

Link Prediction without Graph Neural Networks

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ABSTRACT

Link prediction, which consists of predicting edges based on graph features, is a fundamental task in many graph applications. As for several related problems, Graph Neural Networks (GNNs), which are based on an attribute-centric message-passing paradigm, have become the predominant framework for link prediction. GNNs have consistently outperformed traditional topology-based heuristics, but what contributes to their performance? Are there simpler approaches that achieve comparable or better results? To answer these questions, we first identify important limitations in how GNN-based link prediction methods handle the intrinsic class imbalance of the problem—due to the graph sparsity—in their training and evaluation. Moreover, we propose *Gelato*, a novel topology-centric framework that applies a topological heuristic to a graph enhanced by attribute information via graph learning. Our model is trained end-to-end with an N-pair loss on an unbiased training set to address class imbalance. Experiments show that *Gelato* is 145% more accurate, trains 11 times faster, infers 6,000 times faster, and has less than half of the trainable parameters compared to state-of-the-art GNNs for link prediction.

CCS CONCEPTS

- Computing methodologies → Machine learning algorithms;
- Information systems → Social networks.

KEYWORDS

Link Prediction; Graph Neural Networks; Graph Learning; Topological Heuristics

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1 INTRODUCTION

Machine learning on graphs supports various structured-data applications including social network analysis [38, 60, 73], recommender systems [30, 50, 76], natural language processing [62, 71, 85], and physics modeling [15, 29, 64]. Among the graph-related tasks, one could argue that link prediction [43, 46] is the most fundamental one. This is because link prediction not only has many concrete applications [37, 41, 58] but can also be considered an (implicit or explicit) step of the graph-based machine learning pipeline [3, 45, 78]—as the observed graph is usually noisy and/or incomplete.

In recent years, Graph Neural Networks (GNNs) [24, 35, 74] have emerged as the predominant paradigm for machine learning on graphs. Similar to their great success in node classification [36, 79, 95] and graph classification [51, 86, 90], GNNs have been shown to achieve state-of-the-art link prediction performance [55, 88, 89]. Compared to classical approaches that rely on expert-designed heuristics to extract topological information (e.g., Common Neighbors [52], Adamic-Adar [1], Preferential Attachment [4]), GNNs have the potential to discover new heuristics via supervised learning and the natural advantage of incorporating node attributes.

However, there is little understanding of what factors contribute to the success of GNNs in link prediction, and whether simpler alternatives can achieve comparable performance—as recently found for node classification [26]. GNN-based methods approach link prediction as a binary classification problem. Yet different from other classification problems, link prediction deals with extremely class-imbalanced data due to the sparsity of real-world graphs. We argue that class imbalance should be accounted for in both training and evaluation of link prediction. In addition, GNNs combine topological and attribute information by learning topology-smoothed attributes (embeddings) via message-passing [39]. This attribute-centric mechanism has been proven effective for tasks on the topology such as node classification [44], but link prediction is a task for the topology, which naturally motivates topology-centric paradigms (see Figure 1).

The goal of this paper is to address the key issues raised above. We first show that the evaluation of GNN-based link prediction pictures an overly optimistic view of model performance compared to the (more realistic) imbalanced setting. Class imbalance also prevents the generalization of these models due to bias in their training. Instead, we propose the use of the N-pair loss with an unbiased set of training edges to account for class imbalance. Moreover, we present *Gelato*, a novel framework that combines topological and attribute information for link prediction. As a simpler alternative

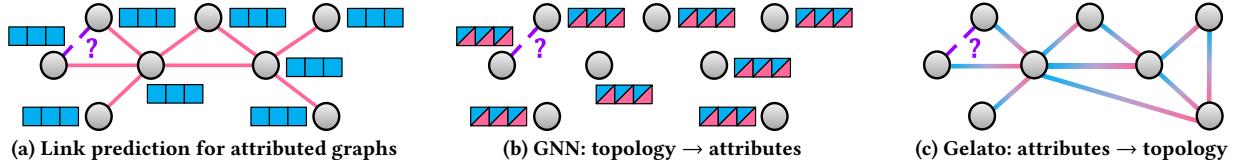


Figure 1: GNN incorporates topology into attributes via message-passing, which is effective for tasks *on* the topology. Link prediction, however, is a task *for* the topology, which motivates the design of Gelato—a novel framework that leverages graph learning to incorporate attributes into topology.

to GNNs, our model applies topology-centric graph learning to incorporate node attributes directly into the graph structure, which is given as input to a topological heuristic, Autocovariance, for link prediction. Extensive experiments demonstrate that our model significantly outperforms state-of-the-art GNN-based methods in both accuracy and scalability.

To summarize, our contributions are:

- We scrutinize the training and evaluation of supervised link prediction methods and identify their limitations in handling class imbalance.
- We propose a simple, effective, and efficient framework to combine topological and attribute information for link prediction without using GNNs.
- We introduce an N-pair link prediction loss combined with an unbiased set of training edges that we show to be more effective at addressing class imbalance.

2 LIMITATIONS IN SUPERVISED LINK PREDICTION EVALUATION AND TRAINING

Supervised link prediction is often formulated as a binary classification problem, where the positive (or negative) class includes node pairs connected (or not connected) by a link. A key difference between link prediction and typical classification problems (e.g., node classification) is that the two classes in link prediction are *extremely* imbalanced, since most real-world graphs of interest are sparse (see Table 1). However, we find that class imbalance is not properly addressed in both evaluation and training of existing supervised link prediction approaches, as discussed below.

Link prediction evaluation. Area Under the Receiver Operating Characteristic Curve (AUC) and Average Precision (AP) are the two most popular evaluation metrics for supervised link prediction [8, 11, 13, 34, 55, 81, 89, 91, 97]. We first argue that, as in other imbalanced classification problems [16, 63], AUC is not an effective evaluation metric for link prediction as it is biased towards the majority class (non-edges). On the other hand, AP and other rank-based metrics such as Hits@ k —used in Open Graph Benchmark (OGB) [25]—are effective for imbalanced classification *if evaluated on a test set that follows the original class distribution*. Yet, existing link prediction methods [8, 34, 55, 89, 97] compute AP on a test set that contains all positive test pairs and only an equal number of random negative pairs. Similarly, OGB computes Hits@ k against a very small subset of random negative pairs. We term these approaches *biased testing* as they highly overestimate the ratio of positive pairs

in the graph. Evaluation metrics based on these biased test sets provide an overly optimistic measurement of the actual performance in *unbiased testing*, where every negative pair is included in the test set. In fact, in real applications where test positive edges are not known *a priori*, it is impossible to construct those biased test sets to begin with. Below, we also present an illustrative example of the misleading performance evaluation based on *biased testing*.

Example: Consider a graph with 10k nodes, 100k edges, and 99.9M disconnected (or negative) pairs. A (bad) model that ranks 1M false positives higher than the true edges achieves 0.99 AUC and 0.95 in AP under *biased testing* with equal negative samples. (Detailed computation in Appendix A.)

The above discussion motivates a *more representative evaluation setting for supervised link prediction*. Specifically, we argue for the use of rank-based evaluation metrics—AP, Precision@ k [43], and Hits@ k [5]—with *unbiased testing*, where positive edges are ranked against all negative pairs. These metrics have been widely applied in related problems, such as unsupervised link prediction [27, 43, 53, 92], knowledge graph completion [5, 72, 82], and information retrieval [66], where class imbalance is also significant. In our experiments, we will illustrate how these evaluation metrics combined with *unbiased testing* provide a drastically different and more informative performance evaluation compared to existing approaches.

Link prediction training. Following the formulation of supervised link prediction as binary classification, most existing models adopt the binary cross entropy loss to optimize their parameters [11, 13, 34, 81, 88, 89, 91, 97]. To deal with class imbalance, these approaches downsample the negative pairs to match the number of positive pairs in the training set (*biased training*). We highlight two drawbacks of *biased training*: (1) it induces the model to overestimate the probability of positive pairs, and (2) it discards potentially useful evidence from most negative pairs. Notice that the first drawback is often hidden by *biased testing*. Instead, this paper proposes the use of *unbiased training*, where the ratio of negative pairs in the training set is the same as in the input graph. To train our model in this highly imbalanced setting, we apply the N-pair loss for link prediction instead of the cross entropy loss (Section 3.3).

3 METHOD

Notation and problem. Consider an attributed graph $G = (V, E, X)$, where V is the set of n nodes, E is the set of m edges (links), and $X = (x_1, \dots, x_n)^T \in \mathbb{R}^{n \times r}$ collects r -dimensional node attributes. The topological (structural) information of the graph is represented by its adjacency matrix $A \in \mathbb{R}^{n \times n}$, with $A_{uv} > 0$ if an edge of weight

A_{uv} connects nodes u and v and $A_{uv} = 0$, otherwise. The (weighted) degree of node u is given as $d_u = \sum_v A_{uv}$ and the corresponding degree vector (matrix) is denoted as $d \in \mathbb{R}^n$ ($D \in \mathbb{R}^{n \times n}$). The volume of the graph is $\text{vol}(G) = \sum_u d_u$. Our goal is to infer missing links in G based on its topological and attribute information, A and X .

Model overview. Figure 2 provides an overview of our link prediction model. It starts with a topology-centric graph learning phase that incorporates node attribute information directly into the graph structure via a Multi-layer Perceptron (MLP). We then apply a topological heuristic, Autocovariance (AC), to the attribute-enhanced graph to obtain a pairwise score matrix. Node pairs with the highest scores are predicted as (positive) links. The scores for training pairs are collected to compute an N-pair loss. Finally, the loss is used to train the MLP parameters in an end-to-end manner. We named our model Gelato (Graph enhancement for link prediction with autocovariance). Gelato represents a paradigm shift in supervised link prediction by combining a graph encoding of attributes with a topological heuristic instead of relying on increasingly popular GNN-based embeddings.

3.1 Graph learning

The goal of graph learning is to generate an enhanced graph that incorporates node attribute information into the topology. This can be considered as the “dual” operation of message-passing in GNNs, which incorporates topological information into attributes (embeddings). We argue that graph learning is the more suitable scheme to combine attributes and topology for link prediction, since link prediction is a task for the topology itself (as opposed to other applications such as node classification).

Specifically, our first step of graph learning is to augment the original edges with a set of node pairs based on their (untrained) attribute similarity (i.e., adding an ϵ -neighborhood graph):

$$\tilde{E} = E + \{(u, v) \mid s(x_u, x_v) > \epsilon_\eta\} \quad (1)$$

where $s(\cdot)$ can be any similarity function (we use cosine in our experiments) and ϵ_η is a threshold that determines the number of added pairs as a ratio η of the original number of edges m .

