

Should Graph Convolution Trust Neighbors? A Simple Causal Inference Method

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ABSTRACT

Recent studies on Graph Convolutional Networks (GCNs) reveal the usefulness of adaptive locality, which enables adjusting the contribution of neighbors to the target node representation. Existing work typically achieves adaptive locality by introducing an additional module such as graph attention, which learns to weigh neighbor nodes. However, such module may not work well in practice, since fitting training data well does not necessarily lead to reasonable adaptive locality, especially when the labeled data are small.

In an orthogonal direction, this work explores how to achieve adaptive locality in the model inference stage, a new perspective that receives little scrutiny. The main advantage of leaving the training stage unchanged is generality — it can be applied to most GCNs and improve their inference accuracy. Given a trained GCN model, the idea is to make a counterfactual prediction by blocking the graph structure, *i.e.*, forcing the model to use each node’s own features to predict its label. By comparing the original prediction with the counterfactual prediction, we can assess the trustworthiness of neighbor nodes. Furthermore, we explore *graph uncertainty* that measures how the prediction would vary with the changes on graph structure, and introduce edge dropout into the inference stage to estimate graph uncertainty. We conduct empirical studies on seven node classification datasets to validate the effectiveness of our methods.

CCS CONCEPTS

- Computing methodologies — Neural networks; • Mathematics of computing — Graph algorithms; • Information systems — Data mining.

KEYWORDS

Graph Convolutional Network, Adaptive Locality

ACM Reference Format:

Fuli Feng, Weiran Huang, Xin Xin, Xiangnan He, and Tat-Seng Chua. 2018. Should Graph Convolution Trust Neighbors? A Simple Causal Inference

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Woodstock ’18, June 03–05, 2018, Woodstock, NY

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ACM ISBN 978-1-4503-9999-9/18/06...\$15.00

<https://doi.org/10.1145/1122445.1122456>

Method. In *Woodstock ’18: ACM Symposium on Neural Gaze Detection, June 03–05, 2018, Woodstock, NY*. ACM, New York, NY, USA, 11 pages. <https://doi.org/10.1145/1122445.1122456>

1 INTRODUCTION

GCN is a promising technique in a wide spectral of graph analytic applications such as user profiling [7, 33], text classification [23, 47], and recommender system [11, 40, 48]. Its main idea is to propagate the representations of neighbors to augment the target node representation, enforcing the smoothness constraint according to connectedness. Generally, graph convolution will increase the representation similarity of nodes in the same category according to the homophily assumption [26]. However, there are some cross-category connections in real-world graphs such as citation networks and social networks [3], *i.e.*, two connected nodes belong to different categories (see node 2 in Figure 1). In such cases, the graph convolution may improperly fuse neighborhood representations with the target node, misleading the prediction. To address this dilemma, it is essential to empower GCN with adaptive locality, *i.e.*, adjusting the effect from neighbor nodes in a node-specific manner.

A surge of attention has been paid on designing adaptive locality module for GCN, most of which focus on the attention mechanism, including neighbor attention [36] and hop attention [24]. The key idea is to assess the trustworthiness of neighbors based on their representations. Ideally, the attention weight should downweight the neighbors that belong to different categories with the target node for reducing their negative impacts. The hop attention weighs the representation of the target node at different GCN layers, which corresponds to the aggregation of neighbors at different hops. Intuitively, the hop attention can eliminate the negative effects of the neighbors by highlighting the own features of the target node. Due to the lack of supervision label for the attention network, it is typically optimized with the overall training objective of GCN, which however may not be reliable in practice [19].

Fitting the training data well does not necessarily lead to accurate assessment of neighbor trustworthiness. Worse still, in order to fit the training data, the graph attention can be distracted by spurious signals. Table 1 provides an empirical evidence on a node classification benchmark dataset OGB-arXiv [13] where representative GCN models are tested with different usage of a trustworthy signal. The trustworthy signal indicates the “ground truth” of whether trusting the neighbors or not (see details in Section 3). In the table, Self+Neighbor_Trust means integrating the trustworthy signal into

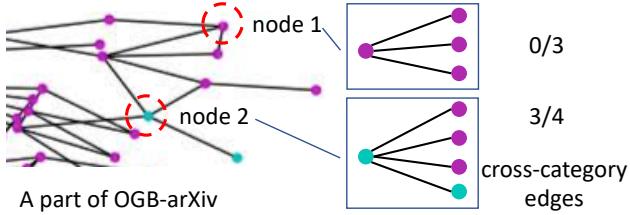


Figure 1: Illustration of cross-category connections in OGB-arXiv [13], a citation graph of papers. Nodes in different colors belong to different categories.

node features for GCN training; Self+Neighbor_Bound means the upper bound performance of using the trustworthy signal in the inference stage. For all the models, there exists a large performance gap between Self+Neighbor_Bound and Self+Neighbor_Trust, indicating that their adaptive locality module cannot fully use the signal to achieve accurate adaptive locality as expected.

This work explores the adaptive locality in the inference stage when a well-trained GCN predicts for unlabeled nodes. Our assumption is that the model output sheds light on the trustworthiness of neighbors and thus can guide the adaptive locality. For instance, we cannot trust the neighbors, if the model is uncertain about its prediction when the neighbors are taken into account. In addition, we can also discard the neighbors if the model is already confident to make prediction with only the target node features. Inherently, both the target node features and neighbors are the causes of the prediction for the target node. By distinguishing the two causal effects, we can revise the model prediction according to the trustworthiness of neighbors. In this way, the adaptive locality is disentangled from model training and can be applied to any GCN model.

To this end, we propose an *adaptive inference mechanism* (AdaInf), which implements the adjustment as a choosing mechanism. In particular, the choice is made between the original prediction of GCN (*i.e.*, trusting neighbors) and a counterfactual prediction with graph structure blocked (*i.e.*, trusting self), based on the confidence and uncertainty of the predictions. Especially, we explore graph uncertainty, aiming to capture how the prediction would vary with the changes on graph structure. To estimate graph uncertainty, we propose *Monte Carlo Edge-drop* (MCE), which performs random edge dropout and evaluates the variance of the predictions. Lastly, we feed the graph uncertainty with other factors that characterize the predictions into a classifier to learn the choice of AdaInf. We demonstrate AdaInf on APPNP [18], a state-of-the-art GCN model for node classification. Extensive experiments on seven datasets of different node classification settings validate the effectiveness of our proposal.

