COUNTERFACTUAL GRAPH LEARNING FOR LINK PREDICTION

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ABSTRACT

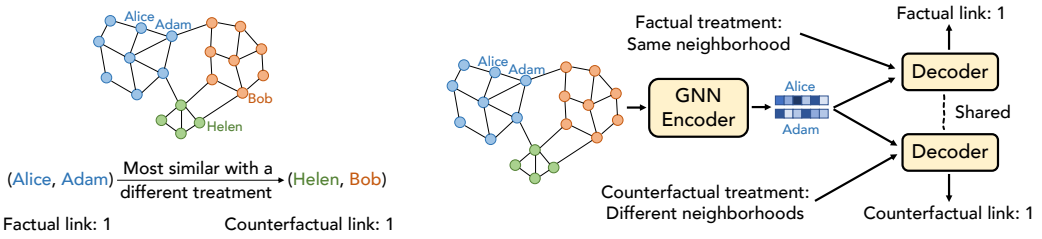
Learning to predict missing links is important for many graph-based applications. Existing methods were designed to learn the association between two sets of variables: (1) the observed graph structure (e.g., clustering effect) and (2) the existence of link between a pair of nodes. However, the causal relationship between these variables was ignored. We visit the possibility of learning it by asking a counterfactual question: "*would the link exist or not if the observed graph structure became different?*" To answer this question, we leverage causal models considering the information of the node pair (i.e., learned graph representations) as context, global graph structural properties as treatment, and link existence as outcome. In this work, we propose a novel link prediction method that enhances graph learning by counterfactual inference. It creates counterfactual links from the observed ones, and learns representations from both the observed and counterfactual links. Experiments on benchmark datasets show that this novel graph learning method achieves state-of-the-art performance on link prediction.

1 INTRODUCTION

Link prediction seeks to predict the likelihood of edge existence between node pairs based on the observed graph. Given the omnipresence of graph-structured data, link prediction has copious applications such as movie recommendation (Bennett et al., 2007), chemical interaction prediction (Stanfield et al., 2017), and knowledge graph completion (Kazemi & Poole, 2018). Graph machine learning methods have been widely applied to solve this problem. Their standard scheme is to first learn the representation vectors of nodes and then learn the *association* between the representations of a pair of nodes and the existence of the link between them. For example, graph neural networks (GNNs) use neighborhood aggregation to create the representation vectors: the representation vector of a node is computed by recursively aggregating and transforming representation vectors of its neighboring nodes (Kipf & Welling, 2016a; Hamilton et al., 2017; Wu et al., 2020). Then the vectors are fed into a binary classification model to learn the *association*. GNN methods have shown predominance in the task of link prediction (Kipf & Welling, 2016b; Zhang et al., 2020a).

Unfortunately, the causal relationship between graph structure and link existence was largely ignored in previous work. Existing methods that learn from association ~~only were~~ are not able to capture essential factors to accurately predict missing links in the *test data*. Take social network as an example. Suppose Alice and Adam live in the same neighborhood and they are close friends. The association between neighborhood belonging and friend closeness could be too strong to discover the essential factors of the friendship such as common interests or family relationship which could be the cause of being living in the same neighborhood. So, our idea is asking a *counterfactual* question: "*would Alice and Adam still be close friends if they were not living in the same neighborhood?*" If a graph learning model could learn the causal relationship by answering the counterfactual questions, it would improve the accuracy of link prediction with the novel knowledge it captured. Generally, the questions can be described as "*would the link exist or not if the graph structure became different?*"

As known to many, counterfactual question is a key component of causal inference and have been well defined in the literature. A counterfactual question is usually framed with three factors: context (as a data point), manipulation (e.g., treatment, intervention, action, strategy), and outcome (van der Laan & Petersen, 2007; Johansson et al., 2016). (To simplify the language, we use "treatment" to refer to the manipulation in this paper, as readers might be familiar more with the word "treatment.")



(a) Find counterfactual link as the most similar node pair with a different treatment.

(b) Train a GNN-based link predictor to predict factual and counterfactual links given the corresponding treatments.

Figure 1: The proposed CFLP learns the causal relationship between the observed graph structure (e.g., neighborhood similarity, considered as treatment variable) and link existence (considered as outcome). In this example, the link predictor would be trained to estimate the individual treatment effect (ITE) as $1 - 1 = 0$ so it looks for factors other than neighborhood to predict the factual link.

Given certain data context, it asks what the outcome would have been if the treatment had not been the observed value. In the scenario of link prediction, we consider the information of a pair of nodes as context, graph structural properties as treatment, and link existence as outcome. Recall the social network example. The context is the representations of Alice and Adam that are learned from their personal attributes and relationships with others on the network. The treatment is living in the same neighborhood, which can be identified by community detection. And the outcome is their friendship. In this work, we present a **c**ounter**f**actual graph learning method for **l**ink **p**rediction (CFLP) that trains graph learning models to answer the counterfactual questions. Figure 1 illustrates this two-step method. Suppose the treatment variable is defined as one type of global graph structure, e.g., the neighborhood assignment discovered by spectral clustering or community detection algorithms. We are wondering how likely the neighborhood distribution makes a difference on the link (non-)existence for each pair of nodes. So, given a pair of nodes (like Alice and Adam) and the treatment value on this pair (in the same neighborhood), we find a pair of nodes (like Helen and Bob) that satisfies two conditions: (1) it has a different treatment (in different neighborhoods) and (2) it is the most similar pair with the given pair of nodes. We call these matched pair of nodes as "counterfactual links." Note that the outcome of the counterfactual link can be either 1 or 0, depending on whether there exists an edge between the matched pair of nodes (Helen and Bob). The counterfactual link provides unobserved outcome to the given pair of nodes (Alice and Adam) under a counterfactual condition (in different neighborhoods). After counterfactual links are created for all (positive and negative) training examples, CFLP trains a link predictor (which can be GNN-based) to learn the representation vectors of nodes to predict both the observed factual links and the counterfactual links. In this Alice-Adam example, the link predictor is trained to estimate the individual treatment effect (ITE) of neighborhood assignment as $1 - 1 = 0$, where ITE is a metric for the effect of treatment on the outcome and zero indicates the given treatment has no effect on the outcome. So, the learner will try to discover the essential factors on the friendship between Alice and Adam. CFLP leverages causal models to find these factors for graph learning models to accurately predict missing links.

Contributions. Our main contributions can be summarized as follows. (1) This is the first work that proposes to improve link prediction by causal inference, specifically, learning to answer counterfactual questions about link existence. (2) This work introduces CFLP that trains GNN-based link predictors to predict both factual and counterfactual links. It learns the causal relationship between global graph structure and link existence. (3) CFLP outperforms competitive baseline methods on several benchmark datasets. We analyze the impact of counterfactual links as well as the choice of treatment variable. This work sheds insights for improving graph machine learning with causal analysis, which has not been extensively studied yet, when the other direction (machine learning for causal inference) has been studied for a long time.

2 Problem Definition

Notations Let $G = (\mathcal{V}, \mathcal{E})$ be an undirected graph of N nodes, where $\mathcal{V} = \{v_1, v_2, \ldots, v_N\}$ is the set of nodes and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ is the set of observed links. We denote the adjacency matrix as

$\mathbf{A} \in \{0,1\}^{N \times N}$, where $A_{i,j} = 1$ indicates nodes v_i and v_j are connected and vice versa. We denote the node feature matrix as $\mathbf{X} \in \mathbb{R}^{N \times F}$, where F is the number of node features and $\mathbf{x}_i$ (bolded) indicates the feature vector of node v_i (the i-th row of $\mathbf{X}$).

In this work, we follow the commonly accepted problem definition of link prediction on graph data (Zhang & Chen, 2018; Zhang et al., 2020a; Cai et al., 2021): Given an observed graph G (with validation and testing links masked off), predict the link existence between every pair of nodes. More specifically, for the GNN-based link prediction methods, they learn low-dimensional node representations $\mathbf{Z} \in \mathbb{R}^{N \times H}$, where H is the dimensional size of latent space such that $H \ll F$, and then use $\mathbf{Z}$ for the prediction of link existence.

3 Proposed Method

3.1 Improving Graph Learning with Causal Model

Leveraging Causal Model(s) Counterfactual causal inference aims to find out the causal relationship between treatment and outcomes by asking the counterfactual questions such as "would the outcome be different if the treatment was different?" (Morgan & Winship, 2015). Figure 2 is a typical example, in which we denote the context (confounder) as $\mathbf{Z}$, treatment as T, and the outcome as Y. Given the context, treatments, and their corresponding outcomes, counterfactual inference methods aim to find the effect of treatment on the outcome, which is usually measured by *individual treatment effect* (ITE) and its expectation *averaged treatment effect* (ATE) (van der Laan & Petersen, 2007; Weiss et al., 2015). For a binary treatment variable $T = \{0,1\}$, denoting $g(\mathbf{z}, T)$ as the outcome of $\mathbf{z}$ given the treatment T, we have $\text{ITE}(\mathbf{z}) = g(\mathbf{z}, 1) - g(\mathbf{z}, 0)$, and $\text{ATE} = \mathbb{E}_{\mathbf{z} \sim \mathbf{Z}} \text{ITE}(\mathbf{z})$.

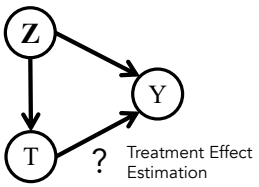


Figure 2: Causal modeling (not the target of our work but related to the idea we propose): Given $\mathbf{Z}$ and observed outcomes, find treatment effect of T on Y.

