Explaining Graph Neural Networks for Node Similarity on Graphs

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Abstract

Similarity search is a fundamental task for exploiting information in various applications dealing with graph data, such as citation networks or knowledge graphs. Prior work on the explainability of graph neural networks (GNNs) has focused on supervised tasks, such as node classification and link prediction. However, the challenge of explaining similarities between node embeddings has been left unaddressed. We take a step towards filling this gap by formulating the problem, identifying desirable properties of explanations of similarity, and proposing intervention-based metrics that qualitatively assess them. Using our framework, we evaluate the performance of representative methods for explaining GNNs, based on the concepts of mutual information (MI) and gradient-based (GB) explanations. We find that unlike MI explanations, GB explanations have three desirable properties. First, they are *actionable*: selecting particular inputs results in predictable changes in similarity scores of corresponding nodes. Second, they are *consistent*: the effect of selecting certain inputs hardly overlaps with the effect of discarding them. Third, they can be pruned significantly to obtain *sparse* explanations that retain the effect on similarity scores. These important findings highlight the utility of our metrics as a framework for evaluating the quality of explanations of node similarities in GNNs.

1 Introduction

Graphs provide a powerful and expressive data structure for modeling relations between objects across diverse domains, such as social networks, biological systems, and knowledge bases (Newman, 2018; Hamilton et al., 2017a; Nickel et al., 2016; Hogan et al., 2021). Additionally, their ability to represent entities and their interactions makes them a natural representation for machine learning methods that seek to learn structural patterns and use them in downstream tasks.

A fundamental problem that arises across domains is similarity search, where the goal is to identify objects that resemble a given query object according to structural or semantic notions of similarity. In particular, we are concerned with similarity search over graphs, where given a query node, the goal is to retrieve a ranked list of similar nodes. Several methods to solve this problem have been proposed in the literature, ranging from heuristic-based methods to data-driven machine learning methods. Heuristics for similarity search on graphs exploit various graph statistics or techniques based on hashing to solve the problem (Shimomura et al., 2021; Shi et al., 2021).

Machine learning methods, on the other hand, avert the need to design handcrafted heuristics or features. Instead, they seek to exploit domain-specific patterns in the graph to learn node representations, or *embeddings*, after which similarities are captured via metrics such as cosine similarity on these representations. Graph neural networks (GNNs), in particular, have become a standard in machine learning approaches that process graph-structured data (Kipf & Welling, 2017; Schlichtkrull et al., 2018; Gilmer et al., 2017).

While GNNs offer several advantages due to their capacity to adapt to specific properties of the graph at hand, these benefits may be compromised when interpretability becomes a necessity (Burkart & Huber, 2021; Arrieta et al., 2020). Given their demonstrated effectiveness on different tasks, there are compelling

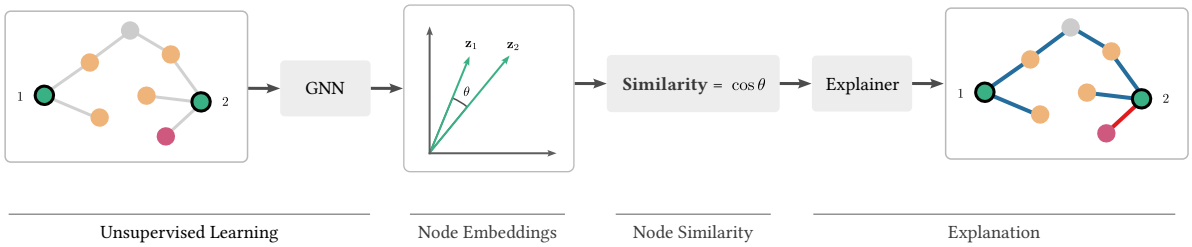


Figure 1: Illustration of the problem we investigate in our work. Given nodes 1 and 2 in a graph, unsupervised learning methods can be used to train a GNN to learn node embeddings, where a score of similarity can be estimated by cosine similarity. We investigate how to create explanations for such scores, that assign values of attributions to edges in the graph. In this example, we show with blue a positive influence in the similarity score, and with red a negative influence.

motivations to explore methods for explaining their predictions (Yuan et al., 2023), which would enable applications that require accountable decision-making to leverage their predictive power.

While extensive works on explaining GNNs exist, the majority of the methods focus on supervised learning problems, where the predicted target is well-defined based on some ground-truth data, as in the case of node classification (Ying et al., 2019; Luo et al., 2020; Lucic et al., 2022; Miao et al., 2022). To the best of our knowledge, the applicability of such methods to the problem of explaining node similarities remains an open question.

Fig. 1 illustrates this problem, where a learning algorithm is used to train a GNN for computing embeddings for nodes 1 and 2. The embeddings are used to compute the cosine similarity that we aim at explaining. The explanation consists of an attribution of values to edges, depending on their influence on the similarity score. In the example, blue edges result in increasing similarity scores and red edges result in decreasing the score. Depending on the explanation method used, the effect of attribution values on similarity scores can be different.

Our work takes a step towards understanding what it means to *explain node similarity* in graph neural networks. This setting differs fundamentally from the supervised tasks for which existing GNN explainers were designed (Yuan et al., 2023). While prior work focuses on discrete predictions, such as node classification or link prediction, explaining *continuous similarity scores* is a fundamentally different problem that has not been addressed by current evaluation protocols. We bridge this gap and provide the following contributions:

- We introduce and study the problem of explaining node similarity in GNNs, which to the best of our knowledge, has not been addressed in prior work.
- Building on principles from explainable AI, we derive three criteria for explanations of node similarity. We then propose model-agnostic metrics that quantify these criteria by measuring how explanations behave under controlled interventions on the graph.
- We demonstrate the utility of our framework by applying it to representative mutual-information and gradient-based methods, yielding several important insights that demonstrate the practical utility of our criteria and metrics.

2 Related work

Similarity learning. The problem of computing node similarities on graphs has been addressed in previous methods that rely on heuristics, rather than representations learned from the data. Some examples of such methods rely on statistics of connectivity (Brin, 1998; Haveliwala, 2002), co-occurrence statistics (Jeh & Widom, 2002), meta-paths in heterogeneous networks (Sun et al., 2011), and metrics for measuring structural similarities (Xu et al., 2007). Other methods employ ideas from hashing techniques to compute

vector representations useful for similarity search (Gionis et al., 1999; Zadeh & Goel, 2013; Shimomura et al., 2021). Such heuristics are beneficial when they are broad enough to be applicable to different graphs. Graph neural networks, on the other hand, are able to adapt to specific signals present in the data, such as domain-specific topological properties and rich multi-modal features like text and images (Markowitz et al., 2022; Gao et al., 2020). Their demonstrated effectiveness for different tasks thus warrants an investigation on how explanations can be provided for them, in the event of applications where rationales for predictions of GNNs are valuable, which is the open question we address in this work.

Unsupervised learning on graphs. In contrast to tasks like node classification or regression where labeled data is available, similarity learning is rarely accompanied with ground truth data. An alternative is concerned with learning representations that capture patterns already present in the graph (Liu et al., 2023a; Xie et al., 2023; Liu et al., 2023b). In the absence of labels that could be used for training, learning in this setting relies on optimization algorithms that produce representations useful for a pretext task. Examples of pretext tasks are maximizing the mutual information between different views of a graph (Velickovic et al., 2019; Sun et al., 2020; Peng et al., 2020), embedding shortest path distances (Bojchevski & Günnemann, 2018; Frogner et al., 2019), reconstructing parts of the input (Kipf & Welling, 2016; Wang et al., 2017a), or maintaining invariance with respect to small changes in the input (Thakoor et al., 2022; Xie et al., 2022b). The resulting representations can then be employed in tasks such as clustering and similarity search.

Most of the research in this area has focused on studying different ways of designing pretext tasks. However, the area of explainability in unsupervised learning on graphs is underexplored (Xie et al., 2023; Liu et al., 2023b). A recently proposed method is Task-Agnostic Graph Explanations (TAGE) (Xie et al., 2022a), which proposes explaining specific dimensions of embeddings obtained via unsupervised learning. The motivation for explaining embedding dimensions is transferring the explainer module of TAGE to supervised learning tasks. The performance of TAGE for generating explanations for problems where labeled data is not available, such as similarity computations, has been so far left unexplored. In our work, we focus on evaluating explanations of similarity in the unsupervised learning setting, which is the problem that has not been explored in TAGE or any prior work on unsupervised learning on graphs.

Explaining graph neural networks. Graph neural networks (GNNs) are neural networks tailored to the irregular structure of graphs, that are able to learn representations of a node in a graph taking into consideration arbitrary subgraphs around it (Zhou et al., 2020; Wu et al., 2021; Ye et al., 2022). A growing number of methods have been proposed in the literature that provide explanations to predictions computed by GNNs, in the form of edges and features responsible for a prediction (Yuan et al., 2023). Existing methods assume a trained GNN and provide *post hoc* mechanisms for explaining their predictions (Ying et al., 2019; Luo et al., 2020; Duval & Malliaros, 2021; Yuan et al., 2021; Muschalik et al., 2025), or propose methods that are explainable a priori (Miao et al., 2022; Lee et al., 2023). Fundamentally, these methods focus on devising mechanisms for explaining supervised tasks, such as node or graph classification. In our work, we instead focus on how this problem differs from the task of node similarity, and how to evaluate such methods for the respective task.

Orthogonally, approaches for *data valuation* have proposed methods for identifying how "valuable" certain parts of a graph (e.g., nodes or edges) are for a GNN, which can be defined in terms of changes to its learned weights (Chen et al., 2023); or its performance for node classification (Song et al., 2023; Chi et al., 2025). Our goal is complementary to these works: rather than studying the effect of graph components on GNN parameter updates or classification performance, we analyze how they influence the computation of individual similarity scores. This constitutes a fundamentally different, label-free setting, where similarity is a continuous quantity and standard notions of prediction correctness or task utility are not as well defined as in accuracy metrics for node classification.

More recently, Piaggesi et al. (2025) proposed metrics for evaluating the interpretability of unsupervised node embeddings. These metrics are designed to assess the semantic structure of the latent space produced by a specific representation learning method, and require ground-truth graph annotations (e.g., communities or motifs). In contrast, our objective is not to evaluate embeddings but rather to evaluate explanations of **similarity scores** produced by arbitrary GNNs. Our metrics are model-agnostic and operate by measuring

the effect of graph interventions; therefore, they quantify the quality of explanations when defined over the structure of the graph rather than the embedding space. As such, the two sets of metrics address complementary but fundamentally different questions.

Knowledge graph embeddings and entity similarity. Knowledge graph embeddings are representations of entities and relation types, which are commonly trained for the *link prediction* task (Nickel et al., 2016; Wang et al., 2017b): Given a query entity and a relation, the embeddings are used to predict a target entity that is likely to form a valid triple with the query entity and relation. KG embeddings have been applied in similarity computations via functions like cosine similarity or the dot product (Liu et al., 2019; Yamada et al., 2020; Gerritse et al., 2020; Daza et al., 2021; Khan et al., 2022), which are not designed to be explainable.

Prior work has explored the problem of explainability for KG embeddings. Some methods have proposed learning embeddings with a predefined structure, such as a set of interpretable concepts (Chandrahas et al., 2020; Xie et al., 2017; Zhang et al., 2021), or via sparsity constraints (Zulaika et al., 2022). The result is an embedding space, where it is possible to identify distinct semantic regions, e.g., "professions" or "cities". This differs from the problem of grounding similarities computed between pairs of entities on known attributes of the entities, which is the focus of our work.

In several other works, given an existing set of KG embeddings trained for link prediction, explanations have takem the form of a subset of supporting triples (Zhang et al., 2019; Pezeshkpour et al., 2019; Betz et al., 2022; Rossi et al., 2022), paths (Gusmão et al., 2018), or Horn rules (Gad-Elrab et al., 2020). While there is empirical evidence for KG embeddings being able to capture notions of similarity (Gad-Elrab et al., 2020), some works have suggested that the link prediction objective is sub-optimal for this task (Ristoski & Paulheim, 2016; Cochez et al., 2017; Ristoski et al., 2019). This motivates our use of GNNs that operate directly on node features and subgraphs, which can serve as explanations for predicted similarity scores.

Another line of work (Petrova et al., 2017; 2019) focused on identifying the reasons behind the similarity of two given entities by extracting SPARQL queries, which have both of the entities as answers. However, unlike in our proposal, in (Petrova et al., 2017; 2019) the authors did not aim at explaining the similarity scores computed by a machine learning method, but rather exclusively relied on the graph structure.

3 Learning and explaining similarities

Let $G = (\mathbf{A}, \mathbf{X})$ be a graph with n nodes, where $\mathbf{A}$ is an $n \times n$ adjacency matrix with $A_{ij} = 1$ if nodes i and j are connected, and 0 otherwise, and $\mathbf{X} \in \mathbb{R}^{n \times m}$ is a feature matrix, where the i-th row $\mathbf{x}_i$ contains the m-dimensional feature vector of the node i. In the following sections, we discuss the problems of learning representations of nodes for the similarity task, and our proposals on how similarity scores can be explained.