A simple MLP then maps the pairwise node attributes into a trained edge weight for every edge in \tilde{E} :

$$w_{uv} = \text{MLP}([x_u; x_v]; \theta) \quad (2)$$

where $[x_u; x_v]$ denotes the concatenation of x_u and x_v and θ contains the trainable parameters. For undirected graphs, we instead use the following permutation invariant operator [12]:

$$w_{uv} = \text{MLP}([x_u + x_v; |x_u - x_v|]; \theta) \quad (3)$$

The final edge weights of the enhanced graph are a weighted combination of the topological weights, the untrained weights, and the trained weights:

$$\tilde{A}_{uv} = \alpha A_{uv} + (1 - \alpha)(\beta w_{uv} + (1 - \beta)s(x_u, x_v)) \quad (4)$$

where α and β are hyperparameters. The enhanced adjacency matrix \tilde{A} is then fed into a topological heuristic for link prediction introduced in the next section. Note that the MLP is not trained directly to predict the links, but instead trained end-to-end to enhance the input graph given to the topological heuristic. Also note that the MLP can be easily replaced by a more powerful model such

as a GNN, but the goal of this paper is to demonstrate the general effectiveness of our framework and we will show that even a simple MLP leads to significant improvement over the base heuristic.

3.2 Topological heuristic

Assuming that the learned adjacency matrix \tilde{A} incorporates structural and attribute information, Gelato applies a topological heuristic to \tilde{A} . Specifically, we adopt Autocovariance, which has been shown to achieve state-of-the-art link prediction results for non-attributed graphs [27].

Autocovariance is a random-walk based similarity metric. Intuitively, it measures the difference between the co-visiting probabilities for a pair of nodes in a truncated walk and in an infinitely long walk. Given the enhanced graph \tilde{G} , the Autocovariance similarity matrix $R \in \mathbb{R}^{n \times n}$ is given as

$$R = \frac{\tilde{D}}{\text{vol}(\tilde{G})} (\tilde{D}^{-1} \tilde{A})^t - \frac{\tilde{d} \tilde{d}^T}{\text{vol}^2(\tilde{G})} \quad (5)$$

where $t \in \mathbb{N}_0$ is the scaling parameter of the truncated walk. Each entry R_{uv} represents a similarity score for node pair (u, v) and top similarity pairs are predicted as links. Note that R_{uv} only depends on the t -hop enclosing subgraph of (u, v) and can be easily differentiated with respect to the edge weights in the subgraph. In fact, Gelato could be applied with any differentiable topological heuristic or even a combination of them. In our experiments (Section 4.2), we will show that Autocovariance alone enables state-of-the-art link prediction performance.

Next, we introduce how to train our model parameters with supervised information.

3.3 N-pair loss and unbiased training

As we have mentioned in Section 2, current supervised link prediction methods rely on *biased training* and the cross entropy loss (CE) to optimize model parameters. Instead, Gelato applies the N-pair loss [70] that is inspired by the metric learning and learning-to-rank literature [10, 49, 61, 77] to train the parameters of our graph learning model (see Section 3.1) from highly imbalanced *unbiased training* data.

The N-pair loss (NP) contrasts each positive training edge (u, v) against a set of negative pairs $N(u, v)$. It is computed as follows:

$$L(\theta) = - \sum_{(u,v) \in E} \log \frac{\exp(R_{uv})}{\exp(R_{uv}) + \sum_{(p,q) \in N(u,v)} \exp(R_{pq})} \quad (6)$$

Intuitively, $L(\theta)$ is minimized when each positive edge (u, v) has a much higher similarity than its contrasted negative pairs: $R_{uv} \gg R_{pq}, \forall (p, q) \in N(u, v)$. Compared to CE, NP is more sensitive to negative pairs that have comparable similarities to those of positive pairs—they are more likely to be false positives. While NP achieves good performance in our experiments, alternative losses from the learning-to-rank literature [6, 20, 80] could also be applied.

Gelato generates negative samples $N(u, v)$ using *unbiased training*. This means that $N(u, v)$ is a random subset of all disconnected pairs in the training graph, and $|N(u, v)|$ is proportional to the ratio of negative pairs over positive ones. In this way, we leverage more information contained in negative pairs compared to *biased training*. Note that, similar to *unbiased training*, (unsupervised) topological

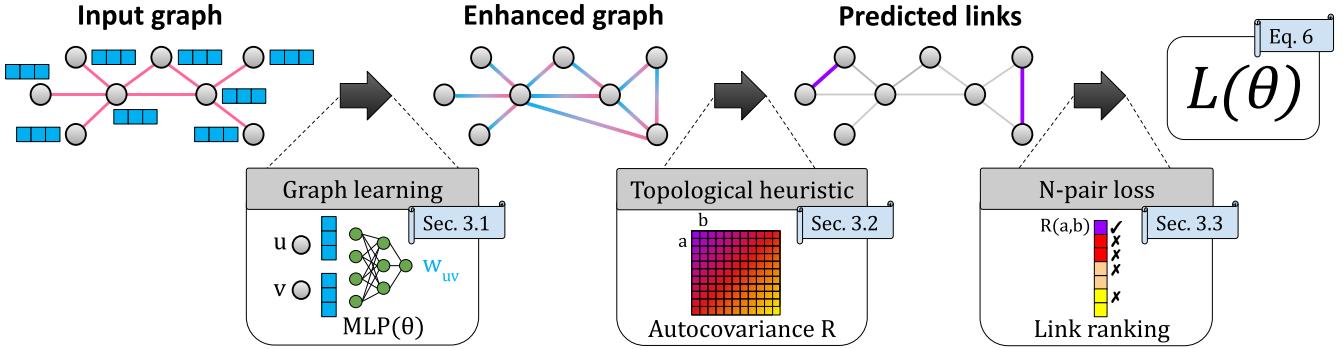


Figure 2: Gelato applies graph learning to incorporate attribute information into the topology via an MLP. The learned graph is given to a topological heuristic that predicts edges between node pairs with high Autocovariance similarity. The parameters of the MLP are optimized end-to-end using the N-pair loss. Experiments show that Gelato outperforms state-of-the-art GNN-based link prediction methods.

heuristics implicitly use information from all edges and non-edges. Also, *unbiased training* can be combined with adversarial negative sampling methods [9, 75] from the knowledge graph embedding literature to increase the quality of contrasted negative pairs.

Complexity analysis. The only trainable component in our model is the graph learning MLP with $O(rh + lh^2)$ parameters—where r is the number of node features, l is the number of hidden layers, and h is the number of neurons per layer. Notice that the number of parameters is independent of the graph size. Constructing the ϵ -neighborhood graph based on cosine similarity can be done efficiently using hashing and pruning [2, 65]. Computing the enhanced adjacency matrix with the MLP takes $O((1+\eta)mr)$ time per epoch—where $m = |E|$ and η is the ratio of edges added to E from the ϵ -neighborhood graph. We apply sparse matrix multiplication to compute k entries of the t -step AC in $O(\max(k, (1+\eta)mt))$ time. Note that unlike recent GNN-based approaches [42, 55, 89] that generate distinctive subgraphs for each link (e.g., via the labeling trick), enclosing subgraphs for links in Gelato share the same information (i.e., learned edge weights), which significantly reduces the computational cost. Our experiments will demonstrate Gelato’s efficiency in training and inference.

4 EXPERIMENTS

We provide empirical evidence for our claims regarding supervised link prediction and demonstrate the accuracy and efficiency of Gelato. Our implementation is anonymously available at <https://anonymous.4open.science/r/Gelato/>.

4.1 Experiment settings

Datasets. Our method is evaluated on five attributed graphs commonly used as link prediction benchmark [11, 13, 55, 81, 91, 97].

Table 1 shows dataset statistics—see Appendix B for dataset details. **Baselines.** For GNN-based link prediction, we include six state-of-the-art methods published in the past two years: LGCN [91], TLC-GNN [81], Neo-GNN [88], NBFNet [97], BScNets [13], and WalkPool [55], as well as three pioneering works—GAE [34], SEAL [89], and HGNC [11]. For topological link prediction heuristics, we

Table 1: A summary of dataset statistics.

	#Nodes	#Edges	#Attrs	Avg. degree	Density
CORA	2,708	5,278	1,433	3.90	0.14%
CITESEER	3,327	4,552	3,703	2.74	0.08%
PUBMED	19,717	44,324	500	4.50	0.02%
PHOTO	7,650	119,081	745	31.13	0.41%
COMPUTERS	13,752	245,861	767	35.76	0.26%

consider Common Neighbors (CN) [52], Adamic Adar (AA) [1], Resource Allocation (RA) [96], and Autocovariance (AC) [27]—the base heuristic in our model. To demonstrate the superiority of the proposed end-to-end model, we also include an MLP trained directly for link prediction, the cosine similarity (Cos) between node attributes, and AC on top of the respective weighted/augmented graphs (i.e., two-stage approaches where the MLP is trained separately for link prediction rather than trained end-to-end) as baselines.

Hyperparameters. For Gelato, we tune the proportion of added edges η from $\{0.0, 0.25, 0.5, 0.75, 1.0\}$, the topological weight α from $\{0.0, 0.25, 0.5, 0.75\}$, and the trained weight β from $\{0.25, 0.5, 0.75, 1.0\}$, with a sensitivity analysis included in Section 4.6. All other settings are fixed across datasets: MLP with one hidden layer of 128 neurons, AC scaling parameter $t = 3$, Adam optimizer [33] with a learning rate of 0.001, a dropout rate of 0.5, and *unbiased training* without downsampling. For baselines, we use the same hyperparameters as in their papers.

Data splits for unbiased training and unbiased testing. Following [11, 13, 34, 55, 89, 91], we adopt 85%/5%/10% ratios for training, validation, and testing. Specifically, for *unbiased training* and *testing*, we first randomly (with seed 0) divide the (positive) edges E of the original graph into E_{train}^+ , E_{valid}^+ , and E_{test}^+ for training, validation, and testing based on the selected ratios. Then, we set the negative pairs in these three sets as (1) $E_{train}^- = E^- + E_{valid}^+ + E_{test}^+$, (2) $E_{valid}^- = E^- + E_{test}^+$, and (3) $E_{test}^- = E^-$, where E^- is the set of all negative pairs (excluding self-loops) in the original graph. Notice that the validation and testing *positive* edges are included in the *negative* training set, and the testing *positive* edges are included

in the *negative* validation set. These inclusions simulate the real-world scenario where the testing edges (and the validation edges) are unobserved during validation (training).

Evaluation metrics. We adopt Precision@ k ($prec@k$)—proportion of positive edges among the top k of all testing pairs, Hits@ k ($hits@k$)—ratio of positive edges individually ranked above k th place against all negative pairs, and Average Precision (AP)—area under the precision-recall curve, as evaluation metrics. We report results from 10 runs with random seeds ranging from 1 to 10.

More detailed experiment settings can be found in Appendix C.