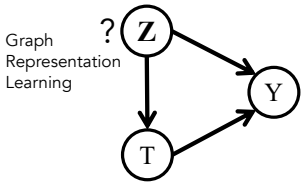


Figure 3: Graph learning with causal model (the proposed idea): leverage the estimated $\text{ATE}(Y|T)$ to improve the learning of $\mathbf{Z}$.

Ideally, we need all possible outcomes of the contexts under all kinds of treatments to study the causal relationships (Morgan & Winship, 2015). However, in reality, the fact that we can only observe one potential outcome under one particular treatment prevents the ITE from being known (Johansson et al., 2016). Traditional causal inference methods use statistical learning approaches such as Neyman–Rubin casual model (BCM) and propensity score matching (PSM) to predict the value of ATE (Rubin, 1974; 2005).

In this work, we look at *link prediction* with graph learning, which is essentially learning the best node representations $\mathbf{Z}$ for the prediction of link existence. Therefore, as shown in Figure 3, where the outcome Y is the link existence, the objective is different from classic causal inference. In graph learning, we can estimate the effect of treatment on the outcome ($\text{ATE}(Y|T)$), and we want to improve the learning of $\mathbf{Z}$ with the estimation. More specifically, in graph learning for link prediction, for each pair of nodes (v_i, v_j), its ITE can be estimated with

$$\text{ITE}_{(v_i, v_j)} = g((\mathbf{z}_i, \mathbf{z}_j), 1) - g((\mathbf{z}_i, \mathbf{z}_j), 0) \tag{1}$$

and we use this information to improve the learning of $\mathbf{Z}$, i.e., $P(\mathbf{Z}|Y)$.

We denote the observed adjacency matrix as the *factual* outcomes $\mathbf{A}$ and the unobserved adjacency matrix when the treatment is different as the *counterfactual* outcomes $\mathbf{A}^{CF}$. We denote $\mathbf{T} \in \{0,1\}^{N \times N}$ as the binary factual treatment matrix, where $T_{i,j}$ indicates the treatment of the node pair (v_i, v_j). We denote $\mathbf{T}^{CF}$ as the counterfactual treatment matrix where $T^{CF}_{i,j} = 1 - T_{i,j}$. We are interested in (1) estimating the counterfactual outcomes $\mathbf{A}^{CF}$ via observed data, (2) learning with the counterfactual adjacency matrix $\mathbf{A}^{CF}$ to enhance link prediction, and (3) learning the causal relationship between graph structural information (treatment) and link existence (outcome).

Treatment Variable Previous work on graph machine learning (Velickovic et al., 2019; Park et al., 2020) showed that the graph's global structural information could improve the quality of representa-

tion vectors of nodes learned by GNNs. This is because the message passing-based GNNs aggregate local information in the algorithm of representation vector generation and the global structural information is complementary with the aggregated information. Therefore, for a pair of nodes, one option of defining the treatment variable is its global structural role in the graph. Without the loss of generality, we use Louvain (Blondel et al., 2008), an unsupervised approach that has been widely used for community detection, as an example. Louvain discovers community structure of a graph and assigns each node to one community. Then we can define the binary treatment variable as whether these two nodes in the pair belong to the same community. Let $c : \mathcal{V} \rightarrow \mathbb{N}$ be any graph mining/clustering method that outputs the index of community/cluster/neighborhood that each node belongs to. The treatment matrix $\mathbf{T}$ is defined as $T_{i,j} = 1$ if $c(v_i) = c(v_j)$, and $T_{i,j} = 0$ otherwise. For the choice of c, we suggest methods that group nodes based on global graph structural information, including but not limited to Louvain (Blondel et al., 2008), K-core (Bader & Hogue, 2003), and spectral clustering (Ng et al., 2001).

3.2 Counterfactual Links

To implement the solution based on above idea, we propose counterfactual links. As aforementioned, for each node pair, the observed data contains only the factual treatment and outcome, meaning that the link existence for the given node pair with an opposite treatment is unknown. Therefore, we use the outcome from the nearest observed context as a substitute. This matching-based idea has been adopted by many causal inference literature (Johansson et al., 2016; Alaa & Van Der Schaar, 2019). That is, we want to find the nearest neighbor with the opposite treatment for each observed node pairs and use the nearest neighbor's outcome as a *counterfactual link*. Formally, $\forall (v_i, v_j) \in \mathcal{V} \times \mathcal{V}$, we want to find its counterfactual link (v_a, v_b) as below:

$$(v_a, v_b) = \underset{v_a, v_b \in \mathcal{V}}{\arg\min} \{h((v_i, v_j), (v_a, v_b)) \mid T_{a,b} = 1 - T_{i,j}\}, \tag{2}$$

where $h(\cdot, \cdot)$ is a metric of measuring the distance between a pair of node pairs (a pair of contexts). Nevertheless, finding the nearest neighbors by computing the distance between all pairs of node pairs is extremely inefficient and infeasible in application, which takes $O(N^4)$ comparisons (as there are totally $O(N^2)$ node pairs). Hence we implement Eq. (2) using node-level embeddings. Specifically, considering that we want to find the nearest node pair based on not only the raw node features but also structural features, we take the state-of-the-art unsupervised graph representation learning method MVGRL (Hassani & Khasahmadi, 2020) to learn the node embeddings $\tilde{\mathbf{X}} \in \mathbb{R}^{N \times \tilde{F}}$ from the observed graph (with validation and testing links masked off). We use $\tilde{\mathbf{X}}$ to find the nearest neighbors of node pairs. Therefore, $\forall (v_i, v_j) \in \mathcal{V} \times \mathcal{V}$, we define its counterfactual link (v_a, v_b) as

$$(v_a, v_b) = \underset{v_a, v_b \in \mathcal{V}}{\arg\min} \{d(\tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_a) + d(\tilde{\mathbf{x}}_j, \tilde{\mathbf{x}}_b) \mid T_{a,b} = 1 - T_{i,j}, d(\tilde{\mathbf{x}}_i, \tilde{\mathbf{x}}_a) + d(\tilde{\mathbf{x}}_j, \tilde{\mathbf{x}}_b) < 2\gamma\}, \tag{3}$$

where $d(\cdot, \cdot)$ is specified as the Euclidean distance on the embedding space of $\tilde{\mathbf{X}}$, and γ is a hyperparameter that defines the maximum distance that two nodes are considered as similar. When no node pair satisfies the above equation (i.e., there does not exist any node pair with opposite treatment that is close enough to the target node pair), we do not assign any nearest neighbor for the given node pair to ensure all the neighbors are similar enough (as substitutes) in the feature space. Thus, the counterfactual treatment matrix $\mathbf{T}^{CF}$ and the counterfactual adjacency matrix $\mathbf{A}^{CF}$ are defined as

$$T^{CF}_{i,j}, A^{CF}_{i,j} = \begin{cases} 1 - T_{i,j}, A_{a,b} & \text{, if } \exists\, (v_a, v_b) \in \mathcal{V} \times \mathcal{V} \text{ satisfies Eq. (3);} \\ T_{i,j}, A_{i,j} & \text{, otherwise.} \end{cases} \tag{4}$$

It is worth noting that the node embeddings $\tilde{\mathbf{X}}$ and the nearest neighbors are computed only once and do not change during the learning process. $\tilde{\mathbf{X}}$ is only used for finding the nearest neighbors.

Learning from Counterfactual Distributions Let P^F be the factual distribution of the observed contexts and treatments, and P^{CF} be the counterfactual distribution that is composed of the observed contexts and opposite treatments. We define the empirical factual distribution $\hat{P}^F \sim P^F$ as $\hat{P}^F = \{(v_i, v_j, T_{i,j})\}_{i,j=1}^N$, and define the empirical counterfactual distribution $\hat{P}^{CF} \sim P^{CF}$ as $\hat{P}^{CF} = \{(v_i, v_j, T^{CF}_{i,j})\}_{i,j=1}^N$. Unlike traditional link prediction methods that take only $\hat{P}^F$ as input and use the observed outcomes $\mathbf{A}$ as the training target, the idea of counterfactual graph learning is to take advantage of the counterfactual distribution by having $\hat{P}^{CF}$ as a complementary input and use the counterfactual outcomes $\mathbf{A}^{CF}$ as the training target for the counterfactual data samples.

3.3 THE COUNTERFACTUAL GRAPH LEARNING MODEL

In this subsection, we present the design of our model as well as the training method. The input of the model in CFLP includes (1) the observed graph data $\mathbf{A}$ and raw feature matrix $\mathbf{X}$, (2) the factual treatments $\mathbf{T}^F$ and counterfactual treatments $\mathbf{T}^{CF}$, and (3) the counterfactual graph data $\mathbf{A}^{CF}$. The output contains link prediction logits in $\widehat{\mathbf{A}}$ and $\widehat{\mathbf{A}}^{CF}$ for the factual and counterfactual adjacency matrices $\mathbf{A}$ and $\mathbf{A}^{CF}$, respectively.