3.1 Learning representations for similarity

Graph neural networks have become a standard architecture for processing graph-structured data, due to their ability to incorporate arbitrary neighborhoods around a node (Kipf & Welling, 2017; Gilmer et al., 2017; Xu et al., 2019; Maron et al., 2019; Corso et al., 2020). They can easily be extended to graphs with rich edge features and multimodal data (Schlichtkrull et al., 2018; Saqur & Narasimhan, 2020; Galkin et al., 2020; Ektefaie et al., 2023). Furthermore, the fact that GNNs implement an explicit function that maps node neighborhoods and features to an embedding offers the opportunity for determining which parts of the input are responsible for a certain output. This is a desirable property when explaining computations such as similarity scores.

A prominent example of a graph neural network is the Graph Convolutional Network (GCN) (Kipf & Welling, 2017). A single layer of the GCN implements the following propagation rule:

$$\mathrm{GCN}(\mathbf{X}, \mathbf{A}) = \sigma\left(\tilde{\mathbf{A}}\mathbf{X}\mathbf{\Theta}\right), \tag{1}$$

where $\tilde{\mathbf{A}}$ is the normalized adjacency matrix, $\tilde{\mathbf{A}} = \hat{\mathbf{D}}^{-\frac{1}{2}}\hat{\mathbf{A}}\hat{\mathbf{D}}^{-\frac{1}{2}}$. Let $\mathbf{I}_n$ be the $n \times n$ identity matrix. Then $\hat{\mathbf{A}} = \mathbf{A} + \mathbf{I}_n$ is the adjacency matrix, adding self-loops, and $\hat{\mathbf{D}}$ is the degree matrix after adding self loops, such that $\hat{D}_{ii} = \sum_j \hat{A}_{ij}$.

The weight matrix $\mathbf{\Theta}$ in Eq. 1 contains the parameters of the layer to be learned during training. When composing together multiple GCN layers, we obtain a function $f_\theta(\mathbf{X}, \mathbf{A}) = \mathbf{Z} \in \mathbb{R}^{n \times d}$ that maps each node and its features to an embedding, conditioned on the features of nodes in its neighborhood.

We approach the problem of training a GNN to learn node embeddings from the perspective of unsupervised learning: In the absence of labeled data containing ground-truth similarity information, we resort to methods that learn node embeddings by capturing patterns existing in the graph, such as communities or structural roles (Hamilton et al., 2017a). The resulting node embeddings are vectors $\mathbf{z}_i \in \mathbb{R}^d$, with $i = 1, \ldots n$, where such patterns are preserved by the geometry of the space. This allows us to address the problem of similarity search for a given query node i, by ranking the rest of the nodes in the graph according to a function such as cosine similarity:

$$y(i, j) = \frac{\mathbf{z}_i^\top \mathbf{z}_j}{\|\mathbf{z}_i\| \|\mathbf{z}_j\|}, \tag{2}$$

where $j = 1, \ldots, n$ and $\|\mathbf{z}_i\|$ is the ℓ^2-norm of $\mathbf{z}_i$.

Several methods are available in the literature for unsupervised learning on graphs (Hamilton et al., 2017a; Liu et al., 2023b; Ju et al., 2023). Examples include Graph Autoencoders and Variational Graph Autoencoders (Kipf & Welling, 2016), which optimize node embeddings so that they are able to reconstruct the adjacency matrix; Deep Graph Infomax (Velickovic et al., 2019), that learns node embeddings by maximizing the mutual information between them and a summarized representation of the graph; and Graph Contrastive Representation Learning (Zhu et al., 2020), which compares different views of a node by perturbing its neighborhood and features.

3.2 Explaining GNNs

The success of GNNs at various tasks has been accompanied by increased interest in explaining the predictions they provide (Yuan et al., 2023). Informally, methods for explaining GNNs aim to determine i) which parts of the input graph $G = (\mathbf{X}, \mathbf{A})$ are responsible for a particular prediction, and ii) how they are responsible. The mechanisms used to answer these questions vary with each method.

A recent survey (Yuan et al., 2023) classifies methods for explaining GNNs into two main groups: instance-level and model-level methods. Instance-level methods produce a distinct explanation for a particular prediction (such as the label predicted for a specific node in the graph), while model-level methods aim to understand the behavior of the GNN under different inputs. Since we are interested in explaining similarity scores computed for specific pairs of nodes, we focus on the class of instance-level explanations.

Examples of instance-level methods are perturbation methods and gradient-based methods (Yuan et al., 2023). They represent an explanation as an assignment of values to parts of the input (for example, edges in the graph or node features), where the values indicate a degree of importance for computing the output of the GNN, as we illustrate in Fig. 1. In this work, the parts of the inputs to the GNN that we consider for explanations are edges between nodes, but our discussion can be easily extended to consider node features.

Formally, we assume that we have access to an already trained GNN. The output $f_\theta(\mathbf{X}, \mathbf{A})$ of the GNN is used to compute a *prediction* $y = g(f_\theta(\mathbf{X}, \mathbf{A}))$, and we wish to compute an explanation for it that describes the degree of influence of an edge in a prediction. For similarity search the prediction is the cosine similarity between two specific node embeddings as defined in Eq. 2.

Explanations over edges in the graph can be defined as a function that maps a prediction to a matrix $\mathbf{M} \in \mathbb{R}^{n \times n}$ containing *explanation values* for each of the (non-zero) entries of the adjacency matrix. For the majority of perturbation methods, the explanation values in $\mathbf{M}$ lie in the interval $[0, 1]$, and they can be interpreted as a *mask*, where values of 1 indicate relevant edges and 0 irrelevant ones. Gradient-based

methods, on the other hand, are unconstrained, providing explanation values over the real numbers that not only carry the magnitude with which an edge influences a prediction, but also its direction (positive or negative) via the sign of the gradient.

Given a matrix $\mathbf{M}$ of explanation values, a subset of the edges in the graph can be selected by defining an *explanation threshold* t. The subset is defined by the entries in the adjacency matrix A_{ij} such that $M_{ij} > t$. The meaning of the selected edges for an explanation of the similarity score depends on whether the matrix is interpreted as a mask, or as a gradient.

Explaining node similarities. Prior work on explaining GNNs has primarily focused on supervised tasks like node classification and link prediction (Yuan et al., 2023), where the goal is to justify a discrete output label. In contrast, node similarity is a continuous, unsupervised quantity, and existing GNN explainers do not come with criteria which a good similarity explanation should satisfy. To address this gap, we revisit principles from the general explainable AI literature and adapt them to the problem of explaining similarity scores. We identify a set of criteria that such explanations should meet and introduce metrics that allow us to quantitatively evaluate them.

4 Criteria for explanations of similarity

Several works in the literature have highlighted the importance of explainability in artificial intelligence systems, particularly when they face human users that could benefit from an understanding of their predictions (Ras et al., 2018; Mueller et al., 2019; Miller, 2019; Arrieta et al., 2020; Yang et al., 2023). These works define a series of properties that explanations should have. For example, they should *"produce details or reasons to make its functioning clear or easy to understand"* (Arrieta et al., 2020), they should be useful for debugging algorithms (Yang et al., 2023), they should provide answers to *why* questions (Miller, 2019) –e.g. *why is this the similarity score?*–; and they should have properties such as fidelity (how much the explanation agrees with the input-output map of the prediction under explanation), low ambiguity, and low complexity, among others (Ras et al., 2018). In the context of node similarity in GNNs, several explanation methods assign a relevance value to each edge involved in the computation. We derive three criteria such explanations should meet:

1. Actionable explanations. We can use the edges whose explanation value is above or below the threshold t to make interventions in the graph that result in a predictable effect on the original similarity score. This facilitates an understanding of the specific effect of some edges on the similarity score, and follows requirements on understanding model decisions (Miller, 2019; Arrieta et al., 2020), interactivity via interventions (Arrieta et al., 2020), model debugging (Yang et al., 2023), and fidelity (Ras et al., 2018).

2. Consistent explanations. Actionability alone does not guarantee that the two sides of the threshold capture *distinct* explanatory behavior. An explanation can be actionable yet non-discriminative: both edges above and below a threshold t may produce the same effect (e.g., both increase similarity). Thus explanations should be consistent: the effect of keeping edges above the threshold is distinct from the effect of discarding them. This implies that the explanations capture specific behaviors of the similarity under explanation, indicating fidelity and low ambiguity (Ras et al., 2018).

3. Sparse explanations. Explanations should admit a principled reduction to a small subset, e.g., selecting the smallest subset that preserves 90% of the effect attributed to the intervention. This does not follow from actionability or consistency, as an explanation may satisfy both yet distribute its effect uniformly across many edges, making it impossible to reduce. Sparsity, therefore, captures the *compressibility* of an explanation while maintaining the effects that define its actionability and consistency. This leads to simpler, parsimonious explanations (Ras et al., 2018) that users can interpret (Miller, 2019).

We now introduce concrete, intervention-based metrics that operationalize these criteria and allow us to evaluate explanation methods quantitatively.

4.1 Metrics for intervention-based evaluation

Given a trained GNN f_θ, we evaluate the properties of explanations for node similarities by measuring quantities that assess changes in the similarity score, after performing interventions in the graph on the basis of the explanation. More concretely, let (i, j) be a pair of nodes in the graph. Given the set of node embeddings $\mathbf{Z} = f_\theta(\mathbf{X}, \mathbf{A})$, we select the embeddings of i and j from it and compute the cosine similarity $y(i, j)$ as defined in Eq. 2. The explanation method is then executed on this value, which results in an explanation matrix $\mathbf{M}$.

Given $\mathbf{M}$, we compute two matrices $\mathbf{M}_a$ and $\mathbf{M}_b$ that select values above or below a threshold t, respectively, such that

$$M_{a,ij} = M_{ij} \quad \text{if } M_{ij} \geq t \text{ else } 0 \tag{3}$$

$$M_{b,ij} = M_{ij} \quad \text{if } M_{ij} < t \text{ else } 0, \tag{4}$$

where the threshold for GNNexplainer is 0.5 and 0 for Gradient Based (GB) methods.

We use these matrices to intervene in the graph, by computing the element-wise multiplication of these matrices with the adjacency matrix, and re-computing the node embeddings, which yields

$$\mathbf{Z}_a = f_\theta(\mathbf{X}, \mathbf{A} \odot \mathbf{M}_a) \tag{5}$$

$$\mathbf{Z}_b = f_\theta(\mathbf{X}, \mathbf{A} \odot \mathbf{M}_b). \tag{6}$$

Given these embeddings, we then re-compute the similarity scores, which for each case we denote as $y_a(i, j)$ and $y_b(i, j)$ respectively.

Measuring actionability. Based on these new similarity scores, we first compute a *fidelity* metric (Ribeiro et al., 2016), which measures the change in the similarity score after the intervention with respect to the original similarity score:

$$\text{Fid}_a = y_a(i, j) - y(i, j) \tag{7}$$

$$\text{Fid}_b = y_b(i, j) - y(i, j) \tag{8}$$

Positive values of Fid_a and Fid_b indicate an increase in similarity, negative values a decrease. If either intervention produces effects in a predictable direction, the explanation is **actionable**. Importantly, Fid_a and Fid_b capture absolute, independent changes, and they do not reveal how the two interventions relate.

Measuring consistency. To evaluate whether explanations induce distinct effects above vs. below the threshold, we consider only the signs of the fidelity values. For each node pair, we count a_1: times where Fid_a is positive; a_2: times where Fid_a is negative; and b_1 and b_2 defined similarly for Fid_b. We then define the Effect Overlap (EO) as the generalized Jaccard similarity between these counts:

$$\text{EO} = \frac{\sum_{i=1}^{2} \min(a_i, b_i)}{\sum_{i=1}^{2} \max(a_i, b_i)}. \tag{9}$$

An explanation method with an EO of zero indicates that the effect observed in Fid_a is always positive, and always negative in Fid_b (or viceversa). This indicates that the effects are distinct and thus the explanations are consistent. The maximum value of EO is 1 and it occurs if the effect is always positive or always negative, leading to an undistinguishable effect. Values between 0 and 1 indicate partial overlap.

EO thus resolves a limitation of fidelity: even if both Fid_a and Fid_b suggest actionability, EO determines whether the two interventions imply complementary effects on node similarity.

Measuring sparsity. Sparsity evaluates whether an explanation can be reduced to a smaller subset of edges while preserving the intervention effects that determine actionability and consistency. Given the explanation matrix $\mathbf{M}$ and the thresholded masks $\mathbf{M}_a$ and $\mathbf{M}_b$, we simulate different sparsity levels by

removing a fraction $s \in [0, 1]$ of the least relevant edges: in $\mathbf{M}_a$ we drop the smallest s-fraction of nonzero values, and in $\mathbf{M}_b$ we drop the largest s-fraction. We then recompute the same fidelity and effect-overlap metrics across increasing values of s.