4.2 Link prediction performance

Table 2 summarizes the link prediction performance in terms of the mean and standard deviation of Average Precision (AP) for all methods. Figure 3 and Figure 4 show results based on $prec@k$ (k as a ratio of test edges) and $hits@k$ (k as the rank) for varying k .

First, we want to highlight the drastically different performance of GNN-based methods compared to those found in the original papers [13, 55, 81, 88, 91, 97] and reproduced in Appendix D. While they achieve AUC/AP scores of often higher than 90% under *biased testing*, here we see most of them underperform even the simplest topological heuristics such as Common Neighbors under *unbiased testing*. These results support our arguments from Section 2 that evaluation metrics based on *biased testing* can produce misleading results compared to *unbiased testing*. The overall best performing GNN model is Neo-GNN, which directly generalizes the pairwise topological heuristics. Yet still, it consistently underperforms AC, a random-walk based heuristic that needs neither node attributes nor supervision/training.

We then look at two-stage combinations of AC and models for attribute information. We observe noticeable performance gains from combining attribute cosine similarity and AC in CORA and CITESEER but not for other datasets. Other two-stage approaches achieve similar or worse performance.

Finally, Gelato significantly outperforms the best GNN-based model with an average relative gain of **145.2%** and AC with a gain of **52.6%** in terms of AP—similar results were obtained for $prec@k$ and $hits@k$. This validates our hypothesis that a simple MLP can effectively incorporate node attribute information into the topology when our model is trained end-to-end. Next, we will provide insights behind these improvements and demonstrate the efficiency of Gelato on training and inference.

4.3 Visualizing Gelato predictions

To better understand the performance of Gelato, we visualize its learned graph, prediction scores, and predicted edges in comparison with AC and the best GNN-based baseline (Neo-GNN) in Figure 5.

Figure 5a shows the input adjacency matrix for the subgraph of PHOTO containing the top 160 nodes belonging to the first class sorted in decreasing order of their (within-class) degree. Figure 5b illustrates the enhanced adjacency matrix learned by Gelato’s MLP. Comparing it with the Euclidean distance between node attributes in Figure 5c, we see that our enhanced adjacency matrix effectively incorporates attribute information. More specifically, we notice the

down-weighting of the edges connecting the high-degree nodes with larger attribute distances (matrix entries 0-40 and especially 0-10) and the up-weighting of those connecting medium-degree nodes with smaller attribute distances (40-80). In Figure 5d and Figure 5e, we see the corresponding AC scores based on the input and the enhanced adjacency matrix (Gelato). Since AC captures the degree distribution of nodes [27], the vanilla AC scores greatly favor high-degree nodes (0-40). By comparison, thanks to the down-weighting, Gelato assigns relatively lower scores to edges connecting them to low-degree nodes (60-160), while still capturing the edge density between high-degree nodes (0-40). The immediate result of this is the significantly improved precision as shown in Figure 5h compared to Figure 5g. Gelato covers as many positive edges in the high-degree region as AC while making far fewer wrong predictions for connections involving low-degree nodes.

The prediction probabilities and predicted edges for Neo-GNN are shown in Figure 5f and Figure 5i, respectively. Note that while it predicts edges connecting high-degree node pairs (0-40) with high probability, similar values are assigned to many low-degree pairs (80-160) as well. Most of those predictions are wrong, both in the low-degree region of Figure 5i and also in other low-degree parts of the graph that are not shown here. This analysis supports our claim that Gelato is more effective at combining node attributes and the graph topology, enabling state-of-the-art link prediction.

4.4 Loss and training setting

In this section, we demonstrate the advantages of the proposed N-pair loss and *unbiased training* for supervised link prediction. Figure 6 shows the training and validation losses and $prec@100\%$ (our validation metric) in training Gelato based on the cross entropy (CE) and N-pair (NP) losses under *biased* and *unbiased training* respectively. The final test AP scores are shown in the titles.

In the first column (CE with *biased training*), different from the training, both loss and precision for (unbiased) validation decrease. This leads to even worse test performance compared to the untrained base model (i.e., AC). In other words, albeit being the most popular loss function for supervised link prediction, CE with *biased training* does not generalize to *unbiased testing*. On the contrary, as shown in the second column, the proposed NP loss with *biased training*—equivalent to the pairwise logistic loss [7]—is a more effective proxy for *unbiased testing* metrics.

The right two columns show results with *unbiased training*, which is better for CE as more negative pairs are present in the training set (with the original class ratio). On the other hand, NP is more consistent with unbiased evaluation metrics, leading to 8.5% better performance. This is because, unlike CE, which optimizes positive and negative pairs independently, NP contrasts negative pairs against positive ones, giving higher importance to negative pairs that are more likely to be false positives.

4.5 Ablation study

We have demonstrated the superiority of Gelato over its individual components and two-stage approaches in Table 2 and analyzed the effect of losses and training settings in Section 4.4. Here, we collect the results with the same hyperparameter setting as Gelato and present a comprehensive ablation study in Table 3. Specifically,

Table 2: Link prediction performance comparison (mean \pm std AP). Gelato consistently outperforms GNN-based methods, topological heuristics, and two-stage approaches combining attributes and topology.

		CORA	CITESEER	PUBMED	PHOTO	COMPUTERS
GNN	GAE	0.27 \pm 0.02	0.66 \pm 0.11	0.26 \pm 0.03	0.28 \pm 0.02	0.30 \pm 0.02
	SEAL	1.89 \pm 0.74	0.91 \pm 0.66	***	10.49 \pm 0.86	6.84*
	HGCN	0.82 \pm 0.03	0.74 \pm 0.10	0.35 \pm 0.01	2.11 \pm 0.10	2.30 \pm 0.14
	LGCN	1.14 \pm 0.04	0.86 \pm 0.09	0.44 \pm 0.01	3.53 \pm 0.05	1.96 \pm 0.03
	TLC-GNN	0.29 \pm 0.09	0.35 \pm 0.18	OOM	1.77 \pm 0.11	OOM
	Neo-GNN	2.05 \pm 0.61	1.61 \pm 0.36	1.21 \pm 0.14	10.83 \pm 1.53	6.75*
	NBFNet	1.36 \pm 0.17	0.77 \pm 0.22	***	11.99 \pm 1.60	***
	BScNets	0.32 \pm 0.08	0.20 \pm 0.06	0.22 \pm 0.08	2.47 \pm 0.18	1.45 \pm 0.10
	WalkPool	2.04 \pm 0.07	1.39 \pm 0.11	1.31*	OOM	OOM
Topological Heuristics	CN	1.10 \pm 0.00	0.74 \pm 0.00	0.36 \pm 0.00	7.73 \pm 0.00	5.09 \pm 0.00
	AA	2.07 \pm 0.00	1.24 \pm 0.00	0.45 \pm 0.00	9.67 \pm 0.00	6.52 \pm 0.00
	RA	2.02 \pm 0.00	1.19 \pm 0.00	0.33 \pm 0.00	10.77 \pm 0.00	7.71 \pm 0.00
	AC	2.43 \pm 0.00	2.65 \pm 0.00	2.50 \pm 0.00	16.63 \pm 0.00	11.64 \pm 0.00
Attributes + Topology	MLP	0.30 \pm 0.05	0.44 \pm 0.09	0.14 \pm 0.06	1.01 \pm 0.26	0.41 \pm 0.23
	Cos	0.42 \pm 0.00	1.89 \pm 0.00	0.07 \pm 0.00	0.11 \pm 0.00	0.07 \pm 0.00
	MLP+AC	3.24 \pm 0.03	1.95 \pm 0.05	2.61 \pm 0.06	15.99 \pm 0.21	11.25 \pm 0.13
	Cos+AC	3.60 \pm 0.00	4.46 \pm 0.00	0.51 \pm 0.00	10.01 \pm 0.00	5.20 \pm 0.00
	MLP+Cos+AC	3.39 \pm 0.06	4.15 \pm 0.14	0.55 \pm 0.03	10.88 \pm 0.09	5.75 \pm 0.11
Gelato		3.90 \pm 0.03	4.55 \pm 0.02	2.88 \pm 0.09	25.68 \pm 0.53	18.77 \pm 0.19

* Run only once as each run takes \sim 100 hrs; *** Each run takes $>$ 1000 hrs; OOM: Out Of Memory.

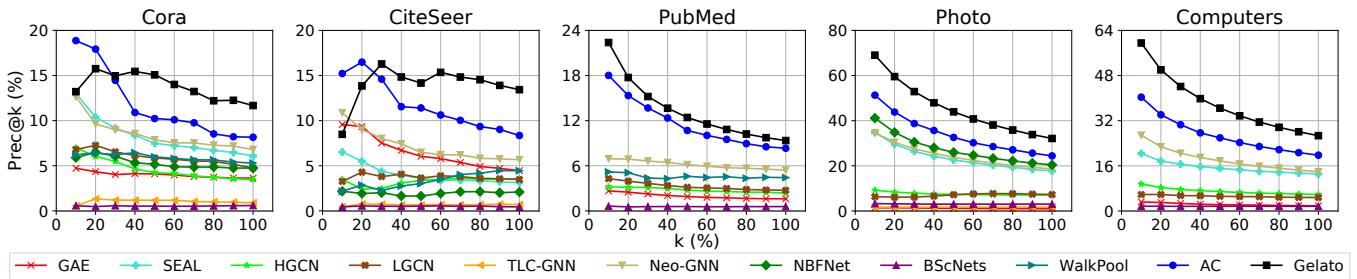


Figure 3: Link prediction performance in terms of prec@k for varying values of k (as percentages of test edges). With few exceptions, Gelato outperforms the baselines across different values of k.

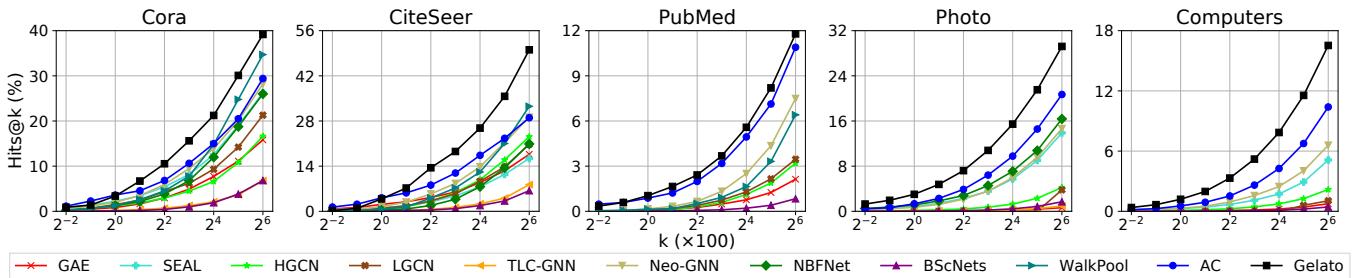


Figure 4: Link prediction performance in terms of hits@k for varying values of k. With few exceptions, Gelato outperforms the baselines across different values of k.

