when the some test data labels are observed.

Comparing the improvement over GCN and TK-GCN, again our model adds more gain to GCN in general, especially on Cora and Pubmed. For example, with 1.52% labels on Pubmed, our method when combining with GCN has an average of 5.62% gains over GCN, 1.49% gains over GraphSage, and 0.54% over truncated Krylov GCN.

Comparison to other relational classifiers We observed similar patterns as in task A with the unlabeled test data. The non-GNN models PL-EM and ICA perform worse than GNN models, with the only exception on Protein where ICA achieved the best performance, with an average accuracy of 84.39%. At the same time, our method is still able to improve the performance of the corresponding GNNs. The performance gap between GNNs and non-GNNs on Protein dataset shows that there is more room for us to learn from the collective learning and inference methods in order to improve the GNN models, especially for inductive semi-supervised tasks.

4.4. Ablation study

To investigate if adding predicted labels in model input adds extra information with partially-labeled test data described in Section 3.2, we tested the performance of a model variant which only use true labels as input with the same node masking procedure. Figure 2 shows two examples on Cora with GCN Figure 2a and Pubmed with TK-GCN Figure 2b, where including predicted labels achieves better performance. We run the model 10 times and calculate the average and standard deviation (shown as shaded area) of classification accuracy at each iteration $t$ as described in Section 3.2. We can see that adding predicted labels starts to improve the performance after the first iteration and achieves consistent gains.

5. Related work

On collective learning and neural networks. There has been work on applying deep learning to collective classification. For example, (Moore & Neville, 2017) proposed to use LSTM-based RNNs for relational classification tasks on graphs. They transform each node and its set of neighbors into an unordered sequence and use an RNN model to predict the class label as the output of that sequence. (Pham et al., 2017) designed a deep learning model for collective classification in multi-relational domains, which learns local and relational features simultaneously to encodes multi-relations between any two instances. The closest work to ours is (Monner & Reggia, 2013), which proposed a recurrent collective classification (RCC) framework, a variant of ICA (Lu & Getoor, 2003) including dynamic relational
The recent interest in semi-supervised learning is, possibly, attributed to representation learning being about understanding the data itself, rather than learning a representation that narrowly performs well in the training data of a particular task. The ease that representation learning can be applied to transfer learning tasks, only reinforces the argument that learning to represent is the key to the low generalization error observed in deep learning. Hence, revisiting the value of semi-supervised learning in graph representation learning is extremely valuable to the research community.

6. Conclusion

In this work, we answer the question “can collective learning and inference techniques improve the expressiveness of

features encoding label information. Unlike our framework, this model stacks multiple recursive steps and is trained end-to-end, also they use a weak local classifier and simple relation features such as average of neighborhood labels instead of GNNs, and no sampling of labels is included. These studies represent different ideas for bringing the power of neural networks to collective classification.

The first and only work applying statistical relational learning to GNNs is Graph Markov Neural Network (GMNN) (Qu et al., 2019), which proposed to model joint label distribution with a conditional random field trained with the variational EM algorithm. GMNN is trained by alternating an E-step and an M-step, and two GCNs are trained for the two steps respectively.

In parallel to our work, (Jia & Benson, 2020) considers regression tasks by modeling the joint GNN residual of a target set \(y - \hat{y}\) as a multivariate Gaussian, defining the loss function as the marginal likelihood only over labeled nodes \(\hat{y}_L\). In contrast, by using the more general foundation of collective classification, our framework can seamlessly model both classification and regression tasks, and include model predictions over the entire graph \(\hat{Y}\) as MCC-GNN’s input, thus affecting both the model prediction and the GNN training in both unlabeled and partially-labeled test data splits.