The main contributions of this work are summarized as follows:

- We achieve achieving adaptive locality during GCN inference and propose an AdaInf mechanism that is model-agnostic.
- We propose MCE to estimate the graph uncertainty for GCN prediction, introducing edge dropout into the inference stage.
- We conduct experiments on seven node classification datasets to demonstrate the rationality of the proposed methods.

2 PRELIMINARIES

Node classification. We represent a graph with N nodes as $G = (A, X)$, *i.e.*, an adjacency matrix $A \in \mathbb{R}^{N \times N}$ associated with a

feature matrix $X = [x_1, x_2, \dots, x_N]^T \in \mathbb{R}^{N \times D}$. A describes the connections between nodes where $A_{ij} = 1$ means there is an edge between node i and j , otherwise $A_{ij} = 0$. D is the dimension of the input node features. Node classification is one of the most popular analytic tasks on graph data. In the general problem setting, the label of M nodes are given $Y = [y_1, y_2, \dots, y_M]^T \in \mathbb{R}^{N \times L}$, where L is the number of node categories and y_1 is a one-hot vector. The target is to learn a classifier $f(X|A, \theta)$ from the labeled nodes where θ denotes the parameter of the classifier. In particular, there are four popular settings with minor differences regarding the observability of testing nodes during model training and the amount of labeled nodes. Without loss of generality, we index the labeled nodes and testing nodes in the range of $[1, M]$ and $(T, N]$, respectively. Specifically,

- *Inductive Full-supervised Learning*: In this setting, testing nodes are not included in the graph used for model training and all training nodes are labeled. That is, $M = T$ and learning the classifier with $f(X_{tr}|A_{tr}, \theta)$ where $X_{tr} \in \mathbb{R}^{M \times D}$ and A_{tr} denotes the features and the subgraph of the training nodes.
- *Inductive Semi-supervised Learning* [10]: In many real-world applications such as text classification [23], it is unaffordable to label all the observed nodes, *i.e.*, only a small portion of the training nodes are labeled (in fact, $M \ll T$).
- *Transductive Full-supervised Learning* [13]: In some cases, the graph is relatively stable, *i.e.*, no new node occurs, where the whole node graph X and A are utilized for model training.
- *Transductive Semi-supervised Learning* [17]: In this setting, the whole graph is available for model training while only a small portion of the training nodes are labeled.

Graph Convolutional Network. Taking the graph as inputs, GCN learns node representations that encodes the graph structure and node features (the last layer makes predictions) [17]. The key operation of GCN is *neighbor aggregation*, which can be abstracted as:

$$\tilde{x} = \mathcal{N}(x, \{x_n | n \in \text{neighbor}(x)\}), \quad (1)$$

where \mathcal{N} denote the node aggregation operation such as a weighted summation [17]. x and $\tilde{x} \in \mathbb{R}^D$ are the origin representation of the target node (node features or representation at the previous layer) and the one after aggregating neighbor node features.

Adaptive locality. In most design of GCN, the target node is equally treated as the neighbor nodes, *i.e.*, no additional operation except adding the edge for self-connection. Aiming to distinguish the contribution from target node and neighbor nodes, a self-weight α is utilized, *i.e.*, $\mathcal{N}(\alpha * \tilde{x}, \{(1 - \alpha) * x_n | n \in \text{neighbor}(x)\})$. More specifically, neighbor attention [36] is introduced to learn node specific weights, *i.e.*, $\mathcal{N}(\alpha \tilde{x}, \{\alpha_n * x_n | n \in \text{neighbor}(x)\})$. The weights α and α_n are calculated by an attention model such as multi-head attention [35] with the node representations \tilde{x} and x_n as inputs. Lastly, hop attention [24] is devised to adaptively aggregate the target node representations at different GCN layers $x^0, \dots, \tilde{x}^k, \dots, \tilde{x}^K$ into a final representation. \tilde{x}^k is the convolution output at the k -th layer which encodes the k -hop neighbors of the target node. For a target node that is expected to trust self more, the hop attention is expected to assign higher weight for x^0 . Most of these adaptive locality models are learned during model training except the self-weight α in GCN models like APPNP which is tuned upon the validation set.

Model	APPNP	JKNet	DAGNN
Self	72.28	72.28	72.28
Self+Neighbor	76.03	75.69	75.28
Self+Neighbor_Trust	78.30	75.71	78.61
Self+Neighbor_Bound	81.40	81.96	82.03

Table 1: Node classification performance of three GCN models: APPNP, JKNet, and DAGNN on OGB-arXiv.

3 PILOT STUDY

To investigate whether the existing adaptive locality methods indeed assess the trustworthiness of neighbors, we conduct a pilot study on OGB-arXiv (see Section 5.1.1 for the details of the dataset) to test whether the model learns to trust self or neighbors. Three representative GCN models with consideration of adaptive locality, APPNP, JKNet, and DAGNN are tested under three different configurations:

- *Self*: The edges in the graph are removed from the model inputs. That is to say, the model trusts the target node itself only.
- *Self+Neighbor*: This is the standard configuration of GCN model that accounts for the graph structure, *i.e.*, trusting neighbors.
- *Self+Neighbor_Trust*: As compared to *Self+Neighbor*, a trustworthy feature is associated with each node, which indicates the “ground truth” of trusting self or neighbors. The trustworthy feature is generated by comparing the prediction under Self and Self+Neighbor with node label, where the value of 1 means Self is correct while Self+Neighbor is wrong, and the value of -1 means the opposite. For the remaining nodes, the value is set as 0.

As a reference, we also study the performance in an ideal case, named *Self+Neighbor_Bound*, which is achieved by selecting the prediction under Self or Self+Neighbor according to the value of the trustworthy feature. It can be seen as the upper bound of performing adaptive locality during model inference.

Table 1 shows the model performance under the node classification setting of inductive full-supervised learning. The performance under the other settings follows the same trend, which are omitted for brevity. From the table, we have the following observations:

- In all cases, the model under *Self+Neighbor* outperforms the one under *Self*, which validates the utility of graph structure in the node classification task.
- As compared to *Self+Neighbor*, all the three models, especially APPNP and DAGNN, achieve better performance under the configuration of *Self+Neighbor_Trust*. It indicates a better usage of the graph structure, which is attributed to the trustworthy feature, highlighting the importance of modeling neighbor trustworthiness.
- However, there is a large gap between *Self+Neighbor_Trust* and *Self+Neighbor_Bound*, which means the underuse of the trustworthy feature by the current adaptive locality methods. We postulate the reason to be the gap between the training objective, *i.e.*, associating node representation with label, and the target of identifying trustworthy neighbors, which is the limitation of considering adaptive locality in model training. The performance under *Self+Neighbor_Bound* also reveals the potential of considering adaptive locality in model inference.