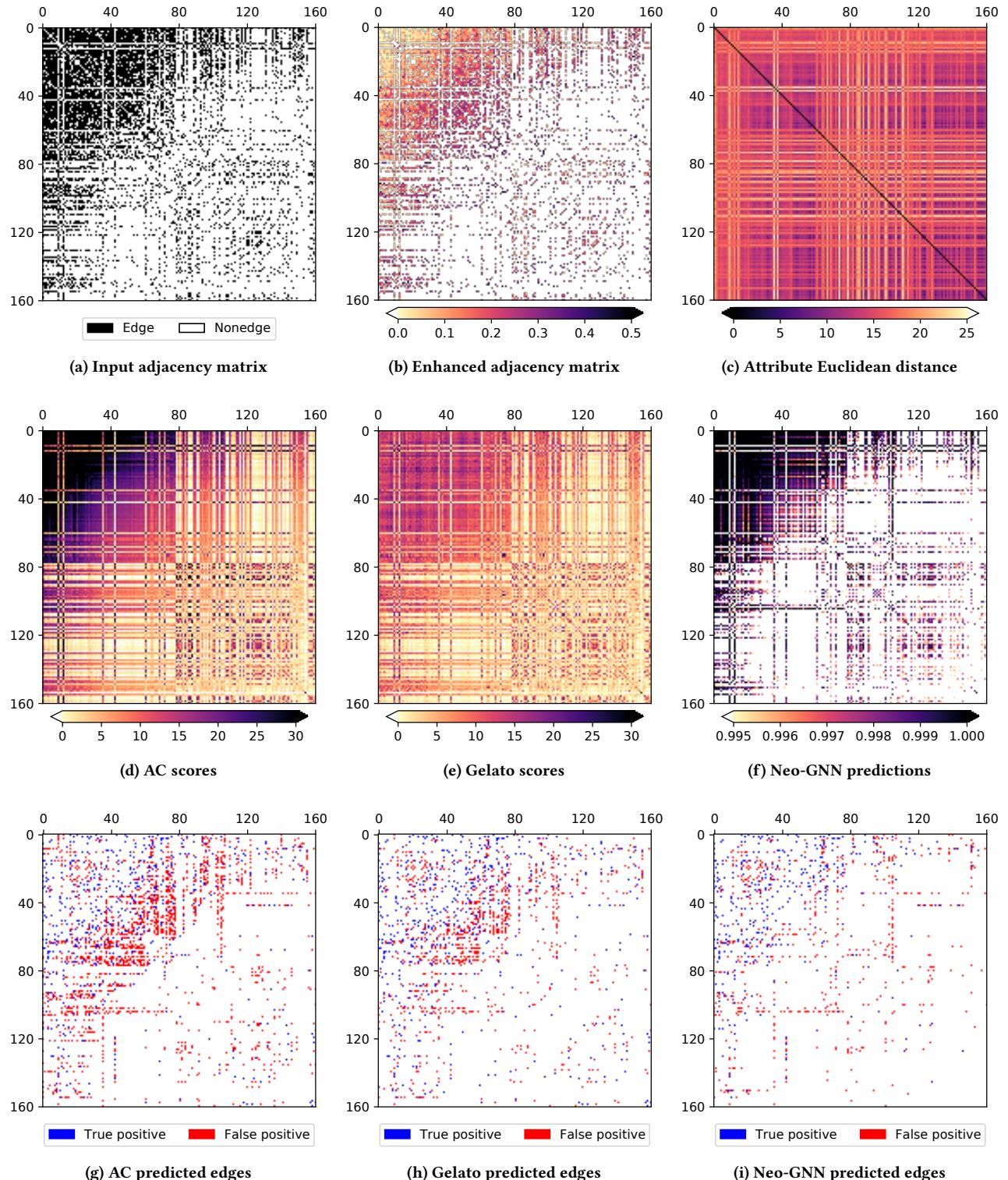


Figure 5: Illustration of the link prediction process of Gelato, AC, and the best GNN-based approach, Neo-GNN, on a subgraph of PHOTO. Gelato effectively incorporates node attributes into the graph structure and leverages topological heuristics to enable state-of-the-art link prediction.

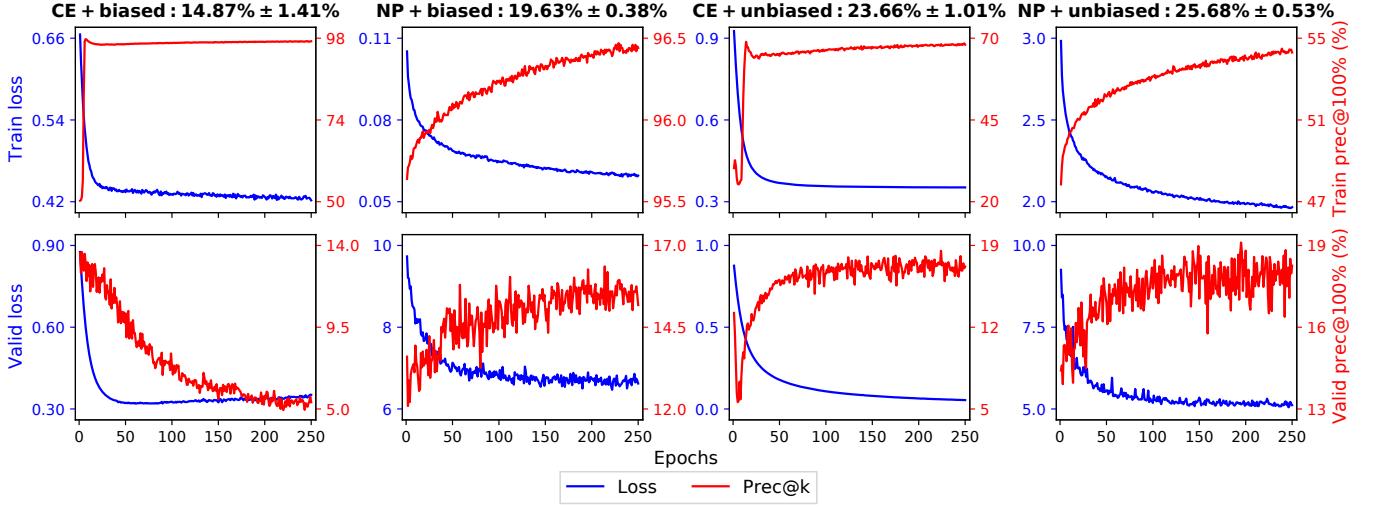


Figure 6: Training of Gelato based on different losses and training settings for PHOTO with test AP (mean \pm std) shown in the titles. Compared with the cross entropy loss, the N-pair loss with *unbiased training* is a more consistent proxy for *unbiased testing* metrics and leads to better peak performance.

Gelato-MLP (AC) represents Gelato without the MLP (Autocovariance) component, i.e., only using Autocovariance (MLP) for link prediction. *Gelato-NP (UT)* replaces the proposed N-pair loss (*unbiased training*) with the cross entropy loss (*biased training*) applied by the baselines. Finally, *Gelato-NP+UT* replaces both the loss and the training setting.

We observe that removing either MLP or Autocovariance leads to inferior performance, as the corresponding attribute or topology information would be missing. Further, to address the class imbalance problem of link prediction, both the N-pair loss and *unbiased training* are crucial for effective training of Gelato.

While all supervised baselines originally adopt *biased training*, we also implement the same *unbiased training* (and N-pair loss) as Gelato for those that are scalable in Appendix E—results are consistent with the ones discussed in Section 4.2.

4.6 Sensitivity analysis

The selected hyperparameters of Gelato for each dataset are recorded in Table 4, and a sensitivity analysis of η , α , and β are shown in Figure 7 and Figure 8 respectively for PHOTO and CORA.

For most datasets, we find that simply setting $\beta = 1.0$ and $\eta = \alpha = 0.0$ leads to the best performance, corresponding to the scenario where no edges based on cosine similarity are added and the edge weights are completely learned by the MLP. For CORA and CITESEER, however, we first notice that adding edges based on untrained cosine similarity alone leads to improved performance (see Table 2), which motivates us to set $\eta = 0.5/0.75$. In addition, we find that a large trainable weight β leads to overfitting of the model as the number of node attributes is large while the number of (positive) edges is small for CORA and CITESEER (see Table 1). We address this by decreasing the relative importance of trained edge weights ($\beta = 0.25/0.5$) and increasing that of the topological edge weights ($\alpha = 0.5$), which leads to better generalization and improved performance.

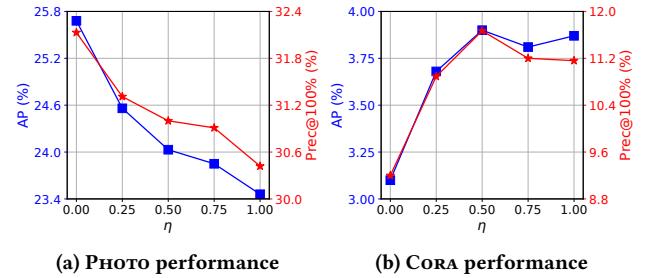


Figure 7: Performance of Gelato with different values of η .

Based on our experiments, these hyperparameters can be easily tuned using simple hyperparameter search techniques, such as line search, using a small validation set.

4.7 Running time comparison

We compare Gelato with other supervised link prediction methods in terms of running time for PHOTO (see details in Appendix F). As the only method that applies *unbiased training*—with more negative samples—Gelato shows a competitive training speed that is 11 \times faster than the best performing GNN-based method, Neo-GNN. In terms of inference time, Gelato is much faster than most baselines with a 6,000 \times speedup compared to Neo-GNN. We further observe more significant efficiency gains for Gelato over Neo-GNN for larger datasets—e.g., 14 \times (training) and 25,000 \times (testing) for COMPUTERS.

5 RELATED WORK

Topological heuristics for link prediction. The early link prediction literature focuses on topology-based heuristics. This includes approaches based on local (e.g., Common Neighbors [52], Adamic

Table 3: Results of the ablation study based on AP scores. Each component of Gelato plays an important role in enabling state-of-the-art link prediction performance.

	CORA	CITESEER	PUBMED	PHOTO	COMPUTERS
<i>Gelato-MLP</i>	2.43 ± 0.00	2.65 ± 0.00	2.50 ± 0.00	16.63 ± 0.00	11.64 ± 0.00
<i>Gelato-AC</i>	1.94 ± 0.18	3.91 ± 0.37	0.83 ± 0.05	7.45 ± 0.44	4.09 ± 0.16
<i>Gelato-NP+UT</i>	2.98 ± 0.20	1.96 ± 0.11	2.35 ± 0.24	14.87 ± 1.41	9.77 ± 2.67
<i>Gelato-NP</i>	1.96 ± 0.01	1.77 ± 0.20	2.32 ± 0.16	19.63 ± 0.38	9.84 ± 4.42
<i>Gelato-UT</i>	3.07 ± 0.01	1.95 ± 0.05	2.52 ± 0.09	23.66 ± 1.01	11.59 ± 0.35
Gelato	3.90 ± 0.03	4.55 ± 0.02	2.88 ± 0.09	25.68 ± 0.53	18.77 ± 0.19

Table 4: Selected hyperparameters of Gelato.