Graph Learning Model The model consist of two trainable components: a graph encoder f and a link decoder g. The graph encoder generates representation vectors of nodes from graph data G. And the link decoder projects the representation vectors of node pairs into the link prediction logits. The choice of the graph encoder f can be any end-to-end GNN model. Without the loss of generality, here we use the commonly used graph convolutional network (GCN) (Kipf & Welling, 2016a). Each layer of GCN is defined as

$$\mathbf{H}^{(l)} = f^{(l)}(\mathbf{A}, \mathbf{H}^{(l-1)}; \mathbf{W}^{(l)}) = \sigma(\tilde{\mathbf{D}}^{-\frac{1}{2}}\tilde{\mathbf{A}}\tilde{\mathbf{D}}^{-\frac{1}{2}}\mathbf{H}^{(l-1)}\mathbf{W}^{(l)}), \tag{5}$$

where l is the layer index, $\tilde{\mathbf{A}} = \mathbf{A} + \mathbf{I}$ is the adjacency matrix with added self-loops, $\tilde{\mathbf{D}}$ is the diagonal degree matrix $\tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$, $\mathbf{H}^{(0)} = \mathbf{X}$, $\mathbf{W}^{(l)}$ is the learnable weight matrix at the l-th layer, and $\sigma(\cdot)$ denotes a nonlinear activation such as ReLU. We denote $\mathbf{Z} = f(\mathbf{A}, \mathbf{X}) \in \mathbb{R}^{N\times H}$ as the output from the encoder's last layer, i.e., the H-dimensional representation vectors of nodes. Following previous work (Zhang et al., 2020a), we compute the representation of a node pair as the Hadamard product of the vectors of the two nodes. That is, the representation for the node pair (v_i, v_j) is $\mathbf{z}_i \odot \mathbf{z}_j \in \mathbb{R}^H$, where $\odot$ stands for the Hadamard product.

For the link decoder that predicts whether a link exists between a pair of nodes, we opt for simplicity and adopt a simple decoder based on multi-layer perceptron (MLP), given the representations of node pairs and their treatments. That is, the decoder g is defined as

$$\widehat{\mathbf{A}} = g(\mathbf{Z}, \mathbf{T}), \text{ where } \widehat{A}_{i,j} = \text{MLP}([\mathbf{z}_i \odot \mathbf{z}_j, T_{i,j}]), \tag{6}$$

$$\widehat{\mathbf{A}}^{CF} = g(\mathbf{Z}, \mathbf{T}^{CF}), \text{ where } \widehat{A}^{CF}_{i,j} = \text{MLP}([\mathbf{z}_i \odot \mathbf{z}_j, T^{CF}_{i,j}]), \tag{7}$$

where $[\cdot,\cdot]$ stands for the concatenation of vectors, and $\widehat{\mathbf{A}}$ and $\widehat{\mathbf{A}}^{CF}$ can be used for estimating the observed ITE as aforementioned in Eq. (1).

During the training process, data samples from the empirical factual distribution $\hat{P}^F$ and the empirical counterfactual distribution $\hat{P}^{CF}$ are fed into decoder g and optimized towards $\mathbf{A}$ and $\mathbf{A}^{CF}$, respectively. That is, for the two distributions, the loss functions are as follows:

$$\mathcal{L}_F = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N} A_{i,j} \cdot \log \widehat{A}_{i,j} + (1 - A_{i,j}) \cdot \log(1 - \widehat{A}_{i,j}), \tag{8}$$

$$\mathcal{L}_{CF} = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N} A^{CF}_{i,j} \cdot \log \widehat{A}^{CF}_{i,j} + (1 - A^{CF}_{i,j}) \cdot \log(1 - \widehat{A}^{CF}_{i,j}). \tag{9}$$

Balancing Counterfactual Learning In the training process, the above loss minimizations train the model on both the empirical factual distribution $\hat{P}^F \sim P^F$ and empirical counterfactual distribution $\hat{P}^{CF} \sim P^{CF}$ that are not necessarily equal – the training examples (node pairs) do not have to be aligned. However, at the stage of inference, the test data contains only observed (factual) samples. Such a gap between the training and testing data distributions exposes the model in the risk of covariant shift, which is a common issue in counterfactual learning (Johansson et al., 2016; Assaad et al., 2021).

To force the distributions of representations of factual distributions and counterfactual distributions to be similar, we use the discrepancy distance (Mansour et al., 2009; Johansson et al., 2016) as another objective to regularize the representation learning. That is, we use the following loss term to minimize the distance between the learned representations from $\hat{P}^F$ and $\hat{P}^{CF}$:

$$\mathcal{L}_{disc} = \text{disc}(\hat{P}^F_f, \hat{P}^{CF}_f), \text{ where } \text{disc}(P, Q) = ||P - Q||_F, \tag{10}$$

where $||\cdot||_F$ denotes the Frobenius Norm, and $\hat{P}_f^F$ and $\hat{P}_f^{CF}$ denote the node pair representations learned by graph encoder f from factual distribution and counterfactual distribution, respectively. That is, the learned representations for $(v_i, v_j, T_{i,j})$ and $(v_i, v_j, T_{i,j}^{CF})$ are $[\mathbf{z}_i \odot \mathbf{z}_j, T_{i,j}]$ (Eq. (6)) and $[\mathbf{z}_i \odot \mathbf{z}_j, T_{i,j}^{CF}]$ (Eq. (7)), respectively.

Training During the training of CFLP, we want the model to be optimized towards three targets: (1) accurate link prediction on the observed outcomes (Eq. (8)), (2) accurate estimation on the counterfactual outcomes (Eq. (9)), and (3) regularization on the representation spaces learned from $\hat{P}^F$ and $\hat{P}^{CF}$ (Eq. (10)). Therefore, the overall training loss of our proposed CFLP is

$$\mathcal{L} = \mathcal{L}_F + \alpha \cdot \mathcal{L}_{CF} + \beta \cdot \mathcal{L}_{disc}, \tag{11}$$

where α and β are hyperparameters to control the weights of counterfactual link prediction (outcome estimation) loss and discrepancy loss.

Summary Algorithm 1 summarizes the whole process of CFLP. The **first step** is to compute the factual and counterfactual treatments $\mathbf{T}$, $\mathbf{T}^{CF}$ as well as the counterfactual outcomes $\mathbf{A}^{CF}$. Then, the **second step** trains the graph learning model on both the observed factual data and created counterfactual data with the integrated loss function (Eq. (11)). Note that the discrepancy loss (Eq. (10)) is computed on the representations of node pairs learned by the graph encoder f, so the decoder g is trained with data from both $\hat{P}^F$ and $\hat{P}^{CF}$ without balancing the constraints. Therefore, after the model is sufficiently trained, we freeze the graph encoder f and fine-tune g with only the factual data. Finally, after the decoder is sufficiently fine-tuned, we output the link prediction logits for both the factual and counterfactual adjacency matrices.

Algorithm 1: CFLP: Counterfactual graph learning for link prediction

Input : f, g, $\mathbf{A}$, $\mathbf{X}$, n_epochs, n_epoch_ft
Compute $\mathbf{T}$ as presented in Section 3.1 ;
Compute $\mathbf{T}^{CF}$, $\mathbf{A}^{CF}$ by Eqs. (3) and (4) ;
`/* model training */`
Initialize Θ_f in f and Θ_g in g ;
for *epoch in range(n_epochs)* **do**
  $\mathbf{Z} = f(\mathbf{A}, \mathbf{X})$;
  Get $\widehat{\mathbf{A}}$ and $\widehat{\mathbf{A}}^{CF}$ via g with Eqs. (6) and (7) ;
  Update Θ_f and Θ_g with $\mathcal{L}$; `// Eq. (11)`
end
`/* decoder fine-tuning */`
Freeze Θ_f and re-initialize Θ_g ;
$\mathbf{Z} = f(\mathbf{A}, \mathbf{X})$;
for *epoch in range(n_epochs_ft)* **do**
  Get $\widehat{\mathbf{A}}$ via g with Eq. (6) ;
  Update Θ_g with $\mathcal{L}_F$; `// Eq. (8)`
end
`/* ~~model inferencing~~ inference */`
$\mathbf{Z} = f(\mathbf{A}, \mathbf{X})$;
Get $\widehat{\mathbf{A}}$ and $\widehat{\mathbf{A}}^{CF}$ via g with Eqs. (6) and (7) ;
Output: $\widehat{\mathbf{A}}$ for link prediction, $\widehat{\mathbf{A}}^{CF}$

Complexity The complexity of the first step (finding counterfactual links with nearest neighbors) is proportional to the number of node pairs. When γ is set as a small value to obtain indeed similar node pairs, this step (Eq. (3)) uses constant time. Moreover, the computation in Eq. (3) can be parallelized. Therefore, the time complexity is $O(N^2/C)$ where C is the number of processes. For the complexity of the second step (training counterfactual learning model), the GNN encoder has time complexity of $O(LH^2N + LH|\mathcal{E}|)$ (Wu et al., 2020), where L is the number of GNN layers and H is the size of node representations. Given that we sample the same number of non-existing links as that of observed links during training, the complexity of a *three-layer MLP* decoder is $O(((H+1) \cdot d_h + d_h \cdot 1)|\mathcal{E}|) = O(d_h(H+2)|\mathcal{E}|)$, where d_h is the number of neurons in the hidden layer. Therefore, the second step has linear time complexity w.r.t. the sum of node and edge counts.

Limitations First, as mentioned above, the computation of finding counterfactual links has a worst-case complexity of $O(N^2)$. Second, CFLP performs counterfactual prediction with only a single treatment; however, there are quite a few kinds of graph structural information that can be considered as treatments. Future work can leverage the rich structural information by bundled treatments (Zou et al., 2020) in counterfactual graph learning.

Table 1: Link prediction performances measured by Hits@20. Best performance and best baseline performance are marked with bold and underline, respectively.