On self-supervised learning. Self-supervised learning is closely related to semi-supervised learning. In fact, self-supervised learning can be seen as a self-imposed semi-supervised learning task, where part of the input is masked (or transformed) and must be predicted back by the model (Doersch et al., 2015; Noroozi & Favaro, 2016; Lee et al., 2017; Misra et al., 2016). Recently, self-supervised learning has been broadly applied to achieve state-of-the-art accuracy in computer vision (Hénaff et al., 2019; Gidaris et al., 2020) and natural language processing (Devlin et al., 2018) supervised learning tasks.

The recent interest in semi-supervised learning is, possibly, attributed to representation learning being about understanding the data itself, rather than learning a representation that narrowly performs well in the training data of a particular task. The ease that representation learning can be applied in transfer learning tasks, only reinforces the argument that learning to represent is the key to the low generalization error observed in deep learning. Hence, revisiting the value of semi-supervised learning in graph representation learning is extremely valuable to the research community.

6. Conclusion

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Table 4. Node classification accuracy with partially labeled test data (%). Not to be compared with Table 3 due to the (required) different train and test data splits. Numbers in bold represent significant improvement in a paired t-test at the \(p < 0.05\) level, and numbers with * represent the best performing method in each column.

| # labels          | Cora                  | Pubmed                  | Friendster           | Facebook            | Protein               |
|-------------------|-----------------------|-------------------------|----------------------|---------------------|-----------------------|
|                   | 85 (3.21%)            | 105 (3.88%)             | 140 (5.17%)          | 300 (1.52%)         | 375 (1.90%)           | 600 (3.04%)           | 641 (1.47%)           | 70 (1.54%)            | 7607 (30%)           |
| Random            | 14.28 (0.00)          | 14.28 (0.00)            | 14.28 (0.00)         | 33.33 (0.00)        | 33.33 (0.00)          | 33.33 (0.00)          | 20.00 (0.00)          | 50.00 (0.00)          | 50.00 (0.00)          |
| GCN\textsuperscript{1}(Kipf & Welling, 2016)\textsuperscript{*}   | +15.69 (3.20)         | +14.02 (3.38)           | +6.31 (0.89)         | +5.62 (1.71)        | +5.06 (3.24)          | +4.60 (2.50)          | +0.90 (0.32)          | +2.95 (0.84)          | +0.75 (0.33)          |
| GS\textsuperscript{1}(Hamrick et al., 2017)\textsuperscript{*}   | -4.82 (0.84)          | +3.06 (0.20)            | +2.18 (0.21)         | +2.42 (0.27)        | +1.49 (0.10)          | +2.67 (0.56)          | +0.73 (0.23)          | +2.05 (0.04)          | +1.47 (0.63)          |
| TK\textsuperscript{1}(Lin et al., 2019)\textsuperscript{*}         | +5.58 (2.08)          | +61.32 (2.45)           | +67.95 (0.45)        | +63.05 (1.51)       | +67.95 (0.45)         | +74.01 (3.58)         | +29.30 (0.15)         | +65.80 (1.16)         | +78.94 (1.50)         |
| PL-EM\textsuperscript{1}(Pfeiffer III et al., 2015)\textsuperscript{*} | -20.35 (0.05)         | 25.25 (0.35)            | 31.45 (1.95)         | 31.70 (4.78)        | 34.92 (5.87)          | 48.70 (5.72)          | 26.30 (0.25)          | 54.56 (6.17)          | 77.95 (1.56)          |
| ICA\textsuperscript{1}(Lu & Getoor, 2003)\textsuperscript{*}       | -31.17 (3.66)         | 42.07 (1.29)            | 57.14 (1.81)         | 33.38 (4.69)        | 45.93 (5.48)          | 46.97 (1.84)          | 25.08 (0.17)          | 59.39 (3.69)          | 84.39 (4.08)          |
| GMNN\textsuperscript{1}(Qu et al., 2019)\textsuperscript{*}       | -36.38 (1.35)         | 48.31 (2.58)            | 64.02 (1.54)         | 54.11 (4.86)        | 56.31 (3.10)          | 68.13 (1.84)          | 28.44 (0.56)          | 63.13 (1.21)          | 77.54 (1.09)          |