An explanation satisfies the sparsity criterion if its actionable and consistent behaviors are preserved as s increases, indicating that the explanatory signal can be concentrated in a compact subset of edges.

5 Experiments

In our experiments, we aim to evaluate the proposed criteria and metrics in practice. To demonstrate this, we apply our framework to representative explanation methods from two major families of methods in the related work: mutual-information methods and gradient-based methods.

5.1 Explainability methods

5.1.1 Mutual information methods

A common approach for identifying explanations for GNNs consists of determining what edges are relevant for computing a prediction, by relying on the concept of Mutual Information (MI)(Ying et al., 2019; Luo et al., 2020; Wang et al., 2021; Miao et al., 2022). Existing works have proposed explaining a prediction $y = g(f_\theta(\mathbf{X}, \mathbf{A}))$ by finding a subgraph from the original graph that has high mutual information with the prediction. This implies that only a region of the graph is relevant for computing a prediction, whereas the rest can be discarded without affecting it. This mechanism for finding an explanation can be formalized by assuming that the matrix $\mathbf{M}$ of explanation values is a sample of a random variable M with values in $\{0, 1\}$, and then maximizing the mutual information between the original prediction (now a random variable Y) and the prediction after "masking" the adjacency matrix with the values in M:

$$\max_{M} I(g(f_\theta(\mathbf{X}, \mathbf{A}); g(f_\theta(\mathbf{X}, \mathbf{A} \odot M)), \tag{10}$$

where $\odot$ indicates element-wise multiplication.

In practice, the problem in Eq. 10 is not tractable. Instead, an approximation leads to the problem of finding a matrix that minimizes the cross-entropy loss (Ying et al., 2019):

$$\mathbf{M}_{\text{MI}} \coloneqq \arg\min_{\mathbf{M}} -\mathbb{E}_Y[\log p(Y|\mathbf{X}, \mathbf{A} \odot \mathbf{M})] \tag{11}$$

This problem is solved by randomly initializing $\mathbf{M}_{\text{MI}}$ and updating it via gradient descent in the direction that minimizes the cross-entropy loss (Ying et al., 2019; Luo et al., 2020; Miao et al., 2022).

Interpreting the explanation matrix. Given the formulation of MI-based methods for explaining GNNs, entries of $\mathbf{M}_{\text{MI}}$ with a value of 1 indicate edges that are relevant for the prediction, and 0 if they are irrelevant. When the matrix contains values in the continuous interval $[0, 1]$, an appropriate threshold for selecting or discarding edges is then $t = 0.5$.

In our experiments, we employ GNNExplainer (Ying et al., 2019) as an instance of MI methods.

5.1.2 Gradient-based methods

An early approach for identifying parts of the inputs relevant for a prediction computed by a neural network is to compute the gradient of the output with respect to the input (Simonyan et al., 2014; Shrikumar et al., 2017; Selvaraju et al., 2017; Sundararajan et al., 2017). This is motivated by the fact that the gradient indicates the direction and rate with which the outputs change with respect to the inputs.

In gradient-based (GB) methods, the extension of this approach to explaining GNNs is natural: the explanation matrix is equal to the gradient of the prediction with respect to the adjacency matrix,

$$\mathbf{M}_{\text{GB}} \coloneqq \nabla_{\mathbf{A}} g(f_\theta(\mathbf{X}, \mathbf{A})). \tag{12}$$

Relying on the gradient alone might become problematic in deep neural networks using non-linearities like the ReLU activation function, whose derivative is zero over half of its domain. To address this issue, more advanced methods based on the gradient have been proposed, such as Guided Backpropagation (Springenberg et al., 2015), which ignores zero gradients, or Integrated Gradients (Sundararajan et al., 2017), which computes the total change from different values of the gradient, rather than relying on a single gradient.

Interpreting the explanation matrix. The values in the explanation matrix $\mathbf{M}_{\text{GB}}$ are unconstrained, and they can take positive or negative values, depending on the sign of the gradient. This means that for each edge in the graph, GB explanations provide a magnitude and direction of influence. In this case, an appropriate threshold for selecting or discarding edges is $t = 0$.

When explaining predictions of node similarity, the (i, j) entry of the explanation matrix indicates i) how much the presence of an edge between nodes i and j influences the similarity score, via the magnitude of the gradient, and ii) the direction of influence –positive or negative– via the sign. Unlike explanations from MI methods, we note that GB explanations are therefore more fine-grained, by providing additional information about how inputs affect changes in similarity scores.

In our experiments with GB methods, we consider direct gradient computation with respect to the adjacency matrix (as defined in Eq. 12), and Integrated Gradients (Sundararajan et al., 2017).

5.2 Node embedding methods

We implement the following unsupervised methods for learning node embeddings: Graph Autoencoders (GAE) and Variational Graph Autoencoders (VGAE) (Kipf & Welling, 2016), Deep Graph Infomax (DGI) (Velickovic et al., 2019), and Graph Contrastive Representation Learning (GRACE) (Zhu et al., 2020). We use them to train a 2-layer GCN (Kipf & Welling, 2017) as defined in Eq. 1. We tune hyperparameters via grid search, selecting the values with the lowest training loss.

5.3 Datasets

We run experiments with six graph datasets of different sizes and domains: Cora, Citeseer, and Pubmed (Sen et al., 2008; Namata et al., 2012; Yang et al., 2016) are citation networks from the computer science and medical domains, where each node corresponds to a scientific publication and an edge indicates that there is a citation from one publication to another. These graphs are known to exhibit high *homophily*: similar nodes (such as publications within the same field) are very likely to be connected (McPherson et al., 2001).

To consider graphs with different structural properties, we also carry out experiments with *heterophilic* graphs where connected nodes are not necessarily similar. Chameleon and Squirrel are graphs obtained from Wikipedia, where each node is a web page and an edge denotes a hyperlink between pages (Rozemberczki et al., 2021). Actor is a graph where each node is an actor, and an edge indicates that two actors co-occur on a Wikipedia page (Tang et al., 2009). Furthermore, we also experiment with the DBpedia50k knowledge graph (Shi & Weninger, 2018), a subset of the DBpedia knowledge graph (Auer et al., 2007). The DBpedia50k graph does not contain node features, therefore for this dataset we also train input node embeddings for the GNN. Statistics of all datasets is presented in Table 1.

5.4 Results

We present the results of the fidelity (Equation (7) and Equation (8)) and effect overlap (Equation (9)) metrics in Tables 2 for the homophilic and heterophilic graphs, and Table 3 for DBpedia50k. We denote GNNExplainer as MI, directly using the gradient as GB1, and Integrated Gradients as GB2.

GB explanations are actionable. The values of Fid_a and Fid_b for GB methods show that across all unsupervised learning methods and datasets, keeping edges above the explanation threshold always results in an increase of the similarity score, while keeping the edges below the threshold always results in a lower score. This means that GB explanations are **actionable**, as they allow interventions that result in a predictable effect on the similarity score. Relying on these explanations would allow to determine what edges contribute

Table 1: Statistics of graphs used in our experiments.

Dataset	Nodes	Edges	Features
Cora	2,708	5,429	1,433
Citeseer	3,327	4,732	3,703
Pubmed	19,717	44,338	500
Chameleon	2,277	36,101	2,325
Actor	7,600	33,544	931
Squirrel	5,201	217,073	2,089
DBpedia50k	30,449	57,161	N/A

Table 2: Results of fidelity metrics (Fid_a and Fid_b) and effect overlap (EO, lower is better) when applying different explanation methods to multiple unsupervised learning methods and graphs. As explanation methods we consider GNNExplainer (Ying et al., 2019) (MI), and two gradient-based methods based on direct computation of the gradient (GB1), and Integrated Gradients (Sundararajan et al., 2017) (GB2).

Method		Cora			Citeseer			Pubmed			Chameleon			Actor			Squirrel		
		Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO
GAE	MI	0.133	0.019	0.451	0.130	0.029	0.406	0.136	0.202	0.532	0.292	0.353	0.531	0.134	0.209	0.521	0.386	0.357	0.411
	GB1	0.118	-0.076	0.033	0.114	-0.026	0.129	0.236	-0.064	0.141	0.355	-0.107	0.125	0.442	-0.146	0.120	0.520	-0.126	0.160
	GB2	0.279	-0.067	**0.013**	0.366	-0.025	**0.098**	0.443	-0.144	**0.011**	0.718	-0.180	**0.030**	0.555	-0.392	**0.008**	0.755	-0.317	**0.038**
VGAE	MI	0.103	0.039	0.504	0.156	0.004	0.397	0.140	0.149	0.502	0.311	0.403	0.540	0.142	0.176	0.506	0.363	0.399	0.450
	GB1	0.149	-0.087	0.045	0.078	-0.054	0.049	0.250	-0.121	0.098	0.412	-0.156	0.105	0.423	-0.203	0.081	0.577	-0.172	0.150
	GB2	0.392	-0.075	**0.007**	0.185	-0.045	**0.023**	0.418	-0.180	**0.017**	0.781	-0.218	**0.030**	0.522	-0.386	**0.009**	0.766	-0.400	**0.042**
DGI	MI	0.015	0.032	0.546	0.039	0.029	0.568	0.061	0.008	0.452	0.322	0.441	0.539	-0.009	-0.000	0.552	0.142	0.162	0.561
	GB1	0.218	-0.118	0.060	0.105	-0.084	0.082	0.023	-0.055	0.254	0.515	-0.196	0.326	-0.009	-0.012	0.511	0.119	-0.400	0.277
	GB2	0.283	-0.161	**0.053**	0.149	-0.122	**0.056**	0.029	-0.043	**0.182**	0.399	-0.299	**0.288**	-0.087	-0.373	**0.491**	0.216	-0.449	**0.273**
GRACE	MI	0.076	0.007	0.536	0.102	0.010	0.475	0.222	0.096	0.513	0.254	0.132	0.535	0.016	-0.185	0.511	0.112	0.020	0.594
	GB1	0.142	-0.057	**0.016**	0.113	-0.030	**0.062**	0.182	-0.016	0.158	0.338	-0.149	0.022	0.124	-0.262	**0.155**	0.253	-0.276	**0.046**
	GB2	0.155	-0.071	0.017	0.140	-0.028	0.063	0.235	-0.041	**0.052**	0.382	-0.154	**0.055**	0.012	-0.443	0.217	0.133	-0.382	0.151

to increase (or decrease) in the score, and to interact with them by re-computing the similarity score with the knowledge provided by the explanation. This property is not observed with GNNExplainer, where the effect of keeping edges above the threshold is not clear, and certain patterns seem to depend on factors such as the model used to learn the embeddings, and the dataset. For example, for GAE and VGAE embeddings, keeping the edges above the threshold increases the similarity score more than keeping the edges below the threshold on Cora and Citeseer, but the opposite happens in the remaining datasets.

GB explanations are consistent. GB methods result in the lowest effect overlap across all learning methods and datasets. In the majority of the cases the overlap is around 0.1 or lower, indicating that the effect of keeping edges above the threshold is distinct from the effect of keeping the edges below the threshold, thus showing that GB explanations are **consistent**. Interestingly, this behavior is not as clear when using DGI embeddings on the heterophilic datasets (Chameleon, Actor, and Squirrel), where the overlap increases. This could be an effect of how the performance of DGI degrades in heterophilic graphs (Xiao et al., 2022), lowering the quality of its embeddings in graphs with these properties and thus becoming sensitive to the interventions required to compute the fidelity and effect overlap metrics. In the case of GNNExplainer, in the majority of the cases, the effect overlap is around 0.4 or even larger than 0.5, indicating that in almost half of the cases keeping the edges above the threshold increases the score, and in the other half the score decreases. We thus cannot rely on its explanations for a consistent effect on similarity scores.

We present further extended results in Appendix A, where we experiment with four additional GNN architectures. These results are consistent with our prior observations, while also showing that in some cases overlap can be low while actionability is limited, indicating the importance of assessing jointly our proposed metrics for explaining node similarities.

Table 3: Results of fidelity metrics (Fid_a and Fid_b) and effect overlap (EO, lower is better) when applying different explanation methods to multiple unsupervised learning methods on the DBpedia50k knowledge graph.

Method		DBpedia50k		
		Fid_a	Fid_b	EO
GAE	MI	0.057	-0.073	0.564
	GB1	0.148	-0.190	0.050
	GB2	0.149	-0.213	**0.028**
VGAE	MI	0.059	-0.054	0.614
	GB1	0.149	-0.185	0.059
	GB2	0.182	-0.187	**0.037**
DGI	MI	-0.035	-0.044	0.618
	GB1	0.107	-0.189	0.065
	GB2	0.121	-0.215	**0.030**
GRACE	MI	-0.120	-0.002	0.541
	GB1	0.055	-0.071	**0.043**
	GB2	0.033	-0.081	0.046

Sparse GB explanations preserve effects. We next evaluate whether explanations preserve their properties when made increasingly sparse. Since previous experiments showed that Integrated Gradients yields actionable and consistent explanations, we focus our study on this method.