	CORA	CITESEER	PUBMED	FACEBOOK	OGB-DDI
Node2Vec	49.96±2.51	47.78±1.72	39.19±1.02	24.24±3.02	23.26±2.09
MVGRL	19.53±2.64	14.07±0.79	14.19±0.85	14.43±0.33	10.02±1.01
VGAE	45.91±3.38	44.04±4.86	23.73±1.61	37.01±0.63	11.71±1.96
SEAL	51.35±2.26	40.90±3.68	28.45±3.81	40.89±5.70	30.56±3.86
LGLP	<u>62.98</u>±0.56	<u>57.43</u>±3.71	–	37.86±2.13	–
GCN	49.06±1.72	55.56±1.32	21.84±3.87	<u>53.89</u>±2.14	37.07±5.07
GSAGE	53.54±2.96	53.67±2.94	<u>39.13</u>±4.41	45.51±3.22	53.90±4.74
JKNet	48.21±3.86	55.60±2.17	25.64±4.11	52.25±1.48	<u>60.56</u>±8.69
Our proposed CFLP with different graph encoders					
CFLP w/ GCN	60.34±2.33	59.45±2.30	34.12±2.72	53.95±2.29	52.51±1.09
CFLP w/ GSAGE	57.33±1.73	53.05±2.07	43.07±2.36	47.28±3.00	75.49±4.33
CFLP w/ JKNet	**65.57**±1.05	**68.09**±1.49	**44.90**±2.00	**55.22**±1.29	**86.08**±1.98

4 EXPERIMENTS

4.1 EXPERIMENTAL SETUP

We conduct experiments on five benchmark datasets including citation networks (CORA, CITESEER, PUBMED (Yang et al., 2016)), social network (FACEBOOK (McAuley & Leskovec, 2012)), and drug-drug interaction network (OGB-DDI (Wishart et al., 2018)) from the Open Graph Benchmark (OGB) (Hu et al., 2020). For the first four datasets, we randomly select 10%/20% of the links and the same numbers of disconnected node pairs as validation/test samples. The links in the validation and test sets are masked off from the training graph. For OGB-DDI, we used the OGB official train/validation/test splits. Statistics and details for the datasets are given in Appendix. We use K-core (Bader & Hogue, 2003) clusters as the default treatment variable. We evaluate CFLP on three commonly used GNN encoders: GCN (Kipf & Welling, 2016a), GSAGE (Hamilton et al., 2017), and JKNet (Xu et al., 2018). We compare the link prediction performance of CFLP against Node2Vec (Grover & Leskovec, 2016), MVGRL (Hassani & Khasahmadi, 2020), VGAE (Kipf & Welling, 2016b), SEAL (Zhang & Chen, 2018), LGLP (Cai et al., 2021), and GNNs with MLP decoder. We report averaged test performance and their standard deviation over 20 runs with different random parameter initializations. Other than the most commonly used of Area Under ROC Curve (AUC), we report Hits@20 (one of the primary metrics on OGB leaderboard) as a more challenging metric, as it expects models to rank positive edges higher than nearly all negative edges.

Besides performance comparison on link prediction, we will answer two questions to suggest a way of choosing a treatment variable for creating counterfactual links: (Q1) Does CFLP sufficiently learn the observed *averaged treatment effect* (ATE) derived from the counterfactual links? (Q2) What is the relationship between the estimated ATE learned in the method and the prediction performance? If the answer to Q1 is yes, then the answer to Q2 will indicate how to choose treatment based on observed ATE. To answer the Q1, we calculate the observed ATE ($\widehat{\text{ATE}}_{obs}$) by comparing the observed links in $\mathbf{A}$ and created counterfactual links $\mathbf{A}^{CF}$ that have opposite treatments. And we calculate the estimated ATE ($\widehat{\text{ATE}}_{est}$) by comparing the predicted links in $\widehat{\mathbf{A}}$ and predicted counterfactual links $\widehat{\mathbf{A}}^{CF}$. Formally, $\widehat{\text{ATE}}_{obs}$ and $\widehat{\text{ATE}}_{est}$ are defined as

$$\widehat{\text{ATE}}_{obs} = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\{\mathbf{T}\odot(\mathbf{A}-\mathbf{A}^{CF}) + (\mathbf{1}_{N\times N}-\mathbf{T})\odot(\mathbf{A}^{CF}-\mathbf{A})\}_{i,j}. \tag{12}$$

$$\widehat{\text{ATE}}_{est} = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\{\mathbf{T}\odot(\widehat{\mathbf{A}}-\widehat{\mathbf{A}}^{CF}) + (\mathbf{1}_{N\times N}-\mathbf{T})\odot(\widehat{\mathbf{A}}^{CF}-\widehat{\mathbf{A}})\}_{i,j}. \tag{13}$$

The treatment variables we will investigate are usually graph clustering or community detection methods, such as K-core (Bader & Hogue, 2003), stochastic block model (SBM) (Karrer & Newman, 2011), spectral clustering (SpecC) (Ng et al., 2001), propagation clustering (PropC) (Raghavan et al., 2007), Louvain (Blondel et al., 2008), common neighbors (CommN), Katz index, and hierarchical clustering (Ward) (Ward Jr, 1963). We use JKNet (Xu et al., 2018) as default graph encoder.

Table 2: Link prediction performances measured by AUC. Best performance and best baseline performance are marked with bold and underline, respectively.

	CORA	CITESEER	PUBMED	FACEBOOK	OGB-DDI
Node2Vec	84.49±0.49	80.00±0.68	80.32±0.29	86.49±4.32	90.83±0.02
MVGRL	75.07±3.63	61.20±0.55	80.78±1.28	79.83±0.30	81.45±0.99
VGAE	88.68±0.40	85.35±0.60	95.80±0.13	98.66±0.04	93.08±0.15
SEAL	92.55±0.50	85.82±0.44	96.36±0.28	**99.60**±0.02	97.85±0.17
LGLP	91.30±0.05	89.41±0.13	–	98.51±0.01	–
GCN	90.25±0.53	71.47±1.40	96.33±0.80	99.43±0.02	99.82±0.05
GSAGE	90.24±0.34	87.38±1.39	96.78±0.11	99.29±0.04	99.93±0.02
JKNet	89.05±0.67	88.58±1.78	96.58±0.23	99.43±0.02	**99.94**±0.01
Our proposed CFLP with different graph encoders					
CFLP w/ GCN	92.55±0.50	89.65±0.20	96.99±0.08	99.38±0.01	99.44±0.05
CFLP w/ GSAGE	92.61±0.52	91.84±0.20	97.01±0.01	99.34±0.10	99.83±0.05
CFLP w/ JKNet	**93.05**±0.24	**92.12**±0.47	**97.53**±0.17	99.31±0.04	**99.94**±0.01

Table 3: Results of CFLP with different treatments on CORA. (sorted by Hits@20)

	Hits@20	$\widehat{\text{ATE}}_{obs}$	$\widehat{\text{ATE}}_{est}$
K-core	65.6±1.1	0.002	0.013±0.003
SBM	64.2±1.1	0.006	0.023±0.015
CommN	62.3±1.6	0.007	0.053±0.021
PropC	61.7±1.4	0.037	0.059±0.065
Ward	61.2±2.3	0.001	0.033±0.012
SpecC	59.3±2.8	0.002	0.033±0.011
Louvain	57.6±1.8	0.025	0.138±0.091
Katz	56.6±3.4	0.740	0.802±0.041

Table 4: Results of CFLP with different treatments on CITESEER. (sorted by Hits@20)

	Hits@20	$\widehat{\text{ATE}}_{obs}$	$\widehat{\text{ATE}}_{est}$
SBM	71.6 ±1.9	0.004	0.005 ±0.001
K-core	68.1±1.5	0.002	0.010±0.002
Ward	67.0±1.7	0.003	0.037±0.009
PropC	64.6±3.6	0.141	0.232±0.113
Louvain	63.3±2.5	0.126	0.151±0.078
SpecC	59.9±1.3	0.009	0.166±0.034
Katz	57.3±0.5	0.245	0.224±0.037
CommN	56.8±4.9	0.678	0.195±0.034

Implementation details and supplementary experimental results (e.g., sensitivity on γ, ablation study on $\mathcal{L}_{CF}$ and $\mathcal{L}_{disc}$) can be found in Appendix. Source code is available in supplementary material.

4.2 EXPERIMENTAL RESULTS

Link Prediction Tables 1 and 2 show the link prediction performance of Hits@20 and AUC by all methods. LGLP on PUBMED and OGB-DDI are missing due to the out of memory error when running the code package from the authors. We observe that our CFLP on different graph encoders achieve similar or better performances compared with baselines. The only exception is the AUC on FACEBOOK where most methods have close-to-perfect AUC. As AUC is a relatively easier metric comparing with Hits@20, most methods achieved good performance on AUC. We observe that CFLP with JKNet almost consistently achieves the best performance and outperforms baselines significantly on Hits@20. Specifically, comparing with the best baseline, CFLP improves relatively by 16.4% and 0.8% on Hits@20 and AUC, respectively. Comparing with the best performing baselines, which are also GNN-based, CFLP benefits from learning with both observed link existence ($\mathbf{A}$) and our defined counterfactual links ($\mathbf{A}^{CF}$).

ATE with Different Treatments Tables 3 and 4 show the link prediction performance, $\widehat{\text{ATE}}_{obs}$, and $\widehat{\text{ATE}}_{est}$ of CFLP (with JKNet) when using different treatments. The treatments in Tables 3 and 4 are sorted by the Hits@20 performance. Bigger ATE indicates stronger causal relationship between the treatment and outcome, and vice versa. We observe: (1) the rankings of $\widehat{\text{ATE}}_{est}$ and $\widehat{\text{ATE}}_{obs}$ are positively correlated with Kendell's ranking coefficient (Abdi, 2007) of 0.67 and 0.57 for CORA and CITESEER, respectively. Hence, CFLP was sufficiently trained to learn the causal relationship between graph structure information and link existence; (2) $\widehat{\text{ATE}}_{obs}$ and $\widehat{\text{ATE}}_{est}$ are both negatively correlated with the link prediction performance, showing that we can pick a proper treatment prior to training a model with CFLP. Using the treatment that has the weakest causal relationship with link existence is likely to train the model to capture more essential factors on the outcome, in a way similar to denoising the unrelated information from the representations.