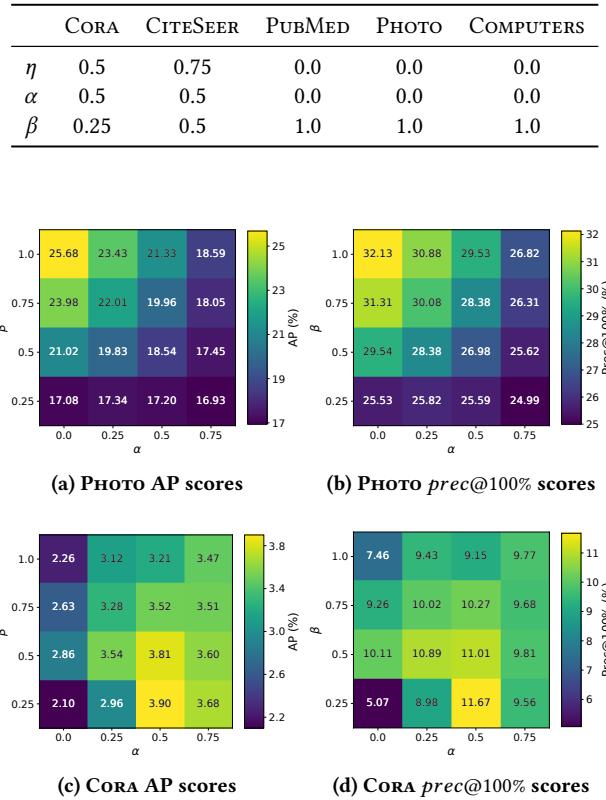


Figure 8: Performance of Gelato with different α and β .

Adar [1], and Resource Allocation [96]) and higher-order (e.g., Katz [32], PageRank [54], and SimRank [31]) information. More recently, random-walk based graph embedding methods, which learn vector representations for nodes [22, 27, 57], have achieved promising results in graph machine learning tasks. Popular embedding approaches, such as DeepWalk [57] and node2vec [22], have been shown to implicitly approximate the Pointwise Mutual Information similarity [59], which can also be used as a link prediction heuristic. This has motivated the investigation of other similarity metrics such as Autocovariance [17, 27, 28]. However, these heuristics are unsupervised and cannot take advantage of data beyond the topology.

Graph Neural Networks for link prediction. GNN-based link prediction addresses the limitations of topological heuristics by training a neural network to combine topological and attribute information and potentially learn new heuristics. GAE [34] combines a graph convolution network [35] and an inner product decoder based on node embeddings for link prediction. SEAL [89] models link prediction as a binary subgraph classification problem (edge/non-edge), and follow-up work (e.g., SHHF [42], WalkPool [55]) investigates different pooling strategies. Other recent approaches for GNN-based link prediction include learning representations in hyperbolic space (e.g., HGCRN [11], LGCN [91]), generalizing topological heuristics (e.g., Neo-GNN [88], NBFNet [97]), and incorporating additional topological features (e.g., TLC-GNN [81], BScNets [13]). Motivated by the growing popularity of GNNs for link prediction, this work investigates key questions regarding their training, evaluation, and ability to learn effective topological heuristics directly from data. We propose Gelato, which is simpler, more accurate, and faster than the state-of-the-art GNN-based link prediction methods.

Graph learning. Gelato learns a graph that combines topological and attribute information. Our goal differs from generative models [23, 40, 87], which learn to sample from a distribution over graphs. Graph learning also enables the application of GNNs when the graph is unavailable, noisy, or incomplete (for a recent survey, see [93]). LDS [19] and GAUG [94] jointly learn a probability distribution over edges and GNN parameters. IDGL [14] and EGLN [83] alternate between optimizing the graph and embeddings for node/graph classification and collaborative filtering. [69] proposes two-stage link prediction by augmenting the graph as a preprocessing step. In comparison, Gelato effectively learns a graph in an end-to-end manner by minimizing the loss of a topological heuristic.

6 CONCLUSION

This work sheds light on key limitations in how GNN-based link prediction methods handle the intrinsic class imbalance of the problem and presents more effective and efficient ways to combine attributes and topology. Our findings might open new research directions on machine learning for graph data, including a better understanding of the advantages of increasingly popular and sophisticated deep learning models compared to more traditional and simpler graph-based solutions.

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REFERENCES

- [1] Lada A Adamic and Eytan Adar. 2003. Friends and neighbors on the web. *Social networks* 25, 3 (2003), 211–230.
- [2] David C Anastasiu and George Karypis. 2014. L2ap: Fast cosine similarity search with prefix l-2 norm bounds. In *ICDE*.
- [3] Ashwin Bahulkar, Boleslaw K Szymanski, N Orkun Baycik, and Thomas C Sharkey. 2018. Community detection with edge augmentation in criminal networks. In *ASONAM*.
- [4] Albert-Laszlo Barabási, Hawoong Jeong, Zoltan Néda, Erzsebet Ravasz, Andras Schubert, and Tamas Vicsek. 2002. Evolution of the social network of scientific collaborations. *Physica A: Statistical mechanics and its applications* 311, 3-4 (2002), 590–614.
- [5] Antoine Bordes, Nicolas Usunier, Alberto García-Durán, Jason Weston, and Oksana Yakhnenko. 2013. Translating Embeddings for Modeling Multi-relational Data. In *NeurIPS*.
- [6] Sebastian Bruch. 2021. An alternative cross entropy loss for learning-to-rank. In *WebConf*.
- [7] Chris Burges, Tal Shaked, Erin Renshaw, Ari Lazier, Matt Deeds, Nicole Hamilton, and Greg Hullender. 2005. Learning to rank using gradient descent. In *ICML*.
- [8] Lei Cai, Jundong Li, Jie Wang, and Shuiwang Ji. 2021. Line graph neural networks for link prediction. *IEEE TPAMI* (2021).
- [9] Liwei Cai and William Yang Wang. 2018. KBGAN: Adversarial Learning for Knowledge Graph Embeddings. In *NAACL*.
- [10] Fatih Cakir, Kun He, Xide Xia, Brian Kulis, and Stan Sclaroff. 2019. Deep metric learning to rank. In *CVPR*.
- [11] Ines Chami, Zhitao Ying, Christopher Ré, and Jure Leskovec. 2019. Hyperbolic graph convolutional neural networks. In *NeurIPS*.
- [12] Xu Chen, Xiuyuan Cheng, and Stéphane Mallat. 2014. Unsupervised deep haar scattering on graphs. In *NeurIPS*.
- [13] Yuzhou Chen, Yulia R Gel, and H Vincent Poor. 2022. BScNets: Block Simplicial Complex Neural Networks. In *AAAI*.
- [14] Yu Chen, Lingfei Wu, and Mohammed Zaki. 2020. Iterative deep graph learning for graph neural networks: Better and robust node embeddings. In *NeurIPS*.
- [15] Arlei Lopes da Silva, Furkan Kocayusufoglu, Saber Jafarpour, Francesco Bullo, Ananthram Swami, and Ambuj Singh. 2020. Combining Physics and Machine Learning for Network Flow Estimation. In *ICLR*.
- [16] Jesse Davis and Mark Goadrich. 2006. The relationship between Precision-Recall and ROC curves. In *ICML*.
- [17] J-C Delvenne, Sophia N Yaliraki, and Mauricio Barahona. 2010. Stability of graph communities across time scales. *PNAS* 107, 29 (2010), 12755–12760.
- [18] Matthias Fey and Jan E. Lenssen. 2019. Fast Graph Representation Learning with PyTorch Geometric. In *ICLR Workshop on Representation Learning on Graphs and Manifolds*.
- [19] Luca Franceschi, Mathias Niepert, Massimiliano Pontil, and Xiao He. 2019. Learning discrete structures for graph neural networks. In *ICML*.
- [20] Yoav Freund, Raj Iyer, Robert E Schapire, and Yoram Singer. 2003. An efficient boosting algorithm for combining preferences. *JMLR* 4, Nov (2003), 933–969.
- [21] C Lee Giles, Kurt D Bollacker, and Steve Lawrence. 1998. CiteSeer: An automatic citation indexing system. In *ACM conference on Digital libraries*.
- [22] Aditya Grover and Jure Leskovec. 2016. node2vec: Scalable feature learning for networks. In *SIGKDD*.
- [23] Aditya Grover, Aaron Zweig, and Stefano Ermon. 2019. Graphite: Iterative generative modeling of graphs. In *ICML*.
- [24] Will Hamilton, Zhitao Ying, and Jure Leskovec. 2017. Inductive representation learning on large graphs. In *NeurIPS*.
- [25] Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and Jure Leskovec. 2020. Open graph benchmark: Datasets for machine learning on graphs. In *NeurIPS*.
- [26] Qian Huang, Horace He, Abhay Singh, Ser-Nam Lim, and Austin R Benson. 2021. Combining label propagation and simple models out-performs graph neural networks. In *ICLR*.
- [27] Zexi Huang, Arlei Silva, and Ambuj Singh. 2021. A Broader Picture of Random-walk Based Graph Embedding. In *SIGKDD*.
- [28] Zexi Huang, Arlei Silva, and Ambuj Singh. 2022. POLE: Polarized Embedding for Signed Networks. In *WSDM*.
- [29] Boris Ivanovic and Marco Pavone. 2019. The trajectron: Probabilistic multi-agent trajectory modeling with dynamic spatiotemporal graphs. In *ICCV*.
- [30] Mohsen Jamali and Martin Ester. 2009. Trustwalker: a random walk model for combining trust-based and item-based recommendation. In *SIGKDD*.
- [31] Glen Jeh and Jennifer Widom. 2002. Simrank: a measure of structural-context similarity. In *SIGKDD*.
- [32] Leo Katz. 1953. A new status index derived from sociometric analysis. *Psychometrika* 18, 1 (1953), 39–43.
- [33] Diederik P Kingma and Jimmy Ba. 2015. Adam: A method for stochastic optimization. In *ICLR*.
- [34] Thomas N Kipf and Max Welling. 2016. Variational graph auto-encoders. *arXiv preprint arXiv:1611.07308* (2016).
- [35] Thomas N Kipf and Max Welling. 2017. Semi-supervised classification with graph convolutional networks. In *ICLR*.
- [36] Johannes Klicpera, Aleksandar Bojchevski, and Stephan Günnemann. 2018. Predict then Propagate: Graph Neural Networks meet Personalized PageRank. In *ICLR*.
- [37] Yehuda Koren, Robert Bell, and Chris Volinsky. 2009. Matrix factorization techniques for recommender systems. *Computer* 42, 8 (2009), 30–37.
- [38] Cheng Li, Jiaqi Ma, Xiaoxiao Guo, and Qiaozhu Mei. 2017. Deepcas: An end-to-end predictor of information cascades. In *WebConf*.
- [39] Qimai Li, Zhichao Han, and Xiao-Ming Wu. 2018. Deeper insights into graph convolutional networks for semi-supervised learning. In *AAAI*.
- [40] Yujia Li, Oriol Vinyals, Chris Dyer, Razvan Pascanu, and Peter Battaglia. 2018. Learning deep generative models of graphs. In *ICML*.
- [41] David Liben-Nowell and Jon Kleinberg. 2007. The link-prediction problem for social networks. *Journal of the American society for information science and technology* 58, 7 (2007), 1019–1031.
- [42] Zheyi Liu, Darong Lai, Chuanyou Li, and Meng Wang. 2020. Feature Fusion Based Subgraph Classification for Link Prediction. In *CIKM*.
- [43] Linyuan Lü and Tao Zhou. 2011. Link prediction in complex networks: A survey. *Physica A: statistical mechanics and its applications* 390, 6 (2011), 1150–1170.
- [44] Jiaqi Ma, Bo Chang, Xuefei Zhang, and Qiaozhu Mei. 2020. CopulaGNN: towards integrating representational and correlational roles of graphs in graph neural networks. In *ICLR*.
- [45] Travis Martin, Brian Ball, and Mark EJ Newman. 2016. Structural inference for uncertain networks. *Physical Review E* 93, 1 (2016), 012306.
- [46] Víctor Martínez, Fernando Berzal, and Juan-Carlos Cubero. 2016. A survey of link prediction in complex networks. *ACM computing surveys (CSUR)* 49, 4 (2016), 1–33.
- [47] Julian McAuley, Christopher Targett, Qinfeng Shi, and Anton Van Den Hengel. 2015. Image-based recommendations on styles and substitutes. In *SIGIR*.
- [48] Andrew Kachites McCallum, Kamal Nigam, Jason Rennie, and Kristie Seymore. 2000. Automating the construction of internet portals with machine learning. *Information Retrieval* 3, 2 (2000), 127–163.
- [49] Brian McFee and Gert Lanckriet. 2010. Metric learning to rank. In *ICML*.
- [50] Federico Monti, Michael Bronstein, and Xavier Bresson. 2017. Geometric matrix completion with recurrent multi-graph neural networks. In *NeurIPS*.
- [51] Christopher Morris, Martin Ritzert, Matthias Fey, William L Hamilton, Jan Eric Lenssen, Gaurav Rattan, and Martin Grohe. 2019. Weisfeiler and leman go neural: Higher-order graph neural networks. In *AAAI*.
- [52] Mark EJ Newman. 2001. Clustering and preferential attachment in growing networks. *Physical review E* 64, 2 (2001), 025102.
- [53] Mingdong Ou, Peng Cui, Jian Pei, Ziwei Zhang, and Wenwu Zhu. 2016. Asymmetric transitivity preserving graph embedding. In *SIGKDD*.
- [54] Lawrence Page, Sergey Brin, Rajeev Motwani, and Terry Winograd. 1999. *The PageRank citation ranking: Bringing order to the web*. Technical Report. Stanford InfoLab.
- [55] Liming Pan, Cheng Shi, and Ivan Dokmanić. 2022. Neural Link Prediction with Walk Pooling. In *ICLR*.
- [56] Adam Paszke, Sam Gross, Francisco Massa, Adam Lerer, James Bradbury, Gregory Chanan, Trevor Killeen, Zeming Lin, Natalia Gimelshein, Luca Antiga, et al. 2019. Pytorch: An imperative style, high-performance deep learning library. In *NeurIPS*.
- [57] Bryan Perozzi, Rami Al-Rfou, and Steven Skiena. 2014. Deepwalk: Online learning of social representations. In *SIGKDD*.
- [58] Yanjun Qi, Ziv Bar-Joseph, and Judith Klein-Seetharaman. 2006. Evaluation of different biological data and computational classification methods for use in protein interaction prediction. *Proteins: Structure, Function, and Bioinformatics* 63, 3 (2006), 490–500.
- [59] Jiezhong Qiu, Yuxiao Dong, Hao Ma, Jian Li, Kuansan Wang, and Jie Tang. 2018. Network embedding as matrix factorization: Unifying deepwalk, line, pte, and node2vec. In *WSDM*.
- [60] Jiezhong Qiu, Jian Tang, Hao Ma, Yuxiao Dong, Kuansan Wang, and Jie Tang. 2018. Deepinf: Social influence prediction with deep learning. In *SIGKDD*.
- [61] Jerome Revaud, Jon Almazán, Rafael S Rezende, and Cesar Roberto de Souza. 2019. Learning with average precision: Training image retrieval with a listwise loss. In *ICCV*.
- [62] Sunil Kumar Sahu, Fenia Christopoulou, Makoto Miwa, and Sophia Ananiadou. 2019. Inter-sentence Relation Extraction with Document-level Graph Convolutional Neural Network. In *ACL*.
- [63] Takaya Saito and Marc Rehmsmeier. 2015. The precision-recall plot is more informative than the ROC plot when evaluating binary classifiers on imbalanced datasets. *PloS one* 10, 3 (2015), e0118432.
- [64] Alvaro Sanchez-Gonzalez, Nicolas Heess, Jost Tobias Springenberg, Josh Merel, Martin Riedmiller, Raia Hadsell, and Peter Battaglia. 2018. Graph networks as learnable physics engines for inference and control. In *ICML*.
- [65] Venu Satuluri and Srinivasan Parthasarathy. 2012. Bayesian Locality Sensitive Hashing for Fast Similarity Search. In *VLDB*.
- [66] Hinrich Schütze, Christopher D Manning, and Prabhakar Raghavan. 2008. *Introduction to information retrieval*. Vol. 39. Cambridge University Press Cambridge.