To carry out this study, instead of taking all values of the explanation matrix above the threshold (as outlined in Eqs. 3 and 4), we drop a fraction s of the smallest values in $\mathbf{M}_a$, and a fraction s of the largest values in $\mathbf{M}_b$, where s is the sparsity level taking values in the interval $[0, 1]$. When $s = 0$ all values in the explanation matrix are used, and we obtain the results previously described in Table 2. As s increases, only the edges with the largest or the smallest values are kept in $\mathbf{M}_a$ and $\mathbf{M}_b$.

We compute the fidelity and effect overlap metrics for different values of sparsity from 0 up to 0.9 with increments of 0.1, when using GAE to learn embeddings. The results are shown in Fig. 2. We observe that the actionable and consistent properties of GB explanations remain almost constant across all datasets. This implies that when obtaining GB explanations, we can further reduce the set of edges in the explanation by up to 90%, and the different effects on the similarity scores will be preserved. This is beneficial for applications in which a more compact explanation is desired.

Examples. We present concrete examples of the explanations obtained by GNNExplainer and Integrated Gradients in Fig. 3. For this case study, we train node embeddings using GAE on the DBpedia50k knowledge graph (Shi & Weninger, 2018). We then select the most relevant edges according to the explanation values assigned by each method. We consider two entities in the graph: *Lilium* and *Dendrobium*, which are two genera of flowering plants. Their similarity is reflected in a cosine similarity value of 0.705. We denote the effect attributed to each edge with colors, with blue indicating an increase in the similarity, red a decrease, and gray indicating little or no effect. When we obtain explanations with GNNExplainer, we observe that a few edges increase the similarity score, and none of them are in the 1-hop neighborhood of the entities, where their similarities are apparent. Both entities belong to the *Plant* kingdom and the *Flowering Plant* division. With gradient-based explanations, we observe that edges containing this information contribute to the increase of the similarity score, with the highest contributions (illustrated with the thickness of the edges) assigned to the relationships with *Plant* and *Flowering Plant*. Conversely, this analytical framework also enables the identification of specific informational elements that exert a negative influence on the calculated similarity score, thereby facilitating diagnostic assessment of dissimilarity factors. Overall, we note that gradient-based explanations are intuitive, by indicating both the magnitude and direction in which inputs affect similarity scores.

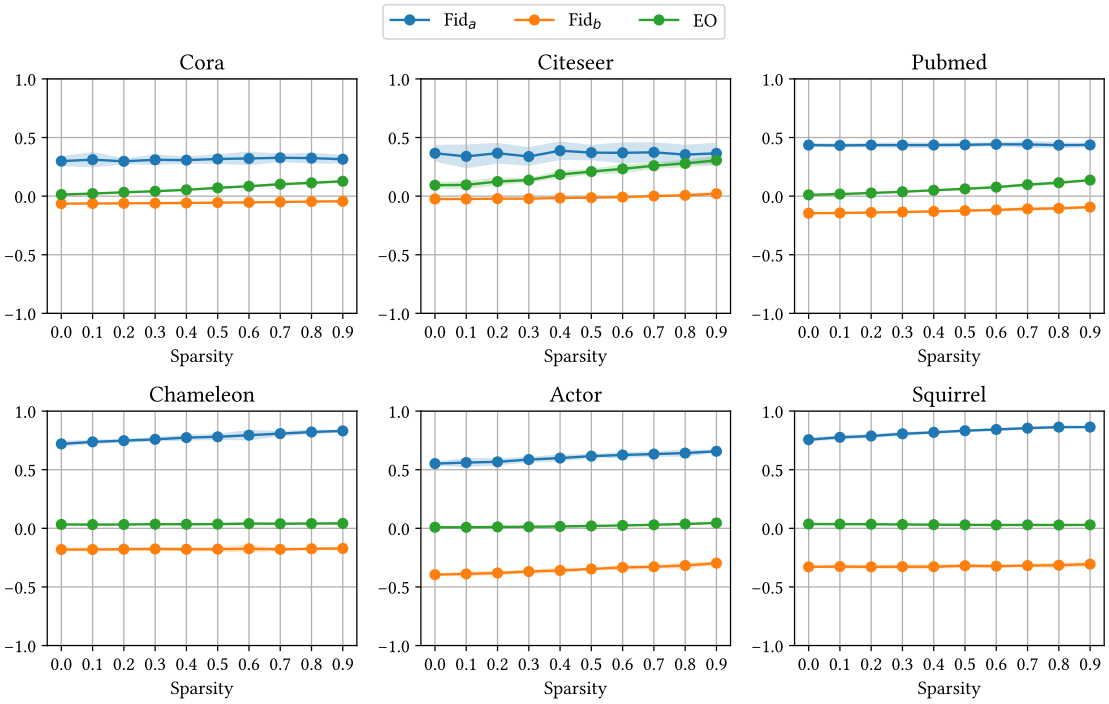


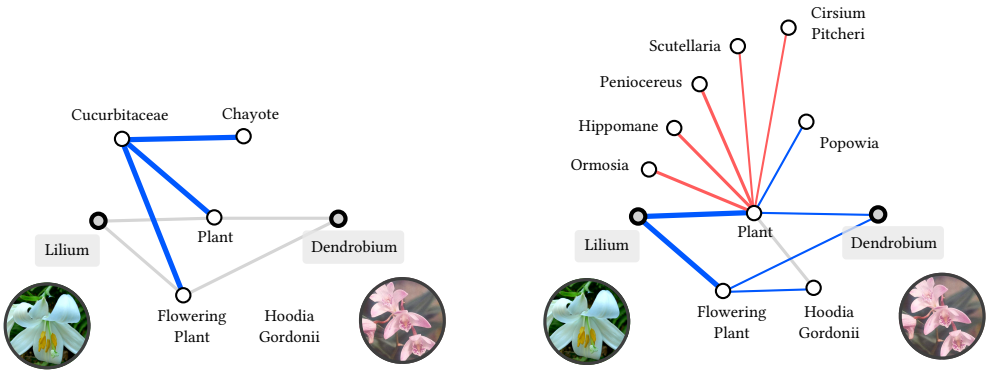
Figure 2: Influence of sparse explanations on fidelity metrics (Fid_a and Fid_b) and effect overlap (EO), evaluated with GAE embeddings across different datasets. At zero sparsity, all edges above (or below) the explanation threshold are kept and used to compute the change in similarity scores Fid_a (or F_b), as well as the effect overlap (EO). Larger values of sparsity indicate the fraction of edges discarded before computing the change in similarity scores. Confidence intervals are shown indicating two standard deviations over 10 runs.

6 Conclusion

We have studied the problem of explaining node similarities computed by graph neural networks, a setting relevant in practice but largely overlooked by prior work on GNN explainability. Building on principles from explainable AI, we introduced criteria that explanations of similarity should satisfy, and we operationalized them through intervention-based metrics. We have demonstrate the utility of our framework by applying it to representative mutual-information and gradient-based methods. Our results reveal that unlike prior results on supervised tasks like node classification (Ying et al., 2019; Luo et al., 2020; Yuan et al., 2023), gradient-based methods are more suitable in the setting of node similarity, by providing explanations with a predictable and consistent effect of increasing or decreasing similarity scores. Furthermore, we observe that the complexity of the explanations can be reduced while maintaining their desirable properties.

In this work, we focused on evaluating explanation methods based on how graph interventions derived from them affect similarity scores. An additional important aspect to be taken into account in the practical choice of an explanation method is its computational complexity. Gradient-based explanations require computing the gradient of a scalar similarity score with respect to the input graph, which amounts to a single backward pass through the GNN and scales linearly with the size of the graph up to constant factors. In contrast, mutual-information–based methods such as GNNExplainer rely on an iterative optimization procedure that repeatedly evaluates and differentiates the GNN over multiple steps, making them strictly more expensive in practice. While computational cost was not the main focus of our empirical study, it represents an additional criterion that may further favor gradient-based explanations in large-scale similarity search settings.

Beyond the specific methods examined here, our criteria and evaluation methodology offer a general foundation for evaluating explanations of similarity on graphs. They can inform the development of new methods



(a) GNNExplainer explanation.

(b) Gradient-based explanation.

Figure 3: Example of explanations provided by GNNExplainer (3a) and Integrated Gradients (3b) for the similarity computed between two entities in the DBpedia50k knowledge graph: *Lilium* and *Dendrobium*, two genera of flowering plants. Edge thickness indicates magnitude, while the color of the edges is associated with the score, i.e., blue edges reflect the score increase, red edges decrease, and gray edges have little effect.

for node similarity, and the design of methods that are explainable *a priori*. Moreover, based on our proposed methodology, further explainers (e.g., PGExplainer Luo et al. (2020), SubgraphX Yuan et al. (2021), PGM-Explainer Vu & Thai (2020)) could be analyzed, which is an interesting direction left for future research.

While we focused on cosine similarity, as it is the standard choice for fast dense similarity search over learned embeddings, our proposed intervention-based metrics are not specific to cosine similarity. They only require a similarity function defined over node embeddings, and can be applied to alternatives such as Euclidean distance without modification. The intervention logic, which measures how explanations predictably affect similarity under controlled graph perturbations, remains the same. We expect the qualitative behavior observed in our study to extend to other commonly used similarity measures without modification. We view these directions as promising avenues for future work.

References

Sami Abu-El-Haija, Bryan Perozzi, Amol Kapoor, Nazanin Alipourfard, Kristina Lerman, Hrayr Harutyunyan, Greg Ver Steeg, and Aram Galstyan. MixHop: Higher-order graph convolutional architectures via sparsified neighborhood mixing. In Kamalika Chaudhuri and Ruslan Salakhutdinov (eds.), *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pp. 21–29. PMLR, 09–15 Jun 2019. URL `https://proceedings.mlr.press/v97/abu-el-haija19a.html`.

Alejandro Barredo Arrieta, Natalia Díaz Rodríguez, Javier Del Ser, Adrien Bennetot, Siham Tabik, Alberto Barbado, Salvador García, Sergio Gil-Lopez, Daniel Molina, Richard Benjamins, Raja Chatila, and Francisco Herrera. Explainable artificial intelligence (XAI): concepts, taxonomies, opportunities and challenges toward responsible AI. *Inf. Fusion*, 58:82–115, 2020. doi: 10.1016/j.inffus.2019.12.012. URL `https://doi.org/10.1016/j.inffus.2019.12.012`.

Sören Auer, Christian Bizer, Georgi Kobilarov, Jens Lehmann, Richard Cyganiak, and Zachary Ives. Dbpedia: A nucleus for a web of open data. In *international semantic web conference*, pp. 722–735. Springer, 2007.

Patrick Betz, Christian Meilicke, and Heiner Stuckenschmidt. Adversarial explanations for knowledge graph embeddings. In Luc De Raedt (ed.), *Proceedings of the Thirty-First International Joint Conference on*

Artificial Intelligence, IJCAI 2022, Vienna, Austria, 23-29 July 2022, pp. 2820–2826. ijcai.org, 2022. doi: 10.24963/ijcai.2022/391. URL https://doi.org/10.24963/ijcai.2022/391.

Aleksandar Bojchevski and Stephan Günnemann. Deep Gaussian embedding of graphs: Unsupervised inductive learning via ranking. In *6th International Conference on Learning Representations, ICLR 2018, Vancouver, BC, Canada, April 30 - May 3, 2018, Conference Track Proceedings*. OpenReview.net, 2018. URL https://openreview.net/forum?id=r1ZdKJ-0W.

Sergey Brin. The pagerank citation ranking: bringing order to the web. *Proceedings of ASIS, 1998*, 98: 161–172, 1998.

Nadia Burkart and Marco F. Huber. A survey on the explainability of supervised machine learning. *J. Artif. Intell. Res.*, 70:245–317, 2021. doi: 10.1613/jair.1.12228. URL https://doi.org/10.1613/jair.1.12228.

. Chandrahas, Tathagata Sengupta, Cibi Pragadeesh, and Partha Talukdar. Inducing interpretability in knowledge graph embeddings. In *Proceedings of the 17th International Conference on Natural Language Processing (ICON)*, pp. 70–75, Indian Institute of Technology Patna, Patna, India, December 2020. NLP Association of India (NLPAI). URL https://aclanthology.org/2020.icon-main.9.

Zizhang Chen, Peizhao Li, Hongfu Liu, and Pengyu Hong. Characterizing the influence of graph elements. In *The Eleventh International Conference on Learning Representations*, 2023. URL https://openreview.net/forum?id=51GXyzOKOp.