5 Related Work

Link Prediction With its wide applications, link prediction has draw attention from many research communities including statistical machine learning and data mining. Stochastic generative methods based on stochastic block models (SBM) are developed to generate links (Mehta et al., 2019). In data mining, matrix factorization (Menon & Elkan, 2011), heuristic methods (Philip et al., 2010; Martínez et al., 2016), and graph embedding methods (Cui et al., 2018) have been applied to predict links in the graph. Heuristic methods compute the similarity score of nodes based on their neighborhoods. These methods can be generally categorized into first-order, second-order, and high-order heuristics based on the maximum distance of the neighbors. Graph embedding methods learn latent node features via embedding lookup and use them for link prediction (Perozzi et al., 2014; Tang et al., 2015; Grover & Leskovec, 2016; Wang et al., 2016).

In the past few years, GNNs have showed promising results on various graph-based tasks with their ability of learning from features and custom aggregations on structures, (Kipf & Welling, 2016a; Hamilton et al., 2017; Xu et al., 2018; Wu et al., 2020). With node pair representations and an attached MLP or inner-product decoder, GNNs can be used for link prediction (Zhang et al., 2020a; Davidson et al., 2018; Yang et al., 2018). For example, VGAE used GCN to learn node representations and reconstruct the graph structure (Kipf & Welling, 2016b). SEAL extracted a local subgraph around each target node pair and then learned graph representation from local subgraph for link prediction (Zhang & Chen, 2018). Following the scheme of SEAL, Cai & Ji (2020) proposed to improve local subgraph representation learning by multi-scale graph representation learning. And LGLP inverted the local subgraphs to line graphs before learning representations (Cai et al., 2021). However, very limited work has studied to use causal inference for improving link prediction.

Counterfactual Prediction As a mean of learning the causality between treatment and outcome, counterfactual prediction has been used for a variety of applications such as recommender systems (Wang et al., 2020; Xu et al., 2020), health care (Alaa & van der Schaar, 2017; Pawlowski et al., 2020), vision-language tasks (Zhang et al., 2020b; Parvaneh et al., 2020), and decision making (Coston et al., 2020; Pitis et al., 2020; Kusner et al., 2017). To infer the causal relationships, previous work usually estimated the ITE via function fitting models (Gelman & Hill, 2006; Chipman et al., 2010; Wager & Athey, 2018; Assaad et al., 2021). Peysakhovich et al. (2019) and Zou et al. (2020) studied counterfactual prediction with multiple agents and bundled treatments, respectively. Sherman & Shpitser (2020) modeled social networks with causal DAGs.

Causal Inference Causal inference methods usually re-weighted samples based on propensity score (Rosenbaum & Rubin, 1983; Austin, 2011; Kuang et al., 2017a;b) to remove confounding bias from binary treatments. Recently, several works studied about learning treatment invariant representation to predict the counterfactual outcomes (Shalit et al., 2017; Li & Fu, 2017; Yao et al., 2018; Yoon et al., 2018; Hassanpour & Greiner, 2019b;a; Bica et al., 2020). When part of unobserved outcomes may mislead the counterfactual prediction, Louizos et al. (2017) attempted to infer the outcomes from proxies, and Hartford et al. (2017) introduced instrumental variable. SITE preserved local similarity to balance the distributions of control and treated groups (Yao et al., 2018). Bevilacqua et al. (2021) tackled graph classification under a counterfactually-driven data shift.

6 Conclusion and Future Work

In this work, we presented a counterfactual graph learning method for link prediction (CFLP). We introduced the idea of counterfactual prediction to improve link prediction on graphs. CFLP accurately predicted the missing links by exploring the causal relationship between global graph structure and link existence. Extensive experiments demonstrated that CFLP achieved the state-of-the-art performance on benchmark datasets. This work sheds insights that a good use of causal models (even basic ones) can greatly improve the performance of (graph) machine learning tasks, which in our case is link prediction. We note that the use of more sophistically designed causal models may lead to larger improvements for other machine learning tasks, which could be a valuable future research direction for the community. Other than our use of global graph structure as treatment, other treatments choices (with both empirical and theoretical analyses) are also worth exploring. Moreover, as CFLP first generates counterfactual links and then learns from both observed and counterfactual link existence, investigating the relationship between counterfactual graph learning and graph data augmentation is also a possible future research direction.

REFERENCES

Hervé Abdi. The kendall rank correlation coefficient. *Encyclopedia of Measurement and Statistics. Sage, Thousand Oaks, CA*, pp. 508–510, 2007.

Ahmed Alaa and Mihaela Van Der Schaar. Validating causal inference models via influence functions. In *International Conference on Machine Learning*, pp. 191–201. PMLR, 2019.

Ahmed M Alaa and Mihaela van der Schaar. Bayesian inference of individualized treatment effects using multi-task gaussian processes. *Advances in Neural Information Processing Systems*, 2017.

Serge Assaad, Shuxi Zeng, Chenyang Tao, Shounak Datta, Nikhil Mehta, Ricardo Henao, Fan Li, and Lawrence Carin Duke. Counterfactual representation learning with balancing weights. In *International Conference on Artificial Intelligence and Statistics*, pp. 1972–1980. PMLR, 2021.

Peter C Austin. An introduction to propensity score methods for reducing the effects of confounding in observational studies. *Multivariate behavioral research*, 46(3):399–424, 2011.

Gary D Bader and Christopher WV Hogue. An automated method for finding molecular complexes in large protein interaction networks. *BMC bioinformatics*, 4(1):1–27, 2003.

James Bennett, Stan Lanning, et al. The netflix prize. In *Proceedings of KDD cup and workshop*, volume 2007, pp. 35. Citeseer, 2007.

Beatrice Bevilacqua, Yangze Zhou, and Bruno Ribeiro. Size-invariant graph representations for graph classification extrapolations. *arXiv preprint arXiv:2103.05045*, 2021.

Ioana Bica, Ahmed M Alaa, James Jordon, and Mihaela van der Schaar. Estimating counterfactual treatment outcomes over time through adversarially balanced representations. *arXiv preprint arXiv:2002.04083*, 2020.

Vincent D Blondel, Jean-Loup Guillaume, Renaud Lambiotte, and Etienne Lefebvre. Fast unfolding of communities in large networks. *Journal of statistical mechanics: theory and experiment*, 2008 (10):P10008, 2008.

Lei Cai and Shuiwang Ji. A multi-scale approach for graph link prediction. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 34, pp. 3308–3315, 2020.

Lei Cai, Jundong Li, Jie Wang, and Shuiwang Ji. Line graph neural networks for link prediction. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2021.

Hugh A Chipman, Edward I George, Robert E McCulloch, et al. Bart: Bayesian additive regression trees. *The Annals of Applied Statistics*, 4(1):266–298, 2010.

Amanda Coston, Edward H Kennedy, and Alexandra Chouldechova. Counterfactual predictions under runtime confounding. *Advances in Neural Information Processing Systems*, 2020.

Peng Cui, Xiao Wang, Jian Pei, and Wenwu Zhu. A survey on network embedding. *IEEE Transactions on Knowledge and Data Engineering*, 31(5):833–852, 2018.

Tim R Davidson, Luca Falorsi, Nicola De Cao, Thomas Kipf, and Jakub M Tomczak. Hyperspherical variational auto-encoders. *arXiv preprint arXiv:1804.00891*, 2018.

Matthias Fey and Jan Eric Lenssen. Fast graph representation learning with pytorch geometric. *arXiv preprint arXiv:1903.02428*, 2019.

Thorben Funke and Till Becker. Stochastic block models: A comparison of variants and inference methods. *PloS one*, 14(4), 2019.

Andrew Gelman and Jennifer Hill. *Data analysis using regression and multilevel/hierarchical models*. Cambridge university press, 2006.

Aditya Grover and Jure Leskovec. node2vec: Scalable feature learning for networks. In *Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 855–864, 2016.

William L Hamilton, Rex Ying, and Jure Leskovec. Inductive representation learning on large graphs. *arXiv preprint arXiv:1706.02216*, 2017.

Jason Hartford, Greg Lewis, Kevin Leyton-Brown, and Matt Taddy. Deep iv: A flexible approach for counterfactual prediction. In *International Conference on Machine Learning*, pp. 1414–1423. PMLR, 2017.

Kaveh Hassani and Amir Hosein Khasahmadi. Contrastive multi-view representation learning on graphs. In *International Conference on Machine Learning*, pp. 4116–4126. PMLR, 2020.

Negar Hassanpour and Russell Greiner. Counterfactual regression with importance sampling weights. In *IJCAI*, pp. 5880–5887, 2019a.

Negar Hassanpour and Russell Greiner. Learning disentangled representations for counterfactual regression. In *International Conference on Learning Representations*, 2019b.

Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and Jure Leskovec. Open graph benchmark: Datasets for machine learning on graphs. *arXiv preprint arXiv:2005.00687*, 2020.

Fredrik Johansson, Uri Shalit, and David Sontag. Learning representations for counterfactual inference. In *International conference on machine learning*, pp. 3020–3029. PMLR, 2016.

Brian Karrer and Mark EJ Newman. Stochastic blockmodels and community structure in networks. *Physical review E*, 83(1):016107, 2011.