- [67] Prithviraj Sen, Galileo Namata, Mustafa Bilgic, Lise Getoor, Brian Galligher, and Tina Eliassi-Rad. 2008. Collective classification in network data. *AI magazine* 29, 3 (2008), 93–93.
- [68] Oleksandr Shchur, Maximilian Mumme, Aleksandar Bojchevski, and Stephan Günnemann. 2018. Pitfalls of graph neural network evaluation. *arXiv preprint arXiv:1811.05868* (2018).
- [69] Abhay Singh, Qian Huang, Sijia Linda Huang, Omkar Bhalerao, Horace He, Ser-Nam Lim, and Austin R Benson. 2021. Edge proposal sets for link prediction. *arXiv preprint arXiv:2106.15810* (2021).
- [70] Kihyuk Sohn. 2016. Improved deep metric learning with multi-class n-pair loss objective. In *NeurIPS*.
- [71] Haitian Sun, Bhuvan Dhingra, Manzil Zaheer, Kathryn Mazaitis, Ruslan Salakhutdinov, and William Cohen. 2018. Open Domain Question Answering Using Early Fusion of Knowledge Bases and Text. In *EMNLP*.
- [72] Zhiqing Sun, Zhi-Hong Deng, Jian-Yun Nie, and Jian Tang. 2018. RotatE: Knowledge Graph Embedding by Relational Rotation in Complex Space. In *ICLR*.
- [73] Jie Tang, Jing Zhang, Limin Yao, Juanzi Li, Li Zhang, and Zhong Su. 2008. Arnetminer: extraction and mining of academic social networks. In *SIGKDD*.
- [74] Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Liò, and Yoshua Bengio. 2018. Graph Attention Networks. In *ICLR*.
- [75] Peifeng Wang, Shuangyin Li, and Rong Pan. 2018. Incorporating gan for negative sampling in knowledge representation learning. In *AAAI*.
- [76] Xiang Wang, Xiangnan He, Yixin Cao, Meng Liu, and Tat-Seng Chua. 2019. Kgat: Knowledge graph attention network for recommendation. In *SIGKDD*.
- [77] Xinshe Wang, Yang Hua, Elyor Kodirov, Guosheng Hu, Romain Garnier, and Neil M Robertson. 2019. Ranked list loss for deep metric learning. In *ICCV*.
- [78] Bryan Wilder, Eric Ewing, Bistra Dilkina, and Milind Tambe. 2019. End to end learning and optimization on graphs. *NeurIPS* (2019).
- [79] Felix Wu, Amauri Souza, Tianyi Zhang, Christopher Fifty, Tao Yu, and Kilian Weinberger. 2019. Simplifying graph convolutional networks. In *ICML*.
- [80] Fen Xia, Tie-Yan Liu, Jue Wang, Wensheng Zhang, and Hang Li. 2008. Listwise approach to learning to rank: theory and algorithm. In *ICML*.
- [81] Zuoyu Yan, Tengfei Ma, Liangcai Gao, Zhi Tang, and Chao Chen. 2021. Link prediction with persistent homology: An interactive view. In *ICML*.
- [82] Bishan Yang, Scott Wen-tau Yih, Xiaodong He, Jianfeng Gao, and Li Deng. 2015. Embedding Entities and Relations for Learning and Inference in Knowledge Bases. In *ICLR*.
- [83] Yonghui Yang, Le Wu, Richang Hong, Kun Zhang, and Meng Wang. 2021. Enhanced graph learning for collaborative filtering via mutual information maximization. In *SIGIR*.
- [84] Zhihui Yang, William Cohen, and Ruslan Salakhudinov. 2016. Revisiting semi-supervised learning with graph embeddings. In *ICML*.
- [85] Liang Yao, Chengsheng Mao, and Yuan Luo. 2019. Graph convolutional networks for text classification. In *AAAI*.
- [86] Zhitao Ying, Jiaxuan You, Christopher Morris, Xiang Ren, Will Hamilton, and Jure Leskovec. 2018. Hierarchical graph representation learning with differentiable pooling. In *NeurIPS*.
- [87] Jiaxuan You, Rex Ying, Xiang Ren, William Hamilton, and Jure Leskovec. 2018. Graphrnn: Generating realistic graphs with deep auto-regressive models. In *ICML*.
- [88] Seongjum Yun, Seoyoon Kim, Junhyun Lee, Jaewoo Kang, and Hyunwoo J Kim. 2021. Neo-GNNs: Neighborhood Overlap-aware Graph Neural Networks for Link Prediction. In *NeurIPS*.
- [89] Muhan Zhang and Yixin Chen. 2018. Link prediction based on graph neural networks. In *NeurIPS*.
- [90] Muhan Zhang, Zhicheng Cui, Marion Neumann, and Yixin Chen. 2018. An end-to-end deep learning architecture for graph classification. In *AAAI*.
- [91] Yiding Zhang, Xiao Wang, Chuan Shi, Nian Liu, and Guojie Song. 2021. Lorentzian graph convolutional networks. In *WebConf*.
- [92] Ziwei Zhang, Peng Cui, Xiao Wang, Jian Pei, Xuanrong Yao, and Wenwu Zhu. 2018. Arbitrary-order proximity preserved network embedding. In *SIGKDD*.
- [93] Tong Zhao, Gang Liu, Stephan Günnemann, and Meng Jiang. 2022. Graph data augmentation for graph machine learning: A survey. *arXiv preprint arXiv:2202.08871* (2022).
- [94] Tong Zhao, Yozen Liu, Leonardo Neves, Oliver Woodford, Meng Jiang, and Neil Shah. 2021. Data augmentation for graph neural networks. In *AAAI*.
- [95] Cheng Zheng, Bo Zong, Wei Cheng, Dongjin Song, Jingchao Ni, Wenchao Yu, Haifeng Chen, and Wei Wang. 2020. Robust graph representation learning via neural sparsification. In *ICML*.
- [96] Tao Zhou, Linyuan Lü, and Yi-Cheng Zhang. 2009. Predicting missing links via local information. *The European Physical Journal B* 71, 4 (2009), 623–630.
- [97] Zhaocheng Zhu, Zuobai Zhang, Louis-Pascal Xhonneux, and Jian Tang. 2021. Neural bellman-ford networks: A general graph neural network framework for link prediction. In *NeurIPS*.