Furthermore, we study the impact of trustworthy feature on model training. Figure 2 illustrates the training loss along the training procedure of the tested models under the configuration of *Self+Neighbor* and *Self+Neighbor_Trust*. It should be noted that we select the

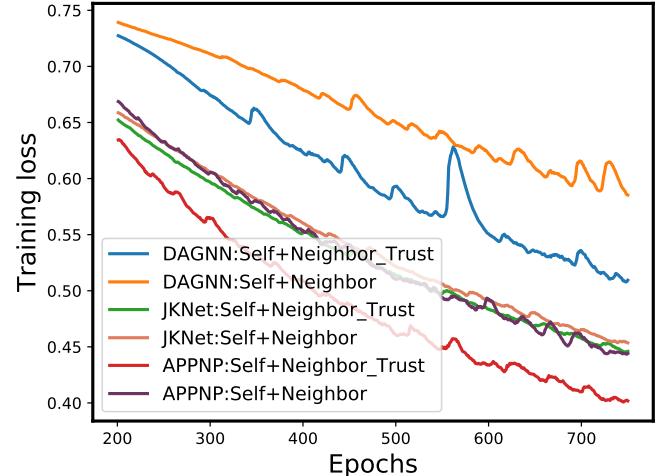


Figure 2: Training loss on OGB-arXiv under the *Self+Neighbor* and *Self+Neighbor_Trust* model configurations.

period from 200 to 750 epochs for better visualization. From the figure, we can see that, in all the three cases, the loss of model under *Self+Neighbor_Trust* is smaller than that under *Self+Neighbor*. The result shows that the trustworthy feature facilitates the GCN model fitting the training data, *i.e.*, capturing the correlation between the node label and the node features as well as the graph structure. However, the adaptive locality module, especially graph attention, is distracted from the target of assessing neighbor trustworthiness. Ideally, the graph attention can achieve the target by recognizing the value of the trustworthy feature. For instance, the hop attention in DAGNN should highlight the target node representation at layer 0 if the trustworthy feature is 1.

It should be noted that the trustworthy feature is not available in real-world applications due to relying on testing labels. As such, neither GCN training nor GCN inference can directly use the feature to perform adaptive locality. Nevertheless, it would be fruitful if observable factors relevant to the trustworthy feature, *i.e.*, reflecting the trustworthiness of neighbor nodes.

4 METHODOLOGY

In this section, we first introduce the proposed AdaInf mechanism, followed by elaborating the recognized factors that can indicate neighbor trustworthiness. Lastly, we shed light on the rationality of the proposed mechanism from a causal-effect view.

4.1 Adaptive Inference Mechanism

Our key intuition is that the model outputs bring additional clues for conducting adaptive locality. Accordingly, our focus is to construct a more precise inference mechanism upon a normal GCN model, which has been optimized over the training nodes according to the following objective function:

$$\hat{\theta} = \min_{\theta} \sum_{i=1}^M (l(\hat{y}_i, y_i)) + \lambda \|\theta\|_F^2, \quad (2)$$

where $l(\cdot)$ denotes a classification loss function such as cross-entropy, $\hat{\mathbf{y}}_i$ denotes the model prediction for node i , and λ is a hyper-parameter to balance the training loss and regularization term for preventing overfitting. Formally, the trained model is denoted as $f(X|A, \hat{\theta})$, which predicts $\hat{\mathbf{y}}_i$ for node i . It should be noted that $\hat{\mathbf{y}}_i$ is a probability distribution over the label space. The final classification z_i corresponds to the category with the largest probability, *i.e.*, $z_i = \max_j \hat{y}_{i,j}, j \leq L$ where $\hat{y}_{i,j}$ is the j -th entry of $\hat{\mathbf{y}}_i$. In the following, the mention of prediction and classification mean the predicted probability distribution ($\hat{\mathbf{y}}_i$) and category (z_i), respectively. Besides, the subscript i will be omitted for brevity.

In addition to the regular inference ($\hat{\mathbf{y}}$) of the trained GCN model with consideration of neighbor nodes, *i.e.*, trusting neighbors, AdaInf conducts an inference with all graph edges removed, *i.e.*, trusting self, which generates the prediction of $\hat{\mathbf{y}}^s$. Note that the corresponding classification is denoted as z^s . Furthermore, aiming to achieve adaptive locality for each testing node, a choice is made between $\hat{\mathbf{y}}$ and $\hat{\mathbf{y}}^s$ according to the characters of these two predictions. Formally, the AdaInf mechanism can be abstracted as:

$$\bar{\mathbf{y}} = g(\hat{\mathbf{y}}, \hat{\mathbf{y}}^s | c), \quad (3)$$

where $\bar{\mathbf{y}}$ denotes the final prediction for the target node and c represents the trustworthiness related factors that lead to the choice. In particular, c is a set of features that characterize the confidence and uncertainty of the two predictions $\hat{\mathbf{y}}$ and $\hat{\mathbf{y}}^s$ (detailed in Section 4.2). Aiming to learn the choosing function $g(\cdot)$, we implement it as a binary classifier that takes c as inputs. Without loss of generality, we set its output space to be $\{-1, 1\}$ where 1 means trusting self, *i.e.*, $\bar{\mathbf{y}} = \hat{\mathbf{y}}^s$, and -1 means trusting neighbors, *i.e.*, $\bar{\mathbf{y}} = \hat{\mathbf{y}}$. The classifier is optimized over the nodes in the validation set with the value of trustworthy feature (see Section 3) as labels. It should be noted that only the nodes with trustworthy feature of 1 or -1 are utilized for the training of $g(\cdot)$. In other words, we learn the choosing function from nodes where the two model predictions are inconsistent. Considering that a few factors are adequate to characterize the model prediction, *i.e.*, the dimension of c is typically small (in fact, < 10), simple classifiers such as Logistic Regression and Support Vector Machine [32] are sufficient to strategy for making choice. As such, there is little overhead in the practical usage of AdaInf.