Seyed Mehran Kazemi and David Poole. Simple embedding for link prediction in knowledge graphs. In *Advances in Neural Information Processing Systems*, volume 31, 2018.

Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. *arXiv preprint arXiv:1609.02907*, 2016a.

Thomas N Kipf and Max Welling. Variational graph auto-encoders. *arXiv preprint arXiv:1611.07308*, 2016b.

Kun Kuang, Peng Cui, Bo Li, Meng Jiang, and Shiqiang Yang. Estimating treatment effect in the wild via differentiated confounder balancing. In *Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pp. 265–274, 2017a.

Kun Kuang, Peng Cui, Bo Li, Meng Jiang, Shiqiang Yang, and Fei Wang. Treatment effect estimation with data-driven variable decomposition. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 31, 2017b.

Matt J Kusner, Joshua R Loftus, Chris Russell, and Ricardo Silva. Counterfactual fairness. *Advances in Neural Information Processing Systems*, 2017.

Sheng Li and Yun Fu. Matching on balanced nonlinear representations for treatment effects estimation. In *Advances in Neural Information Processing Systems*, 2017.

Christos Louizos, Uri Shalit, Joris Mooij, David Sontag, Richard Zemel, and Max Welling. Causal effect inference with deep latent-variable models. *arXiv preprint arXiv:1705.08821*, 2017.

Yishay Mansour, Mehryar Mohri, and Afshin Rostamizadeh. Domain adaptation: Learning bounds and algorithms. *arXiv preprint arXiv:0902.3430*, 2009.

Víctor Martínez, Fernando Berzal, and Juan-Carlos Cubero. A survey of link prediction in complex networks. *ACM computing surveys (CSUR)*, 49(4):1–33, 2016.

Julian J McAuley and Jure Leskovec. Learning to discover social circles in ego networks. In *Advances in Neural Information Processing Systems*, volume 2012, pp. 548–56, 2012.

Nikhil Mehta, Lawrence Carin Duke, and Piyush Rai. Stochastic blockmodels meet graph neural networks. In *International Conference on Machine Learning*, pp. 4466–4474. PMLR, 2019.

Aditya Krishna Menon and Charles Elkan. Link prediction via matrix factorization. In *Joint european conference on machine learning and knowledge discovery in databases*, pp. 437–452. Springer, 2011.

Stephen L Morgan and Christopher Winship. *Counterfactuals and causal inference*. Cambridge University Press, 2015.

Andrew Ng, Michael Jordan, and Yair Weiss. On spectral clustering: Analysis and an algorithm. *Advances in neural information processing systems*, 14:849–856, 2001.

Chanyoung Park, Jiawei Han, and Hwanjo Yu. Deep multiplex graph infomax: Attentive multiplex network embedding using global information. *Knowledge-Based Systems*, 197:105861, 2020.

Amin Parvaneh, Ehsan Abbasnejad, Damien Teney, Qinfeng Shi, and Anton van den Hengel. Counterfactual vision-and-language navigation: Unravelling the unseen. *Advances in Neural Information Processing Systems*, 33, 2020.

Nick Pawlowski, Daniel C Castro, and Ben Glocker. Deep structural causal models for tractable counterfactual inference. *Advances in Neural Information Processing Systems*, 2020.

Bryan Perozzi, Rami Al-Rfou, and Steven Skiena. Deepwalk: Online learning of social representations. In *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 701–710, 2014.

Alexander Peysakhovich, Christian Kroer, and Adam Lerer. Robust multi-agent counterfactual prediction. *Advances in Neural Information Processing Systems*, 2019.

S Yu Philip, Jiawei Han, and Christos Faloutsos. *Link mining: Models, algorithms, and applications*. Springer, 2010.

Silviu Pitis, Elliot Creager, and Animesh Garg. Counterfactual data augmentation using locally factored dynamics. *Advances in Neural Information Processing Systems*, 2020.

Usha Nandini Raghavan, Réka Albert, and Soundar Kumara. Near linear time algorithm to detect community structures in large-scale networks. *Physical review E*, 76(3):036106, 2007.

Paul R Rosenbaum and Donald B Rubin. The central role of the propensity score in observational studies for causal effects. *Biometrika*, 70(1):41–55, 1983.

Donald B Rubin. Estimating causal effects of treatments in randomized and nonrandomized studies. *Journal of educational Psychology*, 66(5):688, 1974.

Donald B Rubin. Causal inference using potential outcomes: Design, modeling, decisions. *Journal of the American Statistical Association*, 100(469):322–331, 2005.

Uri Shalit, Fredrik D Johansson, and David Sontag. Estimating individual treatment effect: generalization bounds and algorithms. In *International Conference on Machine Learning*, pp. 3076–3085. PMLR, 2017.

Eli Sherman and Ilya Shpitser. Intervening on network ties. In *Uncertainty in Artificial Intelligence*, pp. 975–984. PMLR, 2020.

Leslie N Smith. Cyclical learning rates for training neural networks. In *2017 IEEE winter conference on applications of computer vision (WACV)*, pp. 464–472. IEEE, 2017.

Zachary Stanfield, Mustafa Coşkun, and Mehmet Koyutürk. Drug response prediction as a link prediction problem. *Scientific reports*, 7(1):1–13, 2017.

Jian Tang, Meng Qu, Mingzhe Wang, Ming Zhang, Jun Yan, and Qiaozhu Mei. Line: Large-scale information network embedding. In *Proceedings of the 24th international conference on world wide web*, pp. 1067–1077, 2015.

Mark J van der Laan and Maya L Petersen. Causal effect models for realistic individualized treatment and intention to treat rules. *The international journal of biostatistics*, 3(1), 2007.

Petar Veličković, Guillem Cucurull, Arantxa Casanova, Adriana Romero, Pietro Lio, and Yoshua Bengio. Graph attention networks. *arXiv preprint arXiv:1710.10903*, 2017.

Petar Velickovic, William Fedus, William L Hamilton, Pietro Liò, Yoshua Bengio, and R Devon Hjelm. Deep graph infomax. In *ICLR (Poster)*, 2019.

Stefan Wager and Susan Athey. Estimation and inference of heterogeneous treatment effects using random forests. *Journal of the American Statistical Association*, 113(523):1228–1242, 2018.

Daixin Wang, Peng Cui, and Wenwu Zhu. Structural deep network embedding. In *Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 1225–1234, 2016.

Zifeng Wang, Xi Chen, Rui Wen, Shao-Lun Huang, Ercan E Kuruoglu, and Yefeng Zheng. Information theoretic counterfactual learning from missing-not-at-random feedback. *Advances in Neural Information Processing Systems*, 2020.

Joe H Ward Jr. Hierarchical grouping to optimize an objective function. *Journal of the American statistical association*, 58(301):236–244, 1963.

Jeremy Weiss, Finn Kuusisto, Kendrick Boyd, Jie Liu, and David Page. Machine learning for treatment assignment: Improving individualized risk attribution. In *AMIA Annual Symposium Proceedings*, volume 2015, pp. 1306. American Medical Informatics Association, 2015.

David S Wishart, Yannick D Feunang, An C Guo, Elvis J Lo, Ana Marcu, Jason R Grant, Tanvir Sajed, Daniel Johnson, Carin Li, Zinat Sayeeda, et al. Drugbank 5.0: a major update to the drugbank database for 2018. *Nucleic acids research*, 46(D1):D1074–D1082, 2018.

Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and S Yu Philip. A comprehensive survey on graph neural networks. *IEEE transactions on neural networks and learning systems*, 2020.

Da Xu, Chuanwei Ruan, Evren Korpeoglu, Sushant Kumar, and Kannan Achan. Adversarial counterfactual learning and evaluation for recommender system. *Advances in Neural Information Processing Systems*, 2020.

Keyulu Xu, Chengtao Li, Yonglong Tian, Tomohiro Sonobe, Ken-ichi Kawarabayashi, and Stefanie Jegelka. Representation learning on graphs with jumping knowledge networks. In *International Conference on Machine Learning*, pp. 5453–5462. PMLR, 2018.

Hong Yang, Shirui Pan, Peng Zhang, Ling Chen, Defu Lian, and Chengqi Zhang. Binarized attributed network embedding. In *2018 IEEE International Conference on Data Mining (ICDM)*, pp. 1476–1481. IEEE, 2018.

Zhilin Yang, William Cohen, and Ruslan Salakhudinov. Revisiting semi-supervised learning with graph embeddings. In *International conference on machine learning*, pp. 40–48. PMLR, 2016.

Liuyi Yao, Sheng Li, Yaliang Li, Mengdi Huai, Jing Gao, and Aidong Zhang. Representation learning for treatment effect estimation from observational data. *Advances in Neural Information Processing Systems*, 31, 2018.

Jinsung Yoon, James Jordon, and Mihaela Van Der Schaar. Ganite: Estimation of individualized treatment effects using generative adversarial nets. In *International Conference on Learning Representations*, 2018.

Muhan Zhang and Yixin Chen. Link prediction based on graph neural networks. In *Advances in Neural Information Processing Systems*, 2018.

Muhan Zhang, Pan Li, Yinglong Xia, Kai Wang, and Long Jin. Revisiting graph neural networks for link prediction. *arXiv preprint arXiv:2010.16103*, 2020a.

Zhu Zhang, Zhou Zhao, Zhijie Lin, Xiuqiang He, et al. Counterfactual contrastive learning for weakly-supervised vision-language grounding. *Advances in Neural Information Processing Systems*, 33:18123–18134, 2020b.