Figure 2. MCC-GNN performance with and without updating predicted labels on Cora and Pubmed. X-axis refers to iteration number \(t\) in Section 3.2.
state-of-the-art GNNs in supervised and semi-supervised node classification tasks?" We first show that with the most expressive GNNs there is no need to do collective learning; however, since we do not have the most expressive models, we present a collective learning framework that can be combined with any existing GNN architectures to improve model expressiveness. We considered two inductive semi-supervised learning tasks: with and without labeled test data, and showed by extensive empirical study that our collective learning methods significantly improve GNNs performance on both tasks.

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Supplementary Material of collective learning GNN

Proof of Theorem 1

We restate the theorem for completeness.

**Theorem 1** (Collective classification can be unnecessary). Consider the task of predicting node labels when no labels are available in test data. Let \( \Gamma^*(v, G) \) be a most-expressive representation of node \( v \in V \) in graph \( G \). Then, for any collective inference procedure predicting the class label of \( v \in V \), there exists a classifier that takes \( \Gamma^*(v, G) \) as input and predicts the label of \( v \) with equal or higher accuracy.

**Proof.** Let \( \hat{Y}(v) = \varphi(\Gamma^*(v, G)) \) be a classifier function that takes the most expressive representation \( \Gamma^*(v, G) \) of node \( v \) as input and outputs a predicted class label for \( v \).

Let \( \hat{Y}^{(t)} \) be the set of predicted labels at iteration \( t \) of collective classification and let \( Y_v \) be the true label of node \( v \in V \). Then either (1) \( Y_v \perp \perp \varphi(\Gamma^*(v, G), \epsilon_v) \), or (2) \( Y_v \perp \perp \varphi(\Gamma^*(v, G), \epsilon_v, \hat{Y}^{(t)}) \).

Case (1): Given the classifier \( \varphi \) and the most expressive representation \( \Gamma^*(v, G) \), the true label of \( v \) is independent of the labels predicted with collective classification. In this case, the predicted labels of \( v \)'s neighbors offer no additional information and, thus, collective classification is unnecessary.

Case (2): In this case, the true label of \( v \) is not independent of the predicted labels. By Theorem 1 of Srinivasan & Ribeiro (2019), we know that for any random variable \( H_v \) attached to node \( v \in V \), it must be that \( \exists \varphi' \) a measurable function independent of \( G \) s.t.

\[
H_v \overset{a.s.}{=} \varphi'(\Gamma^*(v, G), \epsilon_v),
\]

where \( \epsilon_v \) is an noise source exogenous to \( G \) (pure noise), and a.s. implies almost sure equality. Defining \( H_v := Y_v, \)

\[
\varphi'(\Gamma^*(v, G), \epsilon_v, \hat{Y}^{(t)}),
\]

which means \( \hat{Y}^{(t)} \) must either be dependent on \( \epsilon_v \) or contain domain knowledge information about the function \( \varphi' \) that is not in \( \varphi \). Since \( \hat{Y}^{(t)} \) is a vector of random variables fully determined by \( G \) and \( \varphi' \), it cannot depend on an exogenous variable \( \epsilon_v \). Thus, the predictions must contain domain knowledge of \( \varphi' \). Hence, we can directly incorporate this domain knowledge into another classifier \( \varphi' \) s.t. \( Y_v \perp \perp \varphi(\Gamma^*(v, G), \epsilon_v, \hat{Y}^{(t)}) \), for instance \( \varphi' \) is a function of \( \varphi' \). In this case, \( \varphi' \) will predict the label of \( v \) with equal or higher accuracy than collective classification based on predicted labels \( \hat{Y} \), which finishes our proof.