4.2 Trustworthiness Related Factors

Note that the core of AdaInf is to choose the more reliable prediction from the two candidates. It is thus essential to identify factors that can describe the reliability of predictions, especially the one with consideration of graph structure. Technically, model prediction on a target node is a conditional distribution $p(\mathbf{y}|X, A, \hat{\theta})$ ¹. In most cases, we only pay attention to the mean of the conditional distribution, which corresponds to the model prediction $f(X|A, \hat{\theta})$. To assess its reliability, in addition to the value of the prediction, our belief is to further rely on the character of the corresponding conditional distribution such as the variance, skewness, and kurtosis. Towards this end, we recognize three kinds of factors to form c and describe the two model predictions $\hat{\mathbf{y}}$ and $\hat{\mathbf{y}}^s$.

¹Note that the inference of GCN model is different from normal classifier which only accounts for the features of the testing sample, *i.e.*, $p(\mathbf{y}|\mathbf{x}, \hat{\theta})$

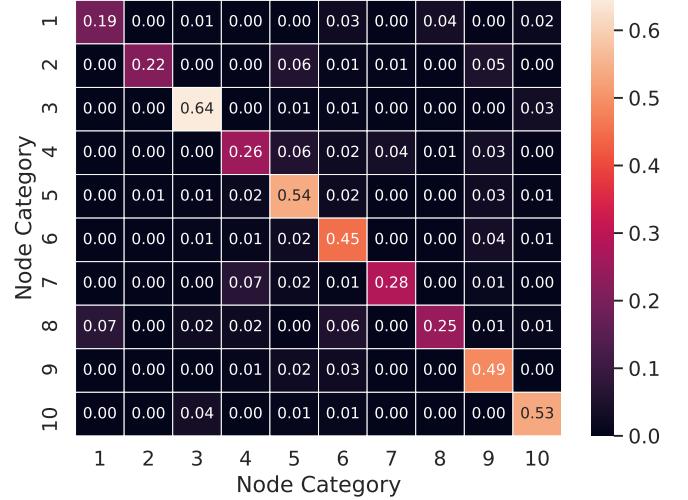


Figure 3: Illustration of the category transition matrix on OGB-arXiv. To save space, we cut the number of categories to ten (see Appendix A for the full matrix with 40 categories).

Prediction confidence. There has been a surge of attention on using the values of model prediction such as model distillation [12] and self-supervised learning [6]. The intuition is that a larger probability indicates higher confidence on the classification. As such, a factor of prediction reliability is the prediction confidence, *i.e.*, trusting the prediction with higher confidence. Formally, we calculate two factors: *self_conf* (\hat{y}_z) and *neighbor_conf* (\hat{y}_{z^s}), where z and z^s correspond to the classification of $\hat{\mathbf{y}}$ and $\hat{\mathbf{y}}^s$, respectively.

Category transition. In fact, the distribution of edges over categories is not uniform. 1) *Intra-category connection.* Nodes in different categories have different probabilities to be connected to nodes in the same category. 2) *Inter-category connection.* Nodes in a category have different probabilities to have edges connecting the other categories. Over the labeled training nodes, we can calculate the probabilities and form a category transition matrix T where $T_{i,j}$ is the ratio of edges between category i and j to the edges connect nodes in category i . Figure 3 illustrates these probabilities on the OGB-arXiv dataset (raw normalized). From the diagonal entries, we can see that the probability of intro-category connection varies in a large range ([0.19, 0.64]). The distribution of inter-category probability is also skewed. Intuitively, such probabilities can be clues for choosing the correct prediction. For instance, $\hat{\mathbf{y}}$ might be trustworthy if $T_{z,z}$ is high. To leverage such inductive bias, we calculate four factors: *self_self* ($T_{z,z}$), *neighbor_neighbor* (T_{z^s,z^s}), *self_neighbor* (T_{z,z^s}), and *neighbor_self* ($T_{z^s,z}$).

Graph uncertainty. Furthermore, we characterize the conditional distribution corresponding to the GCN prediction, *i.e.*, $p(\mathbf{y}|X, A, \hat{\theta})$, and focus on the variance of the distribution, which is typically viewed as the uncertainty of the prediction [9]. As our key objective is the trustworthiness of the neighbors, different from conventional uncertainty estimation that is focused on the uncertainty caused by model parameters, we particularly study the uncertainty caused by the graph structure, named *graph uncertainty*. Monte Carlo dropout

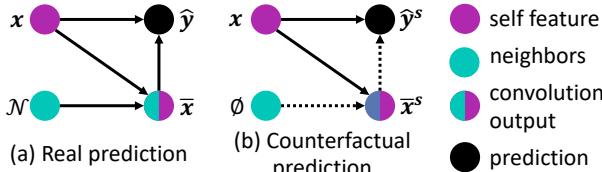


Figure 4: Causal graph of GCN when making original prediction (a) and counterfactual prediction (b). Dashed line means the effect from the predecessor is blocked.

(MCD) [9] has become a promising method to estimate model uncertainty, which repeats K times of model inference with feature dropout performed. In this way, K different predictions are obtained where the variance are treated as the uncertainty of prediction. Intuitively, each repeat can be seen as a sampling over the model space by dropping a portion of parameters. The variance of the resulted predictions approximates the variance of the conditional distribution. We extend the MCD to *Monte Carlo Edge-drop* (MCE) to estimate the prediction uncertainty regarding the graph structure, *i.e.*, A . As A is also parameter of the GCN model, MCE repeats K times of GCN inference with edge dropout [34] performed, *i.e.*, each edge has a probability η to be removed. Formally,

$$\sigma = \text{var}(\{f(X|A_k, \hat{\theta})|k \leq K\}), \quad (4)$$

where $\sigma \in \mathbb{R}^L$ denotes the estimated variance and $\text{var}(\cdot)$ is an element-wise operation that calculates the variance of K values. A_k is the k -th resulted graph after edge dropout. Regarding the original GCN classification z , we account for the graph uncertainty factor $\text{graph_var}(\sigma_z)$, where larger value indicates higher graph uncertainty. Lastly, we include the *degree* of the target node as a factor for the intuition of the majority rule.