Yanqiao Zhu, Yichen Xu, Feng Yu, Qiang Liu, Shu Wu, and Liang Wang. Deep graph contrastive representation learning. *arXiv preprint arXiv:2006.04131*, 2020.

Hao Zou, Peng Cui, Bo Li, Zheyan Shen, Jianxin Ma, Hongxia Yang, and Yue He. Counterfactual prediction for bundle treatment. *Advances in Neural Information Processing Systems*, 33, 2020.

Table 5: Statistics of datasets used in the experiments.

Dataset	CORA	CITESEER	PUBMED	FACEBOOK	OGB-DDI
# nodes	2,708	3,327	19,717	4,039	4,267
# links	5,278	4,552	44,324	88,234	1,334,889
# validation node pairs	1,054	910	8,864	17,646	235,371
# test node pairs	2,110	1,820	17,728	35,292	229,088

APPENDICES

A ADDITIONAL DATASET DETAILS

In this section, we provide some additional dataset details. All the datasets used in this work are publicly available. Statistics for the datasets are shown in Table 5.

Citation Networks CORA, CITESEER, and PUBMED are citation networks that were first used by Yang et al. (2016) and then commonly used as benchmarks in GNN-related literature (Kipf & Welling, 2016a; Veličković et al., 2017). In these citation networks, the nodes are published papers and features are bag-of-word vectors extracted from the corresponding paper. Links represent the citation relation between papers. We loaded the datasets with the `DGL`[1] package.

Social Network The FACEBOOK dataset[2] is a social network constructed from friends lists from Facebook (McAuley & Leskovec, 2012). The nodes are Facebook users and links indicate the friendship relation on Facebook. The node features were constructed from the user profiles and anonymized by McAuley & Leskovec (2012).

Drug-Drug Interaction Network The OGB-DDI dataset was constructed from a public Drug database (Wishart et al., 2018) and provided by the Open Graph Benchmark (OGB) (Hu et al., 2020). Each node in this graph represents an FDA-approved or experimental drug and edges represent the existence of unexpected effect when the two drugs are taken together. This dataset does not contain any node features, and it can be downloaded with the dataloader[3] provided by OGB.

B DETAILS ON IMPLEMENTATION AND HYPERPARAMETERS

All the experiments in this work were conducted on a Linux server with Intel Xeon Gold 6130 Processor (16 Cores @2.1Ghz), 96 GB of RAM, and 4 RTX 2080Ti cards (11 GB of RAM each). Our method are implemented with `Python 3.8.5` with `PyTorch`. Source code is available in the supplementary materials. A list of used packages can be found in `requirements.txt`.

Baseline Methods For baseline methods, we use official code packages from the authors for MVGRL[4] (Hassani & Khasahmadi, 2020), SEAL[5] (Zhang & Chen, 2018), and LGLP[6] (Cai et al., 2021). We use a public implementation for VGAE[7] (Kipf & Welling, 2016b) and OGB implementations[8] for Node2Vec and baseline GNNs. For fair comparison, we set the size of node/link representations to be 256 of all methods.

[1] https://github.com/dmlc/dgl
[2] https://snap.stanford.edu/data/ego-Facebook.html
[3] https://ogb.stanford.edu/docs/linkprop/#data-loader
[4] https://github.com/kavehhassani/mvgrl
[5] https://github.com/facebookresearch/SEAL_OGB
[6] https://github.com/LeiCaiwsu/LGLP
[7] https://github.com/DaehanKim/vgae_pytorch
[8] https://github.com/snap-stanford/ogb/tree/master/examples/linkproppred/ddi

Table 6: Link prediction performances measured by Hits@50. Best performance and best baseline performance are marked with bold and underline, respectively.

	CORA	CITESEER	PUBMED	FACEBOOK	OGB-DDI
Node2Vec	63.64±0.76	54.57±1.40	50.73±1.10	43.91±1.03	24.34±1.67
MVGRL	29.97±3.06	26.48±0.98	16.96±0.56	17.06±0.19	12.03±0.11
VGAE	60.36±2.71	54.68±3.15	41.98±0.31	51.36±0.93	23.00±1.66
SEAL	51.68±2.85	54.55±1.77	42.85±2.03	57.20±1.85	40.85±2.97
LGLP	<u>71.43</u>±0.75	<u>69.98</u>±0.16	–	56.22±0.49	–
GCN	64.93±1.62	63.38±1.73	39.20±6.47	<u>69.90</u>±0.65	73.70±3.99
GSAGE	63.18±3.39	61.71±2.43	<u>54.81</u>±2.67	62.53±4.24	86.83±3.85
JKNet	62.64±1.40	62.26±2.10	45.16±3.18	68.81±1.76	<u>91.48</u>±2.41
Our proposed CFLP with different graph encoders					
CFLP w/ GCN	72.61±0.92	69.85±1.11	55.00±1.95	70.47±0.77	62.47±1.53
CFLP w/ GSAGE	73.25±0.94	64.75±2.27	58.16±1.40	63.89±2.08	83.32±3.61
CFLP w/ JKNet	**75.49**±1.54	**77.01**±1.92	**62.80**±0.79	**71.41**±0.61	**93.07**±1.14

CFLP We use the Adam optimizer with a simple cyclical learning rate scheduler (Smith, 2017), in which the learning rate waves cyclically between the given learning rate (lr) and 1e-4 in every 70 epochs (50 warmup steps and 20 annealing steps). We implement the GNN encoders with `torch_geometric`[9] (Fey & Lenssen, 2019). Same with the baselines, we set the size of all hidden layers and node/link representations of CFLP as 256. The graph encoders all have three layers and JKNet has mean pooling for the final aggregation layer. The decoder is a 3-layer MLP with a hidden layer of size 64 and ELU as the nonlinearity. As the Euclidean distance used in Eq. (3) has a range of $[0, \infty)$, the value of γ depends on the distribution of all-pair node embedding distances, which varies for different datasets. Therefore, we set the value of γ as the γ_{pct}-percentile of all-pair node embedding distances. Commands for reproducing the experiments are included in `README.md`.

Hyperparameter Searching Space We manually tune the following hyperparameters over range: $lr \in \{0.005, 0.01, 0.05, 0.1, 0.2\}$, $\alpha \in \{0.001, 0.01, 0.1, 1, 2\}$, $\beta \in \{0.001, 0.01, 0.1, 1, 2\}$, $\gamma_{pct} \in \{10, 20, 30\}$.

Treatments For the graph clustering or community detection methods we used as treatments, we use the implementation from `scikit-network`[10] for Louvain (Blondel et al., 2008), SpecC (Ng et al., 2001), PropC (Raghavan et al., 2007), and Ward (Ward Jr, 1963). We used implementation of K-core (Bader & Hogue, 2003) from `networkx`.[11] We used SBM (Karrer & Newman, 2011) from a public implementation by Funke & Becker (2019).[12] For CommN and Katz, we set $T_{i,j} = 1$ if the number of common neighbors or Katz index between v_i and v_j are greater or equal to 2 or 2 times the average of all Katz index values, respectively. For SpecC, we set the number of clusters as 16. For SBM, we set the number of communities as 16. These settings are fixed for all datasets.

C ADDITIONAL EXPERIMENTAL RESULTS AND DISCUSSIONS

Link Prediction Tables 6 and 7 show the link prediction performance of Hits@50 and Average Precision (AP) by all methods. LGLP on PUBMED and OGB-DDI are missing due to the out of memory error when running the code package from the authors. Similar to the results in Tables 1 and 2, we observe that our CFLP on different graph encoders achieve similar or better performances compared with baselines, with the only exception of AP on FACEBOOK where most methods have close-to-perfect AP. From Tables 1, 2, 6 and 7, we observe that CFLP achieves improvement over all GNN architectures (averaged across datasets). Specifically, CFLP improves 25.6% (GCN), 12.0% (GSAGE), and 36.3% (JKNet) on Hits@20, 9.6% (GCN), 5.0% (GSAGE), and 17.8% (JKNet)

[9] `https://pytorch-geometric.readthedocs.io/en/latest/`
[10] `https://scikit-network.readthedocs.io/`
[11] `https://networkx.org/documentation/`
[12] `https://github.com/funket/pysbm`

Table 7: Link prediction performances measured by Average Precision (AP). Best performance and best baseline performance are marked with bold and underline, respectively.

	CORA	CITESEER	PUBMED	FACEBOOK	OGB-DDI
Node2Vec	88.53±0.42	84.42±0.48	87.15±0.12	99.07±0.02	98.39±0.04
MVGRL	76.47±3.07	67.40±0.52	82.00±0.97	82.37±0.35	81.12±1.77
VGAE	89.89±0.50	86.97±0.78	95.97±0.16	98.60±0.04	95.28±0.11
SEAL	89.08±0.57	88.55±0.32	96.33±0.28	**99.51**±0.03	98.39±0.21
LGLP	93.05±0.03	91.62±0.09	–	98.62±0.01	–
GCN	91.42±0.45	90.87±0.52	96.19±0.88	99.42±0.02	99.86±0.03
GSAGE	91.52±0.46	89.43±1.15	96.93±0.11	99.27±0.06	99.93±0.01
JKNet	90.50±0.22	90.42±1.34	96.56±0.31	99.41±0.02	99.95±0.01
Our proposed CFLP with different graph encoders					
CFLP w/ GCN	93.77±0.49	91.84±0.20	97.16±0.08	99.40±0.01	99.60±0.03
CFLP w/ GSAGE	93.55±0.49	90.80±0.87	97.10±0.08	99.29±0.06	99.88±0.04
CFLP w/ JKNet	**94.24**±0.28	**93.92**±0.41	**97.69**±0.13	99.35±0.02	**99.96**±0.01

Table 8: Link prediction performance of CFLP (w/ JKNet) on CORA and CITESEER when removing $\mathcal{L}_{CF}$ or $\mathcal{L}_{disc}$ or both versus normal setting.