A ANALYSIS OF LINK PREDICTION EVALUATION METRICS WITH DIFFERENT TEST SETTINGS

In Section 2, we present an example scenario where a bad link prediction model that ranks 1M false positives higher than the 100k true edges achieves good AUC/AP with *biased testing*. Here, we provide the detailed computation steps and compare the results with those based on *unbiased testing*.

Figure 9a and Figure 9b show the receiver operating characteristic (ROC) and precision-recall (PR) curves for the model under *biased testing* with equal negative samples. Due to the downsampling, only 100k (out of 99.9M) negative pairs are included in the test set, among which only $100k/99.9M \times 1M \approx 1k$ pairs are ranked higher than the positive edges. In the ROC curve, this means that once the false positive rate reaches $1k/100k = 0.01$, the true positive rate would reach 1.0, leading to an AUC score of 0.99. Similarly, in the PR curve, when the recall reaches 1.0, the precision is $100k/(1k + 100k) \approx 0.99$, leading to an overall AP score of ~ 0.95 .

By comparison, as shown in Figure 9c, when the recall reaches 1.0, the precision under *unbiased testing* is only $100k/(1M + 100k) \approx 0.09$, leading to an AP score of ~ 0.05 . This demonstrates that evaluation metrics based on *biased testing* provide an overly optimistic measurement of link prediction model performance compared to the more realistic *unbiased testing* setting.

B DESCRIPTION OF DATASETS

We use the following datasets in our experiments (with their statistics in Table 1):

- CORA [48] and CITESEER [21] are citation networks where nodes represent scientific publications (classified into seven and six classes, respectively) and edges represent the citations between them. Attributes of each node is a binary word vector indicating the absence/presence of the corresponding word from a dictionary.
- PUBMED [67] is a citation network where nodes represent scientific publications (classified into three classes) and edges represent the citations between them. Attributes of each node is a TF/IDF weighted word vector.
- PHOTO and COMPUTERS are subgraphs of the Amazon co-purchase graph [47] where nodes represent products (classified into eight and ten classes, respectively) and edges imply that two products are frequently bought together. Attributes of each node is a bag-of-word vector encoding the product review.

We use the publicly available version of the datasets from the pytorch-geometric library [18] (under the MIT licence) curated by [84] and [68].

C DETAILED EXPERIMENT SETTINGS

Positive masking. For *unbiased training*, a trick similar to *negative injection* [89] in *biased training* is needed to guarantee model generalizability. Specifically, we divide the training positive edges into batches and during the training with each batch E_b , we feed in only the residual edges $E - E_b$ as the structural information to the model. This setting simulates the testing phase, where the model

is expected to predict edges without using their own connectivity information. We term this trick *positive masking*.

Other implementation details. We add self-loops to the enhanced adjacency matrix to ensure that each node has a valid transition probability distribution that is used in computing Autocovariance. The self-loops are added to all isolated nodes in the training graph for PUBMED, PHOTO, and COMPUTERS, and to all nodes for CORA and CITESEER. Following the postprocessing of the Autocovariance matrix for embedding in [27], we standardize Gelato similarity scores before computing the loss. For training with the cross entropy loss, we further add a linear layer with the sigmoid activation function to map our prediction score to a probability. We optimize our model with gradient descent via autograd in pytorch [56]. We find that the gradients are sometimes invalid when training our model (especially with the cross entropy loss), and we address this by skipping the parameter updates for batches leading to invalid gradients. Finally, we use *prec@100%* on the (unbiased) validation set as the criteria for selecting the best model from all training epochs. The maximum number of epochs for CORA/CITESEER/PUBMED and PHOTO/COMPUTERS are set to be 100 and 250, respectively.

Experiment environment. We run our experiments in an *a2-highgpu-1g* node of the Google Cloud Compute Engine. It has one NVIDIA A100 GPU with 40GB HBM2 GPU memory and 12 Intel Xeon Scalable Processor (Cascade Lake) 2nd Generation vCPUs with 85GB memory.

Reference of baselines. We list link prediction baselines and their reference repositories we use in our experiments in Table 5. Note that we had to implement the batched training and testing for several baselines as their original implementations do not scale to *unbiased training* and *unbiased testing* without downsampling.

Table 5: Reference of baseline code repositories.

Baseline	Repository
GAE [35]	https://github.com/zfjsail/gae-pytorch
SEAL [89]	https://github.com/facebookresearch/SEAL_OGB
HGCN [11]	https://github.com/HazyResearch/hgcn
LGCN [91]	https://github.com/ydzhang-stormstout/LGCN/
TLC-GNN [81]	https://github.com/pkuyzy/TLC-GNN/
Neo-GNN [88]	https://github.com/seongjunyun/Neo-GNNs
NBFNet [97]	https://github.com/DeepGraphLearning/NBFNet
BScNets [13]	https://github.com/BScNets/BScNets
WalkPool [55]	https://github.com/DaDaCheng/WalkPooling
AC [27]	https://github.com/zexihuang/random-walk-embedding

Number of trainable parameters. The only trainable component in Gelato is the graph learning MLP, which for Photo has 208,130 parameters. By comparison, the best performing GNN-based method, Neo-GNN, has more than twice the number of parameters (455,200).

D RESULTS BASED ON AUC SCORES

As we have argued in Section 2, AUC is not an effective evaluation metric for link prediction (even under *unbiased testing*) as it is biased towards the majority class. In Table 6, we report the AUC scores for different methods under *unbiased testing*. These results,

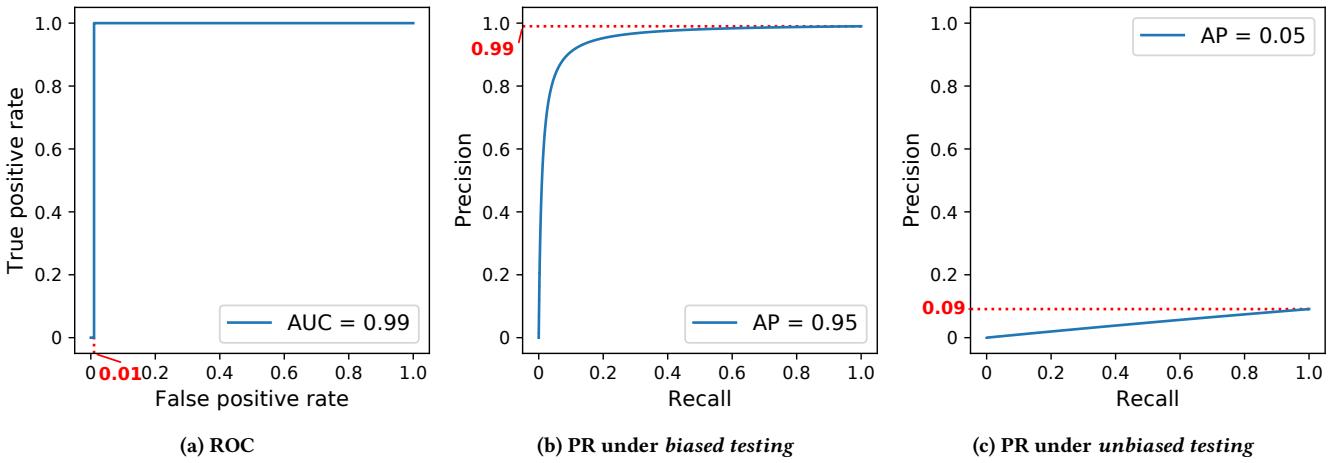


Figure 9: Receiver operating characteristic and precision-recall curves for the bad link prediction model that ranks 1M false positives higher than the 100k true edges. The model achieves 0.99 in AUC and 0.95 AP under *biased testing*, while the more informative performance evaluation metric, Average Precision (AP) under *unbiased testing*, is only 0.05.

while being consistent with those found in the link prediction literature, disagree with those obtained using the rank-based evaluation metrics under *unbiased testing*.

E BASELINE RESULTS WITH UNBIASED TRAINING

Table 7 summarizes the link prediction performance in terms of mean and standard deviation of AP for Gelato and the baselines using *unbiased training* without downsampling and the cross entropy loss, and Figure 10 and Figure 11 show results based on *prec@k* and *hits@k* for varying *k* values.

We first note that *unbiased training* without downsampling brings serious scalability challenges to most GNN-based approaches, making scaling up to larger datasets intractable. For the scalable baselines, *unbiased training* leads to marginal (e.g., Neo-GNN) to significant (e.g., BScNets) gains in performance. However, all of them still underperform the topological heuristic, Autocovariance, in most cases, and achieve much worse performance compared to Gelato. **This supports our claim that the topology-centric graph learning mechanism in Gelato is more effective than the attribute-centric message-passing in GNNs for link prediction, leading to state-of-the-art performance.**

As for the GNN-based baselines using both *unbiased training* and our proposed N-pair loss, we have attempted to modify the training functions of the reference repositories of the baselines and managed to train SEAL, LGCN, Neo-GNN, and BScNet. However, despite our best efforts, we are unable to obtain better link prediction performance using the N-pair loss. We defer the further investigation of the incompatibility of our loss and the baselines to future research. On the other hand, we have observed significantly better performance for MLP with the N-pair loss compared to the cross entropy loss under *unbiased training*. This can be seen by comparing the MLP performance in Table 7 here and the *Gelato-AC* performance in Table 3 in the ablation study. The improvement

shows the potential benefit of applying our training setting and loss to other supervised link prediction methods.