Hongliang Chi, Wei Jin, Charu C. Aggarwal, and Yao Ma. Precedence-constrained winter value for effective graph data valuation. In *The Thirteenth International Conference on Learning Representations*, 2025. URL https://openreview.net/forum?id=tVRVE0OAyb.

Michael Cochez, Petar Ristoski, Simone Paolo Ponzetto, and Heiko Paulheim. Global RDF vector space embeddings. In Claudia d'Amato, Miriam Fernández, Valentina A. M. Tamma, Freddy Lécué, Philippe Cudré-Mauroux, Juan F. Sequeda, Christoph Lange, and Jeff Heflin (eds.), *The Semantic Web - ISWC 2017 - 16th International Semantic Web Conference, Vienna, Austria, October 21-25, 2017, Proceedings, Part I*, volume 10587 of *Lecture Notes in Computer Science*, pp. 190–207. Springer, 2017. doi: 10.1007/978-3-319-68288-4_12. URL https://doi.org/10.1007/978-3-319-68288-4_12.

Gabriele Corso, Luca Cavalleri, Dominique Beaini, Pietro Liò, and Petar Velickovic. Principal neighbourhood aggregation for graph nets. In Hugo Larochelle, Marc'Aurelio Ranzato, Raia Hadsell, Maria-Florina Balcan, and Hsuan-Tien Lin (eds.), *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual*, 2020. URL https://proceedings.neurips.cc/paper/2020/hash/99cad265a1768cc2dd013f0e740300ae-Abstract.html.

Daniel Daza, Michael Cochez, and Paul Groth. Inductive entity representations from text via link prediction. In Jure Leskovec, Marko Grobelnik, Marc Najork, Jie Tang, and Leila Zia (eds.), *WWW '21: The Web Conference 2021, Virtual Event / Ljubljana, Slovenia, April 19-23, 2021*, pp. 798–808. ACM / IW3C2, 2021. doi: 10.1145/3442381.3450141. URL https://doi.org/10.1145/3442381.3450141.

Alexandre Duval and Fragkiskos D Malliaros. GraphSVX: Shapley value explanations for graph neural networks. In *Joint European conference on machine learning and knowledge discovery in databases*, pp. 302–318. Springer, 2021.

Yasha Ektefaie, George Dasoulas, Ayush Noori, Maha Farhat, and Marinka Zitnik. Multimodal learning with graphs. *Nat. Mac. Intell.*, 5(4):340–350, 2023. doi: 10.1038/s42256-023-00624-6. URL https://doi.org/10.1038/s42256-023-00624-6.

Charlie Frogner, Farzaneh Mirzazadeh, and Justin Solomon. Learning embeddings into entropic Wasserstein spaces. In *7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019*. OpenReview.net, 2019. URL https://openreview.net/forum?id=rJg4J3CqFm.

Mohamed H. Gad-Elrab, Daria Stepanova, Trung-Kien Tran, Heike Adel, and Gerhard Weikum. Excut: Explainable embedding-based clustering over knowledge graphs. In Jeff Z. Pan, Valentina A. M. Tamma, Claudia d'Amato, Krzysztof Janowicz, Bo Fu, Axel Polleres, Oshani Seneviratne, and Lalana Kagal (eds.), *The Semantic Web - ISWC 2020 - 19th International Semantic Web Conference, Athens, Greece, November 2-6, 2020, Proceedings, Part I*, volume 12506 of *Lecture Notes in Computer Science*, pp. 218–237. Springer, 2020. doi: 10.1007/978-3-030-62419-4_13. URL https://doi.org/10.1007/978-3-030-62419-4_13.

Mikhail Galkin, Priyansh Trivedi, Gaurav Maheshwari, Ricardo Usbeck, and Jens Lehmann. Message passing for hyper-relational knowledge graphs. In Bonnie Webber, Trevor Cohn, Yulan He, and Yang Liu (eds.), *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing, EMNLP 2020, Online, November 16-20, 2020*, pp. 7346–7359. Association for Computational Linguistics, 2020. doi: 10.18653/v1/2020.emnlp-main.596. URL https://doi.org/10.18653/v1/2020.emnlp-main.596.

Difei Gao, Ke Li, Ruiping Wang, Shiguang Shan, and Xilin Chen. Multi-modal graph neural network for joint reasoning on vision and scene text. In *2020 IEEE/CVF Conference on Computer Vision and Pattern Recognition, CVPR 2020, Seattle, WA, USA, June 13-19, 2020*, pp. 12743–12753. Computer Vision Foundation / IEEE, 2020. doi: 10.1109/CVPR42600.2020.01276. URL https://openaccess.thecvf.com/content_CVPR_2020/html/Gao_Multi-Modal_Graph_Neural_Network_for_Joint_Reasoning_on_Vision_and_CVPR_2020_paper.html.

Emma J. Gerritse, Faegheh Hasibi, and Arjen P. de Vries. Graph-embedding empowered entity retrieval. In Joemon M. Jose, Emine Yilmaz, João Magalhães, Pablo Castells, Nicola Ferro, Mário J. Silva, and Flávio Martins (eds.), *Advances in Information Retrieval - 42nd European Conference on IR Research, ECIR 2020, Lisbon, Portugal, April 14-17, 2020, Proceedings, Part I*, volume 12035 of *Lecture Notes in Computer Science*, pp. 97–110. Springer, 2020. doi: 10.1007/978-3-030-45439-5_7. URL https://doi.org/10.1007/978-3-030-45439-5_7.

Justin Gilmer, Samuel S. Schoenholz, Patrick F. Riley, Oriol Vinyals, and George E. Dahl. Neural message passing for quantum chemistry. In Doina Precup and Yee Whye Teh (eds.), *Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, 6-11 August 2017*, volume 70 of *Proceedings of Machine Learning Research*, pp. 1263–1272. PMLR, 2017. URL http://proceedings.mlr.press/v70/gilmer17a.html.

Aristides Gionis, Piotr Indyk, and Rajeev Motwani. Similarity search in high dimensions via hashing. In Malcolm P. Atkinson, Maria E. Orlowska, Patrick Valduriez, Stanley B. Zdonik, and Michael L. Brodie (eds.), *VLDB'99, Proceedings of 25th International Conference on Very Large Data Bases, September 7-10, 1999, Edinburgh, Scotland, UK*, pp. 518–529. Morgan Kaufmann, 1999. URL http://www.vldb.org/conf/1999/P49.pdf.

Arthur Colombini Gusmão, Alvaro Henrique Chaim Correia, Glauber De Bona, and Fabio Gagliardi Cozman. Interpreting embedding models of knowledge bases: a pedagogical approach. *arXiv preprint arXiv:1806.09504*, 2018.

William L. Hamilton, Rex Ying, and Jure Leskovec. Representation learning on graphs: Methods and applications. *IEEE Data Eng. Bull.*, 40(3):52–74, 2017a. URL http://sites.computer.org/debull/A17sept/p52.pdf.

William L. Hamilton, Zhitao Ying, and Jure Leskovec. Inductive representation learning on large graphs. In Isabelle Guyon, Ulrike von Luxburg, Samy Bengio, Hanna M. Wallach, Rob Fergus, S. V. N. Vishwanathan, and Roman Garnett (eds.), *Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, December 4-9, 2017, Long Beach, CA, USA*, pp. 1024–1034, 2017b. URL https://proceedings.neurips.cc/paper/2017/hash/5dd9db5e033da9c6fb5ba83c7a7ebea9-Abstract.html.

Taher H. Haveliwala. Topic-sensitive pagerank. In David Lassner, David De Roure, and Arun Iyengar (eds.), *Proceedings of the Eleventh International World Wide Web Conference, WWW 2002, May 7-11, 2002, Honolulu, Hawaii, USA*, pp. 517–526. ACM, 2002. doi: 10.1145/511446.511513. URL https://doi.org/10.1145/511446.511513.

Aidan Hogan, Eva Blomqvist, Michael Cochez, Claudia d'Amato, Gerard de Melo, Claudio Gutierrez, Sabrina Kirrane, José Emilio Labra Gayo, Roberto Navigli, Sebastian Neumaier, et al. Knowledge graphs. *ACM Computing Surveys (CSUR)*, 54(4):1–37, 2021.

Glen Jeh and Jennifer Widom. Simrank: a measure of structural-context similarity. In *Proceedings of the Eighth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, July 23-26, 2002, Edmonton, Alberta, Canada*, pp. 538–543. ACM, 2002. doi: 10.1145/775047.775126. URL https://doi.org/10.1145/775047.775126.

Wei Ju, Zheng Fang, Yiyang Gu, Zequn Liu, Qingqing Long, Ziyue Qiao, Yifang Qin, Jianhao Shen, Fang Sun, Zhiping Xiao, Junwei Yang, Jingyang Yuan, Yusheng Zhao, Xiao Luo, and Ming Zhang. A comprehensive survey on deep graph representation learning. *CoRR*, abs/2304.05055, 2023. doi: 10.48550/arXiv.2304.05055. URL https://doi.org/10.48550/arXiv.2304.05055.

Nasrullah Khan, Zongmin Ma, Aman Ullah, and Kemal Polat. Similarity attributed knowledge graph embedding enhancement for item recommendation. *Inf. Sci.*, 613:69–95, 2022. doi: 10.1016/j.ins.2022.08.124. URL https://doi.org/10.1016/j.ins.2022.08.124.

Thomas N. Kipf and Max Welling. Variational graph auto-encoders. *CoRR*, abs/1611.07308, 2016. URL http://arxiv.org/abs/1611.07308.

Thomas N. Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. In *5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings*. OpenReview.net, 2017. URL https://openreview.net/forum?id=SJU4ayYgl.

Namkyeong Lee, Dongmin Hyun, Gyoung S. Na, Sungwon Kim, Junseok Lee, and Chanyoung Park. Conditional graph information bottleneck for molecular relational learning. *CoRR*, abs/2305.01520, 2023. doi: 10.48550/arXiv.2305.01520. URL https://doi.org/10.48550/arXiv.2305.01520.

Xiao Liu, Fanjin Zhang, Zhenyu Hou, Li Mian, Zhaoyu Wang, Jing Zhang, and Jie Tang. Self-supervised learning: Generative or contrastive. *IEEE Trans. Knowl. Data Eng.*, 35(1):857–876, 2023a. doi: 10.1109/TKDE.2021.3090866. URL https://doi.org/10.1109/TKDE.2021.3090866.

Yixin Liu, Ming Jin, Shirui Pan, Chuan Zhou, Yu Zheng, Feng Xia, and Philip S. Yu. Graph self-supervised learning: A survey. *IEEE Trans. Knowl. Data Eng.*, 35(6):5879–5900, 2023b. doi: 10.1109/TKDE.2022.3172903. URL https://doi.org/10.1109/TKDE.2022.3172903.

Zhenghao Liu, Chenyan Xiong, Maosong Sun, and Zhiyuan Liu. Explore entity embedding effectiveness in entity retrieval. In Maosong Sun, Xuanjing Huang, Heng Ji, Zhiyuan Liu, and Yang Liu (eds.), *Chinese Computational Linguistics - 18th China National Conference, CCL 2019, Kunming, China, October 18-20, 2019, Proceedings*, volume 11856 of *Lecture Notes in Computer Science*, pp. 105–116. Springer, 2019. doi: 10.1007/978-3-030-32381-3_9. URL https://doi.org/10.1007/978-3-030-32381-3_9.

Ana Lucic, Maartje A. ter Hoeve, Gabriele Tolomei, Maarten de Rijke, and Fabrizio Silvestri. Cf-gnnexplainer: Counterfactual explanations for graph neural networks. In Gustau Camps-Valls, Francisco J. R. Ruiz, and Isabel Valera (eds.), *International Conference on Artificial Intelligence and Statistics, AISTATS 2022, 28-30 March 2022, Virtual Event*, volume 151 of *Proceedings of Machine Learning Research*, pp. 4499–4511. PMLR, 2022. URL https://proceedings.mlr.press/v151/lucic22a.html.

Dongsheng Luo, Wei Cheng, Dongkuan Xu, Wenchao Yu, Bo Zong, Haifeng Chen, and Xiang Zhang. Parameterized explainer for graph neural network. In Hugo Larochelle, Marc'Aurelio Ranzato, Raia Hadsell, Maria-Florina Balcan, and Hsuan-Tien Lin (eds.), *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual*, 2020. URL https://proceedings.neurips.cc/paper/2020/hash/e37b08dd3015330dcbb5d6663667b8b8-Abstract.html.

Elan Markowitz, Keshav Balasubramanian, Mehrnoosh Mirtaheri, Murali Annavaram, Aram Galstyan, and Greg Ver Steeg. Statik: Structure and text for inductive knowledge graph completion. In Marine Carpuat, Marie-Catherine de Marneffe, and Iván Vladimir Meza Ruíz (eds.), *Findings of the Association for Computational Linguistics: NAACL 2022, Seattle, WA, United States, July 10-15, 2022*, pp. 604–615. Association for Computational Linguistics, 2022. doi: 10.18653/v1/2022.findings-naacl.46. URL https://doi.org/10.18653/v1/2022.findings-naacl.46.