	CORA		CITESEER	
	Hits@20	AUC	Hits@20	AUC
CFLP ($\alpha = 0$)	58.58±0.23	89.16±0.93	65.49±2.18	91.01±0.64
CFLP ($\beta = 0$)	62.27±0.84	92.96±0.34	66.92±1.84	91.98±0.17
CFLP ($\alpha = \beta = 0$)	58.52±0.83	88.79±0.28	64.69±3.25	90.61±0.64
CFLP	**65.57**±1.05	**93.05**±0.24	**68.09**±1.49	**92.12**±0.47

on Hits@50, 5.6% (GCN), 1.6% (GSAGE), and 1.9% (JKNet) on AUC, and 0.8% (GCN), 0.8% (GSAGE), and 1.8% (JKNet) on AP. We note that CFLP with JKNet almost consistently achieves the best performance and outperforms baselines significantly on Hits@50. Specifically, compared with the best baseline, CFLP improves relatively by 6.8% and 0.9% on Hits@50 and AP, respectively.

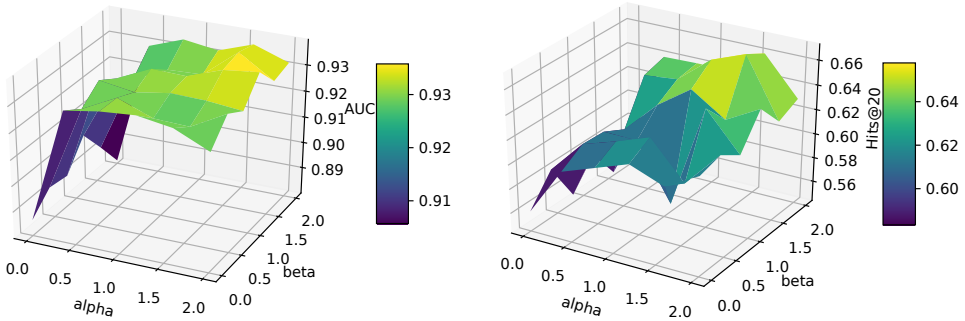
Ablation Study on Losses For the ablative studies of $\mathcal{L}_{CF}$ (Eq. (9)) and $\mathcal{L}_{disc}$ (Eq. (10)), we show their effect by removing them from the integrated loss function (Eq. (11)). Table 8 shows the results of CFLP on CORA and CITESEER under different settings ($\alpha = 0$, $\beta = 0$, $\alpha = \beta = 0$, and original setting). We observe that CFLP in the original setting achieves the best performance. The performance drops significantly when having $\alpha = 0$, i.e., not using any counterfactual data during training. We note that having $\beta = 0$, i.e., not using the discrepancy loss, also lowers the performance. Therefore, both $\mathcal{L}_{CF}$ and $\mathcal{L}_{disc}$ are essential for improving the link prediction performance.

Ablation Study on Node Embedding $\tilde{\mathbf{X}}$ As the node embedding $\tilde{\mathbf{X}}$ is used in the early step of CFLP for finding the counterfactual links, the quality of $\tilde{\mathbf{X}}$ may affect the later learning process. Therefore, we also evaluate CFLP with different state-of-the-art unsupervised graph representation learning methods: MVGRL (Hassani & Khasahmadi, 2020), DGI (Velickovic et al., 2019), and GRACE (Zhu et al., 2020). Table 9 shows the link prediction performance of CFLP (w/ JKNet) on CORA and CITESEER with different node embeddings. We observe that the choice of the method for learning $\tilde{\mathbf{X}}$ does have an impact on the later learning process as well as the link prediction performance. Nevertheless, Table 9 shows CFLP's advantage can be consistently observed with different choices of methods for learning $\tilde{\mathbf{X}}$, as CFLP with $\tilde{\mathbf{X}}$ learned from all three methods showed promising link prediction performance.

Sensitivity Analysis of α and β Figure 4 shows the AUC performance of CFLP on CORA with different combinations of α and β. We observe that the performance is the poorest when $\alpha = \beta = 0$ and gradually improves and gets stable as α and β increase, showing that CFLP is generally robust to the hyperparameters α and β, and the optimal values are easy to locate.

Table 9: Link prediction performance of CFLP (w/ JKNet) on CORA and CITESEER with node embeddings ($\tilde{\mathbf{X}}$) learned from different methods.

	CORA		CITESEER		OGB-DDI	
	Hits@20	AUC	Hits@20	AUC	Hits@20	AUC
(MVGRL)	65.57±1.05	93.05±0.24	68.09±1.49	92.12±0.47	86.08±1.98	99.94±0.01
(GRACE)	62.54±1.41	92.28±0.69	68.68±1.75	93.80±0.36	82.30±3.32	99.93±0.01
(DGI)	61.04±1.52	92.99±0.49	72.17±1.08	93.34±0.51	85.61±1.66	99.94±0.01



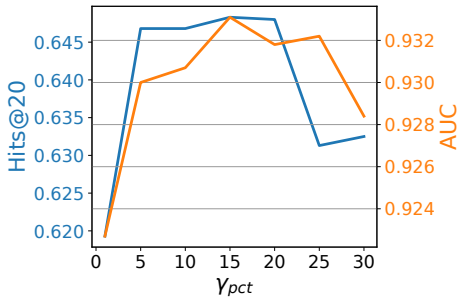
(a) AUC performance. (b) Hits@20 performance.

Figure 4: Performance of CFLP on CORA w.r.t different combinations of α and β.

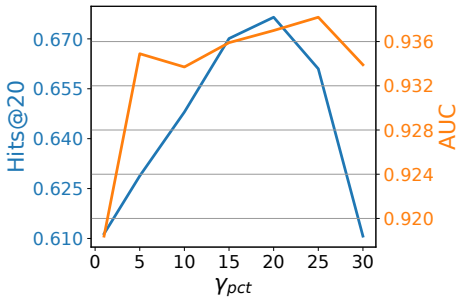
Sensitivity Analysis of γ Figure 5 shows the Hits@20 and AUC performance on link prediction of CFLP (with JKNet) on CORA and CITESEER with different treatments and γ_{pct}. We observe that the performance is generally good when $10 \leq \gamma_{pct} \leq 20$ and gradually get worse when the value of γ_{pct} is too small or too large, showing that CFLP is robust to γ and the optimal γ is easy to find.

Sensitivity to Noisy Data We note that robustness w.r.t. noisy data is not within our claim of technical contributions. Nevertheless, CFLP is not more vulnerable than other link prediction baselines. We conduct experiments with random attacks on the Cora dataset (randomly removing links and adding noisy links). Table 10 shows the AUC performances of our proposed CFLP (w/ JKNet) compared to the strongest baseline methods under different levels of random attacks (0%, 2%, 5%, and 10%). We can observe that as the attack strength goes up, the link prediction performance of all methods go down. We also note that our proposed CFLP still outperforms the baseline methods.

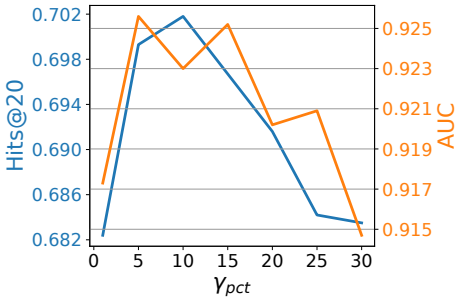
Generalization to Graphs with Weighted Edges As our proposed CFLP uses GNN as the graph encoder and GNNs are usually able to take weighted graph as input (e.g., the adjacency matrix $\mathbf{A}$ for GCN can be weighted), the model should be able to handle weighted graphs as given. Note the link prediction losses (Eqs. (8) and (9)) need to be slightly modified considering the task. When the task is to predict the link existence, the label adjacency matrix used in Eqs. (8) and (9) must be of binary values. When the task is to predict the link weights, the BCE loss functions (Eqs. (8) and (9)) need to be changed to regression loss functions such as MSE.



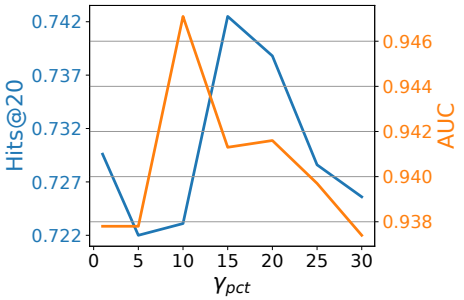
(a) Performances of CFLP on CORA when using K-core as treatment.



(b) Performances of CFLP on CORA when using SBM as treatment.



(c) Performances of CFLP on CITESEER when using K-core as treatment.



(d) Performances of CFLP on CITESEER when using SBM as treatment.

Figure 5: Hits@20 and AUC performances of CFLP (w/ JKNet) on CORA and CITESEER with different treatments w.r.t. different γ_{pct} value.

Table 10: Link prediction performances measured by AUC on CORA when the graph is randomly perturbed at different levels. Best performances are marked with bold.

	0%	2%	5%	10%
SEAL	92.55±0.50	87.81±1.37	87.90±0.79	87.64±0.89
LGLP	91.30±0.05	90.70±0.15	90.38±0.17	88.61±0.15
JKNet	89.05±0.67	88.85±0.75	88.14±0.59	87.64±0.89
CFLP w/ JKNet	**93.05**±0.24	**92.93**±0.17	**92.77**±0.18	**91.58**±0.23