4.3 Causal-effect View

As pointed out by [31], models trained over labeled samples according to a classification loss is mainly empowered with the association ability, *i.e.*, associating the features and labels in a static distribution. The inference of such models, including the GCN models, is thus mainly the estimation of likelihood. Apart from the static distribution and the likelihood, the proposed AdaInf aims to inject extra assumptions on trusting neighbors or self. Particularly, the mechanism is focused on target nodes where considering neighbor nodes lead to classification different from the one from target node features. Essentially, AdaInf assesses to what extent the prediction is affected by the neighbor nodes and whether the effect is trustworthy. By making choice between the two predictions, AdaInf adjusts how the effect from neighbors are fused with the effect from own features so as to achieve a more precise prediction. In the dictionary of causality [30], such effect between two variables are named *causal effect*. To facilitate understanding, we depict the causal graph (see Figure 4) for the inference of GCN model, which represents the causal relations between variables². Functionally speaking, the structure $x \rightarrow \bar{x} \leftarrow A$ corresponds to the graph convolution where both the target node features and neighbor nodes directly affect the convolution output; the structure $x \rightarrow y \leftarrow \bar{x}$ encodes the adaptive

locality module in GCN such as attention which fuses the two effects on the prediction.

Recall that the proposed AdaInf conducts two inferences resulting the prediction of \hat{y} and \hat{y}^s . The two inferences corresponds to the causal graphs in Figure 4(a) and Figure 4(b), respectively. The first inference is upon the static distribution encoded by the trained model, while the second inference is under a counterfactual — *if the target node has no neighbor, what the prediction would be*. Specifically, we perform intervention by setting the neighbor as a reference status (*i.e.*, \emptyset). According to the causality theory [29], the causal effect from neighbors (A) to the prediction can be inferred from \hat{y} and \hat{y}^s . Therefore, choosing \hat{y} or \hat{y}^s for each testing node will adjust the effect from neighbors on the prediction and the fusion of self and neighbor effects. Moreover, characterizing \hat{y} and \hat{y}^s can reveal the trustworthiness of neighbors' effect. As such, we implement AdaInf as a simple classifier with the factors (*i.e.*, c) as inputs.

5 EXPERIMENTS

We conduct experiments on seven node classification datasets to answer the following research questions:

- **RQ1:** How do the trustworthy factors influence the effectiveness of the proposed AdaInf?
- **RQ2:** To what extend the proposed AdaInf facilitates node classification under different problem settings?
- **RQ3:** In which cases the proposed AdaInf mechanism and MCE are more effective?

5.1 Experimental Settings

5.1.1 Dataset. For the full-supervised settings, we use the widely used benchmark dataset of citation network, OGB-arXiv [13], which represents papers and their citation relations as nodes and edges, respectively. Each node has 128 features generated by averaging the embeddings of words in its title and abstract, where the embeddings are learned by the skip-gram model [27]. Considering that the old-fashioned way may not generate representative text features, we replace the node features with a 768-dimensional vector extracted by feeding the title and abstract into RoBERTa [25] (12-layer³), where the representation of [CLS] token at the second last layer is selected.

For the semi-supervised settings, we adopt three widely used citation networks, Cora, Citeseer, and Pubmed, and select the 20-shot data split released by [17], where 500 and 1000 nodes are selected as validation and testing, 20 nodes from each category are labeled for training. Apart from the real-world graphs, we further created three synthetic ones based on Citeseer by intentionally adding cross-category edges on 50% randomly selected nodes. It should be noted that more cross-category edges will make the neighbors less trustworthy. It thus leads to gap between the poisoned nodes and the unaffected ones regarding neighbor trustworthiness, and pushes the GCN models to rely more on adaptive locality. In particular, according to the number of edges in the original Citeseer, we add 10%, 30%, and 50% of cross-category edges, constructing Citeseer(10%), Citeseer(30%), and Citeseer(50%). Note that the data split and node features are unchanged.

²We refer the book [30] for basic concepts of causal graph and causality.

³<https://github.com/huggingface/transformers>.



Figure 5: Illustration of factor influence on AdaInf.

5.1.2 Compared Methods. To justify the proposed AdaInf, we compare it with the representative GCN models, including GraphSAGE [10], GCN [17], GAT [36], JKNet [46], DAGNN [24], and APPNP [18], which adopt normal inference. Apart from GCN models, we also test MLP, which discard the graph structure and treat node classification as normal text classification. Lastly, as AdaInf uses two predictions, we include an ensemble baseline which averages the prediction of APPNP and MLP. For these models, we use the implementations on the OGB leaderboard⁴. If necessary, *e.g.*, under the transductive full-supervised setting, the hyper-parameters are tuned according to the settings in the original paper of the model. For the proposed AdaInf, we apply it to APPNP and adopt the SVM equipped with RBF kernel⁵ to make choice. For the SVM, we tune two hyper-parameters c and γ through 5-fold cross-validation, *i.e.*, splitting the nodes in validation into 5 folds. In addition, for the MCE that estimates graph uncertainty, we set the number of repeats and the edge dropout ratio η as 50 and 0.15, respectively.

5.2 Effects of Trustworthy Factors (RQ1)

We first study the effects of the identified trustworthiness related factors on the AdaInf mechanism. In particular, we compare the factors *w.r.t.* the performance of AdaInf as removing the factor, where lower performance indicates larger contribution of the factor. Note that we report the accuracy regarding whether AdaInf makes the correct choice for testing nodes, rather than the accuracy for node classification. That is to say, here we only consider “conflict” testing nodes where the two inferences of AdaInf have different classifications. Figure 5 shows the performance on OGB-arXiv under the inductive setting, accounting for 6,810 nodes (47,420 nodes in total). We omit the results of other datasets or under different settings, which have a close trend.

From the figure, we have the following observations: 1) Discarding any factor will lead to performance drop as compared to the case with all factors as inputs of the SVM (*i.e.*, All factors). This result indicates the effectiveness of the identified factors on characterizing GCN predictions and facilitating making the correct choice. 2) Among the factors, removing *self_conf* and *neighbor_conf* leads to the largest performance drop, showing that the confidence of prediction is the most informative factor regarding the reliability of the prediction. 3) In all cases, the performance of AdaInf surpasses

⁴https://ogb.stanford.edu/docs/leader_nodeprop/#ogbn-arxiv.

⁵<https://scikit-learn.org/stable/modules/svm.html>.