Haggai Maron, Heli Ben-Hamu, Hadar Serviansky, and Yaron Lipman. Provably powerful graph networks. In Hanna M. Wallach, Hugo Larochelle, Alina Beygelzimer, Florence d'Alché-Buc, Emily B. Fox, and Roman Garnett (eds.), *Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, December 8-14, 2019, Vancouver, BC, Canada*, pp. 2153–2164, 2019. URL https://proceedings.neurips.cc/paper/2019/hash/bb04af0f7ecaee4aae62035497da1387-Abstract.html.

Miller McPherson, Lynn Smith-Lovin, and James M Cook. Birds of a feather: Homophily in social networks. *Annual review of sociology*, 27(1):415–444, 2001.

Siqi Miao, Mia Liu, and Pan Li. Interpretable and generalizable graph learning via stochastic attention mechanism. In Kamalika Chaudhuri, Stefanie Jegelka, Le Song, Csaba Szepesvári, Gang Niu, and Sivan Sabato (eds.), *International Conference on Machine Learning, ICML 2022, 17-23 July 2022, Baltimore, Maryland, USA*, volume 162 of *Proceedings of Machine Learning Research*, pp. 15524–15543. PMLR, 2022. URL https://proceedings.mlr.press/v162/miao22a.html.

Tim Miller. Explanation in artificial intelligence: Insights from the social sciences. *Artif. Intell.*, 267:1–38, 2019. doi: 10.1016/j.artint.2018.07.007. URL https://doi.org/10.1016/j.artint.2018.07.007.

Shane T Mueller, Robert R Hoffman, William Clancey, Abigail Emrey, and Gary Klein. Explanation in human-ai systems: A literature meta-review, synopsis of key ideas and publications, and bibliography for explainable ai. *arXiv preprint arXiv:1902.01876*, 2019.

Maximilian Muschalik, Fabian Fumagalli, Paolo Frazzetto, Janine Strotherm, Luca Hermes, Alessandro Sperduti, Eyke Hüllermeier, and Barbara Hammer. Exact computation of any-order shapley interactions for graph neural networks. In *The Thirteenth International Conference on Learning Representations*, 2025. URL https://openreview.net/forum?id=9tKC0YM8sX.

Galileo Namata, Ben London, Lise Getoor, Bert Huang, and U Edu. Query-driven active surveying for collective classification. In *10th international workshop on mining and learning with graphs*, volume 8, pp. 1, 2012.

Mark Newman. *Networks*. Oxford university press, 2018.

Maximilian Nickel, Kevin Murphy, Volker Tresp, and Evgeniy Gabrilovich. A review of relational machine learning for knowledge graphs. *Proc. IEEE*, 104(1):11–33, 2016. doi: 10.1109/JPROC.2015.2483592. URL https://doi.org/10.1109/JPROC.2015.2483592.

Zhen Peng, Wenbing Huang, Minnan Luo, Qinghua Zheng, Yu Rong, Tingyang Xu, and Junzhou Huang. Graph representation learning via graphical mutual information maximization. In Yennun Huang, Irwin King, Tie-Yan Liu, and Maarten van Steen (eds.), *WWW '20: The Web Conference 2020, Taipei, Taiwan, April 20-24, 2020*, pp. 259–270. ACM / IW3C2, 2020. doi: 10.1145/3366423.3380112. URL https://doi.org/10.1145/3366423.3380112.

Alina Petrova, Evgeny Sherkhonov, Bernardo Cuenca Grau, and Ian Horrocks. Entity comparison in RDF graphs. In *The Semantic Web - ISWC 2017*, volume 10587, pp. 526–541. Springer, 2017.

Alina Petrova, Egor V. Kostylev, Bernardo Cuenca Grau, and Ian Horrocks. Query-based entity comparison in knowledge graphs revisited. In *The Semantic Web - ISWC 2019 - 18th International Semantic Web Conference*, volume 11778, pp. 558–575. Springer, 2019.

Pouya Pezeshkpour, Yifan Tian, and Sameer Singh. Investigating robustness and interpretability of link prediction via adversarial modifications. In Jill Burstein, Christy Doran, and Thamar Solorio (eds.), *Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, NAACL-HLT 2019, Minneapolis, MN, USA, June 2-7, 2019, Volume 1 (Long and Short Papers)*, pp. 3336–3347. Association for Computational Linguistics, 2019. doi: 10.18653/v1/n19-1337. URL https://doi.org/10.18653/v1/n19-1337.

Simone Piaggesi, André Panisson, and Megha Khosla. Disentangled and self-explainable node representation learning. *Trans. Mach. Learn. Res.*, 2025, 2025.

Gabriëlle Ras, Marcel van Gerven, and Pim Haselager. Explanation methods in deep learning: Users, values, concerns and challenges. *Explainable and interpretable models in computer vision and machine learning*, pp. 19–36, 2018.

Marco Túlio Ribeiro, Sameer Singh, and Carlos Guestrin. "why should I trust you?": Explaining the predictions of any classifier. In Balaji Krishnapuram, Mohak Shah, Alexander J. Smola, Charu C. Aggarwal, Dou Shen, and Rajeev Rastogi (eds.), *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, San Francisco, CA, USA, August 13-17, 2016*, pp. 1135–1144. ACM, 2016. doi: 10.1145/2939672.2939778. URL https://doi.org/10.1145/2939672.2939778.

Petar Ristoski and Heiko Paulheim. Rdf2vec: RDF graph embeddings for data mining. In Paul Groth, Elena Simperl, Alasdair J. G. Gray, Marta Sabou, Markus Krötzsch, Freddy Lécué, Fabian Flöck, and Yolanda Gil (eds.), *The Semantic Web - ISWC 2016 - 15th International Semantic Web Conference, Kobe, Japan, October 17-21, 2016, Proceedings, Part I*, volume 9981 of *Lecture Notes in Computer Science*, pp. 498–514, 2016. doi: 10.1007/978-3-319-46523-4_30. URL https://doi.org/10.1007/978-3-319-46523-4_30.

Petar Ristoski, Jessica Rosati, Tommaso Di Noia, Renato De Leone, and Heiko Paulheim. Rdf2vec: RDF graph embeddings and their applications. *Semantic Web*, 10(4):721–752, 2019. doi: 10.3233/SW-180317. URL https://doi.org/10.3233/SW-180317.

Andrea Rossi, Donatella Firmani, Paolo Merialdo, and Tommaso Teofili. Explaining link prediction systems based on knowledge graph embeddings. In Zachary G. Ives, Angela Bonifati, and Amr El Abbadi (eds.), *SIGMOD '22: International Conference on Management of Data, Philadelphia, PA, USA, June 12 - 17, 2022*, pp. 2062–2075. ACM, 2022. doi: 10.1145/3514221.3517887. URL https://doi.org/10.1145/3514221.3517887.

Benedek Rozemberczki, Carl Allen, and Rik Sarkar. Multi-scale attributed node embedding. *J. Complex Networks*, 9(2), 2021. doi: 10.1093/comnet/cnab014. URL https://doi.org/10.1093/comnet/cnab014.

Raeid Saqur and Karthik Narasimhan. Multimodal graph networks for compositional generalization in visual question answering. In Hugo Larochelle, Marc'Aurelio Ranzato, Raia Hadsell, Maria-Florina Balcan, and Hsuan-Tien Lin (eds.), *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual*, 2020. URL https://proceedings.neurips.cc/paper/2020/hash/1fd6c4e41e2c6a6b092eb13ee72bce95-Abstract.html.

Michael Sejr Schlichtkrull, Thomas N. Kipf, Peter Bloem, Rianne van den Berg, Ivan Titov, and Max Welling. Modeling relational data with graph convolutional networks. In Aldo Gangemi, Roberto Navigli, Maria-Esther Vidal, Pascal Hitzler, Raphaël Troncy, Laura Hollink, Anna Tordai, and Mehwish Alam (eds.), *The Semantic Web - 15th International Conference, ESWC 2018, Heraklion, Crete, Greece, June 3-7, 2018, Proceedings*, volume 10843 of *Lecture Notes in Computer Science*, pp. 593–607. Springer, 2018. doi: 10.1007/978-3-319-93417-4_38. URL https://doi.org/10.1007/978-3-319-93417-4_38.

Ramprasaath R. Selvaraju, Michael Cogswell, Abhishek Das, Ramakrishna Vedantam, Devi Parikh, and Dhruv Batra. Grad-cam: Visual explanations from deep networks via gradient-based localization. In *IEEE International Conference on Computer Vision, ICCV 2017, Venice, Italy, October 22-29, 2017*, pp. 618–626. IEEE Computer Society, 2017. doi: 10.1109/ICCV.2017.74. URL https://doi.org/10.1109/ICCV.2017.74.

Prithviraj Sen, Galileo Namata, Mustafa Bilgic, Lise Getoor, Brian Gallagher, and Tina Eliassi-Rad. Collective classification in network data. *AI Mag.*, 29(3):93–106, 2008. doi: 10.1609/aimag.v29i3.2157. URL https://doi.org/10.1609/aimag.v29i3.2157.

Baoxu Shi and Tim Weninger. Open-world knowledge graph completion. In Sheila A. McIlraith and Kilian Q. Weinberger (eds.), *Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence, (AAAI-18), the 30th innovative Applications of Artificial Intelligence (IAAI-18), and the 8th AAAI Symposium on Educational Advances in Artificial Intelligence (EAAI-18), New Orleans, Louisiana, USA, February 2-7, 2018*, pp. 1957–1964. AAAI Press, 2018. doi: 10.1609/aaai.v32i1.11535. URL https://doi.org/10.1609/aaai.v32i1.11535.

Yuxuan Shi, Gong Cheng, Trung-Kien Tran, Jie Tang, and Evgeny Kharlamov. Keyword-based knowledge graph exploration based on quadratic group steiner trees. In *Proceedings of the Thirtieth International Joint Conference on Artificial Intelligence, IJCAI*, pp. 1555–1562, 2021.

Larissa Capobianco Shimomura, Rafael Seidi Oyamada, Marcos R. Vieira, and Daniel S. Kaster. A survey on graph-based methods for similarity searches in metric spaces. *Inf. Syst.*, 95:101507, 2021. doi: 10.1016/j.is.2020.101507. URL https://doi.org/10.1016/j.is.2020.101507.

Avanti Shrikumar, Peyton Greenside, and Anshul Kundaje. Learning important features through propagating activation differences. In Doina Precup and Yee Whye Teh (eds.), *Proceedings of the 34th International Conference on Machine Learning*, volume 70 of *Proceedings of Machine Learning Research*, pp. 3145–3153. PMLR, 06–11 Aug 2017. URL https://proceedings.mlr.press/v70/shrikumar17a.html.

Karen Simonyan, Andrea Vedaldi, and Andrew Zisserman. Deep inside convolutional networks: Visualising image classification models and saliency maps. In Yoshua Bengio and Yann LeCun (eds.), *2nd International Conference on Learning Representations, ICLR 2014, Banff, AB, Canada, April 14-16, 2014, Workshop Track Proceedings*, 2014. URL http://arxiv.org/abs/1312.6034.

Jaeyun Song, SungYub Kim, and Eunho Yang. RGE: A repulsive graph rectification for node classification via influence. In *International Conference on Machine Learning*, pp. 32331–32348. PMLR, 2023.

Jost Tobias Springenberg, Alexey Dosovitskiy, Thomas Brox, and Martin A. Riedmiller. Striving for simplicity: The all convolutional net. In Yoshua Bengio and Yann LeCun (eds.), *3rd International Conference on Learning Representations, ICLR 2015, San Diego, CA, USA, May 7-9, 2015, Workshop Track Proceedings*, 2015. URL http://arxiv.org/abs/1412.6806.

Fan-Yun Sun, Jordan Hoffmann, Vikas Verma, and Jian Tang. Infograph: Unsupervised and semi-supervised graph-level representation learning via mutual information maximization. In *8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020*. OpenReview.net, 2020. URL https://openreview.net/forum?id=r1lfF2NYvH.

Yizhou Sun, Jiawei Han, Xifeng Yan, Philip S. Yu, and Tianyi Wu. Pathsim: Meta path-based top-k similarity search in heterogeneous information networks. *Proc. VLDB Endow.*, 4(11):992–1003, 2011. URL http://www.vldb.org/pvldb/vol4/p992-sun.pdf.

Mukund Sundararajan, Ankur Taly, and Qiqi Yan. Axiomatic attribution for deep networks. In Doina Precup and Yee Whye Teh (eds.), *Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, 6-11 August 2017*, volume 70 of *Proceedings of Machine Learning Research*, pp. 3319–3328. PMLR, 2017. URL http://proceedings.mlr.press/v70/sundararajan17a.html.