Additional ablation study

| # labels | Cora | PubMed | Friendster | Facebook | Protein |
|----------|------|--------|------------|----------|---------|
| Random   | 14.28 (0.00) | 14.28 (0.00) | 14.28 (0.00) | 33.33 (0.00) | 33.33 (0.00) | 33.33 (0.00) | 20.00 (0.00) | 50.00 (0.00) | 50.00 (0.00) |
| GCN      | 45.15 (3.73) | 52.35 (2.01) | 65.11 (1.95) | 53.21 (4.04) | 57.15 (3.61) | 70.81 (3.47) | 29.80 (0.48) | 65.89 (0.68) | 73.03 (2.14) |
| + CL-random | 45.15 (3.73) | 52.35 (2.01) | 65.11 (1.95) | 53.21 (4.04) | 57.15 (3.61) | 70.81 (3.47) | 29.80 (0.48) | 65.89 (0.68) | 73.03 (2.14) |
| GS       | 46.38 (1.62) | 52.87 (1.03) | 63.46 (1.38) | 55.38 (3.48) | 57.61 (4.21) | 68.81 (4.15) | 28.05 (0.56) | 65.20 (0.40) | 71.05 (0.40) |
| + CL-random | 46.38 (1.62) | 52.87 (1.03) | 63.46 (1.38) | 55.38 (3.48) | 57.61 (4.21) | 68.81 (4.15) | 28.05 (0.56) | 65.20 (0.40) | 71.05 (0.40) |
| TK       | 61.99 (3.07) | 67.88 (1.80) | 73.04 (0.42) | 61.00 (4.93) | 61.91 (5.16) | 73.87 (3.99) | 29.44 (0.39) | 67.75 (0.40) | 73.38 (0.57) |
| + CL-random | 61.99 (3.07) | 67.88 (1.80) | 73.04 (0.42) | 61.00 (4.93) | 61.91 (5.16) | 73.87 (3.99) | 29.44 (0.39) | 67.75 (0.40) | 73.38 (0.57) |

Table 5. Node classification accuracy with **unlabeled** test data (%) using uniform sampling. Numbers in bold represent significant improvement in a paired t-test at the \( p < 0.05 \) level.

Creating more expressive GNN representations by averaging out random features was first proposed by Murphy et al. (2019). Murphy et al. (2019) shows a whole-graph classification application, Circulant Skip Links (CSL) graphs, where such randomized feature averaging is provably (and empirically) more expressive than GNNs. Our Monte Carlo collective learning method can be seen as a type of feature averaging GNN representation though, unlike Murphy et al. (2019), the
feature sampling is not at random, but rather driven by our own model recursively. Hence, it is fair to ask if our performance gains are simply because random feature averaging is beneficial to GNN representations? Or does collective learning sampling actually improve performance? We need an ablation study.

Therefore, in this section we investigate whether the gains of our method for unlabeled test data are from incorporating feature randomness, or from sampling w.r.t predicted labels (collective learning). To do so, we replace the samples drawn from previous prediction $\hat{Y}$ as uniformly drawn from the set of class labels at each gradient step in MCC-GNN. The results are shown in Table 5. Clearly, the random features are not able to consistently improve the model performance as our method does (contrast Table 5 with Table 3). In summary, collective learning goes beyond the purely randomized approach of Murphy et al. (2019), providing much larger, statistically significant, gains.

Further notes on experimental setup: Training/test split

As seen in Section 4.2, to approximate an inductive learning setting, we use a different train/test data split procedure (i.e. connected training set) on Cora and Pubmed networks from the public version (i.e. random training set) used in most of the existing GNN models (Kipf & Welling, 2016; Luan et al., 2019). This is illustrated in Figure 3, where the random training set of the traditional GNN evaluation methods (in e.g., (Kipf & Welling, 2016; Luan et al., 2019)) is shown on the left, contrasted with our harder task of connected training set shown on the right. This difference in task is the reason why the model performance reported in our paper is not directly comparable with the reported results in previous GNN papers, even though we used the same implementations and hyperparameter search procedures.

*Figure 3. The different data splits between traditional GNN train/test split evaluation (left) and our—more realistic—connected train/random test split evaluation (right)*