F RUNNING TIME COMPARISON

We compare Gelato with other supervised link prediction methods in terms of running time for Photo in Table 8. As the only method that applies *unbiased training* by default, Gelato shows a competitive training speed that is 11 \times faster than the best performing GNN-based method, Neo-GNN and is 6,000 \times faster for inference.

We also show the training time comparison between different supervised link prediction methods using *unbiased training* without downsampling in Table 9. Gelato is the second fastest model, only slower than the vanilla MLP. This further demonstrates that Gelato is a more efficient alternative compared to GNNs.

Table 6: Link prediction performance comparison (mean \pm std AUC). AUC results conflict with other evaluation metrics, presenting a misleading view of the model performance for link prediction.

		CORA	CITESEER	PUBMED	PHOTO	COMPUTERS
GNN	GAE	87.30 \pm 0.22	87.48 \pm 0.39	94.10 \pm 0.22	77.59 \pm 0.73	79.36 \pm 0.37
	SEAL	91.82 \pm 1.08	90.37 \pm 0.91	***	98.85 \pm 0.04	98.7*
	HGCN	92.60 \pm 0.29	92.39 \pm 0.61	94.40 \pm 0.14	96.08 \pm 0.08	97.86 \pm 0.10
	LGCN	91.60 \pm 0.23	93.07 \pm 0.77	95.80 \pm 0.03	98.36 \pm 0.01	97.81 \pm 0.01
	TLC-GNN	91.57 \pm 0.95	91.18 \pm 0.78	OOM	98.20 \pm 0.08	OOM
	Neo-GNN	91.77 \pm 0.84	90.25 \pm 0.80	90.43 \pm 1.37	98.74 \pm 0.55	98.34*
	NBFNet	86.06 \pm 0.59	85.10 \pm 0.32	***	98.29 \pm 0.35	***
	BScNets	91.59 \pm 0.47	89.62 \pm 1.05	97.48 \pm 0.07	98.68 \pm 0.06	98.41 \pm 0.05
	WalkPool	92.33 \pm 0.30	90.73 \pm 0.42	98.66*	OOM	OOM
Topological Heuristics	CN	71.15 \pm 0.00	66.91 \pm 0.00	64.09 \pm 0.00	96.73 \pm 0.00	96.15 \pm 0.00
	AA	71.22 \pm 0.00	66.92 \pm 0.00	64.09 \pm 0.00	97.02 \pm 0.00	96.58 \pm 0.00
	RA	71.22 \pm 0.00	66.93 \pm 0.00	64.09 \pm 0.00	97.20 \pm 0.00	96.82 \pm 0.00
	AC	75.41 \pm 0.00	72.41 \pm 0.00	67.46 \pm 0.00	98.24 \pm 0.00	96.86 \pm 0.00
Attributes + Topology	MLP	85.43 \pm 0.36	87.89 \pm 2.05	87.89 \pm 2.05	91.24 \pm 1.61	88.84 \pm 2.58
	Cos	79.06 \pm 0.00	89.86 \pm 0.00	89.14 \pm 0.00	71.46 \pm 0.00	71.68 \pm 0.00
	MLP+AC	79.77 \pm 0.03	82.26 \pm 0.29	66.31 \pm 0.74	98.02 \pm 0.05	96.69 \pm 0.05
	Cos+AC	86.34 \pm 0.00	89.29 \pm 0.00	75.56 \pm 0.00	97.28 \pm 0.00	96.26 \pm 0.00
	MLP+Cos+AC	86.90 \pm 0.14	89.42 \pm 0.09	75.78 \pm 0.27	97.27 \pm 0.01	96.24 \pm 0.01
Gelato		83.12 \pm 0.06	88.38 \pm 0.02	64.93 \pm 0.06	98.01 \pm 0.03	96.72 \pm 0.04

* Run only once as each run takes \sim 100 hrs; *** Each run takes $>$ 1000 hrs; OOM: Out Of Memory.

Table 7: Link prediction performance comparison (mean \pm std AP) with supervised link prediction methods using unbiased training. While we observe noticeable improvement for some baselines (e.g., BScNets), Gelato still consistently and significantly outperform the baselines.

		CORA	CITESEER	PUBMED	PHOTO	COMPUTERS
GNN	GAE	0.33 \pm 0.21	0.69 \pm 0.18	0.63*	1.36 \pm 3.38	7.91*
	SEAL	2.24*	1.11*	***	***	***
	HGCN	0.54 \pm 0.23	1.02 \pm 0.05	0.41*	3.27 \pm 2.97	2.60*
	LGCN	1.53 \pm 0.08	1.45 \pm 0.09	0.55*	2.90 \pm 0.26	1.13*
	TLC-GNN	0.68 \pm 0.16	0.61 \pm 0.19	OOM	2.95 \pm 1.50	OOM
	Neo-GNN	2.76 \pm 0.36	1.80 \pm 0.22	***	***	***
	NBFNet	***	***	***	***	***
	BScNets	1.13 \pm 0.25	1.27 \pm 0.20	0.47*	8.54 \pm 1.55	4.40*
	WalkPool	***	***	***	OOM	OOM
Topological Heuristics	CN	1.10 \pm 0.00	0.74 \pm 0.00	0.36 \pm 0.00	7.73 \pm 0.00	5.09 \pm 0.00
	AA	2.07 \pm 0.00	1.24 \pm 0.00	0.45 \pm 0.00	9.67 \pm 0.00	6.52 \pm 0.00
	RA	2.02 \pm 0.00	1.19 \pm 0.00	0.33 \pm 0.00	10.77 \pm 0.00	7.71 \pm 0.00
	AC	2.43 \pm 0.00	2.65 \pm 0.00	2.50 \pm 0.00	16.63 \pm 0.00	11.64 \pm 0.00
Attributes + Topology	MLP	0.22 \pm 0.27	1.17 \pm 0.63	0.44 \pm 0.12	1.15 \pm 0.40	1.19 \pm 0.46
	Cos	0.42 \pm 0.00	1.89 \pm 0.00	0.07 \pm 0.00	0.11 \pm 0.00	0.07 \pm 0.00
	MLP+AC	0.63 \pm 0.32	1.00 \pm 0.43	1.17 \pm 0.44	11.88 \pm 0.83	8.73 \pm 0.45
	Cos+AC	3.60 \pm 0.00	4.46 \pm 0.00	0.51 \pm 0.00	10.01 \pm 0.00	5.20 \pm 0.00
	MLP+Cos+AC	3.80 \pm 0.01	3.94 \pm 0.03	0.77 \pm 0.01	12.80 \pm 0.03	7.57 \pm 0.02
Gelato		3.90 \pm 0.03	4.55 \pm 0.02	2.88 \pm 0.09	25.68 \pm 0.53	18.77 \pm 0.19

* Run only once as each run takes \sim 100 hrs; *** Each run takes $>$ 1000 hrs; OOM: Out Of Memory.

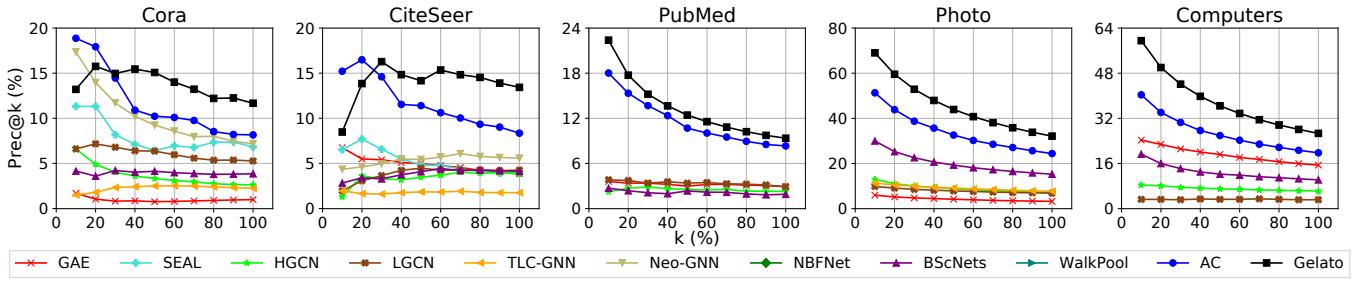


Figure 10: Link prediction performance in terms of $prec@k$ (in percentage) for varying values of k with baselines using *unbiased training*. While we observe noticeable improvement for some baselines (e.g., BScNets), Gelato still consistently and significantly outperform the baselines.

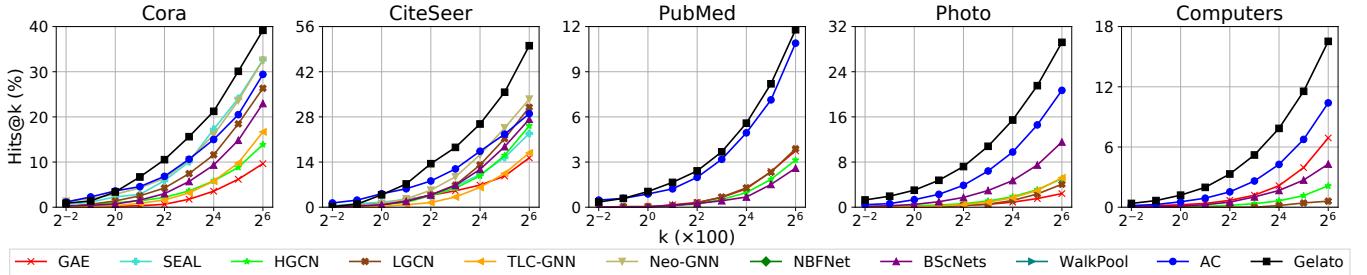


Figure 11: Link prediction performance in terms of $hits@k$ (in percentage) for varying values of k with baselines using *unbiased training*. While we observe noticeable improvement for some baselines (e.g., BScNets), Gelato still consistently and significantly outperform the baselines.

Table 8: Training and inference time comparison between supervised link prediction methods for PHOTO. Gelato has competitive training time (even under *unbiased training*) and is significantly faster than most baselines in terms of inference, especially compared to the best GNN model, Neo-GNN.

	GAE	SEAL	HGCN	LGCN	TLC-GNN	Neo-GNN	NBFNet	BScNets	MLP	Gelato
Training	1,022	11,493	92	56	42,440	14,807	30,896	115	232	1,265
Testing	0.031	380	0.093	0.099	5.722	346	76,737	0.394	1.801	0.057

Table 9: Training time comparison between supervised link prediction methods for PHOTO under *unbiased training*. Gelato, while achieving the best performance, is also the second most efficient method in terms of total training time, slower only than the vanilla MLP.

	GAE	SEAL	HGCN	LGCN	TLC-GNN	Neo-GNN	NBFNet	BScNets	MLP	Gelato
Training	6,361	>450,000	1,668	1,401	53,304	>450,000	>450,000	2,323	744	1,285