Jie Tang, Jimeng Sun, Chi Wang, and Zi Yang. Social influence analysis in large-scale networks. In John F. Elder IV, Françoise Fogelman-Soulié, Peter A. Flach, and Mohammed Javeed Zaki (eds.), *Proceedings of the 15th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, Paris, France, June 28 - July 1, 2009*, pp. 807–816. ACM, 2009. doi: 10.1145/1557019.1557108. URL https://doi.org/10.1145/1557019.1557108.

Shantanu Thakoor, Corentin Tallec, Mohammad Gheshlaghi Azar, Mehdi Azabou, Eva L. Dyer, Rémi Munos, Petar Velickovic, and Michal Valko. Large-scale representation learning on graphs via bootstrapping. In *The Tenth International Conference on Learning Representations, ICLR 2022, Virtual Event, April 25-29, 2022*. OpenReview.net, 2022. URL https://openreview.net/forum?id=0UXT6PpRpW.

Petar Velickovic, William Fedus, William L. Hamilton, Pietro Liò, Yoshua Bengio, and R. Devon Hjelm. Deep graph infomax. In *7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019*. OpenReview.net, 2019. URL https://openreview.net/forum?id=rklz9iAcKQ.

Minh N. Vu and My T. Thai. Pgm-explainer: Probabilistic graphical model explanations for graph neural networks. In *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual*, 2020.

Chun Wang, Shirui Pan, Guodong Long, Xingquan Zhu, and Jing Jiang. MGAE: marginalized graph autoencoder for graph clustering. In Ee-Peng Lim, Marianne Winslett, Mark Sanderson, Ada Wai-Chee Fu, Jimeng Sun, J. Shane Culpepper, Eric Lo, Joyce C. Ho, Debora Donato, Rakesh Agrawal, Yu Zheng, Carlos Castillo, Aixin Sun, Vincent S. Tseng, and Chenliang Li (eds.), *Proceedings of the 2017 ACM on Conference on Information and Knowledge Management, CIKM 2017, Singapore, November 06 - 10, 2017*, pp. 889–898. ACM, 2017a. doi: 10.1145/3132847.3132967. URL https://doi.org/10.1145/3132847.3132967.

Quan Wang, Zhendong Mao, Bin Wang, and Li Guo. Knowledge graph embedding: A survey of approaches and applications. *IEEE Trans. Knowl. Data Eng.*, 29(12):2724–2743, 2017b. doi: 10.1109/TKDE.2017.2754499. URL https://doi.org/10.1109/TKDE.2017.2754499.

Xiang Wang, Ying-Xin Wu, An Zhang, Xiangnan He, and Tat-Seng Chua. Towards multi-grained explainability for graph neural networks. In Marc'Aurelio Ranzato, Alina Beygelzimer, Yann N. Dauphin, Percy Liang, and Jennifer Wortman Vaughan (eds.), *Advances in Neural Information Processing Systems 34: Annual Conference on Neural Information Processing Systems 2021, NeurIPS 2021, December 6-14, 2021, virtual*, pp. 18446–18458, 2021. URL https://proceedings.neurips.cc/paper/2021/hash/99bcfcd754a98ce89cb86f73acc04645-Abstract.html.

Felix Wu, Amauri H. Souza Jr., Tianyi Zhang, Christopher Fifty, Tao Yu, and Kilian Q. Weinberger. Simplifying graph convolutional networks. In Kamalika Chaudhuri and Ruslan Salakhutdinov (eds.), *Proceedings of the 36th International Conference on Machine Learning, ICML 2019, 9-15 June 2019, Long Beach, California, USA*, volume 97 of *Proceedings of Machine Learning Research*, pp. 6861–6871. PMLR, 2019. URL http://proceedings.mlr.press/v97/wu19e.html.

Zonghan Wu, Shirui Pan, Fengwen Chen, Guodong Long, Chengqi Zhang, and Philip S. Yu. A comprehensive survey on graph neural networks. *IEEE Trans. Neural Networks Learn. Syst.*, 32(1):4–24, 2021. doi: 10.1109/TNNLS.2020.2978386. URL https://doi.org/10.1109/TNNLS.2020.2978386.

Teng Xiao, Zhengyu Chen, Zhimeng Guo, Zeyang Zhuang, and Suhang Wang. Decoupled self-supervised learning for graphs. In *NeurIPS*, 2022. URL http://papers.nips.cc/paper_files/paper/2022/hash/040c816286b3844fd78f2124eec75f2e-Abstract-Conference.html.

Qizhe Xie, Xuezhe Ma, Zihang Dai, and Eduard Hovy. An interpretable knowledge transfer model for knowledge base completion. In *Proceedings of the 55th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pp. 950–962, Vancouver, Canada, July 2017. Association for Computational Linguistics. doi: 10.18653/v1/P17-1088. URL https://aclanthology.org/P17-1088.

Yaochen Xie, Sumeet Katariya, Xianfeng Tang, Edward W. Huang, Nikhil Rao, Karthik Subbian, and Shuiwang Ji. Task-agnostic graph explanations. In *NeurIPS*, 2022a. URL http://papers.nips.cc/paper_files/paper/2022/hash/4eb7f0abf16d08e50ed42beb1e22e782-Abstract-Conference.html.

Yaochen Xie, Zhao Xu, and Shuiwang Ji. Self-supervised representation learning via latent graph prediction. In Kamalika Chaudhuri, Stefanie Jegelka, Le Song, Csaba Szepesvári, Gang Niu, and Sivan Sabato (eds.), *International Conference on Machine Learning, ICML 2022, 17-23 July 2022, Baltimore, Maryland, USA*,

volume 162 of *Proceedings of Machine Learning Research*, pp. 24460–24477. PMLR, 2022b. URL https://proceedings.mlr.press/v162/xie22e.html.

Yaochen Xie, Zhao Xu, Jingtun Zhang, Zhengyang Wang, and Shuiwang Ji. Self-supervised learning of graph neural networks: A unified review. *IEEE Trans. Pattern Anal. Mach. Intell.*, 45(2):2412–2429, 2023. doi: 10.1109/TPAMI.2022.3170559. URL https://doi.org/10.1109/TPAMI.2022.3170559.

Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? In *7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019*. OpenReview.net, 2019. URL https://openreview.net/forum?id=ryGs6iA5Km.

Xiaowei Xu, Nurcan Yuruk, Zhidan Feng, and Thomas A. J. Schweiger. SCAN: a structural clustering algorithm for networks. In Pavel Berkhin, Rich Caruana, and Xindong Wu (eds.), *Proceedings of the 13th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, San Jose, California, USA, August 12-15, 2007*, pp. 824–833. ACM, 2007. doi: 10.1145/1281192.1281280. URL https://doi.org/10.1145/1281192.1281280.

Ikuya Yamada, Akari Asai, Jin Sakuma, Hiroyuki Shindo, Hideaki Takeda, Yoshiyasu Takefuji, and Yuji Matsumoto. Wikipedia2vec: An efficient toolkit for learning and visualizing the embeddings of words and entities from wikipedia. In Qun Liu and David Schlangen (eds.), *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing: System Demonstrations, EMNLP 2020 - Demos, Online, November 16-20, 2020*, pp. 23–30. Association for Computational Linguistics, 2020. doi: 10.18653/v1/2020.emnlp-demos.4. URL https://doi.org/10.18653/v1/2020.emnlp-demos.4.

Wenli Yang, Yuchen Wei, Hanyu Wei, Yanyu Chen, Guan Huang, Xiang Li, Renjie Li, Naimeng Yao, Xinyi Wang, Xiaotong Gu, Muhammad Bilal Amin, and Byeong Kang. Survey on explainable AI: from approaches, limitations and applications aspects. *Hum. Centric Intell. Syst.*, 3(3):161–188, 2023. doi: 10.1007/s44230-023-00038-y. URL https://doi.org/10.1007/s44230-023-00038-y.

Zhilin Yang, William W. Cohen, and Ruslan Salakhutdinov. Revisiting semi-supervised learning with graph embeddings. In Maria-Florina Balcan and Kilian Q. Weinberger (eds.), *Proceedings of the 33nd International Conference on Machine Learning, ICML 2016, New York City, NY, USA, June 19-24, 2016*, volume 48 of *JMLR Workshop and Conference Proceedings*, pp. 40–48. JMLR.org, 2016. URL http://proceedings.mlr.press/v48/yanga16.html.

Zi Ye, Yogan Jaya Kumar, Goh Ong Sing, Fengyan Song, and Junsong Wang. A comprehensive survey of graph neural networks for knowledge graphs. *IEEE Access*, 10:75729–75741, 2022. doi: 10.1109/ACCESS.2022.3191784. URL https://doi.org/10.1109/ACCESS.2022.3191784.

Zhitao Ying, Dylan Bourgeois, Jiaxuan You, Marinka Zitnik, and Jure Leskovec. Gnnexplainer: Generating explanations for graph neural networks. In Hanna M. Wallach, Hugo Larochelle, Alina Beygelzimer, Florence d'Alché-Buc, Emily B. Fox, and Roman Garnett (eds.), *Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, December 8-14, 2019, Vancouver, BC, Canada*, pp. 9240–9251, 2019. URL https://proceedings.neurips.cc/paper/2019/hash/d80b7040b773199015de6d3b4293c8ff-Abstract.html.

Hao Yuan, Haiyang Yu, Jie Wang, Kang Li, and Shuiwang Ji. On explainability of graph neural networks via subgraph explorations. In Marina Meila and Tong Zhang (eds.), *Proceedings of the 38th International Conference on Machine Learning, ICML 2021, 18-24 July 2021, Virtual Event*, volume 139 of *Proceedings of Machine Learning Research*, pp. 12241–12252. PMLR, 2021. URL http://proceedings.mlr.press/v139/yuan21c.html.

Hao Yuan, Haiyang Yu, Shurui Gui, and Shuiwang Ji. Explainability in graph neural networks: A taxonomic survey. *IEEE Trans. Pattern Anal. Mach. Intell.*, 45(5):5782–5799, 2023. doi: 10.1109/TPAMI.2022.3204236. URL https://doi.org/10.1109/TPAMI.2022.3204236.

Reza Bosagh Zadeh and Ashish Goel. Dimension independent similarity computation. *J. Mach. Learn. Res.*, 14(1):1605–1626, 2013. doi: 10.5555/2567709.2567715. URL https://dl.acm.org/doi/10.5555/2567709.2567715.

Hengtong Zhang, Tianhang Zheng, Jing Gao, Chenglin Miao, Lu Su, Yaliang Li, and Kui Ren. Data poisoning attack against knowledge graph embedding. In Sarit Kraus (ed.), *Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI 2019, Macao, China, August 10-16, 2019*, pp. 4853–4859. ijcai.org, 2019. doi: 10.24963/ijcai.2019/674. URL https://doi.org/10.24963/ijcai.2019/674.

Zhao Zhang, Fuzhen Zhuang, Meng Qu, Zheng-Yu Niu, Hui Xiong, and Qing He. Knowledge graph embedding with shared latent semantic units. *Neural Networks*, 139:140–148, 2021. doi: 10.1016/j.neunet.2021.02.013. URL https://doi.org/10.1016/j.neunet.2021.02.013.

Jie Zhou, Ganqu Cui, Shengding Hu, Zhengyan Zhang, Cheng Yang, Zhiyuan Liu, Lifeng Wang, Changcheng Li, and Maosong Sun. Graph neural networks: A review of methods and applications. *AI Open*, 1:57–81, 2020. doi: 10.1016/j.aiopen.2021.01.001. URL https://doi.org/10.1016/j.aiopen.2021.01.001.

Yanqiao Zhu, Yichen Xu, Feng Yu, Qiang Liu, Shu Wu, and Liang Wang. Deep graph contrastive representation learning. *CoRR*, abs/2006.04131, 2020. URL https://arxiv.org/abs/2006.04131.

Unai Zulaika, Aitor Almeida, and Diego López-de Ipiña. Regularized online tensor factorization for sparse knowledge graph embeddings. *Neural Comput. Appl.*, 35(1):787–797, sep 2022. ISSN 0941-0643. doi: 10.1007/s00521-022-07796-z. URL https://doi-org.vu-nl.idm.oclc.org/10.1007/s00521-022-07796-z.

Table 4: Results of fidelity metrics (Fid_a and Fid_b) and effect overlap (EO, lower is better) when using an SGC (Wu et al., 2019) as the base GNN architecture.