Feature	Method	Inductive	Transductive
Word2Vec (128)	MLP	$55.84 \pm 0.35\%$	$55.84 \pm 0.35\%$
	GraphSAGE	$71.43 \pm 0.19\%$	$71.52 \pm 0.32\%$
	GCN	$71.83 \pm 0.21\%$	$71.96 \pm 0.15\%$
	GAT	$71.93 \pm 0.33\%$	$72.04 \pm 0.28\%$
	JKNet	$72.25 \pm 0.15\%$	$72.48 \pm 0.22\%$
	DAGNN	$72.07 \pm 0.18\%$	$72.09 \pm 0.09\%$
	APPNP	$71.61 \pm 0.22\%$	$71.67 \pm 0.32\%$
RoBERTa (768)	MLP	72.26%	72.26%
	JKNet	$75.59 \pm 0.10\%$	$75.54 \pm 0.12\%$
	DAGNN	$74.93 \pm 0.35\%$	$74.83 \pm 0.10\%$
	APPNP	$75.74 \pm 0.17\%$	$75.61 \pm 0.13\%$
	Ensemble	76.26%	75.86%
	AdaInf	76.52%	76.07%

Table 2: Performance comparison under full-supervised settings of node classification.

the *Majority class*, which always chooses the original GCN prediction and equals to normal inference. It validates the rationality of additionally considering adaptive locality during GCN inference, *i.e.*, choosing between the original prediction and the counterfactual prediction without consideration of graph structure. Lastly, considering that the “conflict” nodes account for 14.4% in the testing nodes (6,810/47,420) and the accuracy of AdaInf’s choices is 66.53%, there are still a large area for future exploration.

5.3 Performance Comparison (RQ2)

To verify the proposed AdaInf, we conduct performance comparison under both full-supervised and semi-supervised settings.

Full-supervised setting. Recall that there are also inductive and transductive settings regarding whether the testing nodes are observed during model training. We thus test the models under the two settings separately. Table 2 shows the node classification performance of the compared methods on the OGB-arXiv dataset under both settings *w.r.t.* accuracy. Apart from the newly generated RoBERTa features, we also report the performance of baseline models with the original Word2Vec features. From the table, we have the following observations:

- The performance gap between MLP and GCN models will be largely bridged when replacing the Word2Vec features with the more advanced RoBERTa features. In particular, the relative performance improvement of GCN models over MLP shrinks from 27.9% to 3.7%. The result raises a concern that the merit of GCN model might be unintentionally exaggerated [17] due to the low quality of node features.
- Moreover, as compared to APPNP, DAGNN performs better as using the Word2Vec features, while performs worse when using the RoBERTa features. It suggests accounting for feature quality in future research that investigates the capability of GCN or compares different GCN models.
- As to RoBERTa features, Ensemble performs slightly better than its base models, *i.e.*, MLP and APPNP, which is reasonable since the two models can complement each other [52]. As averaging the prediction of MLP and APPNP can also be seen as choosing between trusting self or neighbors by comparing model confidence,

Dataset	Cora	Citeseer	Pubmed
APPNP	81.8%	72.6%	79.8%
APPNP_Self	69.3%	66.5%	75.9%
APPNP_Ensemble	78.0%	71.4%	79.2%
APPNP_AdaInf	82.3%	73.7%	81.0%

Table 3: Performance of APPNP with different inference mechanisms on three semi-supervised node classification datasets w.r.t. the classification accuracy.

the performance gain indicates the benefit of considering adaptive locality during inference under full-supervised setting.

- AdaInf further outperforms Ensemble under both settings, which is attributed to the additional classifier with the identified factors as inputs. This result shows the merit of characterizing the prediction of GCN models with the factors, which enables the extra assumptions on the inference mechanism.
- In all cases, the model achieves comparable performance under the inductive setting and the transductive setting. In the following, the experiment is focused on the inductive setting which is closer to real-world scenarios aiming to serve the upcoming nodes.

Semi-supervised setting. We then investigate the effect of AdaInf under semi-supervised setting by comparing the performance of APPNP that adopts different inference mechanisms: 1) normal GCN inference (APPNP); 2) counterfactual inference without consideration of graph structure (APPNP_Self); 3) ensemble of APPNP and APPNP_Self (APPNP_Ensemble); 4) APPNP_AdaInf. Note that the four inference mechanisms are applied on the same APPNP model with exactly same model parameters. Table 3 shows the node classification performance on Cora, Citeseer, and Pubmed. From the table, we have the following observations:

- On the three datasets, the performance of APPNP_Self is largely worse than APPNP, *i.e.*, omitting graph structure during GCN inference witnesses sharp performance drop under semi-supervised setting, which shows the importance of considering neighbors. Note that the performance of APPNP_Self largely surpasses the performance of MLP reported in [17], which highlights the difference between the counterfactual inference of a GCN model and the inference of MLP which is trained without the consideration of graph structure.
- In all cases, APPNP_Ensemble performs worse than its base model APPNP, which is reasonable due to the huge gap between the performance of APPNP and APPNP_Self. Therefore, under semi-supervised setting, it is inadequate to select the correct prediction, *i.e.*, achieving better adaptive locality, by simply averaging the original prediction and counterfactual prediction, which only accounts for model confidence.
- On the contrary, APPNP_AdaInf outperforms APPNP, where the difference is making choice according to the value of the identified factors rather than simply comparing the confidence of the predictions. Recall that the self_conf and neighbor_conf are the most influential factors (cf. Figure 5), the performance gain is attributed to the choosing function $g(\cdot)$, which is worthwhile for further exploration in future research.

Dataset	Citeseer(10%)	Citeseer(30%)	Citeseer(50%)
APPNP	71.0%	64.4%	64.2%
APPNP_Self	65.1%	62.9%	64.3%
APPNP_AdaInf	71.8%	66.9%	68.6%

Table 4: Performance of APPNP equipped with the proposed AdaInf on the three synthetic datasets w.r.t. accuracy. Note that the requirement of adaptive locality will increase from Citeseer(10%) to Citeseer(50%).