Method		Cora			Citeseer			Pubmed			Chameleon			Actor			Squirrel		
		Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO
GAE	MI	0.020	-0.005	0.916	0.185	0.006	0.832	0.090	0.231	0.978	0.231	-0.069	0.668	0.161	-0.053	0.676	0.042	0.250	0.892
	GB1	0.049	-0.036	**0.067**	0.075	-0.048	0.050	0.214	-0.008	0.232	0.137	-0.191	**0.034**	0.253	-0.254	**0.052**	0.281	-0.005	0.251
	GB2	0.060	-0.040	0.074	0.239	-0.033	**0.049**	0.433	-0.120	**0.012**	0.185	-0.169	0.117	0.209	-0.221	0.095	0.561	-0.233	**0.010**
VGAE	MI	0.072	0.135	0.957	0.179	0.010	0.880	0.066	0.265	0.797	0.312	-0.041	0.678	0.225	-0.044	0.733	-0.014	0.346	0.516
	GB1	0.177	-0.060	0.105	0.098	-0.044	0.076	0.261	-0.043	0.206	0.233	-0.283	**0.030**	0.362	-0.387	**0.039**	0.355	0.013	0.307
	GB2	0.539	-0.063	**0.015**	0.280	-0.035	**0.072**	0.479	-0.166	**0.017**	0.289	-0.245	0.065	0.315	-0.324	0.098	0.603	-0.324	**0.018**
DGI	MI	0.018	0.000	0.955	-0.079	0.005	**0.350**	-0.089	-0.027	**0.417**	-0.010	0.134	0.374	0.017	0.042	0.479	0.008	-0.015	0.823
	GB1	0.017	-0.010	0.015	-0.013	-0.104	0.353	-0.112	-0.096	0.914	0.209	-0.213	**0.110**	0.088	-0.053	**0.055**	-0.208	-0.287	0.682
	GB2	0.018	-0.011	**0.006**	-0.085	-0.338	0.527	-0.110	-0.218	0.553	0.310	-0.261	0.125	0.079	-0.059	0.068	-0.265	-0.403	**0.650**
GRACE	MI	0.007	-0.005	0.837	0.010	-0.002	0.908	0.118	0.106	0.729	0.140	-0.017	0.813	-0.066	-0.064	0.953	0.075	-0.008	0.608
	GB1	0.047	-0.040	0.074	0.030	-0.021	0.095	0.115	-0.045	0.162	0.098	-0.107	**0.033**	0.095	-0.244	**0.027**	0.070	-0.064	0.262
	GB2	0.057	-0.047	**0.050**	0.041	-0.024	**0.085**	0.221	-0.060	**0.045**	0.124	-0.104	0.047	0.015	-0.321	0.200	0.080	-0.189	**0.185**

A Additional results

Our main experimental results are aimed at investigating the effect of the metrics we proposed over different embedding learning algorithms and datasets, when the architecture is designed from GCN layers (Kipf & Welling, 2017).

To determine whether our results generalize to other architectures, here we present extended results where we repeat the experiments using four additional architectures: SGC (Wu et al., 2019), a simplified variant of the GCN that reformulates message passing in multi-layer GNNs as a single matrix multiplication with powers of the adjacency matrix; GraphSAGE (Hamilton et al., 2017b), which for a given node, concatenates embeddings of the node from previous layers during the neighborhood aggregation process (in contrast to the GCN which mixes only embeddings from the same layer); MixHop (Abu-El-Haija et al., 2019), which is designed to capture higher-order patterns by computing at each layer representations from powers of the adjacency matrix; and R-GCN (Schlichtkrull et al., 2018), a variant of the GCN that learns different weight matrices for heterogeneous relation types that arise in knowledge graphs.

We present results with SGC in Table 4, GraphSAGE in Table 5, and MixHop in Table 6. On the DBPedia50k knowledge graph, we present additional results using these three architectures plus the R-GCN in Table 7. The extended results indicate that the behaviour observed with our proposed metrics remains under changes in the architecture in the majority of cases: gradient-based explanations are actionable, as interventions based on them produce predictable effects on the score (either increasing it or decreasing it); and they are consistent, as these effects are distinct, which is demonstrated by the low effect overlap.

A special case is found in the combination of DGI as a learning algorithm, and GraphSAGE as the base GNN (shown in Table 5). Here we note that in virtually all cases, any intervention results in *decreasing* the similarity between two nodes (denoted by the negative values of Fid_a and Fid_b) but the magnitude of changes is larger when using gradient-based explanations, resulting in higher actionability. In contrast, the mutual information (MI) method results in smaller changes, thereby indicating low actionability. In spite of this, the MI method results in lower overlap in several cases, indicating higher consistency than gradient-based methods.

We conclude that EO must be interpreted jointly with fidelity: the lower EO of MI here follows from near-zero effects, whereas gradient-based explanations result in substantially stronger interventions (higher actionability) even though their effects are not sign-separated, which raises EO. Despite occasional cases where MI attains lower EO, gradient-based explanations are preferable for similarity explanation because they provide stronger, controllable interventions; MI's improved overlap in this regime is largely explained by its limited impact on the similarity score. This suggests that on DGI+GraphSAGE, the similarity function is globally fragile (interventions mostly reduce similarity), making sign-based separation difficult for any explainer despite differences in actionability.

Table 5: Results of fidelity metrics (Fid_a and Fid_b) and effect overlap (EO, lower is better) when using GraphSAGE (Hamilton et al., 2017b) as the base GNN architecture.

Method		Cora			Citeseer			Pubmed			Chameleon			Actor			Squirrel		
		Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO
GAE	MI	0.000	0.002	0.496	0.001	0.000	0.724	0.081	0.074	0.908	0.036	0.029	0.720	0.060	0.031	0.810	0.037	0.037	0.969
	GB1	0.012	-0.008	0.159	0.024	-0.022	0.149	0.171	-0.041	0.234	0.082	-0.038	0.103	0.094	-0.035	0.235	0.144	-0.083	0.113
	GB2	0.019	-0.014	**0.080**	0.030	-0.026	**0.083**	0.264	-0.130	**0.046**	0.123	-0.050	**0.070**	0.194	-0.075	**0.105**	0.188	-0.121	**0.028**
VGAE	MI	0.057	0.061	0.892	0.056	0.058	0.832	0.079	0.121	0.944	0.041	0.035	0.898	0.097	0.085	0.967	0.035	0.043	0.919
	GB1	0.116	-0.037	0.103	0.091	-0.021	0.137	0.202	-0.020	0.269	0.151	-0.082	0.106	0.232	-0.077	0.177	0.158	-0.106	0.116
	GB2	0.183	-0.058	**0.026**	0.168	-0.042	**0.082**	0.343	-0.142	**0.053**	0.257	-0.126	**0.022**	0.338	-0.157	**0.068**	0.208	-0.154	**0.030**
DGI	MI	-0.105	-0.236	**0.720**	-0.038	-0.365	**0.626**	0.005	-0.000	0.969	0.000	-0.027	**0.708**	0.013	-0.009	**0.373**	-0.038	-0.017	**0.242**
	GB1	-0.303	-0.410	0.946	-0.464	-0.423	0.878	-0.651	-0.604	0.970	-0.276	-0.433	0.869	-0.133	-0.396	0.634	-0.148	-0.218	0.845
	GB2	-0.475	-0.660	0.959	-0.420	-0.783	0.672	-0.170	-0.213	**0.953**	-0.385	-0.627	0.901	-0.317	-0.556	0.807	-0.251	-0.365	0.862
GRACE	MI	0.001	-0.002	0.754	-0.004	-0.002	0.676	-0.013	-0.004	0.459	0.027	-0.002	0.576	0.016	-0.005	0.556	-0.001	-0.000	0.645
	GB1	0.023	-0.024	0.079	0.010	-0.016	0.075	0.036	-0.056	0.087	0.050	-0.043	0.057	0.054	-0.064	0.045	0.080	-0.108	0.085
	GB2	0.029	-0.028	**0.046**	0.011	-0.017	**0.066**	0.048	-0.061	**0.026**	0.071	-0.050	**0.035**	0.066	-0.077	**0.026**	0.107	-0.146	**0.026**

Table 6: Results of fidelity metrics (Fid_a and Fid_b) and effect overlap (EO, lower is better) when using MixHop (Abu-El-Haija et al., 2019) as the base GNN architecture.

Method		Cora			Citeseer			Pubmed			Chameleon			Actor			Squirrel		
		Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO	Fid_a	Fid_b	EO
GAE	MI	0.002	-0.002	0.558	0.013	0.003	0.604	0.080	0.165	0.912	0.069	-0.098	0.860	0.029	-0.038	0.932	0.057	0.048	0.878
	GB1	0.047	-0.038	0.065	0.027	-0.016	**0.098**	0.198	0.047	0.428	0.113	-0.202	**0.043**	0.170	-0.198	**0.052**	0.239	-0.023	0.294
	GB2	0.055	-0.042	**0.059**	0.032	-0.018	0.117	0.363	-0.144	**0.050**	0.114	-0.226	0.071	0.152	-0.222	0.060	0.272	-0.230	**0.033**
VGAE	MI	0.011	-0.011	0.990	0.006	-0.004	0.908	0.088	0.279	0.942	0.112	0.086	0.921	0.171	0.130	0.800	0.101	0.111	0.784
	GB1	0.079	-0.070	0.072	0.033	-0.029	**0.148**	0.248	0.026	0.355	0.268	-0.130	0.062	0.380	-0.119	0.119	0.272	0.035	0.420
	GB2	0.083	-0.075	**0.064**	0.038	-0.027	0.167	0.425	-0.180	**0.057**	0.361	-0.170	**0.021**	0.499	-0.247	**0.024**	0.376	-0.291	**0.031**
DGI	MI	-0.023	0.002	**0.342**	-0.031	0.011	**0.386**	0.065	0.023	0.757	0.004	0.006	0.596	-0.079	-0.010	**0.370**	0.000	-0.030	**0.656**
	GB1	-0.142	-0.245	0.817	-0.211	-0.349	0.696	-0.037	-0.129	0.652	-0.003	-0.214	**0.360**	-0.227	-0.524	0.762	-0.303	-0.417	0.898
	GB2	-0.070	-0.205	0.711	-0.169	-0.351	0.601	-0.019	-0.097	**0.541**	-0.009	-0.334	0.407	-0.032	-0.138	0.577	-0.212	-0.376	0.773
GRACE	MI	-0.016	-0.024	0.590	-0.014	-0.010	0.584	-0.021	-0.026	0.567	-0.021	-0.033	0.608	-0.114	-0.091	0.587	-0.034	-0.069	0.742
	GB1	0.032	-0.072	**0.083**	0.030	-0.051	0.153	0.006	-0.091	0.324	0.061	-0.149	**0.077**	0.027	-0.257	**0.164**	0.017	-0.120	**0.211**
	GB2	0.031	-0.081	0.100	0.028	-0.058	**0.142**	0.012	-0.094	**0.304**	0.062	-0.156	0.086	-0.047	-0.308	0.382	0.008	-0.133	0.296

Table 7: Results of fidelity metrics (Fid_a and Fid_b) and effect overlap (EO, lower is better) on the DBPedia50k dataset, when using SGC (Wu et al., 2019), GraphSAGE (Hamilton et al., 2017b), MixHop (Abu-El-Haija et al., 2019), and R-GCN (Schlichtkrull et al., 2018) as the base GNN architecture.

Method		SGC			GraphSAGE			MixHop			R-GCN		
		Fid_p	Fid_n	EO	Fid_p	Fid_n	EO	Fid_p	Fid_n	EO	Fid_p	Fid_n	EO
GAE	MI	0.006	-0.112	0.914	0.013	-0.037	0.874	-0.029	-0.079	1.000	-0.014	-0.019	0.970
	GB1	0.124	-0.172	**0.089**	0.051	-0.084	0.241	0.096	-0.166	0.127	0.095	-0.114	0.198
	GB2	0.155	-0.184	0.129	0.094	-0.092	**0.159**	0.110	-0.211	**0.087**	0.116	-0.132	**0.137**
VGAE	MI	-0.009	0.071	0.711	0.012	-0.052	0.833	0.005	-0.055	0.976	-0.014	-0.025	0.929
	GB1	0.166	-0.128	0.153	0.067	-0.081	0.242	0.137	-0.172	0.083	0.071	-0.114	0.186
	GB2	0.375	-0.160	**0.114**	0.081	-0.114	**0.135**	0.156	-0.206	**0.041**	0.089	-0.136	**0.091**
DGI	MI	-0.037	0.273	0.252	-0.087	-0.017	0.753	-0.082	-0.020	**0.239**	-0.041	-0.054	0.850
	GB1	0.264	-0.080	0.140	0.123	-0.324	0.357	-0.146	-0.213	0.843	0.057	-0.171	0.331
	GB2	0.345	-0.113	**0.095**	0.093	-0.508	**0.234**	-0.095	-0.211	0.612	0.064	-0.215	**0.230**
GRACE	MI	0.010	-0.022	0.813	-0.001	-0.007	0.546	-0.015	-0.010	0.373	-0.022	-0.024	0.813
	GB1	0.108	-0.083	0.058	0.017	-0.024	0.074	0.021	-0.043	**0.085**	0.077	-0.072	0.203
	GB2	0.107	-0.089	**0.048**	0.019	-0.030	**0.046**	0.017	-0.045	0.099	0.057	-0.072	**0.201**