5.4 In-depth Analysis (RQ3)

Study on synthetic graphs. Recall that the number of cross-category edges on the target node affects the trustworthiness of neighbors. Adaptive locality is thus essential when the distribution of cross-category edges varies across nodes. We then investigate how the skewness of the distribution of cross-category edges influences the effectiveness of the proposed AdaInf. Table 4 shows the performance of APPNP, APPNP_Self, and APPNP_AdaInf on the three synthetic datasets Citeseer(10%), Citeseer(30%), and Citeseer(50%). Note that the datasets are constructed by adding cross-category edges on a part of the nodes. As such, adding more edges will enlarge the difference between poisoned nodes and the unaffected nodes *w.r.t.* the percentage of cross-category edges, *i.e.*, leading to more skewed distribution of cross-category edges. From the table, we have the following observations:

- As more cross-category edges being added, APPNP witnesses more severe performance drop (cf. Table 3). This is because GCN models are vulnerable to cross-category edges which pushes the representations of node in different categories to be close [4].
- As to APPNP_Self, the performance across the three datasets is comparable to each other, as more cross-category edges are injected. It indicates that the cross-category edges may not hinder the model to encode the association between target node features and the label. Furthermore, on Citeseer(50%), the performance of APPNP_Self is comparable to APPNP, which indicates that purely considering adaptive locality in GCN training is not insufficient in cases whether the distribution of cross-category edges is skewed.
- In all cases, APPNP_AdaInf outperforms APPNP, which further validates the effectiveness of the proposed AdaInf mechanism and the rationality of considering adaptive locality during GCN inference.
- Moreover, the relative improvement over APPNP achieved by APPNP_AdaInf increases from 1.1% to 7.2% as more cross-category edges are injected. It indicates that AdaInf might be more effective on graphs where the distribution of cross-category edges over nodes is more skewed.

Study on graph uncertainty. Recall that we propose a Monte Carlo edge-drop method to estimate the graph uncertainty. We then investigate to what extent the MCE sheds light on the correctness of GCN prediction. Figure 6(a) shows the group-wise performance of APPNP on OGB-arXiv where the testing nodes are ranked according to the value of graph_var in an ascending order and split into ten groups with equal size. Note that we select OGB-arXiv for its relatively large scale where the testing set includes 47,420 nodes. From the figure, we can see a clear trend that the classification performance decreases as the graph uncertainty increases. It means that

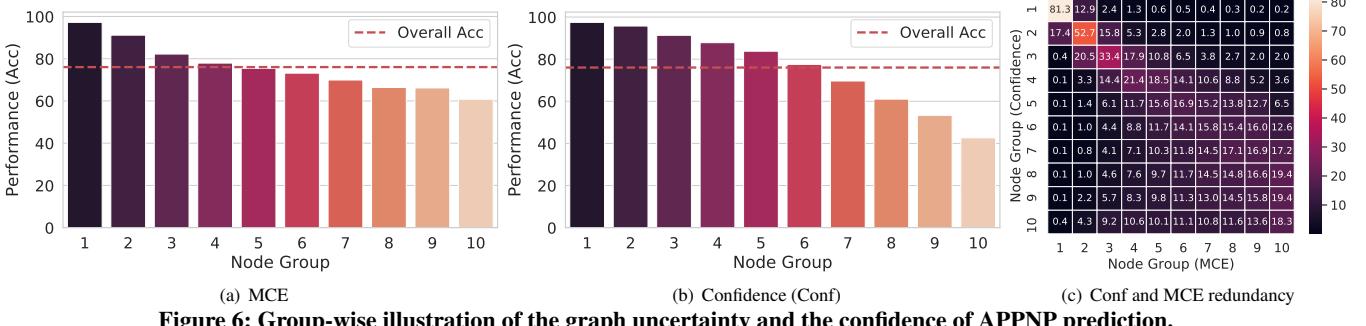


Figure 6: Group-wise illustration of the graph uncertainty and the confidence of APPNP prediction.

the calculated graph uncertainty is informative for the correctness of GCN predictions. For instance, a prediction has higher chance to be correct if its graph uncertainty is relatively low.

As a reference, in Figure 6(b), we further depict the group-wise performance *w.r.t.* the prediction confidence (*i.e.*, neighbor_conf). In particular, the testing nodes are ranked according to the value of neighbor_conf in a descending order. As can be seen, there is also a clear trend of prediction performance regarding the confidence, *i.e.*, the probability of being correct is higher if APPNP is more confident on the prediction. To investigate whether graph uncertainty is redundant, we further calculate the overlap ratio between the groups split by graph_var and the ones split by neighbor_conf. Figure 6(c) illustrates the matrix of overlap ratios. As can be seen, the weights are not dedicated on the diagonal entries. In particular, there are only two group pairs with overlap ratio higher than 0.5, which means that the graph uncertainty reveals the property of GCN prediction complementary to the confidence.

6 RELATED WORK

Graph Convolutional Network. According to the format of the convolution operations, existing GCN models can be divided into two categories: spatial GCN and spectral GCN [51]. Spectral GCN is defined as performing convolution operations in the Fourier domain with spectral node representations [2, 8, 17, 22, 43]. For instance, Bruna *et al.* [2] perform convolution over the eigenvectors of graph Laplacian which are treated as the Fourier basis. Due to the high computational cost of the eigen-decomposition, a line of spectral GCN research has been focused on accelerating the eigen-decomposition with different approximation techniques [8, 17, 22, 43]. However, applying such spectral GCN models on large graphs still raises unaffordable memory cost, which hinders their practical research.

To some extent, the attention on GCN research has been largely dedicated on the spatial GCN, which performs convolution operations directly over the graph structure by aggregating the features from spatially close neighbors to a target node [1, 10, 17, 36, 37, 42, 45]. This line of research mainly focuses on the development of the neighbor aggregation operation. For instance, Kipf and Welling [17] propose to use a linear aggregator (*i.e.*, weighted sum) that uses the reverse of node degree as the coefficient. In addition to aggregating information from directly connected neighbors, augmented aggregators also account for multi-hop neighbors [15, 44]. Moreover, non-linear aggregators are also employed in spatial GNNs such as

capsule [37] and Long Short-Term Memory (LSTM) [10]. Furthermore, there are studies extending the general spatial GNN designed for simple graphs to graphs with heterogeneous nodes [41] and temporal structure [28]. Beyond model design, there are also studies on the model capability analysis [45], model explanation [49], and training schema [14].

However, most of the existing studies are focused on the training stage and blindly adopt the one-time forward propagation for model inference as normal neural networks. This work is in an orthogonal direction, which improve the inference performance with an adaptive mechanism. Moreover, to the best of our knowledge, this work is the first to introduce the edge dropout and counterfactual into GCN inference.

Adaptive Locality. Amongst the GCN research, a surge of attention has been especially dedicated to solving the over-smoothing issue [21]. Adaptive locality has become the promising solution to alleviate the over-smoothing issue, which is typically achieved by the attention mechanism [36, 38, 39, 41, 46, 50] or residual connection [5, 17, 20]. Along the line of research on attention design, integrating context information into the calculation of attention weight is one of the most popular techniques. For instance, Wang *et al.* [39] treats the neighbors at different hops as augmentation of attention inputs. Moreover, to alleviate the issue of lacking direct supervision, Wang *et al.* [38] introduce additional constraints to facilitate attention learning. Similar as Convolutional Neural Networks, residual connection has also been introduced to original design of GCN [17], which connects each layer to the output directly. In addition to the vanilla residual connection, the revised versions are also introduced such as the pre-activation residual [20] and initial residual [5]. Besides, the concept of inception module is also introduced to GCN model [16], which incorporates graph convolutions with different receptive fields. For the existing methods, the adaptive locality mechanism is fixed once the GCN model is trained. Instead, this work explores adaptive locality during model inference, which is in an orthogonal direction.

7 CONCLUSION

This paper revealed that learning an additional model component such as graph attention is insufficient for achieving the adaptive locality of GCN models. Beyond model training, we explored the potential of empowering the GCNs with adaptive locality ability during the inference. In particular, we proposed an adaptive inference mechanism, which leverages the theory of counterfactual inference,

generating a counterfactual prediction when the model only trusts own features, and makes choice between the counterfactual prediction and real prediction. A set of factors are identified to characterize the predictions and taken as inputs for choosing the final prediction. Especially, we explored the graph uncertainty of GCN prediction and proposed the Monte Carlo edge-drop method to estimate the uncertainty. Under three common settings for node classification, we conducted extensive experiments on seven datasets, justifying the effectiveness of the proposed AdaInf.

In the future, we will test the proposed AdaInf on more GCN models such as GAT, JKNet, and DAGNN. Moreover, we will extend the proposed AdaInf from node classification to other graph analytic tasks, such as link prediction. In addition, following the original Monte Carlo dropout, we would like to complete the mathematical derivation of Equation 4, *i.e.*, how the `graph_var` approximates the variance of the prediction distribution. Lastly, we will explore how the property of the classifier $g(\cdot)$ influences the effectiveness of AdaInf, *e.g.*, whether non-linearity is necessary.

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A CATEGORY TRANSITION MATRIX

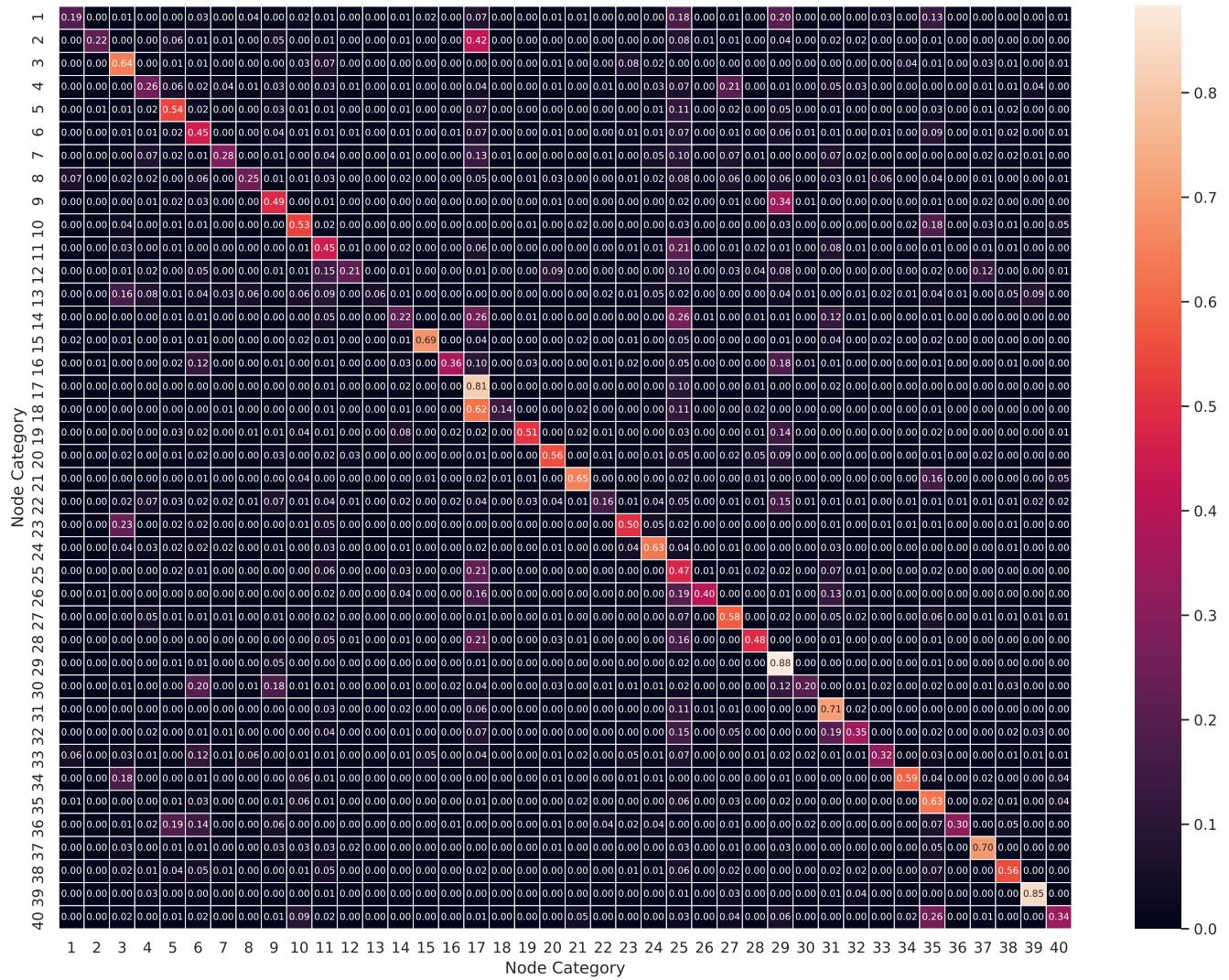


Figure 7: Illustration of the category transition matrix on the OGB-arXiv dataset.